



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:15 PM UTC

PDB ID : 6J3Y / pdb_00006j3y
EMDB ID : EMD-9775
Title : Structure of C2S2-type PSII-FCPII supercomplex from diatom
Authors : Nagao, R.; Kato, K.; Shen, J.R.; Miyazaki, N.; Akita, F.
Deposited on : 2019-01-07
Resolution : 3.30 Å (reported)
Based on initial models : 3WU2, 3JCU

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

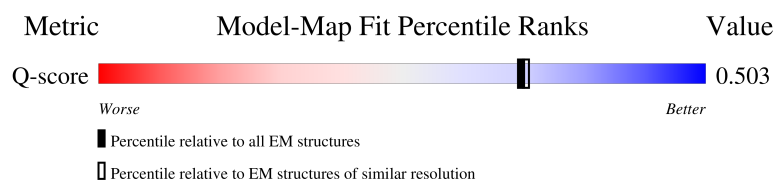
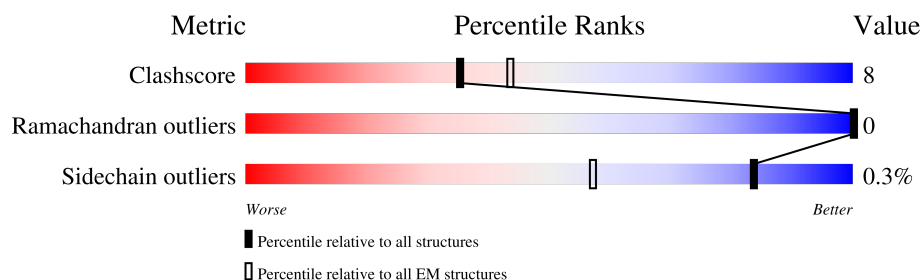
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.



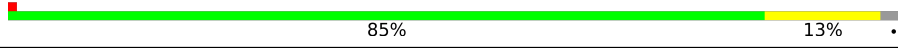
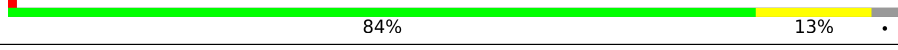
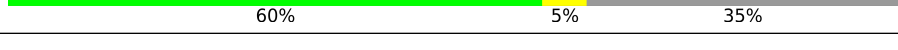
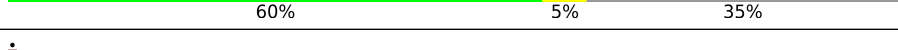
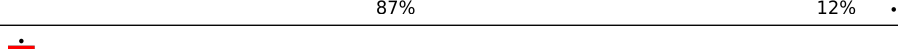
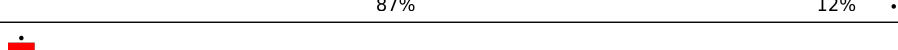
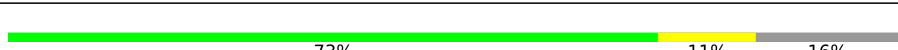
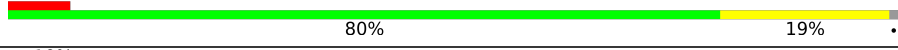
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	
2	B	509	
2	b	509	

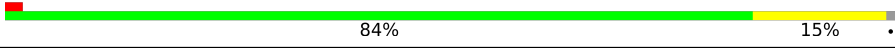
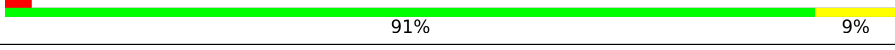
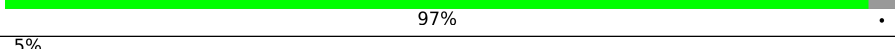
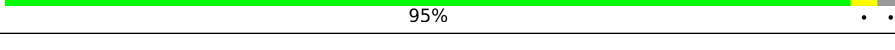
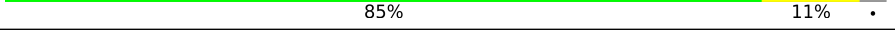
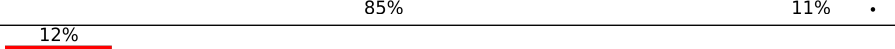
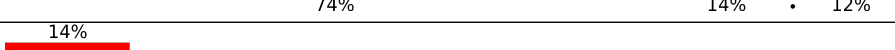
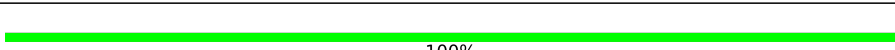
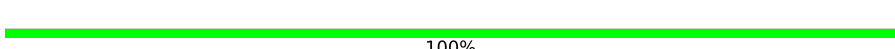
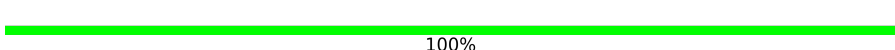
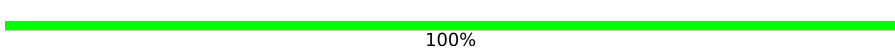
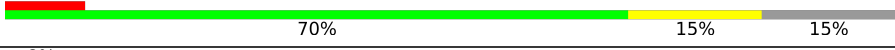
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Mol	Chain	Length	Quality of chain
3	C	471	
3	c	471	
4	D	351	
4	d	351	
5	E	84	
5	e	84	
6	F	43	
6	f	43	
7	H	67	
7	h	67	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	44	
10	k	44	
11	L	38	
11	l	38	
12	M	131	
12	m	131	
13	O	248	
13	o	248	
14	T	31	
14	t	31	
15	U	93	

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Mol	Chain	Length	Quality of chain
15	u	93	
16	V	137	
16	v	137	
17	Y	34	
17	y	34	
18	X	38	
18	x	38	
19	Z	61	
19	z	61	
20	Q	155	
20	q	155	
21	W	72	
21	w	72	
22	0	31	
22	5	31	
23	1	30	
23	6	30	
24	2	10	
24	7	10	
25	11	207	
25	12	207	
25	13	207	
25	14	207	
25	31	207	
25	32	207	

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Mol	Chain	Length	Quality of chain
25	33	207	
25	34	207	

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
27	CLA	11	301	X	-	-	-
27	CLA	11	302	X	-	-	-
27	CLA	11	303	X	-	-	-
27	CLA	11	304	X	-	-	-
27	CLA	11	305	X	-	-	-
27	CLA	11	306	X	-	-	-
27	CLA	11	307	X	-	-	-
27	CLA	11	309	X	-	-	-
27	CLA	11	315	X	-	-	-
27	CLA	12	303	X	-	-	-
27	CLA	12	305	X	-	-	-
27	CLA	12	306	X	-	-	-
27	CLA	12	307	X	-	-	-
27	CLA	12	308	X	-	-	-
27	CLA	12	309	X	-	-	-
27	CLA	12	310	X	-	-	-
27	CLA	12	311	X	-	-	-
27	CLA	12	313	X	-	-	-
27	CLA	13	301	X	-	-	-
27	CLA	13	303	X	-	-	-
27	CLA	13	304	X	-	-	-
27	CLA	13	305	X	-	-	-
27	CLA	13	306	X	-	-	-
27	CLA	13	307	X	-	-	-
27	CLA	13	308	X	-	-	-
27	CLA	13	309	X	-	-	-
27	CLA	13	311	X	-	-	-
27	CLA	14	302	X	-	-	-
27	CLA	14	303	X	-	-	-
27	CLA	14	304	X	-	-	-
27	CLA	14	305	X	-	-	-
27	CLA	14	306	X	-	-	-
27	CLA	14	307	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	14	308	X	-	-	-
27	CLA	14	309	X	-	-	-
27	CLA	14	311	X	-	-	-
27	CLA	31	301	X	-	-	-
27	CLA	31	302	X	-	-	-
27	CLA	31	303	X	-	-	-
27	CLA	31	304	X	-	-	-
27	CLA	31	305	X	-	-	-
27	CLA	31	306	X	-	-	-
27	CLA	31	307	X	-	-	-
27	CLA	31	309	X	-	-	-
27	CLA	31	315	X	-	-	-
27	CLA	32	303	X	-	-	-
27	CLA	32	305	X	-	-	-
27	CLA	32	306	X	-	-	-
27	CLA	32	307	X	-	-	-
27	CLA	32	308	X	-	-	-
27	CLA	32	309	X	-	-	-
27	CLA	32	310	X	-	-	-
27	CLA	32	311	X	-	-	-
27	CLA	32	313	X	-	-	-
27	CLA	33	301	X	-	-	-
27	CLA	33	303	X	-	-	-
27	CLA	33	304	X	-	-	-
27	CLA	33	305	X	-	-	-
27	CLA	33	306	X	-	-	-
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27	CLA	33	308	X	-	-	-
27	CLA	33	309	X	-	-	-
27	CLA	33	311	X	-	-	-
27	CLA	34	302	X	-	-	-
27	CLA	34	304	X	-	-	-
27	CLA	34	305	X	-	-	-
27	CLA	34	306	X	-	-	-
27	CLA	34	307	X	-	-	-
27	CLA	34	308	X	-	-	-
27	CLA	34	309	X	-	-	-
27	CLA	34	310	X	-	-	-
27	CLA	34	312	X	-	-	-
27	CLA	A	402	X	-	-	-
27	CLA	A	404	X	-	-	-
27	CLA	B	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	B	602	X	-	-	-
27	CLA	B	603	X	-	-	-
27	CLA	B	604	X	-	-	-
27	CLA	B	605	X	-	-	-
27	CLA	B	606	X	-	-	-
27	CLA	B	607	X	-	-	-
27	CLA	B	608	X	-	-	-
27	CLA	B	609	X	-	-	-
27	CLA	B	610	X	-	-	-
27	CLA	B	611	X	-	-	-
27	CLA	B	612	X	-	-	-
27	CLA	B	613	X	-	-	-
27	CLA	B	614	X	-	-	-
27	CLA	B	615	X	-	-	-
27	CLA	B	622	X	-	-	-
27	CLA	C	502	X	-	-	-
27	CLA	C	503	X	-	-	-
27	CLA	C	504	X	-	-	-
27	CLA	C	505	X	-	-	-
27	CLA	C	506	X	-	-	-
27	CLA	C	507	X	-	-	-
27	CLA	C	508	X	-	-	-
27	CLA	C	509	X	-	-	-
27	CLA	C	510	X	-	-	-
27	CLA	C	511	X	-	-	-
27	CLA	C	512	X	-	-	-
27	CLA	C	513	X	-	-	-
27	CLA	C	514	X	-	-	-
27	CLA	D	401	X	-	-	-
27	CLA	D	402	X	-	-	-
27	CLA	D	405	X	-	-	-
27	CLA	D	406	X	-	-	-
27	CLA	M	102	X	-	-	-
27	CLA	W	102	X	-	-	-
27	CLA	a	402	X	-	-	-
27	CLA	a	404	X	-	-	-
27	CLA	b	601	X	-	-	-
27	CLA	b	602	X	-	-	-
27	CLA	b	603	X	-	-	-
27	CLA	b	604	X	-	-	-
27	CLA	b	605	X	-	-	-
27	CLA	b	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	b	607	X	-	-	-
27	CLA	b	608	X	-	-	-
27	CLA	b	609	X	-	-	-
27	CLA	b	610	X	-	-	-
27	CLA	b	611	X	-	-	-
27	CLA	b	612	X	-	-	-
27	CLA	b	613	X	-	-	-
27	CLA	b	614	X	-	-	-
27	CLA	b	615	X	-	-	-
27	CLA	b	622	X	-	-	-
27	CLA	c	502	X	-	-	-
27	CLA	c	503	X	-	-	-
27	CLA	c	504	X	-	-	-
27	CLA	c	505	X	-	-	-
27	CLA	c	506	X	-	-	-
27	CLA	c	507	X	-	-	-
27	CLA	c	508	X	-	-	-
27	CLA	c	509	X	-	-	-
27	CLA	c	510	X	-	-	-
27	CLA	c	511	X	-	-	-
27	CLA	c	512	X	-	-	-
27	CLA	c	513	X	-	-	-
27	CLA	c	514	X	-	-	-
27	CLA	d	401	X	-	-	-
27	CLA	d	402	X	-	-	-
27	CLA	d	405	X	-	-	-
27	CLA	d	406	X	-	-	-
27	CLA	m	101	X	-	-	-
27	CLA	w	102	X	-	-	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 70136 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 Photosystem II reaction center protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2618	1712	429	462	15		
1	a	334	Total	C	N	O	S	0	0
			2618	1712	429	462	15		

- Molecule 2 is a protein called Photosystem II chlorophyll protein CP47.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	484	Total	C	N	O	S	0	0
			3812	2494	645	660	13		
2	b	484	Total	C	N	O	S	0	0
			3812	2494	645	660	13		

- Molecule 3 is a protein called Photosystem II chlorophyll protein CP43.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	451	Total	C	N	O	S	0	0
			3504	2289	589	612	14		
3	c	451	Total	C	N	O	S	0	0
			3504	2289	589	612	14		

- Molecule 4 is a protein called Photosystem II reaction center protein D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	0	0
			2697	1781	441	465	10		
4	d	341	Total	C	N	O	S	0	0
			2697	1781	441	465	10		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	75	Total	C	N	O	0	0
			616	401	102	113		
5	e	75	Total	C	N	O	0	0
			616	401	102	113		

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	28	Total	C	N	O	S	0	0
			228	155	39	33	1		
6	f	28	Total	C	N	O	S	0	0
			228	155	39	33	1		

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	66	Total	C	N	O	S	0	0
			513	340	83	88	2		
7	h	66	Total	C	N	O	S	0	0
			513	340	83	88	2		

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	35	Total	C	N	O	S	0	0
			287	194	45	47	1		
8	i	35	Total	C	N	O	S	0	0
			287	194	45	47	1		

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	34	Total	C	N	O	S	0	0
			254	172	38	43	1		
9	j	34	Total	C	N	O	S	0	0
			254	172	38	43	1		

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	37	Total	C	N	O	0	0
			302	212	45	45		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	k	37	Total	C	N	O	0	0
			302	212	45	45		

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	38	Total	C	N	O	S	0	0
			310	208	48	53	1		
11	l	38	Total	C	N	O	S	0	0
			310	208	48	53	1		

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	42	Total	C	N	O	0	0
			316	207	51	58		
12	m	42	Total	C	N	O	0	0
			316	207	51	58		

- Molecule 13 is a protein called Extrinsic protein in photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	245	Total	C	N	O	S	0	0
			1845	1166	306	365	8		
13	o	245	Total	C	N	O	S	0	0
			1845	1166	306	365	8		

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	30	Total	C	N	O	S	0	0
			250	174	36	38	2		
14	t	30	Total	C	N	O	S	0	0
			250	174	36	38	2		

- Molecule 15 is a protein called Extrinsic protein in photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	93	Total	C	N	O	S	0	0
			713	455	119	137	2		
15	u	93	Total	C	N	O	S	0	0
			713	455	119	137	2		

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	136	Total	C	N	O	S	0	0
			1037	647	180	206	4		
16	v	136	Total	C	N	O	S	0	0
			1037	647	180	206	4		

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	34	Total	C	N	O	S	0	0
			250	166	41	40	3		
17	y	34	Total	C	N	O	S	0	0
			250	166	41	40	3		

- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	37	Total	C	N	O	S	0	0
			263	171	45	46	1		
18	x	37	Total	C	N	O	S	0	0
			263	171	45	46	1		

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	59	Total	C	N	O	S	0	0
			447	305	68	73	1		
19	z	59	Total	C	N	O	S	0	0
			447	305	68	73	1		

- Molecule 20 is a protein called Extrinsic protein in photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	137	Total	C	N	O	S	0	0
			1079	684	179	215	1		
20	q	137	Total	C	N	O	S	0	0
			1079	684	179	215	1		

- Molecule 21 is a protein called Photosystem II reaction center protein W.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	W	52	Total	C	N	O	0	0
			422	273	65	84		
21	w	52	Total	C	N	O	0	0
			422	273	65	84		

- Molecule 22 is a protein called Unknown protein 0.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	0	31	Total	C	N	O	0	0
			155	93	31	31		
22	5	31	Total	C	N	O	0	0
			155	93	31	31		

- Molecule 23 is a protein called Unknown protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	1	30	Total	C	N	O	0	0
			150	90	30	30		
23	6	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 24 is a protein called Unknown protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	2	10	Total	C	N	O	0	0
			50	30	10	10		
24	7	10	Total	C	N	O	0	0
			50	30	10	10		

- Molecule 25 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	11	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	12	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	13	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	14	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	31	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		

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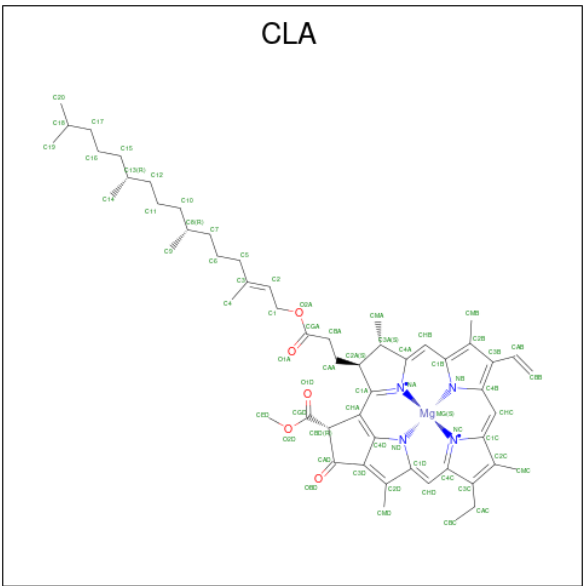
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Mol	Chain	Residues	Atoms					AltConf	Trace
25	32	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	33	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	34	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		

- Molecule 26 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
26	A	1	Total	Fe	0
			1	1	
26	a	1	Total	Fe	0
			1	1	

- Molecule 27 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	M	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	m	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	z	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	w	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	w	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	11	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	14	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	31	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	31	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	31	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	31	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	31	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	31	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	31	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	31	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	31	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	31	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	31	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	32	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	32	1	Total 65	C 55	Mg 1	N 4	O 5	0

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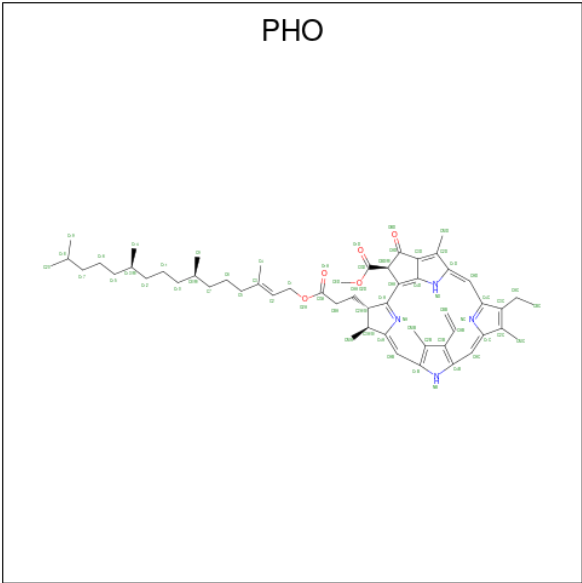
Mol	Chain	Residues	Atoms					AltConf
27	32	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	32	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	32	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	32	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	32	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	32	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	32	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	32	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	32	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	33	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	33	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	33	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	33	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	33	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	33	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	33	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	33	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	33	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	33	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	34	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	34	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	34	1	Total 45	C 35	Mg 1	N 4	O 5	0

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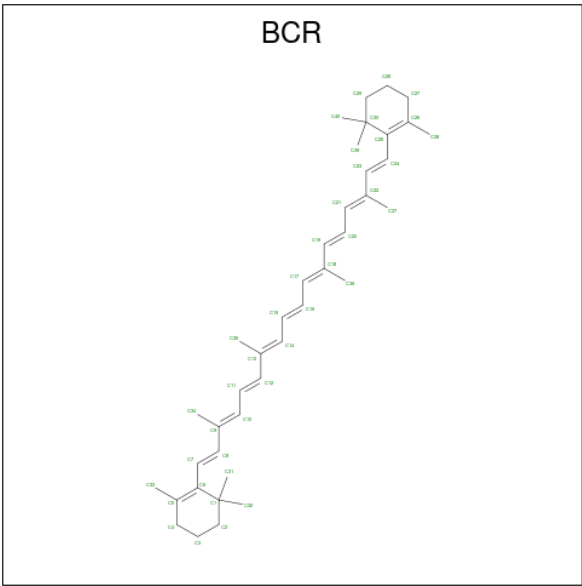
Mol	Chain	Residues	Atoms					AltConf
27	34	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	34	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	34	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	34	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	34	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	34	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	34	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 28 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	N	O	0
			64	55	4	5	
28	D	1	Total	C	N	O	0
			64	55	4	5	
28	a	1	Total	C	N	O	0
			64	55	4	5	
28	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 29 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



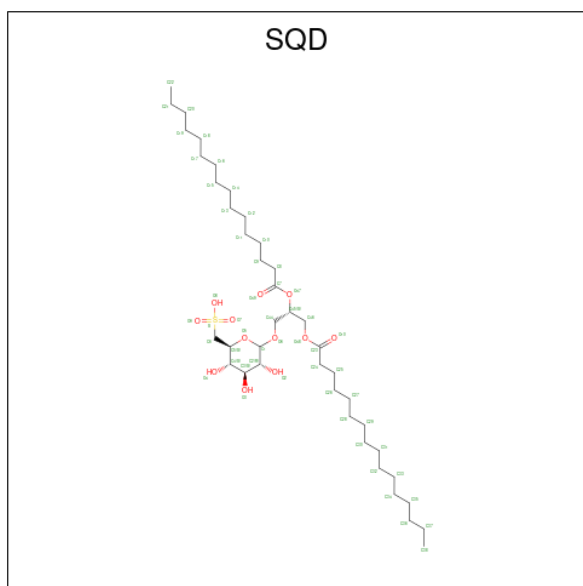
Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	C	1	Total C 40 40	0
29	C	1	Total C 40 40	0
29	C	1	Total C 40 40	0
29	F	1	Total C 40 40	0
29	H	1	Total C 40 40	0
29	M	1	Total C 40 40	0
29	Z	1	Total C 40 40	0
29	a	1	Total C 40 40	0

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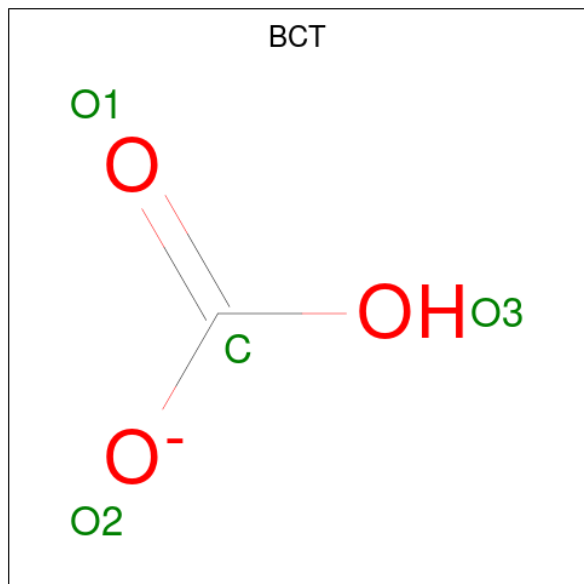
Mol	Chain	Residues	Atoms	AltConf
29	a	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	c	1	Total C 40 40	0
29	c	1	Total C 40 40	0
29	c	1	Total C 40 40	0
29	f	1	Total C 40 40	0
29	h	1	Total C 40 40	0
29	m	1	Total C 40 40	0
29	z	1	Total C 40 40	0

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



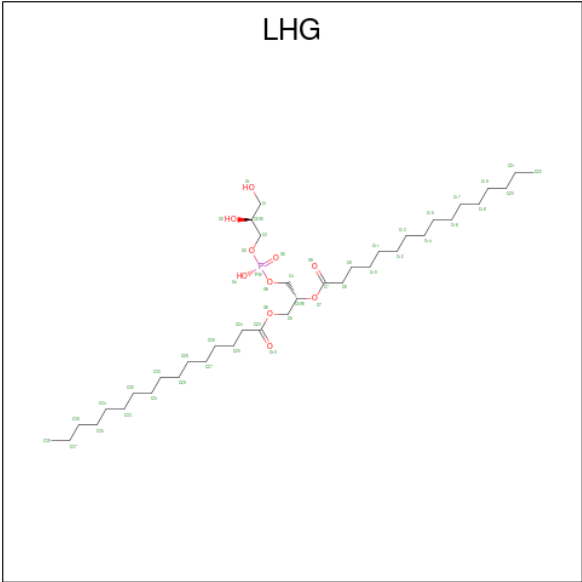
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	S	0
			54	41	12	1	
30	B	1	Total	C	O	S	0
			37	24	12	1	
30	L	1	Total	C	O	S	0
			54	41	12	1	
30	a	1	Total	C	O	S	0
			54	41	12	1	
30	b	1	Total	C	O	S	0
			37	24	12	1	
30	l	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



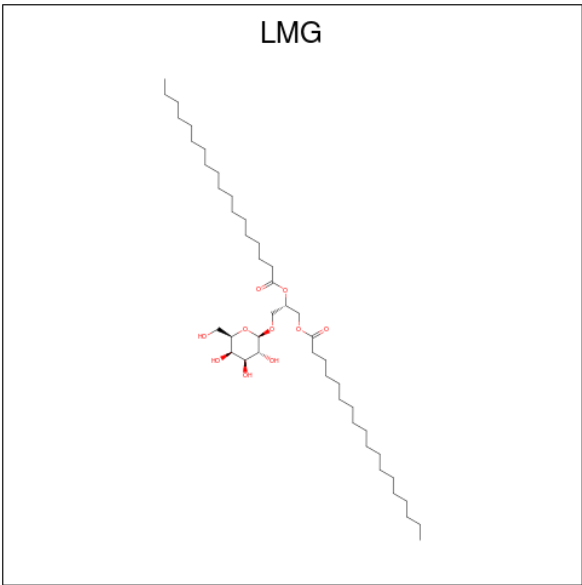
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			4	1	3	
31	a	1	Total	C	O	0
			4	1	3	

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$).



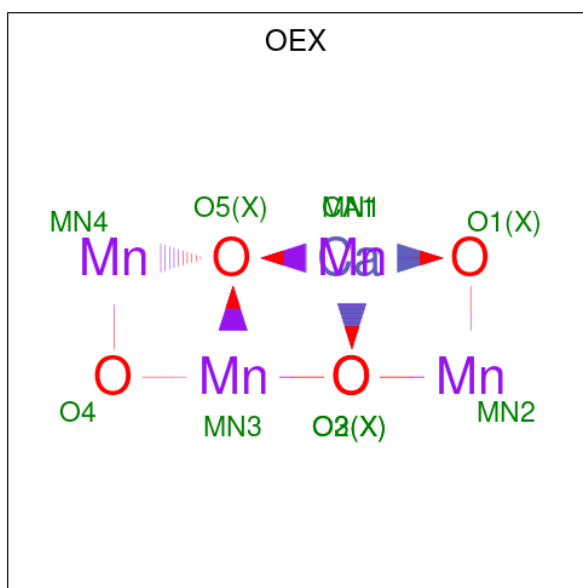
Mol	Chain	Residues	Atoms				AltConf
32	A	1	Total	C	O	P	0
			46	35	10	1	
32	B	1	Total	C	O	P	0
			49	38	10	1	
32	L	1	Total	C	O	P	0
			49	38	10	1	
32	L	1	Total	C	O	P	0
			49	38	10	1	
32	a	1	Total	C	O	P	0
			46	35	10	1	
32	b	1	Total	C	O	P	0
			49	38	10	1	
32	l	1	Total	C	O	P	0
			49	38	10	1	
32	l	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



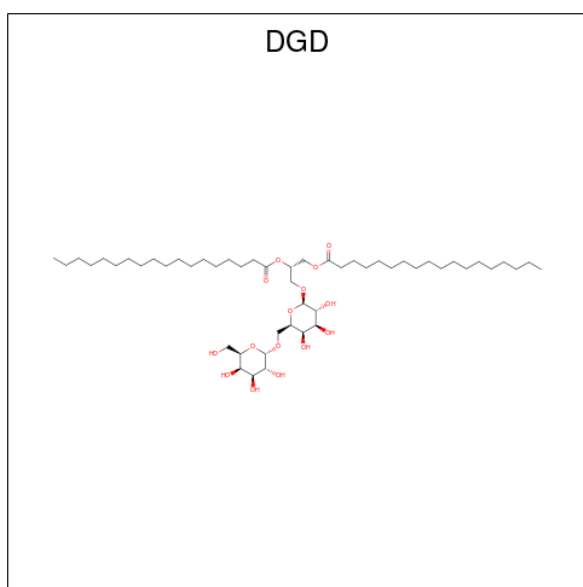
Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			51	41	10	
33	B	1	Total	C	O	0
			51	41	10	
33	C	1	Total	C	O	0
			51	41	10	
33	D	1	Total	C	O	0
			51	41	10	
33	M	1	Total	C	O	0
			40	30	10	
33	W	1	Total	C	O	0
			51	41	10	
33	b	1	Total	C	O	0
			51	41	10	
33	b	1	Total	C	O	0
			51	41	10	
33	d	1	Total	C	O	0
			51	41	10	
33	m	1	Total	C	O	0
			40	30	10	
33	q	1	Total	C	O	0
			51	41	10	
33	w	1	Total	C	O	0
			51	41	10	
33	12	1	Total	C	O	0
			39	29	10	
33	32	1	Total	C	O	0
			39	29	10	

- Molecule 34 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



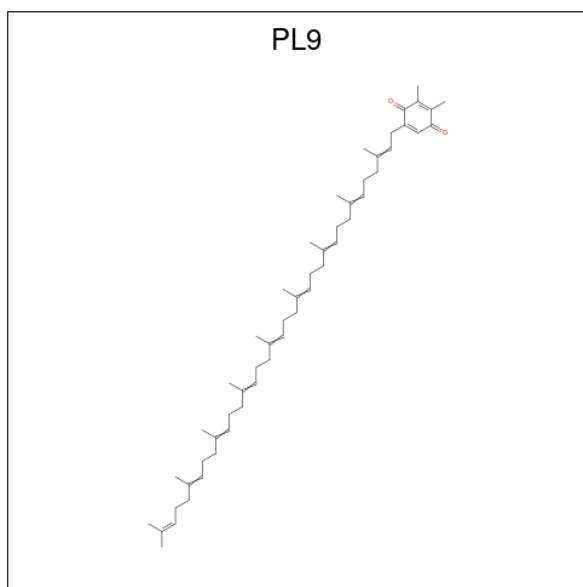
Mol	Chain	Residues	Atoms				AltConf
34	C	1	Total	Ca	Mn	O	0
			10	1	4	5	
34	c	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $\text{C}_{51}\text{H}_{96}\text{O}_{15}$).



Mol	Chain	Residues	Atoms			AltConf
35	C	1	Total	C	O	0
			62	47	15	
35	C	1	Total	C	O	0
			62	47	15	
35	H	1	Total	C	O	0
			62	47	15	
35	J	1	Total	C	O	0
			62	47	15	
35	c	1	Total	C	O	0
			62	47	15	
35	c	1	Total	C	O	0
			62	47	15	
35	h	1	Total	C	O	0
			62	47	15	
35	j	1	Total	C	O	0
			62	47	15	

- Molecule 36 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



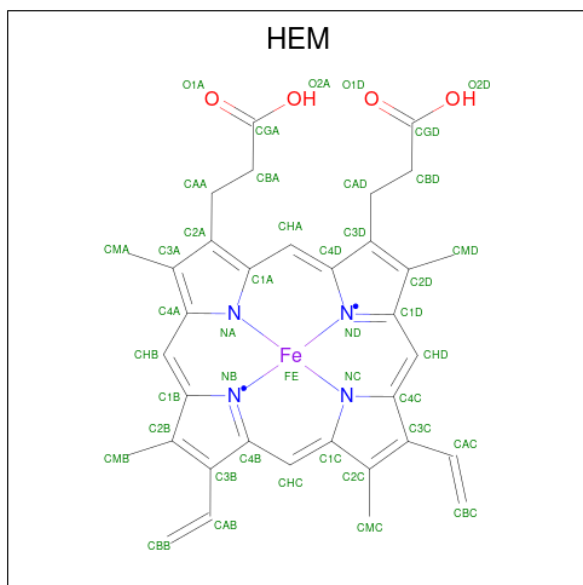
Mol	Chain	Residues	Atoms			AltConf
36	D	1	Total	C	O	0
			55	53	2	
36	D	1	Total	C	O	0
			55	53	2	
36	d	1	Total	C	O	0
			55	53	2	

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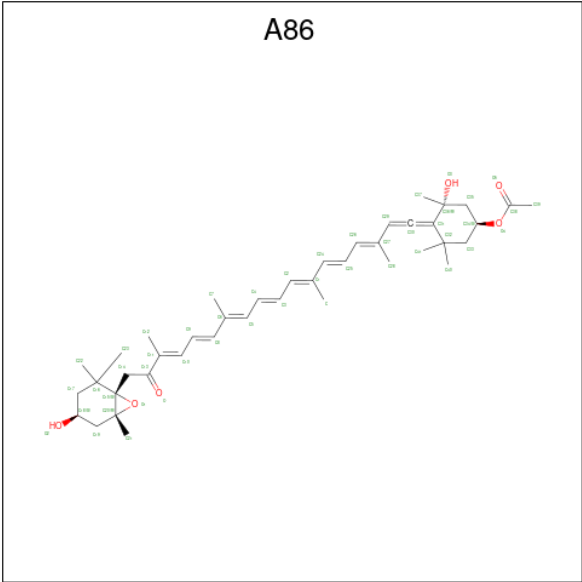
Mol	Chain	Residues	Atoms			AltConf
36	d	1	Total	C	O	0
			55	53	2	

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
37	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
37	V	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
37	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
37	v	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 38 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (CCD ID: A86) (formula: $C_{42}H_{58}O_6$).



Mol	Chain	Residues	Atoms			AltConf
38	11	1	Total	C	O	0
			48	42	6	
38	11	1	Total	C	O	0
			48	42	6	
38	11	1	Total	C	O	0
			48	42	6	
38	11	1	Total	C	O	0
			48	42	6	
38	11	1	Total	C	O	0
			48	42	6	
38	11	1	Total	C	O	0
			48	42	6	
38	12	1	Total	C	O	0
			48	42	6	
38	12	1	Total	C	O	0
			48	42	6	
38	12	1	Total	C	O	0
			48	42	6	
38	12	1	Total	C	O	0
			48	42	6	
38	13	1	Total	C	O	0
			48	42	6	
38	13	1	Total	C	O	0
			48	42	6	
38	13	1	Total	C	O	0
			48	42	6	

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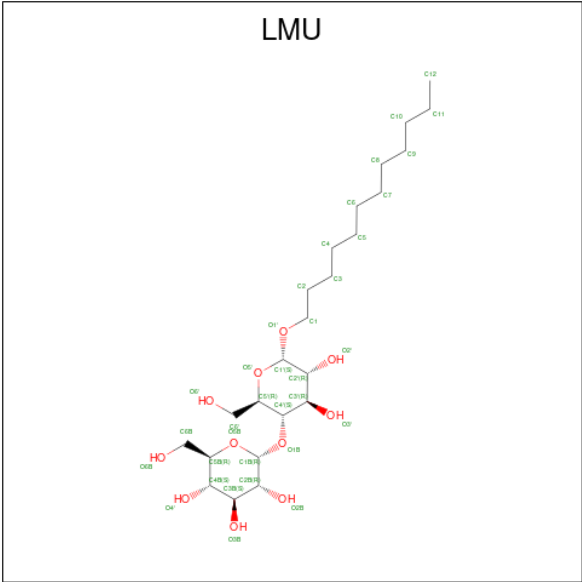
Mol	Chain	Residues	Atoms			AltConf
38	13	1	Total	C	O	0
			48	42	6	
38	13	1	Total	C	O	0
			48	42	6	
38	13	1	Total	C	O	0
			48	42	6	
38	13	1	Total	C	O	0
			48	42	6	
38	14	1	Total	C	O	0
			48	42	6	
38	14	1	Total	C	O	0
			48	42	6	
38	14	1	Total	C	O	0
			48	42	6	
38	14	1	Total	C	O	0
			48	42	6	
38	14	1	Total	C	O	0
			48	42	6	
38	14	1	Total	C	O	0
			48	42	6	
38	31	1	Total	C	O	0
			48	42	6	
38	31	1	Total	C	O	0
			48	42	6	
38	31	1	Total	C	O	0
			48	42	6	
38	31	1	Total	C	O	0
			48	42	6	
38	31	1	Total	C	O	0
			48	42	6	
38	31	1	Total	C	O	0
			48	42	6	
38	32	1	Total	C	O	0
			48	42	6	
38	32	1	Total	C	O	0
			48	42	6	
38	32	1	Total	C	O	0
			48	42	6	
38	32	1	Total	C	O	0
			48	42	6	
38	32	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
38	32	1	Total	C	O	0
			48	42	6	
38	33	1	Total	C	O	0
			48	42	6	
38	33	1	Total	C	O	0
			48	42	6	
38	33	1	Total	C	O	0
			48	42	6	
38	33	1	Total	C	O	0
			48	42	6	
38	33	1	Total	C	O	0
			48	42	6	
38	33	1	Total	C	O	0
			48	42	6	
38	34	1	Total	C	O	0
			48	42	6	
38	34	1	Total	C	O	0
			48	42	6	
38	34	1	Total	C	O	0
			48	42	6	
38	34	1	Total	C	O	0
			48	42	6	
38	34	1	Total	C	O	0
			48	42	6	
38	34	1	Total	C	O	0
			48	42	6	

- Molecule 39 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).

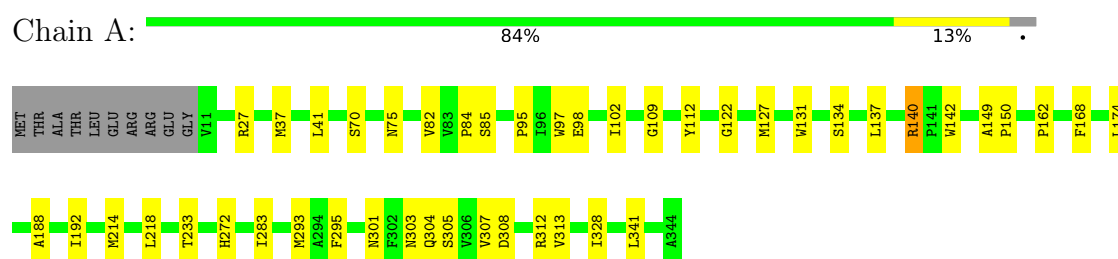


Mol	Chain	Residues	Atoms			AltConf
39	12	1	Total	C	O	0
			32	21	11	
39	32	1	Total	C	O	0
			32	21	11	

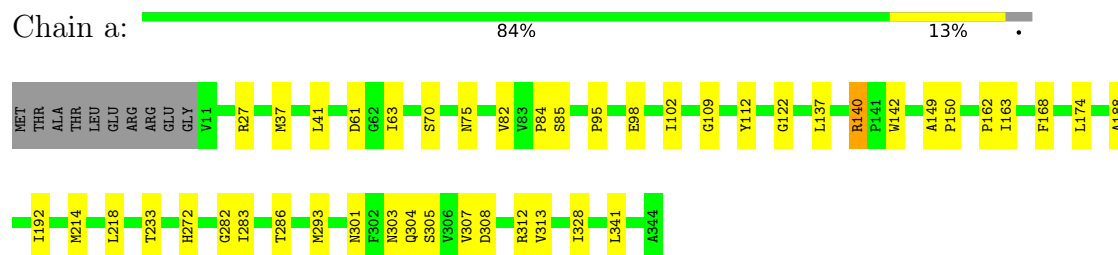
3 Residue-property plots [i](#)

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

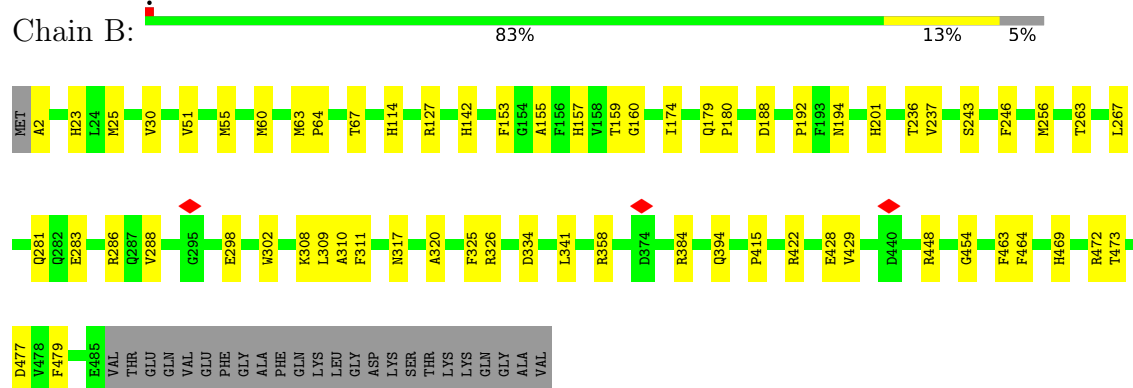
- Molecule 1: Photosystem II reaction center protein D1



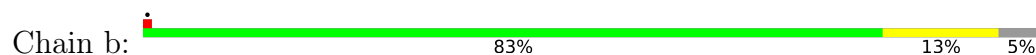
- Molecule 1: Photosystem II reaction center protein D1

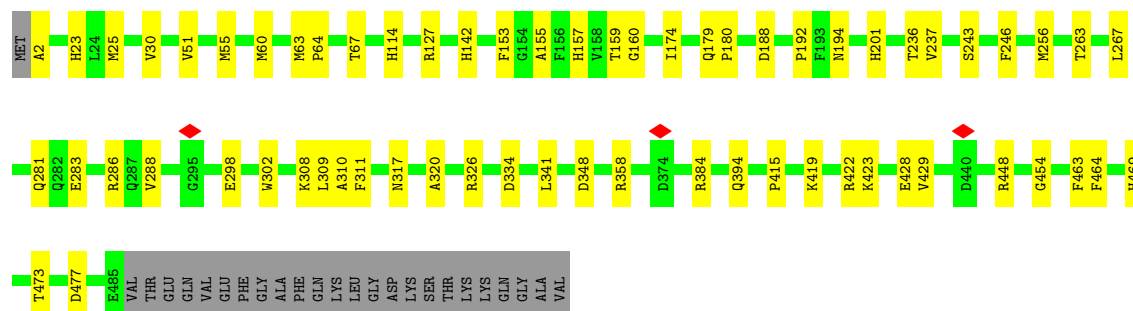


- Molecule 2: Photosystem II chlorophyll protein CP47



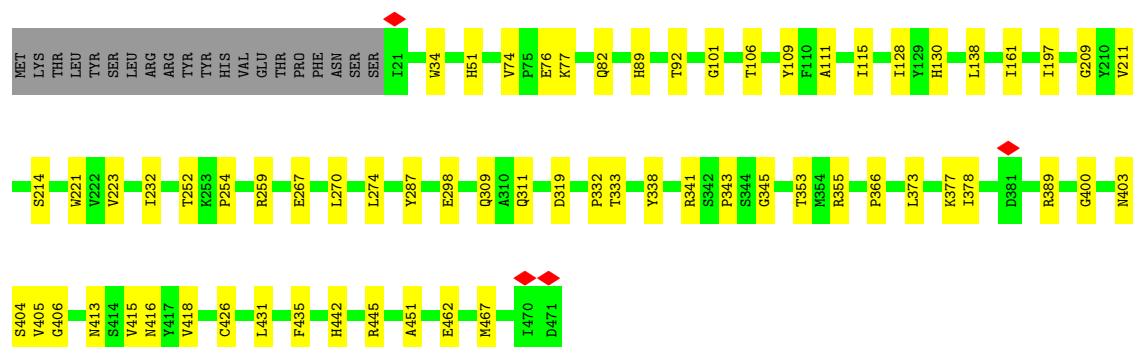
- Molecule 2: Photosystem II chlorophyll protein CP47





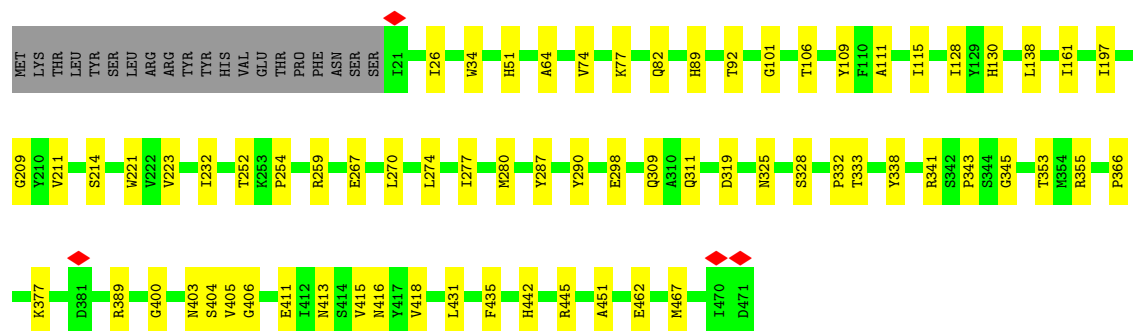
• Molecule 3: Photosystem II chlorophyll protein CP43

Chain C: 82% 14% .



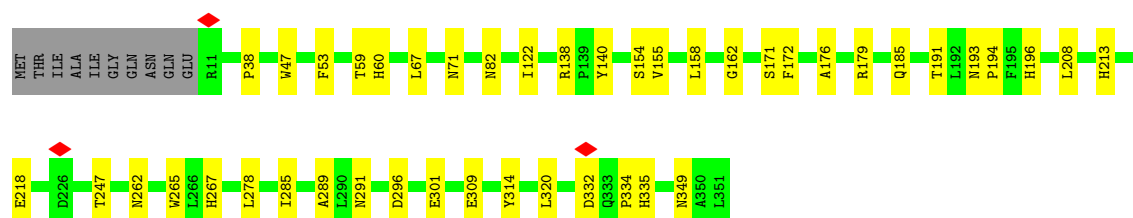
• Molecule 3: Photosystem II chlorophyll protein CP43

Chain c: 81% 15% .

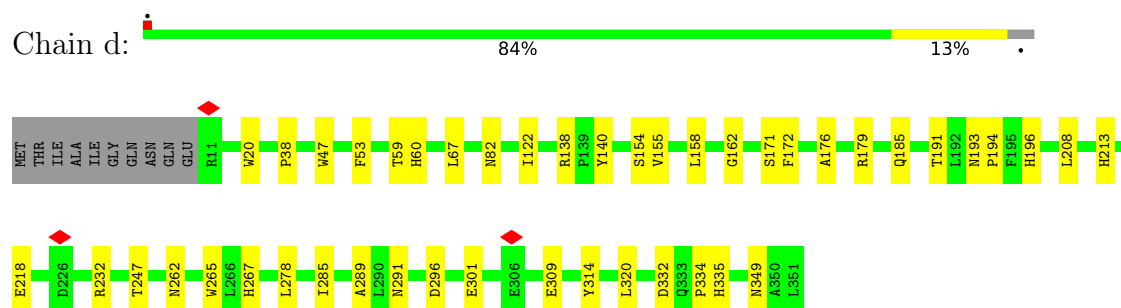


• Molecule 4: Photosystem II reaction center protein D2

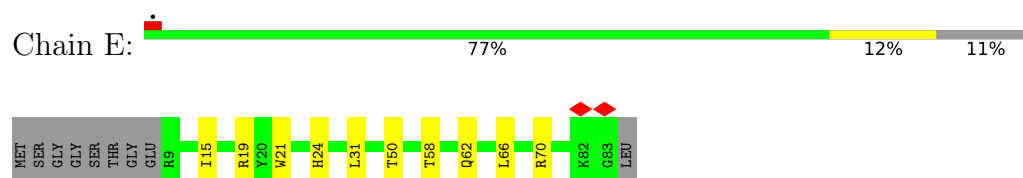
Chain D: 85% 13% .



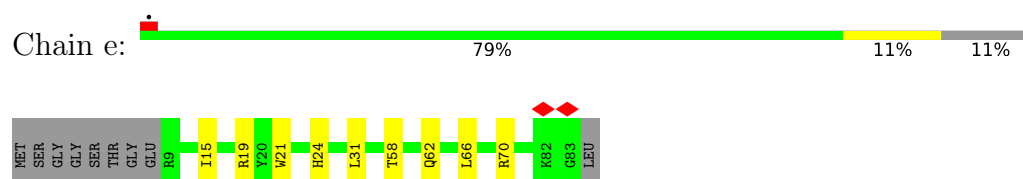
- Molecule 4: Photosystem II reaction center protein D2



- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha



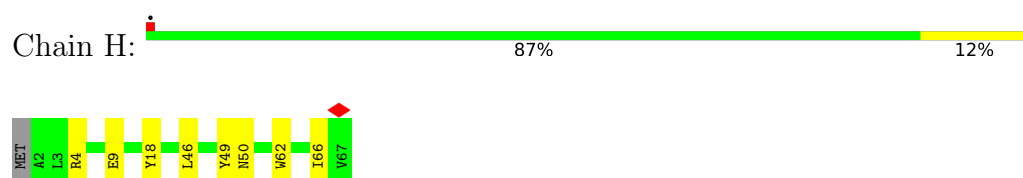
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 6: Cytochrome b559 subunit beta

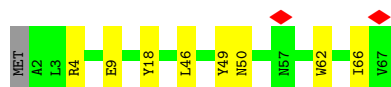


- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H

Chain h:  87% 12%



- Molecule 8: Photosystem II reaction center protein I

Chain I:  74% 18% 8%



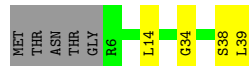
- Molecule 8: Photosystem II reaction center protein I

Chain i:  74% 18% 8%



- Molecule 9: Photosystem II reaction center protein J

Chain J:  77% 10% 13%



- Molecule 9: Photosystem II reaction center protein J

Chain j:  77% 10% 13%



- Molecule 10: Photosystem II reaction center protein K

Chain K:  75% 9% 16%

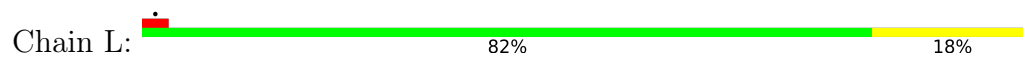


- Molecule 10: Photosystem II reaction center protein K

Chain k:  73% 11% 16%



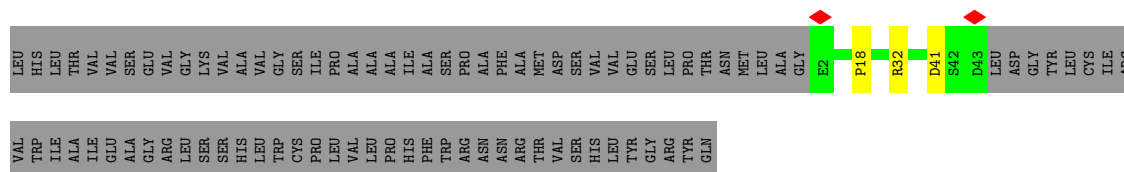
- Molecule 11: Photosystem II reaction center protein L



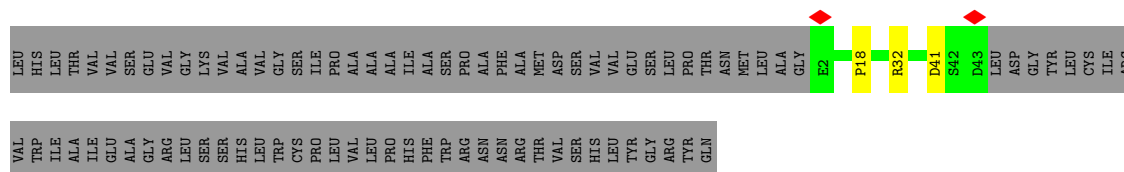
- Molecule 11: Photosystem II reaction center protein L



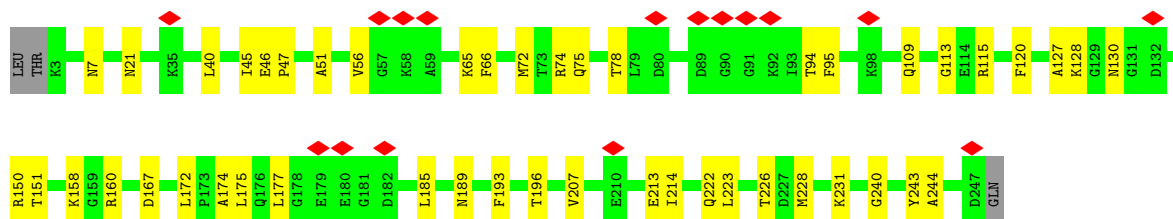
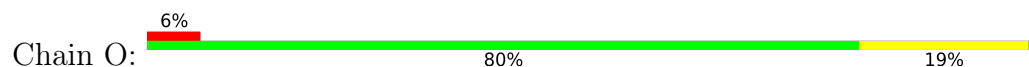
- Molecule 12: Photosystem II reaction center protein M



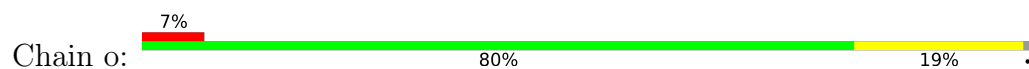
- Molecule 12: Photosystem II reaction center protein M

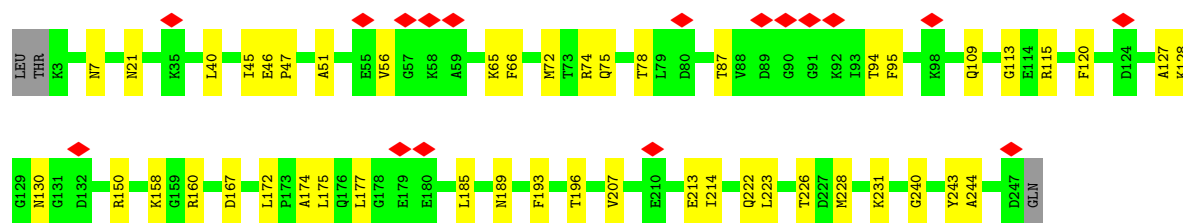


- Molecule 13: Extrinsic protein in photosystem II

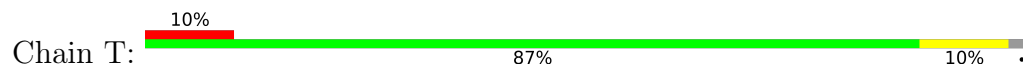


- Molecule 13: Extrinsic protein in photosystem II

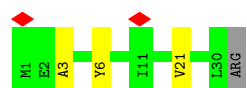
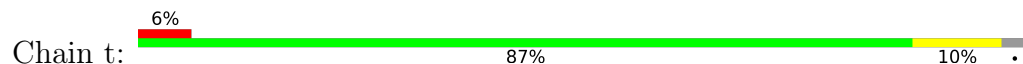




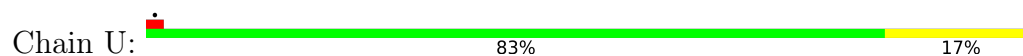
- Molecule 14: Photosystem II reaction center protein T



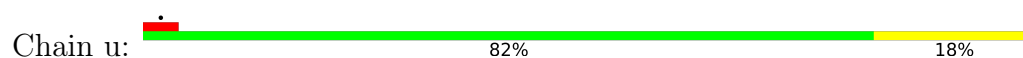
- Molecule 14: Photosystem II reaction center protein T



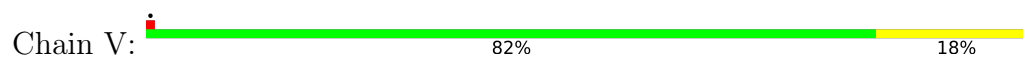
- Molecule 15: Extrinsic protein in photosystem II



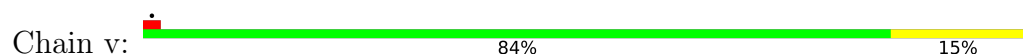
- Molecule 15: Extrinsic protein in photosystem II



- Molecule 16: Cytochrome c-550



- Molecule 16: Cytochrome c-550

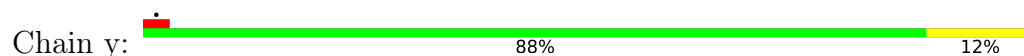




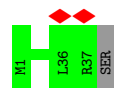
- Molecule 17: Photosystem II reaction center protein Ycf12



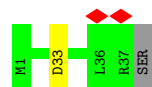
- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center X protein



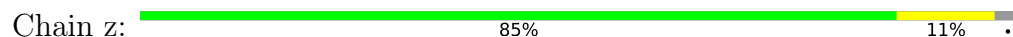
- Molecule 18: Photosystem II reaction center X protein



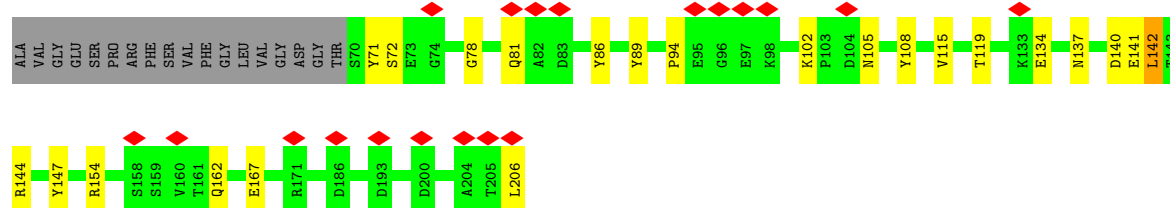
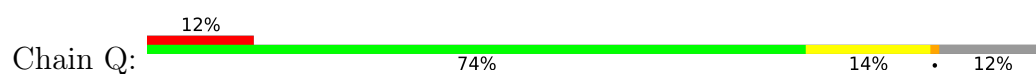
- Molecule 19: Photosystem II reaction center protein Z



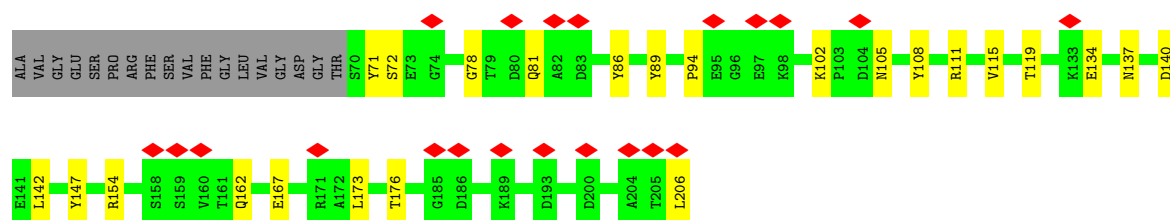
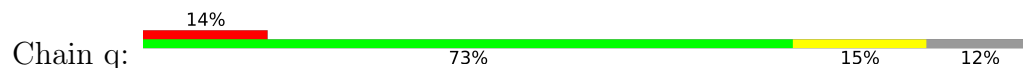
- Molecule 19: Photosystem II reaction center protein Z



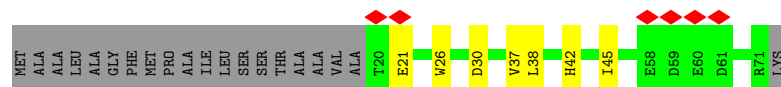
- Molecule 20: Extrinsic protein in photosystem II



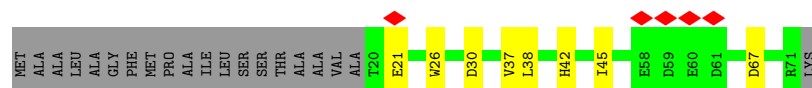
- Molecule 20: Extrinsic protein in photosystem II



- Molecule 21: Photosystem II reaction center protein W



- Molecule 21: Photosystem II reaction center protein W



- Molecule 22: Unknown protein 0



There are no outlier residues recorded for this chain.

- Molecule 22: Unknown protein 0



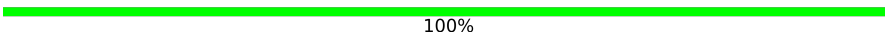
There are no outlier residues recorded for this chain.

- Molecule 23: Unknown protein 1



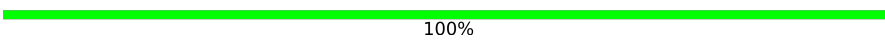
There are no outlier residues recorded for this chain.

- Molecule 23: Unknown protein 1

Chain 6:  100%

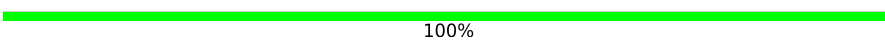
There are no outlier residues recorded for this chain.

- Molecule 24: Unknown protein 2

Chain 2:  100%

There are no outlier residues recorded for this chain.

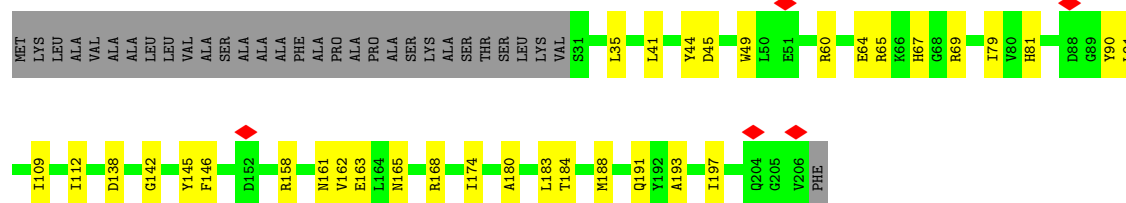
- Molecule 24: Unknown protein 2

Chain 7:  100%

There are no outlier residues recorded for this chain.

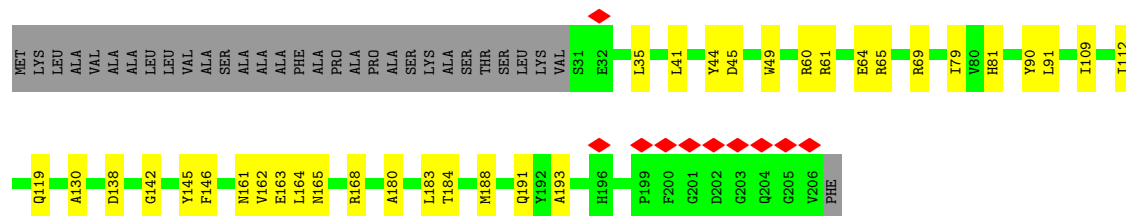
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 11:  69% 16% 15%



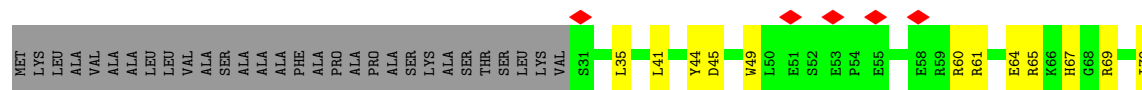
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 12:  5% 69% 16% 15%



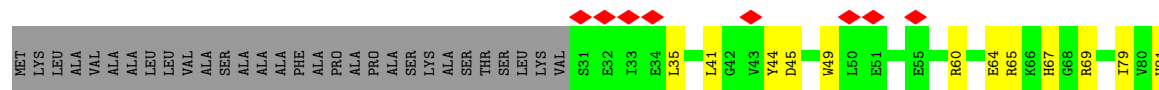
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 13:  9% 70% 15% 15%

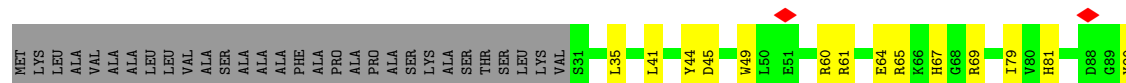




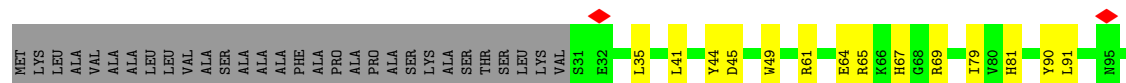
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1



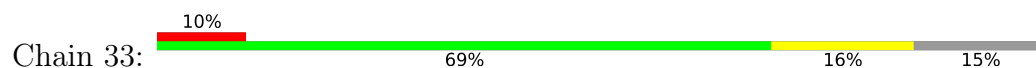
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1



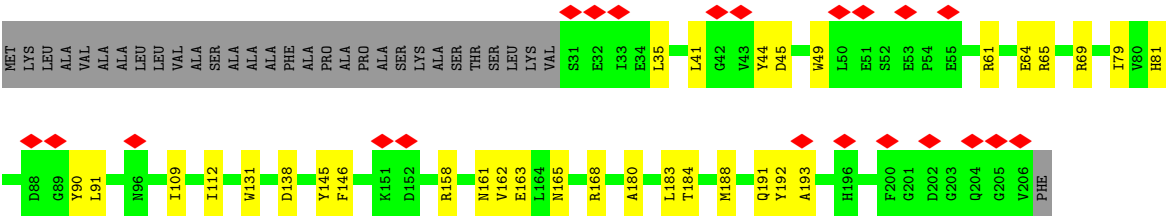
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1



- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1



- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	214939	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.380	Depositor
Minimum map value	-0.155	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	573.44, 573.44, 573.44	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, PHO, OEX, CLA, BCR, LMG, HEM, A86, LMU, BCT, DGD, LHG, SQD, PL9

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.53	0/2701	0.61	0/3682
1	a	0.53	0/2701	0.61	0/3682
2	B	0.51	0/3942	0.60	1/5362 (0.0%)
2	b	0.51	0/3942	0.60	1/5362 (0.0%)
3	C	0.52	0/3620	0.63	2/4933 (0.0%)
3	c	0.52	0/3620	0.63	2/4933 (0.0%)
4	D	0.52	0/2789	0.61	0/3803
4	d	0.52	0/2789	0.61	0/3803
5	E	0.36	0/634	0.55	0/864
5	e	0.36	0/634	0.55	0/864
6	F	0.45	0/235	0.80	0/316
6	f	0.45	0/235	0.80	0/316
7	H	0.44	0/523	0.60	0/714
7	h	0.43	0/523	0.60	0/714
8	I	0.55	0/294	0.78	0/397
8	i	0.55	0/294	0.78	0/397
9	J	0.35	0/260	0.52	0/351
9	j	0.35	0/260	0.52	0/351
10	K	0.49	0/313	1.00	2/429 (0.5%)
10	k	0.49	0/313	1.00	2/429 (0.5%)
11	L	0.52	0/319	0.53	0/433
11	l	0.52	0/319	0.53	0/433
12	M	0.46	0/321	0.66	0/433
12	m	0.46	0/321	0.66	0/433
13	O	0.36	0/1875	0.61	2/2528 (0.1%)
13	o	0.36	0/1875	0.61	2/2528 (0.1%)
14	T	0.38	0/256	0.54	0/346
14	t	0.38	0/256	0.53	0/346
15	U	0.32	0/728	0.62	0/989
15	u	0.32	0/728	0.62	0/989
16	V	0.38	0/1056	0.57	0/1435
16	v	0.38	0/1056	0.57	0/1435

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.29	0/252	0.53	0/341
17	y	0.29	0/252	0.54	0/341
18	X	0.29	0/263	0.52	0/355
18	x	0.29	0/263	0.51	0/355
19	Z	0.34	0/456	0.55	0/624
19	z	0.34	0/456	0.55	0/624
20	Q	0.30	0/1099	0.56	0/1482
20	q	0.30	0/1099	0.56	0/1482
21	W	0.49	0/434	0.66	0/590
21	w	0.49	0/434	0.66	0/590
25	11	0.36	0/1373	0.58	0/1861
25	12	0.36	0/1373	0.58	0/1861
25	13	0.36	0/1373	0.58	0/1861
25	14	0.36	0/1373	0.58	0/1861
25	31	0.36	0/1373	0.58	0/1861
25	32	0.36	0/1373	0.58	0/1861
25	33	0.36	0/1373	0.58	0/1861
25	34	0.36	0/1373	0.58	0/1861
All	All	0.45	0/55724	0.61	14/75702 (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
1	A	0	1
1	a	0	1
16	V	0	1
16	v	0	1
All	All	0	4

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	k	25	ILE	CA-C-N	8.78	125.77	120.24
10	k	25	ILE	C-N-CA	8.78	125.77	120.24
10	K	25	ILE	CA-C-N	8.72	125.73	120.24
10	K	25	ILE	C-N-CA	8.72	125.73	120.24
3	C	252	THR	CA-C-N	6.63	137.18	122.67
3	C	252	THR	C-N-CA	6.63	137.18	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	252	THR	CA-C-N	6.59	137.11	122.67
3	c	252	THR	C-N-CA	6.59	137.11	122.67
13	o	45	ILE	CA-C-N	-5.78	114.82	122.56
13	o	45	ILE	C-N-CA	-5.78	114.82	122.56
13	O	45	ILE	CA-C-N	-5.75	114.86	122.56
13	O	45	ILE	C-N-CA	-5.75	114.86	122.56
2	B	288	VAL	N-CA-C	-5.07	107.89	112.96
2	b	288	VAL	N-CA-C	-5.02	107.94	112.96

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	ARG	Peptide
16	V	63	THR	Peptide
1	a	140	ARG	Peptide
16	v	63	THR	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	A	2618	0	2520	34	0
1	a	2618	0	2520	34	0
2	B	3812	0	3690	48	0
2	b	3812	0	3690	48	0
3	C	3504	0	3410	50	0
3	c	3504	0	3410	54	0
4	D	2697	0	2596	35	0
4	d	2697	0	2596	34	0
5	E	616	0	602	7	0
5	e	616	0	602	6	0
6	F	228	0	234	3	0
6	f	228	0	234	3	0
7	H	513	0	541	8	0
7	h	513	0	541	8	0
8	I	287	0	306	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	i	287	0	306	6	0
9	J	254	0	266	4	0
9	j	254	0	266	4	0
10	K	302	0	316	4	0
10	k	302	0	316	4	0
11	L	310	0	313	8	0
11	l	310	0	313	3	0
12	M	316	0	319	4	0
12	m	316	0	319	4	0
13	O	1845	0	1841	32	0
13	o	1845	0	1841	31	0
14	T	250	0	268	2	0
14	t	250	0	268	2	0
15	U	713	0	715	11	0
15	u	713	0	715	13	0
16	V	1037	0	1033	13	0
16	v	1037	0	1033	13	0
17	Y	250	0	287	3	0
17	y	250	0	287	4	0
18	X	263	0	301	0	0
18	x	263	0	301	1	0
19	Z	447	0	490	7	0
19	z	447	0	490	6	0
20	Q	1079	0	1068	19	0
20	q	1079	0	1068	19	0
21	W	422	0	377	6	0
21	w	422	0	377	8	0
22	0	155	0	34	0	0
22	5	155	0	34	0	0
23	1	150	0	34	0	0
23	6	150	0	34	0	0
24	2	50	0	12	0	0
24	7	50	0	12	0	0
25	11	1343	0	1306	39	0
25	12	1343	0	1305	38	0
25	13	1343	0	1306	33	0
25	14	1343	0	1306	35	0
25	31	1343	0	1306	39	0
25	32	1343	0	1305	39	0
25	33	1343	0	1306	37	0
25	34	1343	0	1306	34	0
26	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	a	1	0	0	0	0
27	11	530	0	486	23	0
27	12	530	0	482	26	0
27	13	530	0	486	22	0
27	14	530	0	486	20	0
27	31	530	0	486	23	0
27	32	530	0	482	24	0
27	33	530	0	486	26	0
27	34	530	0	486	22	0
27	A	130	0	144	8	0
27	B	1040	0	1152	45	0
27	C	845	0	936	33	0
27	D	260	0	288	11	0
27	M	65	0	67	1	0
27	W	130	0	144	7	0
27	Z	65	0	72	2	0
27	a	130	0	144	7	0
27	b	1040	0	1152	46	0
27	c	845	0	936	33	0
27	d	260	0	288	13	0
27	m	65	0	67	2	0
27	w	130	0	144	5	0
27	z	65	0	72	2	0
28	A	64	0	74	0	0
28	D	64	0	74	2	0
28	a	64	0	74	0	0
28	d	64	0	74	2	0
29	A	80	0	112	2	0
29	B	120	0	168	7	0
29	C	120	0	168	6	0
29	F	40	0	56	2	0
29	H	40	0	56	3	0
29	M	40	0	56	2	0
29	Z	40	0	56	2	0
29	a	80	0	112	2	0
29	b	120	0	168	6	0
29	c	120	0	168	8	0
29	f	40	0	56	2	0
29	h	40	0	56	3	0
29	m	40	0	56	3	0
29	z	40	0	56	2	0
30	A	54	0	77	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B	37	0	37	1	0
30	L	54	0	77	3	0
30	a	54	0	77	0	0
30	b	37	0	37	1	0
30	l	54	0	77	3	0
31	A	4	0	0	1	0
31	a	4	0	0	1	0
32	A	46	0	65	6	0
32	B	49	0	74	0	0
32	L	98	0	148	7	0
32	a	46	0	65	6	0
32	b	49	0	74	0	0
32	l	98	0	148	4	0
33	12	39	0	46	3	0
33	32	39	0	46	3	0
33	B	102	0	143	6	0
33	C	51	0	72	2	0
33	D	51	0	72	1	0
33	M	40	0	50	2	0
33	W	51	0	72	4	0
33	b	102	0	143	4	0
33	d	51	0	72	1	0
33	m	40	0	50	3	0
33	q	51	0	72	1	0
33	w	51	0	72	4	0
34	C	10	0	0	1	0
34	c	10	0	0	1	0
35	C	124	0	162	0	0
35	H	62	0	82	5	0
35	J	62	0	82	0	0
35	c	124	0	162	0	0
35	h	62	0	82	3	0
35	j	62	0	82	2	0
36	D	110	0	157	7	0
36	d	110	0	157	6	0
37	E	43	0	30	2	0
37	V	43	0	30	2	0
37	f	43	0	30	2	0
37	v	43	0	30	2	0
38	11	288	0	0	30	0
38	12	240	0	0	25	0
38	13	336	0	0	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	14	288	0	0	23	0
38	31	288	0	0	29	0
38	32	288	0	0	25	0
38	33	288	0	0	29	0
38	34	288	0	0	26	0
39	12	32	0	34	0	0
39	32	32	0	34	0	0
All	All	70136	0	67738	1088	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 (1088) 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)
25:33:146:PHE:HB3	38:33:302:A86:O5	1.23	1.28
25:11:146:PHE:HB3	38:11:316:A86:O5	1.36	1.24
25:13:146:PHE:HB3	38:13:302:A86:O5	1.36	1.23
25:31:146:PHE:HB3	38:31:316:A86:O5	1.39	1.17
25:33:146:PHE:CB	38:33:302:A86:O5	1.93	1.15
25:11:146:PHE:O	38:11:316:A86:O5	1.62	1.15
25:33:146:PHE:O	38:33:302:A86:O5	1.67	1.11
25:12:146:PHE:HB3	38:12:304:A86:O5	1.47	1.10
25:31:146:PHE:O	38:31:316:A86:O5	1.71	1.07
25:34:146:PHE:HB3	38:34:303:A86:O5	1.54	1.07
25:33:146:PHE:HB3	38:33:302:A86:C38	1.86	1.06
25:32:146:PHE:HB3	38:32:304:A86:O5	1.53	1.05
25:33:188:MET:HE3	38:34:303:A86:O	1.58	1.03
25:11:146:PHE:CB	38:11:316:A86:O5	2.05	1.03
25:34:193:ALA:HA	38:34:301:A86:C39	1.88	1.03
25:13:188:MET:HE3	38:13:317:A86:O	1.60	1.02
25:13:146:PHE:O	38:13:302:A86:O5	1.74	1.02
38:13:317:A86:O5	25:14:146:PHE:HB3	1.58	1.00
25:11:188:MET:HE3	38:12:304:A86:O	1.63	0.99
38:11:316:A86:O	25:14:188:MET:HE3	1.64	0.98
25:13:146:PHE:CB	38:13:302:A86:O5	2.11	0.98
25:31:146:PHE:CB	38:31:316:A86:O5	2.12	0.97
25:31:188:MET:HE3	38:32:304:A86:O	1.64	0.97
25:32:188:MET:HE3	38:33:302:A86:O	1.65	0.97
25:12:188:MET:HE3	38:13:302:A86:O	1.64	0.96
38:31:316:A86:O	25:34:188:MET:HE3	1.63	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:11:146:PHE:HB3	38:11:316:A86:C38	1.96	0.95
25:14:193:ALA:HA	38:14:301:A86:C39	1.96	0.95
27:33:303:CLA:H122	38:33:313:A86:C28	1.97	0.95
27:34:304:CLA:H122	38:34:314:A86:C28	1.98	0.93
27:11:301:CLA:H122	38:11:311:A86:C28	1.99	0.93
25:12:193:ALA:HA	38:13:316:A86:C39	1.99	0.92
27:32:305:CLA:H122	38:32:315:A86:C28	1.99	0.92
25:11:193:ALA:HA	38:11:314:A86:C39	2.00	0.91
27:12:305:CLA:H122	38:12:315:A86:C28	2.01	0.91
27:14:303:CLA:H122	38:14:313:A86:C28	2.00	0.91
27:31:301:CLA:H122	38:31:311:A86:C28	2.00	0.90
25:33:193:ALA:HA	38:33:316:A86:C39	2.03	0.88
27:13:303:CLA:H122	38:13:313:A86:C28	2.03	0.87
25:31:146:PHE:HB3	38:31:316:A86:C38	2.04	0.87
27:33:303:CLA:C12	38:33:313:A86:C28	2.54	0.86
27:34:304:CLA:C12	38:34:314:A86:C28	2.55	0.85
27:32:305:CLA:C12	38:32:315:A86:C28	2.56	0.84
25:33:146:PHE:C	38:33:302:A86:O5	2.20	0.84
27:11:301:CLA:C12	38:11:311:A86:C28	2.56	0.84
25:13:146:PHE:HB3	38:13:302:A86:C38	2.06	0.83
27:14:303:CLA:C12	38:14:313:A86:C28	2.57	0.82
27:31:301:CLA:C12	38:31:311:A86:C28	2.57	0.82
27:12:305:CLA:C12	38:12:315:A86:C28	2.58	0.81
2:B:157:HIS:HE1	27:B:606:CLA:NA	1.79	0.80
25:11:146:PHE:C	38:11:316:A86:O5	2.23	0.80
27:13:303:CLA:C12	38:13:313:A86:C28	2.59	0.80
2:b:157:HIS:HE1	27:b:606:CLA:NA	1.79	0.80
27:14:303:CLA:H72	38:14:313:A86:C28	2.14	0.78
25:32:193:ALA:HA	38:32:318:A86:C39	2.13	0.78
27:31:301:CLA:H72	38:31:311:A86:C28	2.14	0.77
27:11:301:CLA:H72	38:11:311:A86:C28	2.14	0.77
27:12:305:CLA:H72	38:12:315:A86:C28	2.14	0.76
25:12:146:PHE:CB	38:12:304:A86:O5	2.32	0.76
27:34:304:CLA:H72	38:34:314:A86:C28	2.15	0.75
27:13:303:CLA:H72	38:13:313:A86:C28	2.17	0.75
27:33:303:CLA:H72	38:33:313:A86:C28	2.16	0.74
25:31:193:ALA:HA	38:31:314:A86:C39	2.17	0.73
25:12:44:TYR:OH	38:12:315:A86:O5	2.07	0.73
27:32:305:CLA:H72	38:32:315:A86:C28	2.19	0.72
25:13:79:ILE:HG23	38:13:317:A86:C12	2.20	0.71
25:13:146:PHE:C	38:13:302:A86:O5	2.32	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:34:146:PHE:CB	38:34:303:A86:O5	2.37	0.71
4:d:196:HIS:HE1	27:d:405:CLA:NC	1.89	0.70
4:D:196:HIS:HE1	27:D:405:CLA:NC	1.89	0.70
25:13:109:ILE:HG13	38:13:313:A86:O2	1.90	0.70
2:b:320:ALA:HB1	4:d:291:ASN:HD22	1.57	0.70
25:31:146:PHE:C	38:31:316:A86:O5	2.34	0.69
31:a:407:BCT:O3	4:d:267:HIS:CE1	2.44	0.69
27:11:301:CLA:H61	38:11:311:A86:C29	2.23	0.69
31:A:407:BCT:O3	4:D:267:HIS:CE1	2.44	0.69
2:B:320:ALA:HB1	4:D:291:ASN:HD22	1.57	0.69
3:c:209:GLY:HA2	21:w:26:TRP:HE1	1.57	0.69
27:14:303:CLA:H61	38:14:313:A86:C29	2.23	0.69
27:a:404:CLA:H2	33:w:101:LMG:H132	1.75	0.69
28:D:403:PHO:H3A	27:D:405:CLA:H142	1.74	0.69
28:d:403:PHO:H3A	27:d:405:CLA:H142	1.73	0.68
27:12:305:CLA:H61	38:12:315:A86:C29	2.23	0.68
25:13:188:MET:CE	38:13:317:A86:O	2.40	0.68
27:31:301:CLA:H61	38:31:311:A86:C29	2.23	0.68
27:A:404:CLA:H2	33:W:101:LMG:H132	1.75	0.68
25:32:44:TYR:OH	38:32:315:A86:O5	2.09	0.68
3:C:274:LEU:HD21	27:C:509:CLA:HAB	1.75	0.68
25:14:44:TYR:OH	38:14:313:A86:O5	2.10	0.68
25:34:44:TYR:OH	38:34:314:A86:O5	2.12	0.68
2:B:394:GLN:HE21	15:U:17:GLY:HA2	1.59	0.67
3:C:161:ILE:HD13	27:C:513:CLA:HBB1	1.76	0.67
25:11:44:TYR:OH	38:11:311:A86:O5	2.12	0.67
25:31:44:TYR:OH	38:31:311:A86:O5	2.10	0.67
25:33:188:MET:CE	38:34:303:A86:O	2.39	0.67
25:33:146:PHE:CA	38:33:302:A86:O5	2.43	0.67
27:33:303:CLA:H61	38:33:313:A86:C29	2.25	0.67
25:32:79:ILE:HG23	38:33:302:A86:C12	2.25	0.67
27:34:304:CLA:H61	38:34:314:A86:C29	2.24	0.67
3:c:274:LEU:HD21	27:c:509:CLA:HAB	1.75	0.66
25:34:193:ALA:CA	38:34:301:A86:C39	2.69	0.66
3:c:161:ILE:HD13	27:c:513:CLA:HBB1	1.76	0.66
25:33:109:ILE:HG13	38:33:313:A86:O2	1.94	0.66
6:F:42:GLN:HB2	20:Q:72:SER:HB3	1.78	0.66
1:a:140:ARG:NH1	4:d:218:GLU:O	2.29	0.66
2:b:394:GLN:HE21	15:u:17:GLY:HA2	1.60	0.66
13:o:109:GLN:HE21	13:o:113:GLY:HA2	1.61	0.66
25:32:109:ILE:HG13	38:32:315:A86:O2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ARG:NH2	32:A:408:LHG:O5	2.29	0.66
25:34:109:ILE:HG13	38:34:314:A86:O2	1.96	0.66
3:c:130:HIS:HE1	27:c:514:CLA:NA	1.93	0.66
25:13:44:TYR:OH	38:13:313:A86:O5	2.09	0.66
3:C:130:HIS:HE1	27:C:514:CLA:NA	1.93	0.65
13:O:109:GLN:HE21	13:O:113:GLY:HA2	1.61	0.65
27:13:303:CLA:H61	38:13:313:A86:C29	2.26	0.65
25:12:119:GLN:NE2	33:12:301:LMG:O9	2.29	0.65
6:f:42:GLN:HB2	20:q:72:SER:HB3	1.78	0.65
27:34:304:CLA:H121	38:34:314:A86:C28	2.27	0.65
27:33:303:CLA:H121	38:33:313:A86:C28	2.26	0.65
4:D:185:GLN:HB2	27:D:405:CLA:HBC1	1.79	0.65
25:31:188:MET:CE	38:32:304:A86:O	2.44	0.65
38:11:316:A86:O	25:14:188:MET:CE	2.44	0.64
29:C:515:BCR:HC7	19:Z:52:ALA:HB2	1.80	0.64
38:11:314:A86:O3	25:12:90:TYR:O	2.15	0.64
25:14:109:ILE:HG13	38:14:313:A86:O2	1.97	0.64
25:11:109:ILE:HG13	38:11:311:A86:O2	1.97	0.64
3:C:404:SER:O	3:C:416:ASN:ND2	2.31	0.64
3:c:404:SER:O	3:c:416:ASN:ND2	2.31	0.64
27:11:301:CLA:H121	38:11:311:A86:C28	2.27	0.64
25:32:188:MET:CE	38:33:302:A86:O	2.45	0.64
25:11:188:MET:CE	38:12:304:A86:O	2.43	0.64
25:12:109:ILE:HG13	38:12:315:A86:O2	1.98	0.64
4:d:185:GLN:HB2	27:d:405:CLA:HBC1	1.79	0.63
1:a:27:ARG:NH2	14:t:21:VAL:O	2.32	0.63
27:32:305:CLA:H61	38:32:315:A86:C29	2.29	0.63
2:b:142:HIS:HE1	27:b:614:CLA:ND	1.96	0.63
25:31:79:ILE:HG23	38:32:304:A86:C12	2.29	0.63
38:11:316:A86:C12	25:14:79:ILE:HG23	2.29	0.63
3:c:332:PRO:HG2	4:d:349:ASN:HD21	1.64	0.63
25:32:146:PHE:O	38:32:304:A86:O5	2.17	0.63
25:11:90:TYR:O	38:14:301:A86:O3	2.17	0.63
25:31:109:ILE:HG13	38:31:311:A86:O2	1.97	0.63
38:31:316:A86:C12	25:34:79:ILE:HG23	2.29	0.63
1:A:85:SER:HA	1:A:109:GLY:HA3	1.81	0.63
1:A:305:SER:HA	9:J:38:SER:HB3	1.81	0.63
2:B:334:ASP:HB3	13:O:174:ALA:HB1	1.81	0.62
25:12:79:ILE:HG23	38:13:302:A86:C12	2.29	0.62
25:11:79:ILE:HG23	38:12:304:A86:C12	2.29	0.62
27:32:305:CLA:H121	38:32:315:A86:C28	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ARG:HH22	32:A:408:LHG:HC41	1.65	0.62
4:d:179:ARG:NH1	4:d:332:ASP:OD1	2.32	0.62
25:32:146:PHE:CB	38:32:304:A86:O5	2.39	0.62
27:14:303:CLA:H121	38:14:313:A86:C28	2.29	0.62
38:33:314:A86:O	27:34:302:CLA:HAC2	2.00	0.62
27:C:510:CLA:H91	27:C:513:CLA:HBD	1.82	0.62
2:b:334:ASP:HB3	13:o:174:ALA:HB1	1.81	0.62
3:C:106:THR:HA	3:C:109:TYR:HD2	1.65	0.62
27:13:307:CLA:HBA1	38:13:315:A86:C9	2.30	0.61
5:E:24:HIS:CD2	37:E:101:HEM:NC	2.69	0.61
1:a:140:ARG:NH2	32:a:408:LHG:O5	2.33	0.61
27:31:301:CLA:H121	38:31:311:A86:C28	2.29	0.61
3:c:106:THR:HA	3:c:109:TYR:HD2	1.65	0.61
27:12:305:CLA:H121	38:12:315:A86:C28	2.31	0.61
2:B:142:HIS:HE1	27:B:614:CLA:ND	1.96	0.61
27:13:303:CLA:H121	38:13:313:A86:C28	2.29	0.61
25:14:90:TYR:O	38:14:316:A86:O3	2.19	0.61
3:c:377:LYS:NZ	20:q:140:ASP:OD2	2.33	0.61
1:a:85:SER:HA	1:a:109:GLY:HA3	1.81	0.61
27:d:402:CLA:H122	36:d:404:PL9:H23	1.82	0.61
25:31:90:TYR:O	38:34:301:A86:O3	2.19	0.61
38:31:316:A86:O	25:34:188:MET:CE	2.43	0.61
4:D:179:ARG:NH1	4:D:332:ASP:OD1	2.32	0.61
27:c:510:CLA:H91	27:c:513:CLA:HBD	1.82	0.61
27:C:514:CLA:H193	27:Z:102:CLA:H201	1.83	0.61
25:12:188:MET:CE	38:13:302:A86:O	2.44	0.60
16:V:27:LYS:HE2	20:Q:71:TYR:HA	1.83	0.60
27:B:604:CLA:HBB1	27:B:613:CLA:HBC2	1.83	0.60
1:a:140:ARG:HH22	32:a:408:LHG:HC41	1.64	0.60
1:a:341:LEU:H	3:c:311:GLN:HE22	1.48	0.60
5:e:24:HIS:CD2	37:f:102:HEM:NC	2.68	0.60
2:B:153:PHE:HB2	27:B:606:CLA:HBB1	1.83	0.60
27:C:503:CLA:H11	27:C:504:CLA:H171	1.83	0.60
27:33:307:CLA:HBA1	38:33:315:A86:C9	2.31	0.60
27:B:604:CLA:H93	27:B:605:CLA:HAB	1.82	0.60
2:b:153:PHE:HB2	27:b:606:CLA:HBB1	1.83	0.60
27:c:503:CLA:H11	27:c:504:CLA:H171	1.83	0.60
27:b:604:CLA:HBB1	27:b:613:CLA:HBC2	1.83	0.60
25:33:79:ILE:HG23	38:34:303:A86:C12	2.31	0.60
2:B:311:PHE:O	2:B:317:ASN:ND2	2.34	0.60
2:b:311:PHE:O	2:b:317:ASN:ND2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:D:402:CLA:H122	36:D:404:PL9:H23	1.82	0.60
3:C:431:LEU:HD21	27:C:509:CLA:H191	1.84	0.59
27:b:604:CLA:H93	27:b:605:CLA:HAB	1.82	0.59
2:B:469:HIS:HE1	27:B:611:CLA:NA	2.00	0.59
1:A:341:LEU:H	3:C:311:GLN:HE22	1.48	0.59
38:32:316:A86:O	27:33:301:CLA:HAC2	2.02	0.59
1:A:27:ARG:NH2	14:T:21:VAL:O	2.35	0.59
1:A:140:ARG:NH1	4:D:218:GLU:O	2.36	0.59
27:34:308:CLA:HBA1	38:34:316:A86:C9	2.33	0.59
3:c:431:LEU:HD21	27:c:509:CLA:H191	1.84	0.59
27:11:305:CLA:HBA1	38:11:313:A86:C9	2.32	0.59
2:b:469:HIS:HE1	27:b:611:CLA:NA	2.00	0.58
25:32:130:ALA:HB1	27:32:303:CLA:C3B	2.33	0.58
27:c:512:CLA:H151	19:z:17:VAL:HG13	1.85	0.58
25:14:35:LEU:O	25:14:161:ASN:ND2	2.37	0.58
25:33:35:LEU:O	25:33:161:ASN:ND2	2.37	0.58
25:11:35:LEU:O	25:11:161:ASN:ND2	2.37	0.58
25:12:35:LEU:O	25:12:161:ASN:ND2	2.37	0.58
25:34:146:PHE:O	38:34:303:A86:O5	2.22	0.58
29:c:515:BCR:HC7	19:z:52:ALA:HB2	1.86	0.58
38:13:317:A86:O5	25:14:146:PHE:CB	2.45	0.58
25:32:35:LEU:O	25:32:161:ASN:ND2	2.37	0.58
25:32:183:LEU:HD21	38:32:317:A86:C21	2.34	0.58
13:O:120:PHE:HA	13:O:222:GLN:HE22	1.69	0.58
13:o:120:PHE:HA	13:o:222:GLN:HE22	1.69	0.58
25:32:119:GLN:NE2	33:32:301:LMG:O9	2.37	0.58
1:a:82:VAL:HB	1:a:174:LEU:HB2	1.86	0.57
13:o:172:LEU:HB3	13:o:175:LEU:HD23	1.86	0.57
25:14:193:ALA:CA	38:14:301:A86:C39	2.79	0.57
25:34:35:LEU:O	25:34:161:ASN:ND2	2.37	0.57
25:12:146:PHE:O	38:12:304:A86:O5	2.22	0.57
25:31:35:LEU:O	25:31:161:ASN:ND2	2.37	0.57
27:31:315:CLA:HAC2	38:34:315:A86:O	2.05	0.57
3:C:333:THR:O	13:O:150:ARG:NH2	2.38	0.57
13:O:172:LEU:HB3	13:O:175:LEU:HD23	1.86	0.57
27:31:305:CLA:HBA1	38:31:313:A86:C9	2.34	0.57
27:c:503:CLA:HBB2	27:c:511:CLA:H151	1.86	0.57
25:13:35:LEU:O	25:13:161:ASN:ND2	2.37	0.57
25:31:192:TYR:HE1	27:32:308:CLA:HMD3	1.68	0.57
38:33:316:A86:O3	25:34:90:TYR:O	2.23	0.57
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:213:GLU:OE1	13:o:243:TYR:OH	2.23	0.57
25:11:146:PHE:CA	38:11:316:A86:O5	2.53	0.57
38:12:316:A86:O	27:13:301:CLA:HAC2	2.04	0.57
3:c:77:LYS:HB2	3:c:82:GLN:HE21	1.70	0.57
27:c:512:CLA:H42	17:y:34:LEU:HA	1.87	0.57
32:l:103:LHG:H312	12:m:18:PRO:HB3	1.87	0.57
30:L:103:SQD:H101	29:m:103:BCR:H24C	1.87	0.56
27:11:315:CLA:HAC2	38:14:314:A86:O	2.04	0.56
25:13:193:ALA:HA	38:14:316:A86:C39	2.35	0.56
27:14:307:CLA:HBA1	38:14:315:A86:C9	2.34	0.56
8:I:5:LYS:NZ	21:W:30:ASP:OD2	2.39	0.56
32:a:408:LHG:H202	27:c:511:CLA:H52	1.88	0.56
8:i:5:LYS:NZ	21:w:30:ASP:OD2	2.38	0.56
25:33:44:TYR:OH	38:33:313:A86:O5	2.19	0.56
4:D:334:PRO:HG2	5:E:66:LEU:HD21	1.87	0.56
29:M:101:BCR:H24C	30:l:101:SQD:H101	1.87	0.56
27:12:309:CLA:HBA1	38:12:317:A86:C9	2.36	0.56
38:31:312:A86:O	27:32:303:CLA:HAC2	2.04	0.56
3:c:333:THR:O	13:o:150:ARG:NH2	2.39	0.56
38:11:312:A86:O	27:12:303:CLA:HAC2	2.05	0.56
27:32:309:CLA:HBA1	38:32:317:A86:C9	2.35	0.56
13:O:213:GLU:OE1	13:O:243:TYR:OH	2.23	0.56
2:b:127:ARG:NH2	7:h:18:TYR:O	2.39	0.56
3:c:451:ALA:O	8:i:33:ASN:ND2	2.39	0.55
27:C:503:CLA:HBB2	27:C:511:CLA:H151	1.86	0.55
16:v:27:LYS:HE2	20:q:71:TYR:HA	1.88	0.55
25:34:146:PHE:HB3	38:34:303:A86:C38	2.34	0.55
3:C:77:LYS:HB2	3:C:82:GLN:HE21	1.70	0.55
14:T:3:ALA:HA	14:T:6:TYR:HD2	1.71	0.55
2:B:422:ARG:NH2	13:O:167:ASP:OD2	2.40	0.55
27:12:305:CLA:H41	38:12:315:A86:C29	2.37	0.55
25:14:162:VAL:HG11	27:14:310:CLA:HAA2	1.89	0.55
25:32:162:VAL:HG11	27:32:312:CLA:HAA2	1.89	0.55
4:D:53:PHE:HA	4:D:67:LEU:HD13	1.88	0.55
7:H:4:ARG:HH11	7:H:9:GLU:HG2	1.72	0.55
20:Q:134:GLU:OE1	20:Q:137:ASN:ND2	2.39	0.55
4:d:334:PRO:HG2	5:e:66:LEU:HD21	1.87	0.55
7:h:4:ARG:HH11	7:h:9:GLU:HG2	1.72	0.55
30:l:101:SQD:H102	27:m:101:CLA:H43	1.89	0.55
25:34:162:VAL:HG11	27:34:311:CLA:HAA2	1.89	0.55
30:L:103:SQD:H102	27:M:102:CLA:H43	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:188:ASP:OD2	2:b:194:ASN:ND2	2.40	0.55
20:q:134:GLU:OE1	20:q:137:ASN:ND2	2.39	0.55
25:31:162:VAL:HG11	27:31:308:CLA:HAA2	1.88	0.55
14:t:3:ALA:HA	14:t:6:TYR:HD2	1.71	0.55
25:12:162:VAL:HG11	27:12:312:CLA:HAA2	1.89	0.55
2:B:188:ASP:OD2	2:B:194:ASN:ND2	2.40	0.55
2:b:422:ARG:NH2	13:o:167:ASP:OD2	2.40	0.55
4:d:53:PHE:HA	4:d:67:LEU:HD13	1.88	0.55
25:13:90:TYR:O	38:13:316:A86:O3	2.25	0.55
38:13:314:A86:O	27:14:302:CLA:HAC2	2.07	0.55
2:B:127:ARG:NH2	7:H:18:TYR:O	2.39	0.54
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.88	0.54
38:32:318:A86:O3	25:33:90:TYR:O	2.25	0.54
3:C:332:PRO:HG2	4:D:349:ASN:HD21	1.72	0.54
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.88	0.54
25:13:162:VAL:HG11	27:13:310:CLA:HAA2	1.89	0.54
25:11:162:VAL:HG11	27:11:308:CLA:HAA2	1.89	0.54
38:13:317:A86:O5	25:14:146:PHE:O	2.25	0.54
38:31:314:A86:O3	25:32:90:TYR:O	2.26	0.54
3:C:214:SER:HB2	33:W:101:LMG:HC72	1.90	0.53
3:C:309:GLN:OE1	3:C:353:THR:OG1	2.27	0.53
25:33:146:PHE:HB3	38:33:302:A86:C39	2.36	0.53
27:14:303:CLA:H41	38:14:313:A86:C29	2.39	0.53
25:34:183:LEU:HD21	38:34:316:A86:C21	2.38	0.53
2:B:384:ARG:NH1	15:U:98:ASN:O	2.42	0.53
27:C:512:CLA:H151	19:Z:17:VAL:HG13	1.90	0.53
4:D:171:SER:HB2	4:D:176:ALA:HB1	1.90	0.53
25:13:65:ARG:NH1	25:13:138:ASP:O	2.42	0.53
25:14:183:LEU:HD21	38:14:315:A86:C21	2.38	0.53
25:31:65:ARG:NH1	25:31:138:ASP:O	2.42	0.53
27:31:301:CLA:H41	38:31:311:A86:C29	2.39	0.53
25:33:162:VAL:HG11	27:33:310:CLA:HAA2	1.89	0.53
3:C:366:PRO:HA	20:Q:140:ASP:HB2	1.90	0.53
25:12:183:LEU:HD21	38:12:317:A86:C21	2.38	0.53
27:B:607:CLA:H42	33:B:618:LMG:H152	1.91	0.53
25:12:65:ARG:NH1	25:12:138:ASP:O	2.42	0.53
1:a:142:TRP:HZ2	3:c:445:ARG:HB2	1.73	0.53
1:a:328:ILE:HG23	4:d:320:LEU:HD22	1.91	0.53
13:o:46:GLU:HB3	13:o:78:THR:HG23	1.91	0.53
25:11:183:LEU:HD21	38:11:313:A86:C21	2.38	0.53
27:11:304:CLA:HAA2	27:11:315:CLA:H192	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:34:65:ARG:NH1	25:34:138:ASP:O	2.42	0.53
32:a:408:LHG:H281	32:a:408:LHG:H181	1.91	0.53
27:13:303:CLA:H41	38:13:313:A86:C29	2.39	0.53
2:b:23:HIS:CD2	27:b:612:CLA:NA	2.77	0.53
30:B:620:SQD:H2	1:a:102:ILE:HD12	1.91	0.53
10:k:26:ILE:HD11	17:y:16:ILE:HD13	1.91	0.53
25:14:65:ARG:NH1	25:14:138:ASP:O	2.42	0.53
27:B:622:CLA:HAC1	27:32:310:CLA:HBB1	1.91	0.53
13:O:74:ARG:NH1	21:W:21:GLU:OE2	2.43	0.53
16:V:36:THR:HA	16:V:103:ARG:HD3	1.91	0.53
3:c:128:ILE:HG22	19:z:24:LEU:HD12	1.90	0.53
25:31:183:LEU:HD21	38:31:313:A86:C21	2.38	0.53
25:33:183:LEU:HD21	38:33:315:A86:C21	2.39	0.53
3:C:51:HIS:CD2	27:C:510:CLA:NA	2.78	0.52
27:b:607:CLA:H42	33:b:618:LMG:H152	1.90	0.52
25:32:65:ARG:NH1	25:32:138:ASP:O	2.42	0.52
3:c:74:VAL:O	3:c:82:GLN:NE2	2.32	0.52
4:d:47:TRP:NE1	4:d:172:PHE:O	2.32	0.52
25:33:65:ARG:NH1	25:33:138:ASP:O	2.42	0.52
27:c:514:CLA:H193	27:z:102:CLA:H201	1.91	0.52
27:11:301:CLA:H41	38:11:311:A86:C29	2.39	0.52
1:A:328:ILE:HG23	4:D:320:LEU:HD22	1.91	0.52
3:c:51:HIS:CD2	27:c:510:CLA:NA	2.78	0.52
27:c:509:CLA:H192	33:q:301:LMG:H412	1.92	0.52
25:11:65:ARG:NH1	25:11:138:ASP:O	2.42	0.52
2:B:23:HIS:CD2	27:B:612:CLA:NA	2.77	0.52
25:11:193:ALA:CA	38:11:314:A86:C39	2.82	0.52
10:K:26:ILE:HD11	17:Y:16:ILE:HD13	1.91	0.52
5:E:58:THR:O	5:E:62:GLN:NE2	2.43	0.52
13:O:46:GLU:HB3	13:O:78:THR:HG23	1.91	0.52
27:b:622:CLA:HAC1	27:12:310:CLA:HBB1	1.91	0.52
3:c:309:GLN:OE1	3:c:353:THR:OG1	2.26	0.52
25:12:193:ALA:CA	38:13:316:A86:C39	2.82	0.52
32:A:408:LHG:H181	32:A:408:LHG:H281	1.91	0.52
11:L:25:ILE:HD13	12:M:18:PRO:HB2	1.92	0.52
13:O:7:ASN:HB3	20:Q:134:GLU:HG2	1.92	0.52
13:O:207:VAL:HG13	13:O:214:ILE:HG22	1.92	0.52
4:d:278:LEU:HD22	28:d:403:PHO:HBC3	1.92	0.52
5:e:58:THR:O	5:e:62:GLN:NE2	2.43	0.52
13:o:7:ASN:HB3	20:q:134:GLU:HG2	1.92	0.52
25:12:130:ALA:HB1	27:12:303:CLA:C3B	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:509:CLA:H192	33:C:519:LMG:H412	1.92	0.52
4:d:171:SER:HB2	4:d:176:ALA:HB1	1.90	0.52
33:12:301:LMG:HC71	27:12:308:CLA:HBC3	1.91	0.52
16:v:36:THR:HA	16:v:103:ARG:HD3	1.91	0.51
16:V:28:ARG:NH1	16:V:111:ASP:OD1	2.44	0.51
16:v:28:ARG:NH1	16:v:111:ASP:OD1	2.44	0.51
3:c:389:ARG:NH2	20:q:147:TYR:OH	2.38	0.51
25:33:69:ARG:NE	25:33:163:GLU:OE2	2.38	0.51
27:B:607:CLA:H43	33:B:618:LMG:H311	1.93	0.51
3:C:197:ILE:HG13	3:C:232:ILE:HG13	1.93	0.51
16:V:8:ARG:NH1	16:V:21:LEU:O	2.39	0.51
27:12:303:CLA:H192	27:12:308:CLA:HAA2	1.93	0.51
25:13:69:ARG:NE	25:13:163:GLU:OE2	2.38	0.51
27:34:304:CLA:H41	38:34:314:A86:C29	2.41	0.51
1:A:301:ASN:H	3:C:403:ASN:HD21	1.59	0.51
2:b:55:MET:HE1	2:b:67:THR:HG21	1.92	0.51
4:d:309:GLU:OE2	13:o:231:LYS:NZ	2.40	0.51
32:L:102:LHG:H312	12:M:18:PRO:HB3	1.92	0.51
2:b:454:GLY:HA2	33:b:618:LMG:H212	1.92	0.51
25:11:69:ARG:NE	25:11:163:GLU:OE2	2.38	0.51
25:12:146:PHE:HB3	38:12:304:A86:C38	2.30	0.51
3:c:197:ILE:HG13	3:c:232:ILE:HG13	1.93	0.51
25:13:183:LEU:HD21	38:13:315:A86:C21	2.40	0.51
25:31:81:HIS:HE1	27:31:303:CLA:NB	2.09	0.51
25:34:81:HIS:HE1	27:34:306:CLA:NB	2.08	0.51
2:B:55:MET:HE1	2:B:67:THR:HG21	1.92	0.51
27:c:509:CLA:H193	27:c:511:CLA:H112	1.93	0.51
25:12:81:HIS:HE1	27:12:307:CLA:NB	2.08	0.51
27:B:602:CLA:H203	35:H:102:DGD:HA72	1.93	0.51
27:b:607:CLA:H43	33:b:618:LMG:H311	1.93	0.50
25:13:81:HIS:HE1	27:13:305:CLA:NB	2.09	0.50
25:11:142:GLY:O	25:14:158:ARG:NH1	2.44	0.50
25:31:69:ARG:NE	25:31:163:GLU:OE2	2.38	0.50
20:Q:115:VAL:O	20:Q:119:THR:OG1	2.28	0.50
25:11:81:HIS:HE1	27:11:303:CLA:NB	2.09	0.50
2:B:60:MET:HB3	2:B:63:MET:HB3	1.94	0.50
2:B:454:GLY:HA2	33:B:618:LMG:H212	1.92	0.50
27:B:604:CLA:H112	27:B:614:CLA:H42	1.94	0.50
1:A:142:TRP:HZ2	3:C:445:ARG:HB2	1.76	0.50
36:D:407:PL9:H401	32:L:101:LHG:H223	1.94	0.50
3:c:406:GLY:H	3:c:415:VAL:HG23	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:33:81:HIS:HE1	27:33:305:CLA:NB	2.08	0.50
25:11:146:PHE:HB3	38:11:316:A86:C39	2.42	0.50
1:A:214:MET:HE3	1:A:218:LEU:HD11	1.93	0.50
27:a:404:CLA:HAA2	33:w:101:LMG:H111	1.93	0.50
27:b:602:CLA:H71	7:h:46:LEU:HD12	1.94	0.50
13:o:207:VAL:HG13	13:o:214:ILE:HG22	1.92	0.50
25:14:81:HIS:HE1	27:14:305:CLA:NB	2.09	0.50
4:d:154:SER:HA	4:d:158:LEU:HB2	1.94	0.50
27:B:602:CLA:H71	7:H:46:LEU:HD12	1.93	0.50
8:I:13:ILE:HD12	21:W:38:LEU:HD22	1.94	0.50
3:c:214:SER:HB2	33:w:101:LMG:HC72	1.93	0.50
3:c:366:PRO:HA	20:q:140:ASP:HB2	1.94	0.50
15:u:48:LYS:NZ	15:u:66:GLY:O	2.37	0.50
2:B:341:LEU:HD12	2:B:429:VAL:HG12	1.94	0.49
3:C:451:ALA:O	8:I:33:ASN:ND2	2.45	0.49
3:c:267:GLU:OE2	3:c:442:HIS:ND1	2.40	0.49
27:11:315:CLA:O1D	25:14:165:ASN:ND2	2.39	0.49
25:32:81:HIS:HE1	27:32:307:CLA:NB	2.09	0.49
25:34:41:LEU:CD1	38:34:315:A86:C22	2.90	0.49
27:A:404:CLA:HAA2	33:W:101:LMG:H111	1.93	0.49
3:C:406:GLY:H	3:C:415:VAL:HG23	1.77	0.49
3:C:462:GLU:OE2	4:D:247:THR:OG1	2.29	0.49
4:D:154:SER:HA	4:D:158:LEU:HB2	1.94	0.49
13:O:150:ARG:HB2	13:O:228:MET:HE3	1.94	0.49
25:32:49:TRP:HH2	38:32:317:A86:C39	2.25	0.49
27:C:509:CLA:H193	27:C:511:CLA:H112	1.93	0.49
27:b:614:CLA:H91	27:b:614:CLA:H171	1.94	0.49
5:e:19:ARG:NH1	37:f:102:HEM:O2A	2.45	0.49
25:14:41:LEU:CD1	38:14:314:A86:C22	2.91	0.49
27:b:602:CLA:H203	35:h:102:DGD:HA72	1.94	0.49
13:o:150:ARG:HB2	13:o:228:MET:HE3	1.94	0.49
25:12:41:LEU:CD1	38:12:316:A86:C22	2.90	0.49
27:12:305:CLA:HMC1	38:12:315:A86:C24	2.43	0.49
27:B:614:CLA:H91	27:B:614:CLA:H171	1.94	0.49
27:11:304:CLA:HMD3	25:14:192:TYR:HE1	1.78	0.49
17:y:9:GLN:NE2	20:q:89:TYR:OH	2.45	0.49
25:13:49:TRP:HH2	38:13:315:A86:C39	2.25	0.49
2:B:2:ALA:N	11:L:10:ALA:O	2.46	0.49
2:B:179:GLN:NE2	7:H:66:ILE:O	2.46	0.49
4:D:208:LEU:HD13	27:D:401:CLA:H42	1.93	0.49
25:11:41:LEU:CD1	38:11:312:A86:C22	2.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:33:303:CLA:H41	38:33:313:A86:C29	2.43	0.49
3:C:101:GLY:HA3	3:C:298:GLU:HB3	1.95	0.49
17:Y:9:GLN:NE2	20:Q:89:TYR:OH	2.46	0.49
1:a:214:MET:HE3	1:a:218:LEU:HD11	1.93	0.49
3:c:101:GLY:HA3	3:c:298:GLU:HB3	1.95	0.49
3:C:74:VAL:O	3:C:82:GLN:NE2	2.32	0.49
13:o:72:MET:HE1	13:o:115:ARG:HG2	1.95	0.49
4:D:162:GLY:HA3	4:D:289:ALA:HB1	1.94	0.49
2:b:60:MET:HB3	2:b:63:MET:HB3	1.94	0.49
27:b:604:CLA:H112	27:b:614:CLA:H42	1.94	0.49
25:31:41:LEU:CD1	38:31:312:A86:C22	2.91	0.49
5:E:19:ARG:NH1	37:E:101:HEM:O2A	2.45	0.48
3:c:77:LYS:HE3	3:c:82:GLN:HG2	1.95	0.48
16:v:8:ARG:NH1	16:v:21:LEU:O	2.39	0.48
25:13:145:TYR:HB2	27:13:309:CLA:HAA1	1.95	0.48
25:31:145:TYR:HB2	27:31:307:CLA:HAA1	1.95	0.48
33:32:301:LMG:HC71	27:32:308:CLA:HBC3	1.95	0.48
3:C:209:GLY:HA2	21:W:26:TRP:HE1	1.78	0.48
33:M:103:LMG:O5	33:M:103:LMG:O4	2.26	0.48
16:V:9:THR:O	16:V:124:LYS:NZ	2.46	0.48
1:a:70:SER:O	1:a:75:ASN:ND2	2.43	0.48
2:b:64:PRO:HB3	2:b:267:LEU:HB3	1.96	0.48
27:w:103:CLA:H162	27:w:103:CLA:H122	1.53	0.48
25:12:165:ASN:ND2	27:13:301:CLA:O1D	2.39	0.48
25:14:145:TYR:HB2	27:14:309:CLA:HAA1	1.95	0.48
13:O:72:MET:HE1	13:O:115:ARG:HG2	1.95	0.48
2:b:341:LEU:HD12	2:b:429:VAL:HG12	1.94	0.48
15:u:12:ASP:OD1	15:u:12:ASP:N	2.42	0.48
25:32:165:ASN:ND2	27:33:301:CLA:O1D	2.39	0.48
2:B:157:HIS:HE1	27:B:606:CLA:C1A	2.27	0.48
2:b:179:GLN:NE2	7:h:66:ILE:O	2.46	0.48
36:d:407:PL9:H401	32:l:102:LHG:H223	1.94	0.48
15:u:58:VAL:HA	15:u:61:LEU:HD23	1.95	0.48
25:13:146:PHE:CA	38:13:302:A86:O5	2.60	0.48
25:31:158:ARG:NH1	25:32:142:GLY:O	2.46	0.48
25:32:145:TYR:HB2	27:32:311:CLA:HAA1	1.96	0.48
2:B:256:MET:O	2:B:448:ARG:NH1	2.45	0.48
2:B:155:ALA:O	2:B:159:THR:OG1	2.31	0.48
3:C:254:PRO:O	3:C:259:ARG:NH1	2.47	0.48
3:c:211:VAL:O	3:c:221:TRP:NE1	2.38	0.48
3:c:254:PRO:O	3:c:259:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:9:THR:O	16:v:124:LYS:NZ	2.47	0.48
25:11:145:TYR:HB2	27:11:307:CLA:HAA1	1.95	0.48
25:12:49:TRP:HH2	38:12:317:A86:C39	2.27	0.48
27:32:303:CLA:H192	27:32:308:CLA:HAA2	1.95	0.48
27:32:305:CLA:H41	38:32:315:A86:C29	2.44	0.48
3:C:77:LYS:HE3	3:C:82:GLN:HG2	1.95	0.48
3:C:254:PRO:HA	27:C:507:CLA:HED3	1.96	0.48
3:C:377:LYS:NZ	20:Q:140:ASP:OD2	2.46	0.48
11:L:16:THR:HG23	32:L:101:LHG:HC62	1.96	0.48
13:o:21:ASN:ND2	13:o:75:GLN:OE1	2.44	0.48
30:L:103:SQD:H222	29:b:616:BCR:H19C	1.95	0.48
16:V:49:ASN:ND2	37:V:201:HEM:O1D	2.47	0.48
4:d:162:GLY:HA3	4:d:289:ALA:HB1	1.94	0.48
21:w:42:HIS:CD2	27:w:102:CLA:ND	2.81	0.48
21:w:67:ASP:OD1	21:w:67:ASP:N	2.47	0.48
27:32:305:CLA:HMC1	38:32:315:A86:C24	2.43	0.48
3:C:332:PRO:HA	13:O:151:THR:HB	1.96	0.48
21:W:42:HIS:CD2	27:W:102:CLA:ND	2.81	0.48
1:A:70:SER:O	1:A:75:ASN:ND2	2.43	0.48
1:A:102:ILE:HD12	30:b:620:SQD:H2	1.96	0.48
15:U:58:VAL:HA	15:U:61:LEU:HD23	1.95	0.48
8:i:13:ILE:HD12	21:w:38:LEU:HD22	1.95	0.48
25:12:145:TYR:HB2	27:12:311:CLA:HAA1	1.95	0.48
25:34:41:LEU:HD11	38:34:315:A86:C22	2.44	0.48
2:b:157:HIS:HE1	27:b:606:CLA:C1A	2.27	0.47
3:c:355:ARG:NH2	34:c:501:OEX:O4	2.47	0.47
37:v:201:HEM:HBC2	37:v:201:HEM:HHH	1.96	0.47
20:q:102:LYS:O	20:q:105:ASN:ND2	2.47	0.47
25:33:145:TYR:HB2	27:33:309:CLA:HAA1	1.96	0.47
3:C:355:ARG:NH2	34:C:501:OEX:O4	2.47	0.47
20:q:105:ASN:HB2	20:q:108:TYR:HD2	1.79	0.47
27:31:315:CLA:O1D	25:34:165:ASN:ND2	2.40	0.47
2:B:243:SER:HA	2:B:246:PHE:CE1	2.50	0.47
20:Q:105:ASN:HB2	20:Q:108:TYR:HD2	1.79	0.47
2:b:51:VAL:HG13	2:b:308:LYS:HB2	1.97	0.47
16:v:49:ASN:ND2	37:v:201:HEM:O1D	2.47	0.47
13:O:47:PRO:HA	13:O:240:GLY:HA3	1.96	0.47
27:W:103:CLA:H162	27:W:103:CLA:H122	1.53	0.47
2:b:155:ALA:O	2:b:159:THR:OG1	2.31	0.47
25:32:158:ARG:NH1	25:33:142:GLY:O	2.48	0.47
27:B:608:CLA:HBB2	4:D:122:ILE:HG12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:155:VAL:HG22	4:D:285:ILE:HG12	1.97	0.47
10:K:13:TYR:HE1	19:Z:6:VAL:HG21	1.80	0.47
20:Q:102:LYS:O	20:Q:105:ASN:ND2	2.47	0.47
27:b:610:CLA:H43	27:b:612:CLA:H51	1.97	0.47
27:14:303:CLA:HMC1	38:14:313:A86:C24	2.44	0.47
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.97	0.47
27:C:507:CLA:H203	27:C:507:CLA:H122	1.96	0.47
9:J:14:LEU:HD11	17:Y:21:PRO:HB3	1.97	0.47
16:V:89:ALA:O	16:V:97:SER:OG	2.31	0.47
25:11:158:ARG:NH1	25:12:142:GLY:O	2.47	0.47
25:33:41:LEU:CD1	38:33:314:A86:C22	2.92	0.47
25:34:145:TYR:HB2	27:34:310:CLA:HAA1	1.96	0.47
2:B:64:PRO:HB3	2:B:267:LEU:HB3	1.96	0.47
29:B:616:BCR:H19C	30:l:101:SQD:H222	1.95	0.47
12:M:32:ARG:NH1	12:m:41:ASP:O	2.48	0.47
29:a:409:BCR:H342	32:l:102:LHG:H362	1.97	0.47
3:c:254:PRO:HA	27:c:507:CLA:HED3	1.96	0.47
27:c:507:CLA:H203	27:c:507:CLA:H122	1.96	0.47
4:d:155:VAL:HG22	4:d:285:ILE:HG12	1.97	0.47
27:13:307:CLA:HBA1	38:13:315:A86:C10	2.45	0.47
25:14:41:LEU:HD11	38:14:314:A86:C22	2.45	0.47
27:31:301:CLA:HMC1	38:31:311:A86:C24	2.44	0.47
27:31:304:CLA:HAA2	27:31:315:CLA:H192	1.96	0.47
25:33:45:ASP:OD1	25:33:45:ASP:N	2.48	0.47
25:33:49:TRP:HH2	38:33:315:A86:C39	2.28	0.47
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.97	0.47
3:C:267:GLU:OE2	3:C:442:HIS:ND1	2.40	0.47
4:D:53:PHE:O	5:E:50:THR:OG1	2.28	0.47
4:D:278:LEU:HD22	28:D:403:PHO:HBC3	1.95	0.47
1:a:95:PRO:HD2	1:a:98:GLU:HB2	1.97	0.47
27:13:303:CLA:HMC1	38:13:313:A86:C24	2.45	0.47
25:14:49:TRP:HH2	38:14:315:A86:C39	2.28	0.47
25:33:41:LEU:HD11	38:33:314:A86:C22	2.45	0.47
27:34:304:CLA:HMC1	38:34:314:A86:C24	2.45	0.47
27:B:610:CLA:H43	27:B:612:CLA:H51	1.97	0.47
27:B:612:CLA:H102	27:B:612:CLA:H61	1.59	0.47
1:a:162:PRO:HB3	1:a:168:PHE:HA	1.97	0.47
13:o:193:PHE:HB2	15:u:90:ASP:HB3	1.97	0.47
25:11:41:LEU:HD11	38:11:312:A86:C22	2.45	0.47
27:12:306:CLA:HBC1	27:12:310:CLA:HBC2	1.97	0.47
3:C:274:LEU:HD22	3:C:435:PHE:HD1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:334:ASP:OD1	2:b:334:ASP:N	2.47	0.47
3:c:64:ALA:HB1	10:k:23:LEU:HB3	1.97	0.47
13:o:47:PRO:HA	13:o:240:GLY:HA3	1.96	0.47
20:q:154:ARG:NH2	20:q:167:GLU:OE2	2.47	0.47
25:11:45:ASP:N	25:11:45:ASP:OD1	2.48	0.47
27:11:302:CLA:HBC1	27:11:306:CLA:HBC2	1.97	0.47
2:b:30:VAL:HG11	27:b:612:CLA:H112	1.97	0.46
27:b:608:CLA:HBB2	4:d:122:ILE:HG12	1.95	0.46
27:c:502:CLA:HBB1	29:c:516:BCR:H21C	1.97	0.46
25:31:41:LEU:HD11	38:31:312:A86:C22	2.45	0.46
25:31:49:TRP:HH2	38:31:313:A86:C39	2.28	0.46
27:34:305:CLA:HBC1	27:34:309:CLA:HBC2	1.97	0.46
32:A:408:LHG:H202	27:C:511:CLA:H52	1.98	0.46
2:b:243:SER:HA	2:b:246:PHE:CE1	2.50	0.46
10:k:21:ASP:OD2	20:q:89:TYR:OH	2.24	0.46
27:33:304:CLA:HBC1	27:33:308:CLA:HBC2	1.97	0.46
2:B:192:PRO:HG3	7:H:49:TYR:CD1	2.50	0.46
2:b:192:PRO:HG3	7:h:49:TYR:CD1	2.50	0.46
27:11:301:CLA:HMC1	38:11:311:A86:C24	2.45	0.46
25:12:45:ASP:OD1	25:12:45:ASP:N	2.48	0.46
2:B:30:VAL:HG11	27:B:612:CLA:H112	1.97	0.46
27:11:301:CLA:H3A	27:11:301:CLA:HBA2	1.38	0.46
27:32:306:CLA:HBC1	27:32:310:CLA:HBC2	1.97	0.46
20:Q:162:GLN:HE21	20:Q:206:LEU:HD13	1.80	0.46
27:a:404:CLA:HBB2	8:i:15:PHE:HB2	1.98	0.46
3:c:89:HIS:NE2	27:c:503:CLA:O1D	2.44	0.46
15:u:50:VAL:HG13	15:u:95:ARG:HB3	1.97	0.46
25:12:41:LEU:HD11	38:12:316:A86:C22	2.45	0.46
25:13:45:ASP:OD1	25:13:45:ASP:N	2.48	0.46
27:33:303:CLA:HMC1	38:33:313:A86:C24	2.46	0.46
27:B:602:CLA:H62	27:B:602:CLA:H41	1.66	0.46
27:B:613:CLA:H41	27:B:613:CLA:H62	1.72	0.46
3:C:89:HIS:NE2	27:C:503:CLA:O1D	2.44	0.46
2:b:2:ALA:N	11:l:10:ALA:O	2.49	0.46
27:b:602:CLA:H62	27:b:602:CLA:H41	1.66	0.46
27:d:402:CLA:H143	27:d:405:CLA:H172	1.98	0.46
20:q:162:GLN:HE21	20:q:206:LEU:HD13	1.80	0.46
27:14:304:CLA:HBC1	27:14:308:CLA:HBC2	1.97	0.46
27:C:502:CLA:HBB1	29:C:516:BCR:H21C	1.97	0.46
16:v:89:ALA:O	16:v:97:SER:OG	2.31	0.46
25:32:69:ARG:NE	25:32:163:GLU:OE2	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:34:64:GLU:OE2	25:34:168:ARG:NE	2.49	0.46
1:A:95:PRO:HD2	1:A:98:GLU:HB2	1.97	0.46
4:D:262:ASN:HB3	4:D:265:TRP:HB3	1.98	0.46
4:d:191:THR:HG23	27:d:405:CLA:HBC2	1.98	0.46
25:32:61:ARG:NH2	27:32:305:CLA:O1D	2.40	0.46
27:33:301:CLA:H192	27:33:306:CLA:HAA2	1.97	0.46
25:34:45:ASP:OD1	25:34:45:ASP:N	2.48	0.46
29:A:409:BCR:H342	32:L:101:LHG:H362	1.97	0.46
29:B:616:BCR:H15C	29:B:616:BCR:H351	1.82	0.46
27:C:504:CLA:H193	27:C:511:CLA:HBB2	1.97	0.46
6:F:43:ARG:NH2	9:J:39:LEU:OXT	2.49	0.46
37:V:201:HEM:HBC2	37:V:201:HEM:HHD	1.96	0.46
2:b:114:HIS:CE1	27:b:615:CLA:ND	2.83	0.46
3:c:274:LEU:HD22	3:c:435:PHE:HD1	1.79	0.46
27:c:502:CLA:H122	27:c:508:CLA:H61	1.98	0.46
27:w:103:CLA:H2	27:w:103:CLA:HAA1	1.98	0.46
25:12:64:GLU:OE2	25:12:168:ARG:NE	2.49	0.46
25:31:45:ASP:N	25:31:45:ASP:OD1	2.48	0.46
25:32:41:LEU:CD1	38:32:316:A86:C22	2.94	0.46
29:A:409:BCR:H15C	29:A:409:BCR:H351	1.84	0.46
2:B:114:HIS:CE1	27:B:615:CLA:ND	2.83	0.46
2:B:237:VAL:HG22	27:B:610:CLA:HBC2	1.98	0.46
16:V:43:GLY:O	16:V:131:GLY:N	2.44	0.46
1:a:301:ASN:ND2	3:c:411:GLU:O	2.45	0.46
36:d:404:PL9:H28	36:d:404:PL9:H322	1.77	0.46
27:13:301:CLA:H151	27:13:306:CLA:HBA1	1.96	0.46
27:13:304:CLA:HBC1	27:13:308:CLA:HBC2	1.97	0.46
25:32:64:GLU:OE2	25:32:168:ARG:NE	2.49	0.46
25:33:165:ASN:ND2	27:34:302:CLA:O1D	2.35	0.46
27:A:404:CLA:HBB2	8:I:15:PHE:HB2	1.97	0.45
15:U:50:VAL:HG13	15:U:95:ARG:HB3	1.97	0.45
2:b:160:GLY:HA3	2:b:180:PRO:HB3	1.98	0.45
27:c:513:CLA:H3A	27:c:513:CLA:HBA1	1.54	0.45
2:B:283:GLU:OE2	2:B:286:ARG:NH2	2.46	0.45
11:L:20:TRP:HH2	32:L:101:LHG:H101	1.80	0.45
1:a:188:ALA:HB2	1:a:328:ILE:HB	1.98	0.45
29:f:101:BCR:H20C	29:f:101:BCR:H361	1.78	0.45
25:14:45:ASP:N	25:14:45:ASP:OD1	2.48	0.45
25:32:45:ASP:OD1	25:32:45:ASP:N	2.48	0.45
2:B:464:PHE:HD2	27:B:611:CLA:HAC2	1.80	0.45
2:b:283:GLU:OE2	2:b:286:ARG:NH2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:464:PHE:HD2	27:b:611:CLA:HAC2	1.80	0.45
19:z:10:VAL:HG13	29:z:101:BCR:HC21	1.99	0.45
25:12:69:ARG:NE	25:12:163:GLU:OE2	2.38	0.45
27:13:303:CLA:H3A	27:13:303:CLA:HBA2	1.38	0.45
1:A:301:ASN:OD1	1:A:303:ASN:ND2	2.50	0.45
27:A:404:CLA:H171	27:C:507:CLA:H41	1.97	0.45
2:B:334:ASP:N	2:B:334:ASP:OD1	2.47	0.45
4:D:191:THR:HG23	27:D:405:CLA:HBC2	1.98	0.45
13:O:21:ASN:ND2	13:O:75:GLN:OE1	2.44	0.45
1:a:272:HIS:CD2	4:d:213:HIS:NE2	2.84	0.45
27:b:613:CLA:H41	27:b:613:CLA:H62	1.72	0.45
4:d:208:LEU:HD13	27:d:401:CLA:H42	1.97	0.45
25:11:49:TRP:HH2	38:11:313:A86:C39	2.30	0.45
27:31:302:CLA:HBC1	27:31:306:CLA:HBC2	1.97	0.45
2:B:298:GLU:OE2	2:B:302:TRP:NE1	2.46	0.45
35:H:102:DGD:O5D	35:H:102:DGD:O4D	2.25	0.45
8:I:6:ILE:HG23	21:W:37:VAL:HG21	1.99	0.45
1:a:301:ASN:OD1	1:a:303:ASN:ND2	2.50	0.45
27:b:615:CLA:H142	27:b:615:CLA:H112	1.78	0.45
25:14:64:GLU:OE2	25:14:168:ARG:NE	2.49	0.45
1:A:188:ALA:HB2	1:A:328:ILE:HB	1.98	0.45
2:B:179:GLN:HE22	7:H:66:ILE:HB	1.82	0.45
13:o:40:LEU:HD11	13:o:244:ALA:HB1	1.99	0.45
27:B:601:CLA:H2	29:B:623:BCR:H323	1.99	0.45
27:B:601:CLA:H52	27:B:601:CLA:H12	1.85	0.45
3:C:128:ILE:HD11	29:C:520:BCR:H21C	1.99	0.45
27:C:502:CLA:H122	27:C:508:CLA:H61	1.98	0.45
13:O:51:ALA:HB1	13:O:66:PHE:HB3	1.98	0.45
27:c:504:CLA:H193	27:c:511:CLA:HBB2	1.97	0.45
25:11:64:GLU:OE2	25:11:168:ARG:NE	2.49	0.45
1:A:233:THR:HG21	4:D:138:ARG:HH12	1.82	0.45
2:B:160:GLY:HA3	2:B:180:PRO:HB3	1.98	0.45
27:C:513:CLA:HBA1	27:C:513:CLA:H3A	1.54	0.45
2:b:298:GLU:OE2	2:b:302:TRP:NE1	2.46	0.45
25:33:64:GLU:OE2	25:33:168:ARG:NE	2.49	0.45
27:C:507:CLA:H172	27:W:102:CLA:H72	1.98	0.45
4:D:301:GLU:OE1	13:O:158:LYS:NZ	2.50	0.45
33:D:408:LMG:H352	29:F:101:BCR:H19C	1.99	0.45
15:U:12:ASP:OD1	15:U:12:ASP:N	2.42	0.45
27:b:604:CLA:H111	27:b:604:CLA:H91	1.76	0.45
4:d:262:ASN:HB3	4:d:265:TRP:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:301:GLU:OE1	13:o:158:LYS:NZ	2.50	0.45
13:o:196:THR:HG21	13:o:223:LEU:HD23	1.99	0.45
16:v:97:SER:HA	20:q:111:ARG:HH12	1.82	0.45
1:A:37:MET:SD	1:A:41:LEU:HD12	2.57	0.45
1:A:307:VAL:HG21	6:F:43:ARG:HH21	1.82	0.45
3:C:319:ASP:OD2	3:C:338:TYR:OH	2.34	0.45
1:a:301:ASN:H	3:c:403:ASN:HD21	1.64	0.45
29:b:616:BCR:H15C	29:b:616:BCR:H351	1.82	0.45
25:14:69:ARG:NE	25:14:163:GLU:OE2	2.38	0.45
27:D:401:CLA:H111	27:D:401:CLA:H152	1.75	0.44
16:V:73:VAL:HG12	16:V:77:LYS:HZ2	1.81	0.44
27:W:102:CLA:H152	27:W:102:CLA:H111	1.70	0.44
2:b:281:GLN:HB2	2:b:358:ARG:HH12	1.82	0.44
27:b:604:CLA:H111	27:b:604:CLA:H152	1.79	0.44
27:c:502:CLA:H41	27:c:502:CLA:H61	1.74	0.44
33:d:408:LMG:H352	29:f:101:BCR:H19C	1.99	0.44
13:o:94:THR:HG22	13:o:128:LYS:HG2	1.99	0.44
25:34:49:TRP:HH2	38:34:316:A86:C39	2.30	0.44
1:a:305:SER:HA	9:j:38:SER:HB3	1.98	0.44
3:c:319:ASP:OD2	3:c:338:TYR:OH	2.34	0.44
9:j:34:GLY:O	20:q:72:SER:OG	2.29	0.44
13:o:95:PHE:HB3	13:o:127:ALA:HB3	1.99	0.44
25:32:146:PHE:HB3	38:32:304:A86:C38	2.38	0.44
13:O:95:PHE:HB3	13:O:127:ALA:HB3	1.99	0.44
2:b:237:VAL:HG22	27:b:610:CLA:HBC2	1.98	0.44
27:w:102:CLA:H202	27:w:102:CLA:H162	1.82	0.44
25:32:41:LEU:HD11	38:32:316:A86:C22	2.48	0.44
27:C:507:CLA:H192	27:C:507:CLA:H102	1.99	0.44
4:D:194:PRO:HG3	11:L:35:TYR:CE2	2.51	0.44
11:L:9:GLN:O	33:M:103:LMG:O3	2.33	0.44
13:O:226:THR:OG1	13:O:231:LYS:O	2.34	0.44
27:a:404:CLA:H3A	33:w:101:LMG:H131	2.00	0.44
27:d:401:CLA:H91	36:d:407:PL9:H402	1.99	0.44
25:12:60:ARG:NH2	38:12:317:A86:O3	2.51	0.44
4:D:82:ASN:HD22	4:D:335:HIS:CD2	2.36	0.44
11:L:23:LEU:HD22	32:L:101:LHG:H261	1.99	0.44
32:a:408:LHG:H281	32:a:408:LHG:H212	2.00	0.44
25:13:64:GLU:OE2	25:13:168:ARG:NE	2.49	0.44
25:33:180:ALA:O	25:33:191:GLN:NE2	2.51	0.44
4:D:309:GLU:OE2	13:O:231:LYS:NZ	2.40	0.44
9:J:34:GLY:O	20:Q:72:SER:OG	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:W:103:CLA:H2	27:W:103:CLA:HAA1	1.98	0.44
1:a:37:MET:SD	1:a:41:LEU:HD12	2.57	0.44
1:a:163:ILE:O	3:c:290:TYR:OH	2.36	0.44
27:d:401:CLA:H41	36:d:407:PL9:H162	1.99	0.44
13:o:51:ALA:HB1	13:o:66:PHE:HB3	1.98	0.44
15:u:33:ARG:NH1	16:v:51:ASN:OD1	2.50	0.44
25:31:64:GLU:OE2	25:31:168:ARG:NE	2.49	0.44
25:31:180:ALA:O	25:31:191:GLN:NE2	2.51	0.44
27:B:604:CLA:H193	29:B:617:BCR:HC8	2.00	0.44
13:O:40:LEU:HD11	13:O:244:ALA:HB1	1.99	0.44
13:O:94:THR:HG22	13:O:128:LYS:HG2	1.99	0.44
1:a:233:THR:HG21	4:d:138:ARG:HH12	1.81	0.44
2:b:179:GLN:HE22	7:h:66:ILE:HB	1.82	0.44
16:v:43:GLY:O	16:v:131:GLY:N	2.44	0.44
1:A:84:PRO:HA	1:A:112:TYR:CG	2.53	0.44
32:A:408:LHG:H281	32:A:408:LHG:H212	2.00	0.44
3:C:405:VAL:HG21	3:C:413:ASN:HA	2.00	0.44
27:D:401:CLA:H41	36:D:407:PL9:H162	2.00	0.44
13:O:196:THR:HG21	13:O:223:LEU:HD23	1.99	0.44
15:U:48:LYS:NZ	15:U:66:GLY:O	2.37	0.44
15:U:68:SER:OG	15:U:69:SER:N	2.51	0.44
2:b:384:ARG:NH1	15:u:98:ASN:O	2.50	0.44
8:i:6:ILE:HG23	21:w:37:VAL:HG21	1.99	0.44
27:33:307:CLA:HBA1	38:33:315:A86:C10	2.47	0.44
27:34:302:CLA:H71	27:34:302:CLA:H112	1.82	0.44
27:b:601:CLA:H151	27:b:601:CLA:HBB1	2.00	0.43
3:c:405:VAL:HG21	3:c:413:ASN:HA	2.00	0.43
27:c:514:CLA:H143	27:c:514:CLA:H111	1.82	0.43
25:11:197:ILE:HD13	27:12:308:CLA:HMD3	2.00	0.43
27:A:404:CLA:H3A	33:W:101:LMG:H131	2.00	0.43
2:B:281:GLN:HB2	2:B:358:ARG:HH12	1.82	0.43
3:C:343:PRO:HB3	13:O:74:ARG:HD3	1.99	0.43
4:D:47:TRP:NE1	4:D:172:PHE:O	2.32	0.43
32:a:408:LHG:HC31	3:c:34:TRP:HH2	1.83	0.43
3:c:89:HIS:O	3:c:92:THR:OG1	2.33	0.43
3:c:343:PRO:HB3	13:o:74:ARG:HD3	2.00	0.43
25:11:165:ASN:ND2	27:12:303:CLA:O1D	2.39	0.43
25:11:180:ALA:O	25:11:191:GLN:NE2	2.51	0.43
27:33:303:CLA:HBA2	27:33:303:CLA:H3A	1.38	0.43
25:34:180:ALA:O	25:34:191:GLN:NE2	2.51	0.43
1:A:304:GLN:HG2	1:A:313:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:211:VAL:O	3:C:221:TRP:NE1	2.38	0.43
27:C:509:CLA:H193	27:C:509:CLA:H161	1.81	0.43
27:b:602:CLA:H202	35:h:102:DGD:HB82	2.00	0.43
15:u:68:SER:OG	15:u:69:SER:N	2.51	0.43
25:12:180:ALA:O	25:12:191:GLN:NE2	2.51	0.43
25:34:131:TRP:CD1	27:34:302:CLA:NB	2.86	0.43
36:D:404:PL9:H322	36:D:404:PL9:H28	1.76	0.43
10:K:36:VAL:HG21	29:Z:101:BCR:H19C	2.00	0.43
4:d:20:TRP:CD1	18:x:33:ASP:HB3	2.53	0.43
4:d:138:ARG:NH2	4:d:140:TYR:OH	2.51	0.43
11:l:23:LEU:HD22	32:l:102:LHG:H261	2.01	0.43
25:32:180:ALA:O	25:32:191:GLN:NE2	2.51	0.43
25:33:174:ILE:HD13	25:33:174:ILE:HA	1.90	0.43
27:33:301:CLA:H151	27:33:306:CLA:HBA1	1.99	0.43
25:34:69:ARG:NE	25:34:163:GLU:OE2	2.38	0.43
2:B:310:ALA:HB1	2:B:428:GLU:HG3	2.01	0.43
27:B:605:CLA:H61	27:B:605:CLA:H41	1.84	0.43
5:E:70:ARG:NH2	7:H:50:ASN:O	2.52	0.43
13:O:193:PHE:HB2	15:U:90:ASP:HB3	2.00	0.43
27:b:612:CLA:H102	27:b:612:CLA:H61	1.59	0.43
3:c:442:HIS:HE1	27:c:509:CLA:NA	2.12	0.43
25:13:180:ALA:O	25:13:191:GLN:NE2	2.51	0.43
25:31:61:ARG:NH2	27:31:301:CLA:O1D	2.40	0.43
25:31:146:PHE:CA	38:31:316:A86:O5	2.64	0.43
3:C:111:ALA:O	3:C:115:ILE:HG12	2.19	0.43
27:c:507:CLA:H102	27:c:507:CLA:H192	1.99	0.43
9:j:14:LEU:HD11	17:y:21:PRO:HB3	1.99	0.43
25:14:180:ALA:O	25:14:191:GLN:NE2	2.51	0.43
3:c:462:GLU:OE2	4:d:247:THR:OG1	2.36	0.43
4:d:82:ASN:HD22	4:d:335:HIS:CD2	2.36	0.43
25:13:61:ARG:NH2	27:13:303:CLA:O1D	2.40	0.43
25:32:112:ILE:HD11	27:32:307:CLA:H3A	2.01	0.43
2:B:326:ARG:NH2	4:D:296:ASP:OD1	2.52	0.43
2:B:415:PRO:HG3	15:U:12:ASP:HB2	2.00	0.43
3:C:128:ILE:HG22	19:Z:24:LEU:HD12	2.00	0.43
27:C:507:CLA:H203	27:C:507:CLA:H162	1.85	0.43
4:D:138:ARG:NH2	4:D:140:TYR:OH	2.51	0.43
27:b:601:CLA:HBB2	29:h:101:BCR:H16C	2.01	0.43
27:b:604:CLA:H193	29:b:617:BCR:HC8	2.00	0.43
27:c:505:CLA:H141	27:c:505:CLA:H161	1.77	0.43
5:e:70:ARG:NH2	7:h:50:ASN:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:34:308:CLA:HBA1	38:34:316:A86:C10	2.49	0.43
27:b:601:CLA:CBB	29:h:101:BCR:H16C	2.49	0.43
3:c:223:VAL:HA	3:c:287:TYR:CE1	2.54	0.43
25:14:112:ILE:HD11	27:14:305:CLA:H3A	2.01	0.43
29:B:617:BCR:H20C	29:B:617:BCR:H361	1.85	0.43
33:B:619:LMG:H421	33:B:619:LMG:H391	1.86	0.43
3:C:89:HIS:O	3:C:92:THR:OG1	2.32	0.43
4:D:193:ASN:HD22	4:D:194:PRO:HD2	1.84	0.43
29:b:617:BCR:H20C	29:b:617:BCR:H361	1.85	0.43
25:31:165:ASN:ND2	27:32:303:CLA:O1D	2.39	0.43
1:a:84:PRO:HA	1:a:112:TYR:CG	2.53	0.42
2:b:256:MET:HA	2:b:263:THR:HG21	2.00	0.42
2:b:310:ALA:HB1	2:b:428:GLU:HG3	2.00	0.42
2:b:477:ASP:OD1	2:b:477:ASP:N	2.51	0.42
3:c:111:ALA:O	3:c:115:ILE:HG12	2.19	0.42
27:c:510:CLA:H92	27:c:510:CLA:H62	1.87	0.42
27:11:305:CLA:HBA1	38:11:313:A86:C10	2.49	0.42
25:32:119:GLN:NE2	33:32:301:LMG:HC8	2.34	0.42
1:A:295:PHE:HB2	3:C:426:CYS:SG	2.59	0.42
2:B:174:ILE:HD11	2:B:309:LEU:HB2	2.01	0.42
33:B:619:LMG:H412	33:B:619:LMG:H381	1.90	0.42
35:H:102:DGD:HB91	35:H:102:DGD:HB62	1.71	0.42
15:U:88:SER:HA	15:U:89:PRO:HD3	1.87	0.42
2:b:174:ILE:HD11	2:b:309:LEU:HB2	2.01	0.42
2:b:201:HIS:HE1	27:b:602:CLA:C1D	2.31	0.42
4:d:193:ASN:HD22	4:d:194:PRO:HD2	1.84	0.42
13:o:74:ARG:NH1	21:w:21:GLU:OE2	2.52	0.42
25:12:61:ARG:NH2	27:12:305:CLA:O1D	2.40	0.42
27:12:305:CLA:H3A	27:12:305:CLA:HBA2	1.38	0.42
2:B:256:MET:HA	2:B:263:THR:HG21	2.00	0.42
4:D:38:PRO:HB2	27:D:406:CLA:HAB	2.01	0.42
36:D:404:PL9:H121	36:D:404:PL9:HC8	1.74	0.42
16:V:76:ILE:HD13	16:V:112:LEU:HD22	2.01	0.42
3:c:26:ILE:HG21	4:d:232:ARG:HH12	1.84	0.42
27:c:509:CLA:H193	27:c:509:CLA:H161	1.81	0.42
25:14:60:ARG:NH2	38:14:315:A86:O3	2.52	0.42
1:A:137:LEU:HD23	3:C:467:MET:HE1	2.01	0.42
1:A:149:ALA:HB1	1:A:283:ILE:HB	2.02	0.42
27:B:602:CLA:H62	27:B:602:CLA:H92	1.80	0.42
3:C:341:ARG:NH1	3:C:345:GLY:O	2.52	0.42
27:D:401:CLA:H91	36:D:407:PL9:H402	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Q:86:TYR:HA	20:Q:94:PRO:HG3	2.01	0.42
1:a:282:GLY:O	1:a:286:THR:OG1	2.34	0.42
29:c:515:BCR:H11C	29:c:515:BCR:H341	1.91	0.42
6:f:43:ARG:NH2	9:j:39:LEU:OXT	2.52	0.42
25:11:112:ILE:HD11	27:11:303:CLA:H3A	2.01	0.42
25:11:184:THR:OG1	25:11:191:GLN:NE2	2.52	0.42
25:13:60:ARG:NH2	38:13:315:A86:O3	2.53	0.42
25:31:112:ILE:HD11	27:31:303:CLA:H3A	2.01	0.42
27:33:301:CLA:H112	27:33:301:CLA:H71	1.83	0.42
27:B:601:CLA:HBB2	29:H:101:BCR:H16C	2.01	0.42
3:C:400:GLY:HA3	3:C:418:VAL:HG22	2.00	0.42
29:C:515:BCR:H11C	29:C:515:BCR:H341	1.91	0.42
1:a:137:LEU:HD23	3:c:467:MET:HE1	2.01	0.42
2:b:419:LYS:O	2:b:423:LYS:NZ	2.42	0.42
3:c:341:ARG:NH1	3:c:345:GLY:O	2.52	0.42
10:k:36:VAL:HG21	29:z:101:BCR:H19C	2.00	0.42
13:o:56:VAL:HG11	13:o:65:LYS:HD3	2.02	0.42
25:13:165:ASN:ND2	27:14:302:CLA:O1D	2.39	0.42
25:31:60:ARG:NH2	38:31:313:A86:O3	2.52	0.42
27:31:305:CLA:HBA1	38:31:313:A86:C10	2.50	0.42
2:B:325:PHE:CG	11:L:35:TYR:HB3	2.54	0.42
3:C:223:VAL:HA	3:C:287:TYR:CE1	2.54	0.42
2:b:256:MET:O	2:b:448:ARG:NH1	2.45	0.42
2:b:463:PHE:CZ	27:b:608:CLA:HBB1	2.55	0.42
29:c:515:BCR:H343	19:z:48:VAL:HG12	2.02	0.42
25:13:112:ILE:HD11	27:13:305:CLA:H3A	2.01	0.42
25:32:202:ASP:HB3	38:32:316:A86:C29	2.50	0.42
25:33:112:ILE:HD11	27:33:305:CLA:H3A	2.01	0.42
27:B:622:CLA:H143	27:B:622:CLA:H111	1.89	0.42
1:a:149:ALA:HB1	1:a:283:ILE:HB	2.02	0.42
1:a:304:GLN:HG2	1:a:313:VAL:HG11	2.01	0.42
27:b:622:CLA:H11	29:b:623:BCR:H23C	2.02	0.42
29:c:519:BCR:H15C	29:c:519:BCR:H351	1.89	0.42
25:32:67:HIS:HE1	27:32:306:CLA:ND	2.16	0.42
25:34:112:ILE:HD11	27:34:306:CLA:H3A	2.01	0.42
27:A:404:CLA:H92	27:A:404:CLA:H62	1.89	0.42
2:B:236:THR:HB	2:B:473:THR:HG21	2.02	0.42
27:B:615:CLA:H112	27:B:615:CLA:H142	1.78	0.42
1:a:307:VAL:HG21	6:f:43:ARG:HH21	1.84	0.42
4:d:38:PRO:HB2	27:d:406:CLA:HAB	2.01	0.42
36:d:407:PL9:HC8	36:d:407:PL9:HC2	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:76:ILE:HD13	16:v:112:LEU:HD22	2.01	0.42
27:B:601:CLA:HBB1	27:B:601:CLA:H151	2.00	0.42
27:C:504:CLA:H102	27:C:504:CLA:H62	1.64	0.42
4:D:59:THR:OG1	4:D:60:HIS:N	2.53	0.42
4:D:71:ASN:OD1	4:D:71:ASN:N	2.52	0.42
27:a:404:CLA:H93	27:a:404:CLA:H111	1.82	0.42
27:b:602:CLA:H102	27:b:609:CLA:H202	2.01	0.42
29:b:617:BCR:H11C	29:b:617:BCR:H341	1.93	0.42
19:z:34:LYS:O	19:z:38:ASN:N	2.46	0.42
25:13:112:ILE:HD11	27:13:305:CLA:HAA2	2.01	0.42
27:14:307:CLA:HBA1	38:14:315:A86:C10	2.50	0.42
25:31:112:ILE:HD11	27:31:303:CLA:HAA2	2.01	0.42
25:32:112:ILE:HD11	27:32:307:CLA:HAA2	2.01	0.42
2:B:201:HIS:HE1	27:B:602:CLA:C1D	2.31	0.42
3:C:442:HIS:HE1	27:C:509:CLA:NA	2.12	0.42
5:E:15:ILE:O	5:E:21:TRP:NE1	2.48	0.42
3:c:400:GLY:HA3	3:c:418:VAL:HG22	2.00	0.42
25:11:174:ILE:HD13	25:11:174:ILE:HA	1.89	0.42
25:14:184:THR:OG1	25:14:191:GLN:NE2	2.52	0.42
27:31:304:CLA:HMD3	25:34:192:TYR:HE1	1.84	0.42
27:B:602:CLA:H202	35:H:102:DGD:HB82	2.01	0.41
27:W:103:CLA:H112	27:W:103:CLA:H72	1.89	0.41
1:a:308:ASP:OD1	1:a:312:ARG:N	2.53	0.41
29:a:405:BCR:H24C	29:a:405:BCR:H371	1.75	0.41
4:d:59:THR:OG1	4:d:60:HIS:N	2.53	0.41
20:q:86:TYR:HA	20:q:94:PRO:HG3	2.01	0.41
3:C:389:ARG:NH2	20:Q:147:TYR:OH	2.39	0.41
27:C:506:CLA:H72	27:C:506:CLA:H112	1.83	0.41
27:C:514:CLA:H143	27:C:514:CLA:H111	1.82	0.41
16:V:5:GLU:O	16:V:9:THR:OG1	2.34	0.41
19:Z:10:VAL:HG13	29:Z:101:BCR:HC21	2.02	0.41
2:b:25:MET:HG2	29:m:103:BCR:H23C	2.02	0.41
2:b:326:ARG:NH2	4:d:296:ASP:OD1	2.52	0.41
27:b:614:CLA:H2	27:b:615:CLA:HBB2	2.02	0.41
29:c:515:BCR:H20C	29:c:515:BCR:H361	1.89	0.41
13:o:185:LEU:HD12	13:o:189:ASN:HD21	1.85	0.41
20:q:78:GLY:HA2	20:q:81:GLN:HE22	1.85	0.41
1:A:308:ASP:OD1	1:A:312:ARG:N	2.53	0.41
32:A:408:LHG:HC31	3:C:34:TRP:HH2	1.85	0.41
27:B:607:CLA:H142	27:B:607:CLA:H111	1.93	0.41
29:B:616:BCR:H20C	29:B:616:BCR:H361	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:C:516:BCR:H20C	29:C:516:BCR:H361	1.91	0.41
29:F:101:BCR:H20C	29:F:101:BCR:H361	1.78	0.41
20:Q:154:ARG:NH2	20:Q:167:GLU:OE2	2.47	0.41
2:b:415:PRO:HG3	15:u:12:ASP:HB2	2.02	0.41
27:b:605:CLA:H61	27:b:605:CLA:H41	1.84	0.41
33:b:619:LMG:H402	33:b:619:LMG:H371	1.82	0.41
20:q:115:VAL:O	20:q:119:THR:OG1	2.27	0.41
25:14:112:ILE:HD11	27:14:305:CLA:HAA2	2.01	0.41
25:32:184:THR:OG1	25:32:191:GLN:NE2	2.52	0.41
25:33:61:ARG:NH2	27:33:303:CLA:O1D	2.36	0.41
25:33:112:ILE:HD11	27:33:305:CLA:HAA2	2.01	0.41
27:B:601:CLA:CBB	29:H:101:BCR:H16C	2.49	0.41
27:B:611:CLA:H112	27:B:611:CLA:H72	1.93	0.41
33:B:618:LMG:H361	33:B:618:LMG:H332	1.79	0.41
33:C:519:LMG:H132	33:C:519:LMG:H161	1.88	0.41
4:D:296:ASP:HA	4:D:314:TYR:OH	2.21	0.41
36:D:407:PL9:H462	36:D:407:PL9:H422	1.89	0.41
19:Z:34:LYS:O	19:Z:38:ASN:N	2.46	0.41
27:b:614:CLA:HBA1	27:b:614:CLA:H3A	1.89	0.41
29:m:103:BCR:H20C	29:m:103:BCR:H361	1.93	0.41
15:u:90:ASP:OD1	15:u:90:ASP:N	2.50	0.41
27:12:303:CLA:H71	27:12:303:CLA:H112	1.82	0.41
25:13:41:LEU:CD1	38:13:314:A86:C22	2.98	0.41
25:34:61:ARG:NH2	27:34:304:CLA:O1D	2.40	0.41
2:B:463:PHE:CZ	27:B:608:CLA:HBB1	2.55	0.41
27:B:601:CLA:H142	27:B:601:CLA:H112	1.93	0.41
27:B:609:CLA:H92	27:B:609:CLA:H62	1.82	0.41
27:B:615:CLA:H143	27:B:615:CLA:H161	1.86	0.41
27:C:505:CLA:H141	27:C:505:CLA:H161	1.77	0.41
12:M:41:ASP:O	12:m:32:ARG:NH1	2.53	0.41
13:O:160:ARG:NH1	13:O:189:ASN:OD1	2.51	0.41
13:O:177:LEU:HD13	13:O:177:LEU:HA	1.97	0.41
27:W:102:CLA:H202	27:W:102:CLA:H162	1.82	0.41
4:d:296:ASP:HA	4:d:314:TYR:OH	2.21	0.41
27:d:405:CLA:H143	27:d:405:CLA:H161	1.95	0.41
25:32:164:LEU:O	25:32:168:ARG:N	2.47	0.41
25:33:60:ARG:NH2	38:33:315:A86:O3	2.53	0.41
27:Z:102:CLA:H93	27:Z:102:CLA:H111	1.91	0.41
27:b:603:CLA:H91	27:b:603:CLA:H112	1.86	0.41
33:m:102:LMG:H111	33:m:102:LMG:H141	1.88	0.41
13:o:160:ARG:NH1	13:o:189:ASN:OD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:11:67:HIS:HE1	27:11:302:CLA:ND	2.16	0.41
25:12:112:ILE:HD11	27:12:307:CLA:HAA2	2.01	0.41
25:12:184:THR:OG1	25:12:191:GLN:NE2	2.52	0.41
25:14:163:GLU:HB2	27:14:309:CLA:C1B	2.51	0.41
25:34:112:ILE:HD11	27:34:306:CLA:HAA2	2.01	0.41
27:A:404:CLA:H93	27:A:404:CLA:H111	1.82	0.41
2:B:477:ASP:OD1	2:B:477:ASP:N	2.51	0.41
27:B:603:CLA:H91	27:B:603:CLA:H112	1.86	0.41
13:O:130:ASN:N	13:O:130:ASN:OD1	2.53	0.41
2:b:236:THR:HB	2:b:473:THR:HG21	2.02	0.41
2:b:348:ASP:OD1	2:b:348:ASP:N	2.53	0.41
29:c:516:BCR:H15C	29:c:516:BCR:H351	1.91	0.41
29:c:519:BCR:H20C	29:c:519:BCR:H361	1.82	0.41
27:m:101:CLA:H62	27:m:101:CLA:H41	1.83	0.41
25:13:163:GLU:HB2	27:13:309:CLA:C1B	2.51	0.41
25:13:184:THR:OG1	25:13:191:GLN:NE2	2.52	0.41
25:14:67:HIS:HE1	27:14:304:CLA:ND	2.16	0.41
25:31:163:GLU:HB2	27:31:307:CLA:C1B	2.51	0.41
25:32:163:GLU:HB2	27:32:311:CLA:C1B	2.51	0.41
27:C:513:CLA:H141	27:C:513:CLA:H162	1.89	0.41
27:b:609:CLA:H92	27:b:609:CLA:H62	1.82	0.41
16:v:81:THR:OG1	16:v:83:ASP:OD1	2.38	0.41
25:12:41:LEU:HD12	38:12:316:A86:C22	2.50	0.41
25:12:112:ILE:HD11	27:12:307:CLA:H3A	2.01	0.41
1:A:41:LEU:HG	1:A:122:GLY:HA3	2.03	0.41
1:A:272:HIS:CD2	4:D:213:HIS:NE2	2.89	0.41
2:B:25:MET:HG2	29:M:101:BCR:H23C	2.02	0.41
27:B:614:CLA:H2	27:B:615:CLA:HBB2	2.02	0.41
29:B:623:BCR:H341	29:B:623:BCR:H11C	1.85	0.41
3:C:373:LEU:HB3	3:C:378:ILE:HD11	2.03	0.41
29:C:516:BCR:H11C	29:C:516:BCR:H341	1.91	0.41
16:V:81:THR:OG1	16:V:83:ASP:OD1	2.38	0.41
20:Q:78:GLY:HA2	20:Q:81:GLN:NE2	2.36	0.41
20:Q:141:GLU:OE1	20:Q:144:ARG:NH1	2.54	0.41
3:c:209:GLY:HA2	21:w:26:TRP:NE1	2.30	0.41
3:c:280:MET:HG2	27:c:502:CLA:H72	2.03	0.41
5:e:15:ILE:O	5:e:21:TRP:NE1	2.48	0.41
29:h:101:BCR:H361	29:h:101:BCR:H20C	1.76	0.41
13:o:130:ASN:N	13:o:130:ASN:OD1	2.53	0.41
13:o:226:THR:OG1	13:o:231:LYS:O	2.34	0.41
15:u:88:SER:HA	15:u:89:PRO:HD3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:99:ASP:N	16:v:99:ASP:OD1	2.53	0.41
27:z:102:CLA:H93	27:z:102:CLA:H111	1.91	0.41
25:11:60:ARG:NH2	38:11:313:A86:O3	2.54	0.41
25:11:163:GLU:HB2	27:11:307:CLA:C1B	2.51	0.41
27:33:303:CLA:H141	27:33:303:CLA:H162	1.95	0.41
27:33:303:CLA:H18	27:33:303:CLA:H151	1.92	0.41
25:34:163:GLU:HB2	27:34:310:CLA:C1B	2.51	0.41
2:B:472:ARG:HA	2:B:479:PHE:CE2	2.56	0.41
27:C:508:CLA:H92	27:C:508:CLA:H62	1.91	0.41
7:H:62:TRP:HE1	35:H:102:DGD:HO5E	1.69	0.41
13:O:56:VAL:HG11	13:O:65:LYS:HD3	2.02	0.41
15:U:97:ASN:ND2	15:U:101:TYR:OH	2.49	0.41
27:b:613:CLA:H92	27:b:613:CLA:H61	1.84	0.41
3:c:277:ILE:HD13	3:c:277:ILE:HG21	1.90	0.41
25:12:163:GLU:HB2	27:12:311:CLA:C1B	2.51	0.41
27:14:302:CLA:H71	27:14:302:CLA:H112	1.82	0.41
1:A:97:TRP:CD1	1:A:98:GLU:HG2	2.56	0.40
27:C:511:CLA:H161	27:C:511:CLA:H121	1.99	0.40
27:D:402:CLA:H143	27:D:405:CLA:H172	2.03	0.40
29:H:101:BCR:H20C	29:H:101:BCR:H361	1.77	0.40
13:O:185:LEU:HD12	13:O:189:ASN:HD21	1.85	0.40
16:V:123:PRO:HG3	16:V:130:TRP:CD1	2.56	0.40
20:Q:78:GLY:HA2	20:Q:81:GLN:HE22	1.85	0.40
27:b:604:CLA:H62	27:b:604:CLA:H41	1.80	0.40
27:b:613:CLA:H111	27:b:613:CLA:H152	1.87	0.40
7:h:62:TRP:HE1	35:h:102:DGD:HO5E	1.67	0.40
25:11:112:ILE:HD11	27:11:303:CLA:HAA2	2.01	0.40
27:34:304:CLA:H151	27:34:304:CLA:H18	1.92	0.40
1:A:127:MET:HE2	1:A:127:MET:HB3	1.92	0.40
8:I:7:LEU:O	8:I:10:THR:OG1	2.39	0.40
10:K:13:TYR:CE1	19:Z:6:VAL:HG21	2.56	0.40
1:a:41:LEU:HG	1:a:122:GLY:HA3	2.03	0.40
1:a:61:ASP:HB2	1:a:63:ILE:HG12	2.04	0.40
27:a:404:CLA:H171	27:c:507:CLA:H41	2.03	0.40
27:c:505:CLA:H91	27:c:505:CLA:H112	1.86	0.40
27:d:401:CLA:H152	27:d:401:CLA:H111	1.75	0.40
11:l:9:GLN:O	33:m:102:LMG:O3	2.35	0.40
13:o:174:ALA:HA	13:o:177:LEU:HD23	2.03	0.40
25:14:41:LEU:HD12	38:14:314:A86:C22	2.51	0.40
25:31:142:GLY:O	25:34:158:ARG:NH1	2.53	0.40
25:31:174:ILE:HG22	25:31:178:MET:HE2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:32:174:ILE:HG22	25:32:178:MET:HE2	2.04	0.40
25:33:163:GLU:HB2	27:33:309:CLA:C1B	2.51	0.40
25:33:180:ALA:O	25:33:184:THR:OG1	2.34	0.40
27:B:602:CLA:H102	27:B:609:CLA:H202	2.02	0.40
3:C:74:VAL:HG12	3:C:76:GLU:H	1.86	0.40
32:L:101:LHG:H281	32:L:101:LHG:H132	2.04	0.40
27:c:508:CLA:H142	27:c:508:CLA:H112	1.83	0.40
13:o:87:THR:OG1	13:o:94:THR:OG1	2.39	0.40
20:q:173:LEU:O	20:q:176:THR:OG1	2.35	0.40
25:14:174:ILE:HG22	25:14:178:MET:HE2	2.03	0.40
25:31:41:LEU:HD12	38:31:312:A86:C22	2.51	0.40
25:31:67:HIS:HE1	27:31:302:CLA:ND	2.16	0.40
1:A:131:TRP:O	1:A:134:SER:OG	2.30	0.40
13:O:174:ALA:HA	13:O:177:LEU:HD23	2.03	0.40
20:Q:142:LEU:H	20:Q:142:LEU:HG	1.74	0.40
1:a:150:PRO:HB2	27:a:402:CLA:H92	2.02	0.40
27:b:605:CLA:H141	27:b:605:CLA:H161	1.87	0.40
27:b:606:CLA:H152	27:b:606:CLA:H111	1.85	0.40
3:c:325:ASN:ND2	3:c:328:SER:OG	2.55	0.40
27:c:507:CLA:H172	27:w:102:CLA:H72	2.02	0.40
8:i:7:LEU:O	8:i:10:THR:OG1	2.39	0.40
35:j:101:DGD:HAH1	35:j:101:DGD:HAT1	1.93	0.40
27:12:309:CLA:HBA1	38:12:317:A86:C10	2.51	0.40
25:13:67:HIS:HE1	27:13:304:CLA:ND	2.16	0.40
27:31:301:CLA:H92	27:31:301:CLA:H62	1.94	0.40
25:34:184:THR:OG1	25:34:191:GLN:NE2	2.52	0.40
1:A:150:PRO:HB2	27:A:402:CLA:H92	2.02	0.40
3:c:403:ASN:OD1	3:c:403:ASN:N	2.54	0.40
27:d:402:CLA:HMB2	27:d:405:CLA:H102	2.02	0.40
35:j:101:DGD:HAE2	35:j:101:DGD:HAF1	1.84	0.40
12:m:32:ARG:HH22	33:m:102:LMG:HO4	1.67	0.40
15:u:97:ASN:ND2	15:u:101:TYR:OH	2.49	0.40
27:11:315:CLA:H112	27:11:315:CLA:H71	1.82	0.40
25:12:119:GLN:NE2	33:12:301:LMG:HC8	2.36	0.40
25:12:164:LEU:O	25:12:168:ARG:N	2.47	0.40
25:31:184:THR:OG1	25:31:191:GLN:NE2	2.52	0.40
25:33:67:HIS:HE1	27:33:304:CLA:ND	2.16	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	322 (97%)	10 (3%)	0	100	100
1	a	332/344 (96%)	321 (97%)	11 (3%)	0	100	100
2	B	482/509 (95%)	467 (97%)	15 (3%)	0	100	100
2	b	482/509 (95%)	466 (97%)	16 (3%)	0	100	100
3	C	449/471 (95%)	429 (96%)	20 (4%)	0	100	100
3	c	449/471 (95%)	429 (96%)	20 (4%)	0	100	100
4	D	339/351 (97%)	324 (96%)	15 (4%)	0	100	100
4	d	339/351 (97%)	324 (96%)	15 (4%)	0	100	100
5	E	73/84 (87%)	72 (99%)	1 (1%)	0	100	100
5	e	73/84 (87%)	72 (99%)	1 (1%)	0	100	100
6	F	26/43 (60%)	26 (100%)	0	0	100	100
6	f	26/43 (60%)	26 (100%)	0	0	100	100
7	H	64/67 (96%)	62 (97%)	2 (3%)	0	100	100
7	h	64/67 (96%)	62 (97%)	2 (3%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
9	J	32/39 (82%)	32 (100%)	0	0	100	100
9	j	32/39 (82%)	32 (100%)	0	0	100	100
10	K	35/44 (80%)	35 (100%)	0	0	100	100
10	k	35/44 (80%)	35 (100%)	0	0	100	100
11	L	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
11	l	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	M	40/131 (30%)	37 (92%)	3 (8%)	0	100	100
12	m	40/131 (30%)	37 (92%)	3 (8%)	0	100	100
13	O	243/248 (98%)	231 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	243/248 (98%)	231 (95%)	12 (5%)	0	100	100
14	T	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
14	t	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
15	U	91/93 (98%)	85 (93%)	6 (7%)	0	100	100
15	u	91/93 (98%)	85 (93%)	6 (7%)	0	100	100
16	V	134/137 (98%)	126 (94%)	8 (6%)	0	100	100
16	v	134/137 (98%)	126 (94%)	8 (6%)	0	100	100
17	Y	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
17	y	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
18	X	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
18	x	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
19	Z	57/61 (93%)	56 (98%)	1 (2%)	0	100	100
19	z	57/61 (93%)	56 (98%)	1 (2%)	0	100	100
20	Q	135/155 (87%)	126 (93%)	9 (7%)	0	100	100
20	q	135/155 (87%)	126 (93%)	9 (7%)	0	100	100
21	W	50/72 (69%)	46 (92%)	4 (8%)	0	100	100
21	w	50/72 (69%)	46 (92%)	4 (8%)	0	100	100
25	11	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	12	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	13	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	14	174/207 (84%)	168 (97%)	6 (3%)	0	100	100
25	31	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	32	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	33	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	34	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
All	All	6884/7712 (89%)	6603 (96%)	281 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	272/280 (97%)	272 (100%)	0	100	100
1	a	272/280 (97%)	272 (100%)	0	100	100
2	B	385/405 (95%)	385 (100%)	0	100	100
2	b	385/405 (95%)	385 (100%)	0	100	100
3	C	356/376 (95%)	354 (99%)	2 (1%)	78	81
3	c	356/376 (95%)	354 (99%)	2 (1%)	78	81
4	D	273/281 (97%)	273 (100%)	0	100	100
4	d	273/281 (97%)	273 (100%)	0	100	100
5	E	69/75 (92%)	68 (99%)	1 (1%)	59	73
5	e	69/75 (92%)	68 (99%)	1 (1%)	59	73
6	F	22/36 (61%)	22 (100%)	0	100	100
6	f	22/36 (61%)	22 (100%)	0	100	100
7	H	55/56 (98%)	55 (100%)	0	100	100
7	h	55/56 (98%)	55 (100%)	0	100	100
8	I	34/37 (92%)	34 (100%)	0	100	100
8	i	34/37 (92%)	34 (100%)	0	100	100
9	J	27/31 (87%)	27 (100%)	0	100	100
9	j	27/31 (87%)	27 (100%)	0	100	100
10	K	32/38 (84%)	32 (100%)	0	100	100
10	k	32/38 (84%)	32 (100%)	0	100	100
11	L	34/34 (100%)	34 (100%)	0	100	100
11	l	34/34 (100%)	34 (100%)	0	100	100
12	M	31/104 (30%)	31 (100%)	0	100	100
12	m	31/104 (30%)	31 (100%)	0	100	100
13	O	196/201 (98%)	196 (100%)	0	100	100
13	o	196/201 (98%)	196 (100%)	0	100	100
14	T	27/28 (96%)	27 (100%)	0	100	100
14	t	27/28 (96%)	27 (100%)	0	100	100
15	U	77/77 (100%)	77 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	u	77/77 (100%)	77 (100%)	0	100	100
16	V	114/115 (99%)	114 (100%)	0	100	100
16	v	114/115 (99%)	114 (100%)	0	100	100
17	Y	27/27 (100%)	27 (100%)	0	100	100
17	y	27/27 (100%)	27 (100%)	0	100	100
18	X	29/30 (97%)	29 (100%)	0	100	100
18	x	29/30 (97%)	29 (100%)	0	100	100
19	Z	48/50 (96%)	48 (100%)	0	100	100
19	z	48/50 (96%)	48 (100%)	0	100	100
20	Q	111/124 (90%)	110 (99%)	1 (1%)	70	78
20	q	111/124 (90%)	110 (99%)	1 (1%)	70	78
21	W	43/55 (78%)	42 (98%)	1 (2%)	44	66
21	w	43/55 (78%)	42 (98%)	1 (2%)	44	66
25	11	138/158 (87%)	137 (99%)	1 (1%)	76	80
25	12	138/158 (87%)	137 (99%)	1 (1%)	76	80
25	13	138/158 (87%)	137 (99%)	1 (1%)	76	80
25	14	138/158 (87%)	137 (99%)	1 (1%)	76	80
25	31	138/158 (87%)	137 (99%)	1 (1%)	76	80
25	32	138/158 (87%)	137 (99%)	1 (1%)	76	80
25	33	138/158 (87%)	137 (99%)	1 (1%)	76	80
25	34	138/158 (87%)	137 (99%)	1 (1%)	76	80
All	All	5628/6184 (91%)	5610 (100%)	18 (0%)	84	86

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	138	LEU
3	C	270	LEU
5	E	31	LEU
20	Q	142	LEU
21	W	45	ILE
3	c	138	LEU
3	c	270	LEU
5	e	31	LEU
20	q	142	LEU

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Mol	Chain	Res	Type
21	w	45	ILE
25	11	91	LEU
25	12	91	LEU
25	13	91	LEU
25	14	91	LEU
25	31	91	LEU
25	32	91	LEU
25	33	91	LEU
25	34	91	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	303	ASN
2	B	87	ASN
2	B	179	GLN
2	B	394	GLN
2	B	457	ASN
3	C	325	ASN
3	C	416	ASN
4	D	82	ASN
4	D	185	GLN
4	D	193	ASN
4	D	229	ASN
4	D	349	ASN
10	K	38	GLN
13	O	7	ASN
13	O	109	GLN
13	O	197	GLN
13	O	208	ASN
13	O	222	GLN
15	U	29	ASN
16	V	68	ASN
17	Y	9	GLN
20	Q	105	ASN
20	Q	162	GLN
1	a	26	ASN
1	a	303	ASN
2	b	87	ASN
2	b	179	GLN
2	b	394	GLN

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Mol	Chain	Res	Type
2	b	457	ASN
3	c	325	ASN
3	c	371	ASN
3	c	416	ASN
4	d	82	ASN
4	d	193	ASN
4	d	229	ASN
4	d	291	ASN
4	d	349	ASN
11	l	9	GLN
13	o	109	GLN
13	o	197	GLN
13	o	208	ASN
13	o	222	GLN
15	u	29	ASN
16	v	68	ASN
17	y	9	GLN
20	q	105	ASN
20	q	162	GLN
25	11	82	ASN
25	11	161	ASN
25	12	82	ASN
25	12	161	ASN
25	13	82	ASN
25	13	161	ASN
25	14	82	ASN
25	14	161	ASN
25	31	82	ASN
25	31	161	ASN
25	32	82	ASN
25	32	161	ASN
25	33	82	ASN
25	33	161	ASN
25	34	82	ASN
25	34	161	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 286 ligands modelled in this entry, 2 are monoatomic - leaving 284 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
27	CLA	b	601	-	69,73,73	1.16	9 (13%)	82,113,113	1.40	6 (7%)
27	CLA	b	613	-	69,73,73	1.23	8 (11%)	82,113,113	1.47	10 (12%)
27	CLA	32	308	25,33	49,53,73	1.40	9 (18%)	58,89,113	1.81	14 (24%)
27	CLA	34	310	25	69,73,73	1.20	10 (14%)	82,113,113	1.42	12 (14%)
27	CLA	B	605	-	69,73,73	1.18	8 (11%)	82,113,113	1.38	6 (7%)
27	CLA	d	402	-	69,73,73	1.16	8 (11%)	82,113,113	1.40	5 (6%)
33	LMG	C	519	-	51,51,55	0.99	4 (7%)	59,59,63	1.46	8 (13%)
29	BCR	Z	101	-	41,41,41	1.26	4 (9%)	56,56,56	1.46	9 (16%)
38	A86	32	315	-	47,50,50	4.21	23 (48%)	51,76,76	6.59	17 (33%)
27	CLA	11	302	-	49,53,73	1.35	9 (18%)	58,89,113	1.59	7 (12%)
27	CLA	c	509	-	69,73,73	1.22	8 (11%)	82,113,113	1.51	9 (10%)
27	CLA	B	603	-	69,73,73	1.16	8 (11%)	82,113,113	1.50	10 (12%)
27	CLA	C	506	-	69,73,73	1.17	8 (11%)	82,113,113	1.43	10 (12%)
27	CLA	c	513	-	69,73,73	1.15	10 (14%)	82,113,113	1.37	6 (7%)
27	CLA	B	609	-	69,73,73	1.15	8 (11%)	82,113,113	1.42	9 (10%)
27	CLA	11	315	-	69,73,73	1.18	9 (13%)	82,113,113	1.37	6 (7%)
29	BCR	B	617	-	41,41,41	1.23	2 (4%)	56,56,56	1.44	10 (17%)
38	A86	31	312	-	47,50,50	4.27	23 (48%)	51,76,76	6.47	18 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	A86	33	302	-	47,50,50	4.24	24 (51%)	51,76,76	6.23	17 (33%)
29	BCR	C	515	-	41,41,41	1.32	3 (7%)	56,56,56	1.43	8 (14%)
33	LMG	m	102	27	40,40,55	0.95	2 (5%)	48,48,63	1.35	7 (14%)
27	CLA	33	309	25	69,73,73	1.22	10 (14%)	82,113,113	1.43	12 (14%)
27	CLA	B	610	-	69,73,73	1.23	8 (11%)	82,113,113	1.42	8 (9%)
27	CLA	34	305	-	49,53,73	1.34	8 (16%)	58,89,113	1.59	7 (12%)
27	CLA	d	405	-	69,73,73	1.22	9 (13%)	82,113,113	1.45	10 (12%)
27	CLA	34	307	25	49,53,73	1.40	9 (18%)	58,89,113	1.82	14 (24%)
28	PHO	d	403	-	58,69,69	1.98	12 (20%)	55,99,99	1.73	8 (14%)
27	CLA	b	622	-	69,73,73	1.18	8 (11%)	82,113,113	1.51	12 (14%)
27	CLA	32	311	25	69,73,73	1.18	9 (13%)	82,113,113	1.43	12 (14%)
29	BCR	b	616	-	41,41,41	1.20	2 (4%)	56,56,56	1.38	9 (16%)
27	CLA	C	509	-	69,73,73	1.22	8 (11%)	82,113,113	1.51	9 (10%)
27	CLA	11	301	25	69,73,73	1.15	9 (13%)	82,113,113	1.58	7 (8%)
27	CLA	b	607	-	69,73,73	1.16	8 (11%)	82,113,113	1.40	8 (9%)
27	CLA	12	313	-	49,53,73	1.36	9 (18%)	58,89,113	1.50	5 (8%)
38	A86	34	314	-	47,50,50	4.20	23 (48%)	51,76,76	6.60	17 (33%)
27	CLA	14	302	-	69,73,73	1.18	9 (13%)	82,113,113	1.37	6 (7%)
33	LMG	b	618	-	51,51,55	0.91	4 (7%)	59,59,63	1.43	8 (13%)
33	LMG	q	301	-	51,51,55	0.98	4 (7%)	59,59,63	1.46	9 (15%)
27	CLA	B	613	-	69,73,73	1.22	8 (11%)	82,113,113	1.45	10 (12%)
38	A86	13	314	-	47,50,50	4.28	23 (48%)	51,76,76	6.47	18 (35%)
38	A86	31	314	-	47,50,50	4.15	23 (48%)	51,76,76	6.58	18 (35%)
38	A86	14	312	-	47,50,50	4.16	23 (48%)	51,76,76	6.93	18 (35%)
32	LHG	b	621	-	48,48,48	0.77	1 (2%)	51,54,54	1.32	6 (11%)
27	CLA	c	512	3	69,73,73	1.21	11 (15%)	82,113,113	1.50	13 (15%)
33	LMG	d	408	-	51,51,55	0.91	3 (5%)	59,59,63	1.43	8 (13%)
27	CLA	32	303	-	69,73,73	1.18	9 (13%)	82,113,113	1.37	6 (7%)
27	CLA	13	308	25	49,53,73	1.36	6 (12%)	58,89,113	1.68	7 (12%)
27	CLA	b	614	-	69,73,73	1.15	9 (13%)	82,113,113	1.46	7 (8%)
30	SQD	A	406	-	52,54,54	0.97	6 (11%)	62,65,65	1.55	11 (17%)
38	A86	33	314	-	47,50,50	4.27	24 (51%)	51,76,76	6.47	19 (37%)
27	CLA	32	312	25	49,53,73	1.39	9 (18%)	58,89,113	1.58	7 (12%)
38	A86	11	313	-	47,50,50	4.25	23 (48%)	51,76,76	6.84	20 (39%)
27	CLA	13	305	-	69,73,73	1.13	9 (13%)	82,113,113	1.47	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	11	307	25	69,73,73	1.18	9 (13%)	82,113,113	1.43	12 (14%)
38	A86	12	314	-	47,50,50	4.16	23 (48%)	51,76,76	6.93	18 (35%)
27	CLA	c	502	-	69,73,73	1.14	10 (14%)	82,113,113	1.51	11 (13%)
27	CLA	d	401	-	69,73,73	1.21	8 (11%)	82,113,113	1.42	10 (12%)
29	BCR	C	516	-	41,41,41	1.30	5 (12%)	56,56,56	1.43	10 (17%)
27	CLA	M	102	33	69,73,73	1.15	10 (14%)	82,113,113	1.26	5 (6%)
27	CLA	14	303	25	69,73,73	1.15	9 (13%)	82,113,113	1.56	7 (8%)
27	CLA	D	402	-	69,73,73	1.16	8 (11%)	82,113,113	1.40	5 (6%)
30	SQD	a	406	-	52,54,54	0.96	6 (11%)	62,65,65	1.55	11 (17%)
33	LMG	b	619	-	51,51,55	0.99	5 (9%)	59,59,63	1.44	9 (15%)
38	A86	13	317	-	47,50,50	4.25	24 (51%)	51,76,76	6.22	17 (33%)
34	OEX	c	501	3,1	0,15,15	-	-	-	-	-
38	A86	14	314	-	47,50,50	4.28	24 (51%)	51,76,76	6.47	18 (35%)
27	CLA	32	310	25	49,53,73	1.36	7 (14%)	58,89,113	1.66	7 (12%)
27	CLA	33	304	-	49,53,73	1.34	9 (18%)	58,89,113	1.60	7 (12%)
35	DGD	h	102	-	63,63,67	0.94	1 (1%)	77,77,81	1.42	8 (10%)
38	A86	33	312	-	47,50,50	4.16	23 (48%)	51,76,76	6.93	18 (35%)
29	BCR	c	519	-	41,41,41	1.27	2 (4%)	56,56,56	1.39	7 (12%)
29	BCR	B	623	-	41,41,41	1.14	3 (7%)	56,56,56	1.32	6 (10%)
27	CLA	B	601	-	69,73,73	1.15	9 (13%)	82,113,113	1.40	6 (7%)
27	CLA	11	303	-	69,73,73	1.14	9 (13%)	82,113,113	1.46	8 (9%)
27	CLA	14	308	25	49,53,73	1.36	6 (12%)	58,89,113	1.66	8 (13%)
27	CLA	31	315	-	69,73,73	1.18	9 (13%)	82,113,113	1.37	6 (7%)
27	CLA	w	103	-	69,73,73	1.17	8 (11%)	82,113,113	1.29	6 (7%)
38	A86	32	318	-	47,50,50	4.15	24 (51%)	51,76,76	6.57	18 (35%)
27	CLA	31	308	25	49,53,73	1.39	9 (18%)	58,89,113	1.58	7 (12%)
27	CLA	11	306	25	49,53,73	1.36	6 (12%)	58,89,113	1.68	7 (12%)
27	CLA	33	303	25	69,73,73	1.16	9 (13%)	82,113,113	1.57	7 (8%)
38	A86	34	301	-	47,50,50	4.14	23 (48%)	51,76,76	6.57	17 (33%)
27	CLA	32	309	-	49,53,73	1.34	8 (16%)	58,89,113	1.51	7 (12%)
27	CLA	D	405	-	69,73,73	1.22	9 (13%)	82,113,113	1.45	10 (12%)
30	SQD	b	620	-	35,37,54	1.21	6 (17%)	45,48,65	1.57	9 (20%)
38	A86	32	304	-	47,50,50	4.25	24 (51%)	51,76,76	6.22	17 (33%)
27	CLA	32	306	39	49,53,73	1.35	9 (18%)	58,89,113	1.60	7 (12%)
35	DGD	C	517	-	63,63,67	1.05	7 (11%)	77,77,81	1.59	15 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	c	508	-	69,73,73	1.19	10 (14%)	82,113,113	1.53	10 (12%)
27	CLA	12	309	-	49,53,73	1.34	8 (16%)	58,89,113	1.52	7 (12%)
31	BCT	a	407	26	3,3,3	1.15	0	2,3,3	3.99	2 (100%)
27	CLA	31	307	25	69,73,73	1.18	9 (13%)	82,113,113	1.43	12 (14%)
27	CLA	34	304	25	69,73,73	1.15	9 (13%)	82,113,113	1.56	7 (8%)
27	CLA	14	311	-	49,53,73	1.37	9 (18%)	58,89,113	1.51	5 (8%)
27	CLA	13	304	-	49,53,73	1.35	9 (18%)	58,89,113	1.60	7 (12%)
27	CLA	13	303	25	69,73,73	1.15	8 (11%)	82,113,113	1.57	6 (7%)
27	CLA	11	309	-	49,53,73	1.36	9 (18%)	58,89,113	1.50	5 (8%)
38	A86	32	316	-	47,50,50	4.27	23 (48%)	51,76,76	6.47	18 (35%)
27	CLA	31	305	-	49,53,73	1.35	9 (18%)	58,89,113	1.52	7 (12%)
27	CLA	B	608	-	69,73,73	1.14	8 (11%)	82,113,113	1.37	6 (7%)
33	LMG	B	618	-	51,51,55	0.91	4 (7%)	59,59,63	1.43	8 (13%)
27	CLA	13	310	25	49,53,73	1.39	9 (18%)	58,89,113	1.58	7 (12%)
27	CLA	C	508	-	69,73,73	1.20	10 (14%)	82,113,113	1.54	10 (12%)
27	CLA	c	510	-	69,73,73	1.22	8 (11%)	82,113,113	1.60	10 (12%)
27	CLA	B	612	-	69,73,73	1.26	8 (11%)	82,113,113	1.66	11 (13%)
27	CLA	C	514	-	69,73,73	1.14	9 (13%)	82,113,113	1.46	9 (10%)
38	A86	12	315	-	47,50,50	4.21	23 (48%)	51,76,76	6.60	17 (33%)
36	PL9	d	407	-	55,55,55	2.29	18 (32%)	68,69,69	1.42	12 (17%)
27	CLA	12	305	25	69,73,73	1.15	9 (13%)	82,113,113	1.57	7 (8%)
27	CLA	11	308	25	49,53,73	1.38	9 (18%)	58,89,113	1.58	7 (12%)
35	DGD	c	518	-	63,63,67	1.26	9 (14%)	77,77,81	1.52	14 (18%)
27	CLA	b	604	-	69,73,73	1.23	10 (14%)	82,113,113	1.56	13 (15%)
38	A86	14	316	-	47,50,50	4.14	23 (48%)	51,76,76	6.57	17 (33%)
27	CLA	33	310	25	49,53,73	1.38	8 (16%)	58,89,113	1.58	7 (12%)
27	CLA	A	404	-	69,73,73	1.16	6 (8%)	82,113,113	1.48	9 (10%)
27	CLA	13	307	-	49,53,73	1.34	9 (18%)	58,89,113	1.52	7 (12%)
27	CLA	11	305	-	49,53,73	1.35	9 (18%)	58,89,113	1.52	7 (12%)
28	PHO	A	403	-	58,69,69	2.06	14 (24%)	55,99,99	1.78	11 (20%)
27	CLA	B	611	-	69,73,73	1.23	8 (11%)	82,113,113	1.47	9 (10%)
27	CLA	12	307	-	69,73,73	1.14	9 (13%)	82,113,113	1.46	8 (9%)
32	LHG	l	103	-	48,48,48	0.79	1 (2%)	51,54,54	1.33	6 (11%)
34	OEX	C	501	3,1	0,15,15	-	-	-	-	-
37	HEM	f	102	6,5	50,50,50	1.36	4 (8%)	67,82,82	1.13	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	A86	31	316	-	47,50,50	4.25	24 (51%)	51,76,76	6.22	18 (35%)
27	CLA	C	507	-	69,73,73	1.20	8 (11%)	82,113,113	1.43	10 (12%)
27	CLA	m	101	33	69,73,73	1.15	9 (13%)	82,113,113	1.26	5 (6%)
27	CLA	B	606	-	69,73,73	1.26	12 (17%)	82,113,113	1.48	9 (10%)
27	CLA	13	309	25	69,73,73	1.18	9 (13%)	82,113,113	1.43	12 (14%)
33	LMG	B	619	-	51,51,55	0.99	5 (9%)	59,59,63	1.44	8 (13%)
27	CLA	W	103	-	69,73,73	1.17	8 (11%)	82,113,113	1.29	6 (7%)
38	A86	31	310	-	47,50,50	4.16	23 (48%)	51,76,76	6.92	18 (35%)
38	A86	31	311	-	47,50,50	4.21	23 (48%)	51,76,76	6.59	17 (33%)
39	LMU	32	302	27	33,33,36	1.28	3 (9%)	44,44,47	1.60	8 (18%)
27	CLA	b	608	-	69,73,73	1.14	8 (11%)	82,113,113	1.37	6 (7%)
27	CLA	Z	102	-	69,73,73	1.18	9 (13%)	82,113,113	1.40	7 (8%)
27	CLA	12	311	25	69,73,73	1.18	9 (13%)	82,113,113	1.42	12 (14%)
27	CLA	z	102	-	69,73,73	1.18	9 (13%)	82,113,113	1.39	6 (7%)
27	CLA	34	306	-	69,73,73	1.13	8 (11%)	82,113,113	1.47	8 (9%)
27	CLA	b	610	-	69,73,73	1.23	8 (11%)	82,113,113	1.42	8 (9%)
37	HEM	v	201	16	50,50,50	1.33	5 (10%)	67,82,82	1.28	6 (8%)
27	CLA	12	306	39	49,53,73	1.35	9 (18%)	58,89,113	1.59	7 (12%)
27	CLA	C	511	-	69,73,73	1.27	10 (14%)	82,113,113	1.44	12 (14%)
38	A86	32	317	-	47,50,50	4.24	23 (48%)	51,76,76	6.84	20 (39%)
27	CLA	C	504	-	69,73,73	1.19	9 (13%)	82,113,113	1.45	9 (10%)
27	CLA	B	607	-	69,73,73	1.16	8 (11%)	82,113,113	1.40	8 (9%)
27	CLA	a	402	-	69,73,73	1.18	8 (11%)	82,113,113	1.45	9 (10%)
27	CLA	b	612	-	69,73,73	1.27	8 (11%)	82,113,113	1.65	11 (13%)
38	A86	13	315	-	47,50,50	4.24	23 (48%)	51,76,76	6.84	20 (39%)
27	CLA	11	304	25	49,53,73	1.41	9 (18%)	58,89,113	1.80	13 (22%)
27	CLA	33	308	25	49,53,73	1.37	6 (12%)	58,89,113	1.68	7 (12%)
38	A86	32	314	-	47,50,50	4.16	23 (48%)	51,76,76	6.93	18 (35%)
27	CLA	34	309	25	49,53,73	1.36	6 (12%)	58,89,113	1.67	7 (12%)
38	A86	13	316	-	47,50,50	4.14	23 (48%)	51,76,76	6.58	17 (33%)
27	CLA	31	304	25	49,53,73	1.41	9 (18%)	58,89,113	1.81	13 (22%)
35	DGD	H	102	-	63,63,67	0.93	1 (1%)	77,77,81	1.42	8 (10%)
27	CLA	31	309	-	49,53,73	1.37	9 (18%)	58,89,113	1.50	5 (8%)
27	CLA	12	303	-	69,73,73	1.18	9 (13%)	82,113,113	1.37	6 (7%)
38	A86	33	315	-	47,50,50	4.25	23 (48%)	51,76,76	6.84	20 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	A86	33	313	-	47,50,50	4.20	23 (48%)	51,76,76	6.59	17 (33%)
38	A86	33	316	-	47,50,50	4.16	23 (48%)	51,76,76	6.57	18 (35%)
27	CLA	12	310	25	49,53,73	1.36	6 (12%)	58,89,113	1.67	7 (12%)
38	A86	13	312	-	47,50,50	4.16	23 (48%)	51,76,76	6.93	18 (35%)
27	CLA	B	614	-	69,73,73	1.15	9 (13%)	82,113,113	1.46	7 (8%)
27	CLA	c	506	-	69,73,73	1.17	7 (10%)	82,113,113	1.43	10 (12%)
29	BCR	M	101	-	41,41,41	1.31	2 (4%)	56,56,56	1.41	9 (16%)
27	CLA	d	406	-	69,73,73	1.14	8 (11%)	82,113,113	1.49	5 (6%)
38	A86	13	302	-	47,50,50	4.24	24 (51%)	51,76,76	6.22	18 (35%)
27	CLA	D	401	-	69,73,73	1.22	8 (11%)	82,113,113	1.42	11 (13%)
29	BCR	m	103	-	41,41,41	1.31	2 (4%)	56,56,56	1.41	9 (16%)
38	A86	14	315	-	47,50,50	4.24	23 (48%)	51,76,76	6.84	20 (39%)
38	A86	14	313	-	47,50,50	4.21	23 (48%)	51,76,76	6.60	17 (33%)
27	CLA	C	502	-	69,73,73	1.15	10 (14%)	82,113,113	1.51	11 (13%)
27	CLA	33	311	-	49,53,73	1.36	9 (18%)	58,89,113	1.51	5 (8%)
27	CLA	14	307	-	49,53,73	1.34	9 (18%)	58,89,113	1.52	7 (12%)
33	LMG	M	103	27	40,40,55	0.95	2 (5%)	48,48,63	1.35	7 (14%)
27	CLA	C	505	-	69,73,73	1.16	9 (13%)	82,113,113	1.53	8 (9%)
35	DGD	C	518	-	63,63,67	1.26	9 (14%)	77,77,81	1.52	14 (18%)
27	CLA	31	306	25	49,53,73	1.36	6 (12%)	58,89,113	1.66	8 (13%)
32	LHG	A	408	-	45,45,48	0.80	2 (4%)	48,51,54	1.37	7 (14%)
29	BCR	a	405	-	41,41,41	1.28	3 (7%)	56,56,56	1.40	6 (10%)
27	CLA	34	312	-	49,53,73	1.36	9 (18%)	58,89,113	1.51	5 (8%)
27	CLA	w	102	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	7 (8%)
29	BCR	f	101	-	41,41,41	1.15	3 (7%)	56,56,56	1.33	9 (16%)
38	A86	31	313	-	47,50,50	4.24	23 (48%)	51,76,76	6.84	20 (39%)
27	CLA	12	312	25	49,53,73	1.38	9 (18%)	58,89,113	1.59	7 (12%)
30	SQD	l	101	-	52,54,54	0.93	3 (5%)	62,65,65	1.78	10 (16%)
29	BCR	H	101	-	41,41,41	1.27	4 (9%)	56,56,56	1.31	8 (14%)
29	BCR	A	409	-	41,41,41	1.16	3 (7%)	56,56,56	1.30	5 (8%)
38	A86	12	304	-	47,50,50	4.25	24 (51%)	51,76,76	6.22	18 (35%)
33	LMG	12	301	27	39,39,55	1.01	4 (10%)	47,47,63	1.21	5 (10%)
32	LHG	a	408	-	45,45,48	0.80	2 (4%)	48,51,54	1.37	7 (14%)
33	LMG	32	301	27	39,39,55	1.00	4 (10%)	47,47,63	1.19	4 (8%)
35	DGD	J	101	-	63,63,67	1.11	8 (12%)	77,77,81	1.55	15 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	b	602	-	69,73,73	1.18	8 (11%)	82,113,113	1.39	8 (9%)
27	CLA	D	406	-	69,73,73	1.15	8 (11%)	82,113,113	1.49	5 (6%)
27	CLA	33	306	25	49,53,73	1.41	9 (18%)	58,89,113	1.81	13 (22%)
37	HEM	E	101	6,5	50,50,50	1.36	4 (8%)	67,82,82	1.13	4 (5%)
38	A86	11	316	-	47,50,50	4.24	24 (51%)	51,76,76	6.22	17 (33%)
27	CLA	32	305	25	69,73,73	1.15	9 (13%)	82,113,113	1.57	7 (8%)
27	CLA	c	511	-	69,73,73	1.27	10 (14%)	82,113,113	1.44	12 (14%)
27	CLA	34	311	25	49,53,73	1.39	9 (18%)	58,89,113	1.57	7 (12%)
27	CLA	c	504	-	69,73,73	1.18	9 (13%)	82,113,113	1.44	8 (9%)
27	CLA	32	307	-	69,73,73	1.14	9 (13%)	82,113,113	1.47	8 (9%)
27	CLA	b	611	-	69,73,73	1.24	8 (11%)	82,113,113	1.47	9 (10%)
27	CLA	C	503	-	69,73,73	1.28	10 (14%)	82,113,113	1.43	8 (9%)
27	CLA	34	308	-	49,53,73	1.34	8 (16%)	58,89,113	1.51	7 (12%)
29	BCR	C	520	-	41,41,41	1.27	2 (4%)	56,56,56	1.39	7 (12%)
29	BCR	a	409	-	41,41,41	1.16	3 (7%)	56,56,56	1.30	5 (8%)
31	BCT	A	407	26	3,3,3	1.15	0	2,3,3	3.97	2 (100%)
27	CLA	13	311	-	49,53,73	1.37	9 (18%)	58,89,113	1.51	5 (8%)
27	CLA	31	302	-	49,53,73	1.35	9 (18%)	58,89,113	1.59	7 (12%)
27	CLA	b	609	-	69,73,73	1.16	8 (11%)	82,113,113	1.42	9 (10%)
29	BCR	b	617	-	41,41,41	1.23	2 (4%)	56,56,56	1.43	10 (17%)
29	BCR	c	515	-	41,41,41	1.32	3 (7%)	56,56,56	1.43	8 (14%)
36	PL9	D	404	-	55,55,55	1.29	6 (10%)	68,69,69	1.45	13 (19%)
27	CLA	31	303	-	69,73,73	1.13	9 (13%)	82,113,113	1.46	8 (9%)
27	CLA	c	507	-	69,73,73	1.21	8 (11%)	82,113,113	1.43	10 (12%)
27	CLA	14	306	25	49,53,73	1.40	9 (18%)	58,89,113	1.81	13 (22%)
29	BCR	h	101	-	41,41,41	1.28	4 (9%)	56,56,56	1.32	8 (14%)
27	CLA	a	404	-	69,73,73	1.16	6 (8%)	82,113,113	1.48	9 (10%)
29	BCR	c	516	-	41,41,41	1.30	5 (12%)	56,56,56	1.42	10 (17%)
38	A86	11	312	-	47,50,50	4.27	23 (48%)	51,76,76	6.48	19 (37%)
38	A86	34	315	-	47,50,50	4.26	23 (48%)	51,76,76	6.47	18 (35%)
29	BCR	b	623	-	41,41,41	1.14	3 (7%)	56,56,56	1.29	6 (10%)
38	A86	34	313	-	47,50,50	4.16	23 (48%)	51,76,76	6.93	18 (35%)
27	CLA	C	513	-	69,73,73	1.15	10 (14%)	82,113,113	1.37	6 (7%)
27	CLA	c	503	-	69,73,73	1.28	10 (14%)	82,113,113	1.43	8 (9%)
28	PHO	D	403	-	58,69,69	1.99	12 (20%)	55,99,99	1.74	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	PHO	a	403	-	58,69,69	2.06	14 (24%)	55,99,99	1.79	11 (20%)
38	A86	34	316	-	47,50,50	4.25	23 (48%)	51,76,76	6.83	20 (39%)
33	LMG	W	101	-	51,51,55	0.90	2 (3%)	59,59,63	1.41	7 (11%)
27	CLA	b	615	-	69,73,73	1.23	10 (14%)	82,113,113	1.36	11 (13%)
29	BCR	F	101	-	41,41,41	1.15	3 (7%)	56,56,56	1.33	9 (16%)
32	LHG	L	102	-	48,48,48	0.79	1 (2%)	51,54,54	1.33	6 (11%)
38	A86	12	316	-	47,50,50	4.28	23 (48%)	51,76,76	6.47	18 (35%)
27	CLA	13	301	-	69,73,73	1.18	9 (13%)	82,113,113	1.37	6 (7%)
27	CLA	31	301	25	69,73,73	1.15	9 (13%)	82,113,113	1.56	7 (8%)
38	A86	11	310	-	47,50,50	4.15	23 (48%)	51,76,76	6.93	18 (35%)
38	A86	11	311	-	47,50,50	4.21	23 (48%)	51,76,76	6.59	17 (33%)
30	SQD	B	620	-	35,37,54	1.20	6 (17%)	45,48,65	1.57	9 (20%)
33	LMG	w	101	-	51,51,55	0.90	2 (3%)	59,59,63	1.41	7 (11%)
27	CLA	12	308	25,33	49,53,73	1.40	9 (18%)	58,89,113	1.81	13 (22%)
27	CLA	14	310	25	49,53,73	1.39	8 (16%)	58,89,113	1.58	7 (12%)
27	CLA	b	605	-	69,73,73	1.17	8 (11%)	82,113,113	1.37	5 (6%)
29	BCR	A	405	-	41,41,41	1.27	3 (7%)	56,56,56	1.40	6 (10%)
32	LHG	l	102	-	48,48,48	0.85	1 (2%)	51,54,54	1.29	5 (9%)
37	HEM	V	201	16	50,50,50	1.33	5 (10%)	67,82,82	1.29	6 (8%)
27	CLA	33	301	-	69,73,73	1.18	9 (13%)	82,113,113	1.37	6 (7%)
33	LMG	D	408	-	51,51,55	0.91	3 (5%)	59,59,63	1.42	8 (13%)
35	DGD	j	101	-	63,63,67	1.10	10 (15%)	77,77,81	1.55	15 (19%)
27	CLA	33	305	-	69,73,73	1.14	9 (13%)	82,113,113	1.47	8 (9%)
38	A86	11	314	-	47,50,50	4.15	23 (48%)	51,76,76	6.58	18 (35%)
36	PL9	d	404	-	55,55,55	1.30	6 (10%)	68,69,69	1.46	13 (19%)
38	A86	34	303	-	47,50,50	4.24	24 (51%)	51,76,76	6.22	18 (35%)
27	CLA	b	603	-	69,73,73	1.17	8 (11%)	82,113,113	1.50	10 (12%)
38	A86	14	301	-	47,50,50	4.14	23 (48%)	51,76,76	6.58	18 (35%)
27	CLA	B	602	-	69,73,73	1.17	8 (11%)	82,113,113	1.39	7 (8%)
39	LMU	12	302	27	33,33,36	1.29	3 (9%)	44,44,47	1.58	7 (15%)
27	CLA	W	102	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	7 (8%)
27	CLA	b	606	-	69,73,73	1.26	12 (17%)	82,113,113	1.47	10 (12%)
27	CLA	C	512	3	69,73,73	1.21	11 (15%)	82,113,113	1.51	12 (14%)
27	CLA	c	505	-	69,73,73	1.16	9 (13%)	82,113,113	1.54	8 (9%)
30	SQD	L	103	-	52,54,54	0.93	4 (7%)	62,65,65	1.78	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LHG	B	621	-	48,48,48	0.77	1 (2%)	51,54,54	1.32	6 (11%)
32	LHG	L	101	-	48,48,48	0.84	1 (2%)	51,54,54	1.29	5 (9%)
38	A86	12	317	-	47,50,50	4.24	23 (48%)	51,76,76	6.84	20 (39%)
35	DGD	c	517	-	63,63,67	1.05	8 (12%)	77,77,81	1.59	14 (18%)
27	CLA	14	305	-	69,73,73	1.13	9 (13%)	82,113,113	1.47	8 (9%)
27	CLA	14	304	-	49,53,73	1.34	9 (18%)	58,89,113	1.60	7 (12%)
27	CLA	C	510	-	69,73,73	1.22	8 (11%)	82,113,113	1.59	10 (12%)
27	CLA	B	604	-	69,73,73	1.23	10 (14%)	82,113,113	1.55	14 (17%)
27	CLA	c	514	-	69,73,73	1.14	9 (13%)	82,113,113	1.46	9 (10%)
27	CLA	A	402	-	69,73,73	1.18	8 (11%)	82,113,113	1.46	9 (10%)
27	CLA	13	306	25	49,53,73	1.40	9 (18%)	58,89,113	1.80	13 (22%)
27	CLA	B	615	-	69,73,73	1.23	10 (14%)	82,113,113	1.36	11 (13%)
27	CLA	14	309	25	69,73,73	1.17	9 (13%)	82,113,113	1.43	12 (14%)
27	CLA	32	313	-	49,53,73	1.37	9 (18%)	58,89,113	1.50	5 (8%)
27	CLA	33	307	-	49,53,73	1.35	8 (16%)	58,89,113	1.51	7 (12%)
27	CLA	34	302	-	69,73,73	1.17	9 (13%)	82,113,113	1.36	6 (7%)
29	BCR	z	101	-	41,41,41	1.27	3 (7%)	56,56,56	1.47	10 (17%)
36	PL9	D	407	-	55,55,55	2.29	18 (32%)	68,69,69	1.42	12 (17%)
27	CLA	B	622	-	69,73,73	1.17	9 (13%)	82,113,113	1.50	12 (14%)
29	BCR	B	616	-	41,41,41	1.19	2 (4%)	56,56,56	1.37	8 (14%)
38	A86	13	313	-	47,50,50	4.20	23 (48%)	51,76,76	6.60	17 (33%)

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
27	CLA	b	601	-	1/1/15/20	18/39/115/115	-
27	CLA	b	613	-	1/1/15/20	7/39/115/115	-
27	CLA	32	308	25,33	1/1/11/20	9/15/91/115	-
27	CLA	34	310	25	1/1/15/20	14/39/115/115	-
27	CLA	B	605	-	1/1/15/20	19/39/115/115	-
27	CLA	d	402	-	1/1/15/20	13/39/115/115	-
33	LMG	C	519	-	-	22/46/66/70	0/1/1/1
29	BCR	Z	101	-	-	16/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	A86	32	315	-	-	3/34/90/90	0/3/3/3
27	CLA	11	302	-	1/1/11/20	3/15/91/115	-
27	CLA	c	509	-	1/1/15/20	10/39/115/115	-
27	CLA	B	603	-	1/1/15/20	12/39/115/115	-
27	CLA	C	506	-	1/1/15/20	15/39/115/115	-
27	CLA	c	513	-	1/1/15/20	16/39/115/115	-
27	CLA	B	609	-	1/1/15/20	9/39/115/115	-
27	CLA	11	315	-	1/1/15/20	11/39/115/115	-
29	BCR	B	617	-	-	7/29/63/63	0/2/2/2
38	A86	31	312	-	-	9/34/90/90	0/3/3/3
29	BCR	C	515	-	-	15/29/63/63	0/2/2/2
33	LMG	m	102	27	-	11/35/55/70	0/1/1/1
27	CLA	33	309	25	1/1/15/20	14/39/115/115	-
27	CLA	B	610	-	1/1/15/20	16/39/115/115	-
27	CLA	34	305	-	1/1/11/20	3/15/91/115	-
27	CLA	d	405	-	1/1/15/20	8/39/115/115	-
27	CLA	34	307	25	1/1/11/20	9/15/91/115	-
28	PHO	d	403	-	-	8/37/103/103	0/5/6/6
27	CLA	b	622	-	1/1/15/20	16/39/115/115	-
27	CLA	32	311	25	1/1/15/20	14/39/115/115	-
29	BCR	b	616	-	-	8/29/63/63	0/2/2/2
27	CLA	C	509	-	1/1/15/20	10/39/115/115	-
27	CLA	11	301	25	1/1/15/20	13/39/115/115	-
27	CLA	b	607	-	1/1/15/20	10/39/115/115	-
27	CLA	12	313	-	1/1/11/20	9/15/91/115	-
38	A86	34	314	-	-	3/34/90/90	0/3/3/3
27	CLA	14	302	-	1/1/15/20	11/39/115/115	-
33	LMG	b	618	-	-	18/46/66/70	0/1/1/1
33	LMG	q	301	-	-	22/46/66/70	0/1/1/1
27	CLA	B	613	-	1/1/15/20	7/39/115/115	-
38	A86	13	314	-	-	10/34/90/90	0/3/3/3
38	A86	31	314	-	-	7/34/90/90	0/3/3/3
38	A86	14	312	-	-	7/34/90/90	0/3/3/3
32	LHG	b	621	-	-	20/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	c	512	3	1/1/15/20	8/39/115/115	-
33	LMG	d	408	-	-	14/46/66/70	0/1/1/1
27	CLA	32	303	-	1/1/15/20	11/39/115/115	-
27	CLA	13	308	25	1/1/11/20	10/15/91/115	-
27	CLA	b	614	-	1/1/15/20	6/39/115/115	-
30	SQD	A	406	-	-	13/49/69/69	0/1/1/1
38	A86	33	314	-	-	9/34/90/90	0/3/3/3
27	CLA	32	312	25	-	8/15/91/115	-
38	A86	11	313	-	-	9/34/90/90	0/3/3/3
27	CLA	13	305	-	1/1/15/20	13/39/115/115	-
27	CLA	11	307	25	1/1/15/20	14/39/115/115	-
38	A86	12	314	-	-	7/34/90/90	0/3/3/3
27	CLA	c	502	-	1/1/15/20	13/39/115/115	-
27	CLA	d	401	-	1/1/15/20	12/39/115/115	-
29	BCR	C	516	-	-	7/29/63/63	0/2/2/2
27	CLA	M	102	33	1/1/15/20	19/39/115/115	-
27	CLA	14	303	25	1/1/15/20	13/39/115/115	-
27	CLA	D	402	-	1/1/15/20	13/39/115/115	-
30	SQD	a	406	-	-	13/49/69/69	0/1/1/1
33	LMG	b	619	-	-	20/46/66/70	0/1/1/1
38	A86	13	317	-	-	15/34/90/90	0/3/3/3
38	A86	14	314	-	-	9/34/90/90	0/3/3/3
27	CLA	32	310	25	1/1/11/20	10/15/91/115	-
27	CLA	33	304	-	1/1/11/20	3/15/91/115	-
35	DGD	h	102	-	-	23/51/91/95	0/2/2/2
38	A86	33	312	-	-	7/34/90/90	0/3/3/3
29	BCR	c	519	-	-	8/29/63/63	0/2/2/2
29	BCR	B	623	-	-	16/29/63/63	0/2/2/2
27	CLA	B	601	-	1/1/15/20	18/39/115/115	-
27	CLA	11	303	-	1/1/15/20	13/39/115/115	-
27	CLA	14	308	25	1/1/11/20	10/15/91/115	-
27	CLA	31	315	-	1/1/15/20	11/39/115/115	-
27	CLA	w	103	-	-	21/39/115/115	-
38	A86	32	318	-	-	7/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	33	303	25	1/1/15/20	13/39/115/115	-
27	CLA	11	306	25	1/1/11/20	10/15/91/115	-
27	CLA	31	308	25	-	8/15/91/115	-
38	A86	34	301	-	-	7/34/90/90	0/3/3/3
27	CLA	32	309	-	1/1/11/20	9/15/91/115	-
27	CLA	D	405	-	1/1/15/20	8/39/115/115	-
30	SQD	b	620	-	-	9/32/52/69	0/1/1/1
38	A86	32	304	-	-	15/34/90/90	0/3/3/3
27	CLA	32	306	39	1/1/11/20	3/15/91/115	-
35	DGD	C	517	-	-	19/51/91/95	0/2/2/2
27	CLA	c	508	-	1/1/15/20	16/39/115/115	-
27	CLA	12	309	-	1/1/11/20	9/15/91/115	-
27	CLA	31	307	25	1/1/15/20	14/39/115/115	-
27	CLA	34	304	25	1/1/15/20	13/39/115/115	-
27	CLA	14	311	-	1/1/11/20	9/15/91/115	-
27	CLA	13	304	-	1/1/11/20	3/15/91/115	-
27	CLA	13	303	25	1/1/15/20	13/39/115/115	-
27	CLA	11	309	-	1/1/11/20	9/15/91/115	-
38	A86	32	316	-	-	9/34/90/90	0/3/3/3
27	CLA	31	305	-	1/1/11/20	9/15/91/115	-
27	CLA	B	608	-	1/1/15/20	7/39/115/115	-
33	LMG	B	618	-	-	18/46/66/70	0/1/1/1
27	CLA	13	310	25	-	8/15/91/115	-
27	CLA	C	508	-	1/1/15/20	16/39/115/115	-
27	CLA	c	510	-	1/1/15/20	11/39/115/115	-
27	CLA	B	612	-	1/1/15/20	12/39/115/115	-
27	CLA	C	514	-	1/1/15/20	11/39/115/115	-
38	A86	12	315	-	-	3/34/90/90	0/3/3/3
36	PL9	d	407	-	-	11/53/73/73	0/1/1/1
27	CLA	12	305	25	1/1/15/20	13/39/115/115	-
27	CLA	11	308	25	-	8/15/91/115	-
35	DGD	c	518	-	-	22/51/91/95	0/2/2/2
27	CLA	b	604	-	1/1/15/20	13/39/115/115	-
38	A86	14	316	-	-	7/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	33	310	25	-	8/15/91/115	-
27	CLA	A	404	-	1/1/15/20	11/39/115/115	-
27	CLA	13	307	-	1/1/11/20	9/15/91/115	-
27	CLA	11	305	-	1/1/11/20	9/15/91/115	-
28	PHO	A	403	-	-	10/37/103/103	0/5/6/6
27	CLA	B	611	-	1/1/15/20	12/39/115/115	-
27	CLA	12	307	-	1/1/15/20	13/39/115/115	-
32	LHG	l	103	-	-	22/53/53/53	-
37	HEM	f	102	6,5	-	7/14/54/54	-
38	A86	33	302	-	-	15/34/90/90	0/3/3/3
38	A86	31	316	-	-	15/34/90/90	0/3/3/3
27	CLA	C	507	-	1/1/15/20	18/39/115/115	-
27	CLA	m	101	33	1/1/15/20	19/39/115/115	-
27	CLA	B	606	-	1/1/15/20	7/39/115/115	-
27	CLA	13	309	25	1/1/15/20	14/39/115/115	-
33	LMG	B	619	-	-	20/46/66/70	0/1/1/1
27	CLA	W	103	-	-	21/39/115/115	-
38	A86	31	310	-	-	7/34/90/90	0/3/3/3
38	A86	31	311	-	-	3/34/90/90	0/3/3/3
39	LMU	32	302	27	-	7/18/58/61	0/2/2/2
27	CLA	b	608	-	1/1/15/20	7/39/115/115	-
27	CLA	Z	102	-	-	22/39/115/115	-
27	CLA	12	311	25	1/1/15/20	14/39/115/115	-
27	CLA	z	102	-	-	22/39/115/115	-
27	CLA	34	306	-	1/1/15/20	13/39/115/115	-
27	CLA	b	610	-	1/1/15/20	16/39/115/115	-
37	HEM	v	201	16	-	1/14/54/54	-
27	CLA	12	306	39	1/1/11/20	3/15/91/115	-
27	CLA	C	511	-	1/1/15/20	11/39/115/115	-
38	A86	32	317	-	-	9/34/90/90	0/3/3/3
27	CLA	C	504	-	1/1/15/20	17/39/115/115	-
27	CLA	B	607	-	1/1/15/20	10/39/115/115	-
27	CLA	a	402	-	1/1/15/20	8/39/115/115	-
27	CLA	b	612	-	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	A86	13	315	-	-	9/34/90/90	0/3/3/3
27	CLA	11	304	25	1/1/11/20	9/15/91/115	-
27	CLA	33	308	25	1/1/11/20	10/15/91/115	-
38	A86	32	314	-	-	7/34/90/90	0/3/3/3
27	CLA	34	309	25	1/1/11/20	10/15/91/115	-
38	A86	13	316	-	-	7/34/90/90	0/3/3/3
27	CLA	31	304	25	1/1/11/20	9/15/91/115	-
35	DGD	H	102	-	-	23/51/91/95	0/2/2/2
27	CLA	31	309	-	1/1/11/20	9/15/91/115	-
27	CLA	12	303	-	1/1/15/20	11/39/115/115	-
38	A86	33	315	-	-	9/34/90/90	0/3/3/3
38	A86	33	313	-	-	3/34/90/90	0/3/3/3
38	A86	33	316	-	-	7/34/90/90	0/3/3/3
27	CLA	12	310	25	1/1/11/20	10/15/91/115	-
38	A86	13	312	-	-	7/34/90/90	0/3/3/3
27	CLA	B	614	-	1/1/15/20	6/39/115/115	-
27	CLA	c	506	-	1/1/15/20	14/39/115/115	-
29	BCR	M	101	-	-	8/29/63/63	0/2/2/2
27	CLA	d	406	-	1/1/15/20	6/39/115/115	-
38	A86	13	302	-	-	15/34/90/90	0/3/3/3
27	CLA	D	401	-	1/1/15/20	12/39/115/115	-
29	BCR	m	103	-	-	8/29/63/63	0/2/2/2
38	A86	14	315	-	-	9/34/90/90	0/3/3/3
38	A86	14	313	-	-	3/34/90/90	0/3/3/3
27	CLA	C	502	-	1/1/15/20	13/39/115/115	-
27	CLA	33	311	-	1/1/11/20	9/15/91/115	-
27	CLA	14	307	-	1/1/11/20	9/15/91/115	-
33	LMG	M	103	27	-	11/35/55/70	0/1/1/1
27	CLA	C	505	-	1/1/15/20	18/39/115/115	-
35	DGD	C	518	-	-	22/51/91/95	0/2/2/2
27	CLA	31	306	25	1/1/11/20	10/15/91/115	-
32	LHG	A	408	-	-	23/50/50/53	-
29	BCR	a	405	-	-	12/29/63/63	0/2/2/2
27	CLA	34	312	-	1/1/11/20	9/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	w	102	-	1/1/15/20	16/39/115/115	-
29	BCR	f	101	-	-	15/29/63/63	0/2/2/2
38	A86	31	313	-	-	9/34/90/90	0/3/3/3
27	CLA	12	312	25	-	8/15/91/115	-
30	SQD	l	101	-	-	21/49/69/69	0/1/1/1
29	BCR	H	101	-	-	8/29/63/63	0/2/2/2
29	BCR	A	409	-	-	9/29/63/63	0/2/2/2
38	A86	12	304	-	-	15/34/90/90	0/3/3/3
33	LMG	12	301	27	-	17/34/54/70	0/1/1/1
32	LHG	a	408	-	-	23/50/50/53	-
33	LMG	32	301	27	-	13/34/54/70	0/1/1/1
35	DGD	J	101	-	-	15/51/91/95	0/2/2/2
27	CLA	b	602	-	1/1/15/20	15/39/115/115	-
27	CLA	D	406	-	1/1/15/20	6/39/115/115	-
27	CLA	33	306	25	1/1/11/20	9/15/91/115	-
37	HEM	E	101	6,5	-	7/14/54/54	-
38	A86	11	316	-	-	15/34/90/90	0/3/3/3
27	CLA	32	305	25	1/1/15/20	13/39/115/115	-
27	CLA	c	511	-	1/1/15/20	12/39/115/115	-
27	CLA	34	311	25	-	8/15/91/115	-
27	CLA	c	504	-	1/1/15/20	17/39/115/115	-
27	CLA	32	307	-	1/1/15/20	13/39/115/115	-
27	CLA	b	611	-	1/1/15/20	12/39/115/115	-
27	CLA	C	503	-	1/1/15/20	12/39/115/115	-
27	CLA	34	308	-	1/1/11/20	9/15/91/115	-
29	BCR	C	520	-	-	8/29/63/63	0/2/2/2
29	BCR	a	409	-	-	9/29/63/63	0/2/2/2
37	HEM	V	201	16	-	1/14/54/54	-
27	CLA	13	311	-	1/1/11/20	9/15/91/115	-
27	CLA	31	302	-	1/1/11/20	3/15/91/115	-
27	CLA	b	609	-	1/1/15/20	9/39/115/115	-
29	BCR	b	617	-	-	7/29/63/63	0/2/2/2
29	BCR	c	515	-	-	15/29/63/63	0/2/2/2
36	PL9	D	404	-	-	17/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	31	303	-	1/1/15/20	13/39/115/115	-
27	CLA	c	507	-	1/1/15/20	18/39/115/115	-
27	CLA	14	306	25	1/1/11/20	9/15/91/115	-
29	BCR	h	101	-	-	8/29/63/63	0/2/2/2
27	CLA	a	404	-	1/1/15/20	11/39/115/115	-
29	BCR	c	516	-	-	7/29/63/63	0/2/2/2
38	A86	11	312	-	-	9/34/90/90	0/3/3/3
38	A86	34	315	-	-	10/34/90/90	0/3/3/3
29	BCR	b	623	-	-	16/29/63/63	0/2/2/2
38	A86	34	313	-	-	7/34/90/90	0/3/3/3
27	CLA	C	513	-	1/1/15/20	16/39/115/115	-
27	CLA	c	503	-	1/1/15/20	12/39/115/115	-
28	PHO	D	403	-	-	8/37/103/103	0/5/6/6
28	PHO	a	403	-	-	10/37/103/103	0/5/6/6
38	A86	34	316	-	-	9/34/90/90	0/3/3/3
33	LMG	W	101	-	-	28/46/66/70	0/1/1/1
27	CLA	b	615	-	1/1/15/20	13/39/115/115	-
29	BCR	F	101	-	-	15/29/63/63	0/2/2/2
32	LHG	L	102	-	-	22/53/53/53	-
38	A86	12	316	-	-	10/34/90/90	0/3/3/3
27	CLA	13	301	-	1/1/15/20	11/39/115/115	-
27	CLA	31	301	25	1/1/15/20	13/39/115/115	-
38	A86	11	310	-	-	7/34/90/90	0/3/3/3
38	A86	11	311	-	-	3/34/90/90	0/3/3/3
30	SQD	B	620	-	-	9/32/52/69	0/1/1/1
33	LMG	w	101	-	-	28/46/66/70	0/1/1/1
27	CLA	12	308	25,33	1/1/11/20	9/15/91/115	-
27	CLA	14	310	25	-	8/15/91/115	-
27	CLA	b	605	-	1/1/15/20	19/39/115/115	-
29	BCR	A	405	-	-	12/29/63/63	0/2/2/2
32	LHG	l	102	-	-	29/53/53/53	-
27	CLA	33	301	-	1/1/15/20	11/39/115/115	-
33	LMG	D	408	-	-	14/46/66/70	0/1/1/1
35	DGD	j	101	-	-	15/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	33	305	-	1/1/15/20	13/39/115/115	-
38	A86	11	314	-	-	7/34/90/90	0/3/3/3
36	PL9	d	404	-	-	17/53/73/73	0/1/1/1
38	A86	34	303	-	-	15/34/90/90	0/3/3/3
27	CLA	b	603	-	1/1/15/20	12/39/115/115	-
38	A86	14	301	-	-	7/34/90/90	0/3/3/3
27	CLA	B	602	-	1/1/15/20	15/39/115/115	-
39	LMU	12	302	27	-	7/18/58/61	0/2/2/2
27	CLA	W	102	-	1/1/15/20	16/39/115/115	-
27	CLA	b	606	-	1/1/15/20	7/39/115/115	-
27	CLA	C	512	3	1/1/15/20	8/39/115/115	-
27	CLA	c	505	-	1/1/15/20	18/39/115/115	-
30	SQD	L	103	-	-	21/49/69/69	0/1/1/1
32	LHG	B	621	-	-	20/53/53/53	-
32	LHG	L	101	-	-	29/53/53/53	-
38	A86	12	317	-	-	9/34/90/90	0/3/3/3
35	DGD	c	517	-	-	19/51/91/95	0/2/2/2
27	CLA	14	305	-	1/1/15/20	13/39/115/115	-
27	CLA	14	304	-	1/1/11/20	3/15/91/115	-
27	CLA	C	510	-	1/1/15/20	11/39/115/115	-
27	CLA	B	604	-	1/1/15/20	13/39/115/115	-
27	CLA	c	514	-	1/1/15/20	11/39/115/115	-
27	CLA	A	402	-	1/1/15/20	8/39/115/115	-
27	CLA	13	306	25	1/1/11/20	9/15/91/115	-
27	CLA	B	615	-	1/1/15/20	13/39/115/115	-
27	CLA	14	309	25	1/1/15/20	14/39/115/115	-
27	CLA	32	313	-	1/1/11/20	9/15/91/115	-
27	CLA	33	307	-	1/1/11/20	9/15/91/115	-
27	CLA	34	302	-	1/1/15/20	11/39/115/115	-
29	BCR	z	101	-	-	16/29/63/63	0/2/2/2
36	PL9	D	407	-	-	11/53/73/73	0/1/1/1
27	CLA	B	622	-	1/1/15/20	17/39/115/115	-
29	BCR	B	616	-	-	8/29/63/63	0/2/2/2
38	A86	13	313	-	-	3/34/90/90	0/3/3/3

All (2823) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	34	316	A86	C14-C13	15.27	1.68	1.51
38	11	313	A86	C14-C13	15.20	1.68	1.51
38	13	315	A86	C14-C13	15.17	1.68	1.51
38	12	317	A86	C14-C13	15.17	1.68	1.51
38	31	313	A86	C14-C13	15.16	1.68	1.51
38	32	317	A86	C14-C13	15.16	1.68	1.51
38	33	315	A86	C14-C13	15.16	1.68	1.51
38	14	315	A86	C14-C13	15.14	1.68	1.51
38	33	316	A86	C14-C13	15.13	1.68	1.51
38	13	314	A86	C14-C13	15.08	1.68	1.51
38	32	318	A86	C14-C13	15.07	1.68	1.51
38	11	312	A86	C14-C13	15.06	1.68	1.51
38	11	314	A86	C14-C13	15.05	1.68	1.51
38	12	316	A86	C14-C13	15.04	1.68	1.51
38	31	314	A86	C14-C13	15.04	1.68	1.51
38	32	316	A86	C14-C13	15.04	1.68	1.51
38	14	314	A86	C14-C13	15.03	1.68	1.51
38	14	316	A86	C14-C13	15.02	1.68	1.51
38	14	301	A86	C14-C13	15.01	1.68	1.51
38	13	316	A86	C14-C13	15.00	1.68	1.51
38	33	314	A86	C14-C13	15.00	1.68	1.51
38	31	312	A86	C14-C13	14.99	1.68	1.51
38	34	301	A86	C14-C13	14.98	1.67	1.51
38	12	314	A86	C14-C13	14.97	1.67	1.51
38	34	315	A86	C14-C13	14.95	1.67	1.51
38	14	312	A86	C14-C13	14.95	1.67	1.51
38	31	316	A86	C14-C13	14.94	1.67	1.51
38	32	314	A86	C14-C13	14.94	1.67	1.51
38	11	310	A86	C14-C13	14.94	1.67	1.51
38	33	312	A86	C14-C13	14.93	1.67	1.51
38	13	312	A86	C14-C13	14.92	1.67	1.51
38	34	313	A86	C14-C13	14.91	1.67	1.51
38	31	310	A86	C14-C13	14.91	1.67	1.51
38	32	304	A86	C14-C13	14.90	1.67	1.51
38	13	317	A86	C14-C13	14.88	1.67	1.51
38	12	304	A86	C14-C13	14.87	1.67	1.51
38	34	303	A86	C14-C13	14.86	1.67	1.51
38	33	302	A86	C14-C13	14.85	1.67	1.51
38	11	316	A86	C14-C13	14.83	1.67	1.51
38	13	302	A86	C14-C13	14.82	1.67	1.51
38	31	311	A86	C14-C13	14.81	1.67	1.51
38	12	315	A86	C14-C13	14.81	1.67	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	32	315	A86	C14-C13	14.80	1.67	1.51
38	14	313	A86	C14-C13	14.78	1.67	1.51
38	13	313	A86	C14-C13	14.77	1.67	1.51
38	34	314	A86	C14-C13	14.76	1.67	1.51
38	33	313	A86	C14-C13	14.76	1.67	1.51
38	11	311	A86	C14-C13	14.76	1.67	1.51
38	13	317	A86	C30-C31	11.27	1.43	1.30
38	12	304	A86	C30-C31	11.25	1.43	1.30
38	32	304	A86	C30-C31	11.25	1.43	1.30
38	13	302	A86	C30-C31	11.25	1.43	1.30
38	33	302	A86	C30-C31	11.25	1.43	1.30
38	31	316	A86	C30-C31	11.24	1.43	1.30
38	34	303	A86	C30-C31	11.24	1.43	1.30
38	11	316	A86	C30-C31	11.23	1.43	1.30
38	12	316	A86	C30-C31	11.21	1.43	1.30
38	13	314	A86	C30-C31	11.19	1.43	1.30
38	14	314	A86	C30-C31	11.19	1.43	1.30
38	32	316	A86	C30-C31	11.18	1.43	1.30
38	11	312	A86	C30-C31	11.16	1.43	1.30
38	31	312	A86	C30-C31	11.14	1.43	1.30
38	34	315	A86	C30-C31	11.12	1.43	1.30
38	33	314	A86	C30-C31	11.08	1.43	1.30
38	12	315	A86	C30-C31	10.88	1.43	1.30
38	14	313	A86	C30-C31	10.86	1.43	1.30
38	33	313	A86	C30-C31	10.84	1.43	1.30
38	33	315	A86	C30-C31	10.84	1.43	1.30
38	34	314	A86	C30-C31	10.81	1.43	1.30
38	13	313	A86	C30-C31	10.81	1.43	1.30
38	11	311	A86	C30-C31	10.80	1.43	1.30
38	11	313	A86	C30-C31	10.78	1.43	1.30
38	32	315	A86	C30-C31	10.77	1.43	1.30
38	13	315	A86	C30-C31	10.76	1.43	1.30
38	32	317	A86	C30-C31	10.75	1.43	1.30
38	31	311	A86	C30-C31	10.74	1.43	1.30
38	14	315	A86	C30-C31	10.72	1.43	1.30
38	31	313	A86	C30-C31	10.72	1.43	1.30
38	34	316	A86	C30-C31	10.69	1.43	1.30
38	12	317	A86	C30-C31	10.68	1.43	1.30
38	33	312	A86	C30-C31	10.56	1.42	1.30
38	14	312	A86	C30-C31	10.52	1.42	1.30
38	31	310	A86	C30-C31	10.48	1.42	1.30
38	13	312	A86	C30-C31	10.47	1.42	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	12	314	A86	C30-C31	10.46	1.42	1.30
38	11	310	A86	C30-C31	10.45	1.42	1.30
38	34	313	A86	C30-C31	10.43	1.42	1.30
38	32	314	A86	C30-C31	10.41	1.42	1.30
38	33	316	A86	C30-C31	10.27	1.42	1.30
38	11	314	A86	C30-C31	10.25	1.42	1.30
38	34	301	A86	C30-C31	10.24	1.42	1.30
38	31	314	A86	C30-C31	10.24	1.42	1.30
38	32	318	A86	C30-C31	10.23	1.42	1.30
38	14	301	A86	C30-C31	10.22	1.42	1.30
38	14	316	A86	C30-C31	10.19	1.42	1.30
38	13	316	A86	C30-C31	10.16	1.42	1.30
38	31	316	A86	C30-C29	9.17	1.46	1.31
38	12	304	A86	C30-C29	9.15	1.46	1.31
38	32	304	A86	C30-C29	9.15	1.46	1.31
38	33	302	A86	C30-C29	9.14	1.46	1.31
38	34	303	A86	C30-C29	9.14	1.46	1.31
38	13	317	A86	C30-C29	9.14	1.46	1.31
38	11	316	A86	C30-C29	9.13	1.46	1.31
38	13	302	A86	C30-C29	9.12	1.46	1.31
38	32	316	A86	C30-C29	8.98	1.46	1.31
38	33	314	A86	C30-C29	8.97	1.46	1.31
38	31	311	A86	C30-C29	8.96	1.46	1.31
38	11	312	A86	C30-C29	8.95	1.46	1.31
38	14	314	A86	C30-C29	8.95	1.46	1.31
38	12	316	A86	C30-C29	8.95	1.46	1.31
38	13	313	A86	C30-C29	8.95	1.46	1.31
38	34	315	A86	C30-C29	8.94	1.46	1.31
38	32	315	A86	C30-C29	8.94	1.46	1.31
38	31	312	A86	C30-C29	8.94	1.46	1.31
38	11	311	A86	C30-C29	8.93	1.46	1.31
38	13	314	A86	C30-C29	8.92	1.46	1.31
38	14	313	A86	C30-C29	8.91	1.46	1.31
38	12	315	A86	C30-C29	8.90	1.46	1.31
38	33	313	A86	C30-C29	8.89	1.46	1.31
38	34	314	A86	C30-C29	8.88	1.46	1.31
38	12	317	A86	C30-C29	8.86	1.46	1.31
38	31	313	A86	C30-C29	8.85	1.46	1.31
38	33	315	A86	C30-C29	8.84	1.46	1.31
38	11	313	A86	C30-C29	8.84	1.46	1.31
38	34	316	A86	C30-C29	8.84	1.46	1.31
38	32	317	A86	C30-C29	8.82	1.46	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	14	315	A86	C30-C29	8.81	1.46	1.31
38	13	315	A86	C30-C29	8.80	1.46	1.31
38	32	314	A86	C30-C29	8.80	1.46	1.31
38	31	310	A86	C30-C29	8.77	1.46	1.31
38	34	313	A86	C30-C29	8.77	1.46	1.31
38	12	314	A86	C30-C29	8.75	1.46	1.31
38	33	312	A86	C30-C29	8.75	1.46	1.31
38	14	312	A86	C30-C29	8.75	1.46	1.31
38	11	310	A86	C30-C29	8.73	1.46	1.31
38	13	312	A86	C30-C29	8.73	1.46	1.31
38	14	301	A86	C30-C29	8.57	1.45	1.31
38	14	316	A86	C30-C29	8.57	1.45	1.31
38	13	316	A86	C30-C29	8.56	1.45	1.31
38	11	314	A86	C30-C29	8.55	1.45	1.31
38	31	314	A86	C30-C29	8.55	1.45	1.31
38	34	301	A86	C30-C29	8.52	1.45	1.31
38	33	316	A86	C30-C29	8.50	1.45	1.31
38	32	318	A86	C30-C29	8.50	1.45	1.31
28	D	403	PHO	C1B-C2B	8.48	1.48	1.39
28	d	403	PHO	C1B-C2B	8.46	1.48	1.39
28	a	403	PHO	C1B-C2B	8.45	1.48	1.39
28	A	403	PHO	C1B-C2B	8.43	1.48	1.39
38	32	304	A86	C4-C5	7.59	1.66	1.43
38	33	302	A86	C4-C5	7.57	1.66	1.43
38	11	316	A86	C4-C5	7.57	1.66	1.43
38	13	317	A86	C4-C5	7.56	1.66	1.43
38	12	304	A86	C4-C5	7.56	1.66	1.43
38	34	303	A86	C4-C5	7.55	1.66	1.43
38	13	302	A86	C4-C5	7.55	1.66	1.43
38	31	316	A86	C4-C5	7.54	1.66	1.43
38	13	314	A86	C4-C5	7.48	1.66	1.43
38	14	314	A86	C4-C5	7.48	1.66	1.43
38	12	316	A86	C4-C5	7.47	1.66	1.43
38	31	312	A86	C4-C5	7.47	1.66	1.43
38	32	316	A86	C4-C5	7.47	1.66	1.43
38	12	304	A86	C8-C6	7.47	1.61	1.46
38	11	312	A86	C4-C5	7.46	1.66	1.43
38	33	314	A86	C4-C5	7.46	1.66	1.43
28	A	403	PHO	C3B-C4B	7.46	1.49	1.41
28	a	403	PHO	C3B-C4B	7.45	1.49	1.41
38	34	315	A86	C4-C5	7.44	1.66	1.43
38	32	304	A86	C8-C6	7.44	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	11	316	A86	C8-C6	7.44	1.61	1.46
38	13	317	A86	C8-C6	7.44	1.61	1.46
38	31	316	A86	C8-C6	7.43	1.61	1.46
38	13	302	A86	C8-C6	7.43	1.61	1.46
38	33	302	A86	C8-C6	7.42	1.61	1.46
38	11	314	A86	C4-C5	7.40	1.66	1.43
38	34	303	A86	C8-C6	7.40	1.61	1.46
38	31	314	A86	C4-C5	7.39	1.66	1.43
38	32	318	A86	C4-C5	7.39	1.66	1.43
38	32	315	A86	C4-C5	7.38	1.66	1.43
38	11	311	A86	C4-C5	7.38	1.66	1.43
38	33	315	A86	C4-C5	7.38	1.66	1.43
38	11	313	A86	C4-C5	7.38	1.66	1.43
38	32	317	A86	C4-C5	7.38	1.66	1.43
38	14	301	A86	C4-C5	7.38	1.66	1.43
38	12	315	A86	C4-C5	7.38	1.66	1.43
38	13	316	A86	C4-C5	7.38	1.66	1.43
38	31	311	A86	C4-C5	7.38	1.66	1.43
38	14	315	A86	C4-C5	7.37	1.66	1.43
38	33	316	A86	C4-C5	7.37	1.66	1.43
38	13	315	A86	C4-C5	7.37	1.66	1.43
38	34	314	A86	C4-C5	7.37	1.66	1.43
38	34	316	A86	C4-C5	7.37	1.66	1.43
38	13	313	A86	C4-C5	7.37	1.66	1.43
38	14	313	A86	C4-C5	7.36	1.66	1.43
38	14	316	A86	C4-C5	7.36	1.66	1.43
38	34	301	A86	C4-C5	7.36	1.66	1.43
38	12	317	A86	C4-C5	7.36	1.66	1.43
36	d	407	PL9	C3-C4	-7.35	1.38	1.49
38	33	313	A86	C4-C5	7.35	1.66	1.43
38	31	313	A86	C4-C5	7.34	1.65	1.43
38	14	312	A86	C4-C5	7.34	1.65	1.43
38	11	310	A86	C4-C5	7.33	1.65	1.43
38	33	312	A86	C4-C5	7.33	1.65	1.43
36	D	407	PL9	C3-C4	-7.33	1.38	1.49
38	13	312	A86	C4-C5	7.33	1.65	1.43
38	32	314	A86	C4-C5	7.32	1.65	1.43
38	12	314	A86	C4-C5	7.32	1.65	1.43
38	31	310	A86	C4-C5	7.32	1.65	1.43
38	34	313	A86	C4-C5	7.32	1.65	1.43
38	13	314	A86	C8-C6	7.27	1.61	1.46
38	14	314	A86	C8-C6	7.27	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	33	314	A86	C8-C6	7.27	1.61	1.46
38	31	312	A86	C8-C6	7.27	1.61	1.46
38	11	312	A86	C8-C6	7.26	1.61	1.46
38	34	315	A86	C8-C6	7.26	1.61	1.46
28	D	403	PHO	C3B-C4B	7.26	1.48	1.41
38	32	316	A86	C8-C6	7.26	1.61	1.46
38	12	316	A86	C8-C6	7.25	1.61	1.46
28	d	403	PHO	C3B-C4B	7.25	1.48	1.41
38	14	315	A86	C8-C6	7.16	1.61	1.46
38	11	313	A86	C8-C6	7.15	1.61	1.46
38	11	313	A86	C19-C20	7.15	1.62	1.52
38	34	316	A86	C19-C20	7.15	1.62	1.52
38	14	315	A86	C19-C20	7.14	1.62	1.52
38	32	317	A86	C8-C6	7.13	1.61	1.46
38	31	313	A86	C19-C20	7.12	1.62	1.52
38	34	316	A86	C8-C6	7.12	1.61	1.46
38	13	315	A86	C8-C6	7.12	1.61	1.46
38	31	313	A86	C8-C6	7.12	1.61	1.46
38	12	317	A86	C19-C20	7.11	1.62	1.52
38	32	317	A86	C19-C20	7.11	1.62	1.52
38	33	315	A86	C8-C6	7.11	1.61	1.46
38	12	317	A86	C8-C6	7.08	1.61	1.46
38	12	315	A86	C8-C6	7.08	1.61	1.46
38	13	315	A86	C19-C20	7.08	1.62	1.52
38	13	313	A86	C8-C6	7.06	1.61	1.46
38	33	313	A86	C8-C6	7.06	1.61	1.46
38	11	311	A86	C8-C6	7.05	1.61	1.46
38	33	315	A86	C19-C20	7.05	1.62	1.52
38	34	314	A86	C8-C6	7.04	1.61	1.46
38	31	311	A86	C8-C6	7.03	1.61	1.46
38	11	314	A86	C8-C6	7.01	1.61	1.46
38	14	313	A86	C8-C6	7.01	1.61	1.46
38	32	315	A86	C8-C6	7.01	1.60	1.46
38	14	316	A86	C8-C6	7.00	1.60	1.46
38	34	301	A86	C8-C6	7.00	1.60	1.46
38	31	314	A86	C8-C6	6.99	1.60	1.46
38	14	301	A86	C8-C6	6.98	1.60	1.46
38	13	316	A86	C8-C6	6.98	1.60	1.46
38	33	312	A86	C8-C6	6.97	1.60	1.46
38	33	316	A86	C8-C6	6.97	1.60	1.46
38	32	318	A86	C8-C6	6.97	1.60	1.46
38	31	310	A86	C8-C6	6.95	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	11	310	A86	C8-C6	6.95	1.60	1.46
38	13	312	A86	C8-C6	6.95	1.60	1.46
38	32	314	A86	C8-C6	6.94	1.60	1.46
38	34	313	A86	C8-C6	6.91	1.60	1.46
38	14	312	A86	C8-C6	6.91	1.60	1.46
38	12	314	A86	C8-C6	6.90	1.60	1.46
38	33	313	A86	C25-C26	6.89	1.64	1.43
38	13	313	A86	C25-C26	6.88	1.64	1.43
36	d	407	PL9	C6-C1	-6.88	1.37	1.48
38	31	311	A86	C25-C26	6.88	1.64	1.43
38	11	311	A86	C25-C26	6.87	1.64	1.43
38	14	313	A86	C25-C26	6.87	1.64	1.43
38	12	315	A86	C25-C26	6.87	1.64	1.43
38	34	314	A86	C25-C26	6.86	1.64	1.43
38	11	311	A86	C19-C20	6.84	1.61	1.52
36	D	407	PL9	C6-C1	-6.84	1.37	1.48
38	32	315	A86	C25-C26	6.84	1.64	1.43
38	12	315	A86	C19-C20	6.84	1.61	1.52
38	33	313	A86	C19-C20	6.83	1.61	1.52
38	13	314	A86	C25-C26	6.83	1.64	1.43
38	32	315	A86	C19-C20	6.83	1.61	1.52
38	33	314	A86	C25-C26	6.83	1.64	1.43
38	13	312	A86	C19-C20	6.83	1.61	1.52
38	33	302	A86	C25-C26	6.83	1.64	1.43
38	14	312	A86	C19-C20	6.83	1.61	1.52
38	31	316	A86	C25-C26	6.82	1.64	1.43
38	14	314	A86	C25-C26	6.82	1.64	1.43
38	31	312	A86	C25-C26	6.82	1.64	1.43
38	34	315	A86	C25-C26	6.82	1.64	1.43
38	12	316	A86	C25-C26	6.82	1.64	1.43
38	13	302	A86	C25-C26	6.81	1.64	1.43
38	34	303	A86	C25-C26	6.81	1.64	1.43
38	12	304	A86	C25-C26	6.81	1.64	1.43
38	13	317	A86	C25-C26	6.81	1.64	1.43
38	11	316	A86	C25-C26	6.81	1.64	1.43
38	11	310	A86	C19-C20	6.81	1.61	1.52
38	12	314	A86	C19-C20	6.81	1.61	1.52
38	34	313	A86	C19-C20	6.81	1.61	1.52
38	32	316	A86	C25-C26	6.81	1.64	1.43
38	11	312	A86	C25-C26	6.80	1.64	1.43
38	31	311	A86	C19-C20	6.80	1.61	1.52
38	34	314	A86	C19-C20	6.80	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	13	313	A86	C19-C20	6.79	1.61	1.52
38	31	310	A86	C19-C20	6.79	1.61	1.52
38	33	312	A86	C19-C20	6.79	1.61	1.52
38	32	304	A86	C25-C26	6.79	1.64	1.43
38	32	314	A86	C19-C20	6.77	1.61	1.52
38	14	313	A86	C19-C20	6.73	1.61	1.52
38	33	316	A86	C25-C26	6.71	1.64	1.43
38	14	316	A86	C25-C26	6.69	1.63	1.43
38	34	301	A86	C25-C26	6.69	1.63	1.43
38	32	318	A86	C25-C26	6.68	1.63	1.43
38	11	314	A86	C25-C26	6.68	1.63	1.43
38	31	314	A86	C25-C26	6.68	1.63	1.43
38	14	301	A86	C25-C26	6.68	1.63	1.43
38	13	316	A86	C25-C26	6.67	1.63	1.43
38	33	315	A86	C25-C26	6.67	1.63	1.43
38	11	310	A86	C25-C26	6.65	1.63	1.43
38	34	313	A86	C25-C26	6.65	1.63	1.43
38	11	313	A86	C25-C26	6.64	1.63	1.43
38	31	310	A86	C25-C26	6.64	1.63	1.43
38	13	315	A86	C25-C26	6.64	1.63	1.43
38	34	316	A86	C25-C26	6.64	1.63	1.43
38	32	314	A86	C25-C26	6.63	1.63	1.43
38	12	317	A86	C25-C26	6.63	1.63	1.43
38	32	317	A86	C25-C26	6.63	1.63	1.43
38	31	313	A86	C25-C26	6.63	1.63	1.43
38	13	312	A86	C25-C26	6.63	1.63	1.43
38	33	312	A86	C25-C26	6.63	1.63	1.43
38	14	315	A86	C25-C26	6.62	1.63	1.43
38	14	312	A86	C25-C26	6.61	1.63	1.43
38	12	314	A86	C25-C26	6.61	1.63	1.43
38	33	314	A86	C19-C20	6.59	1.61	1.52
38	13	314	A86	C19-C20	6.58	1.61	1.52
38	11	312	A86	C19-C20	6.54	1.61	1.52
38	14	314	A86	C19-C20	6.54	1.61	1.52
38	32	316	A86	C19-C20	6.51	1.61	1.52
38	12	316	A86	C19-C20	6.51	1.61	1.52
38	34	315	A86	C19-C20	6.50	1.61	1.52
38	31	312	A86	C19-C20	6.50	1.61	1.52
38	13	316	A86	C19-C20	6.40	1.61	1.52
38	31	314	A86	C19-C20	6.37	1.61	1.52
38	33	316	A86	C19-C20	6.36	1.61	1.52
38	11	314	A86	C19-C20	6.36	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	32	318	A86	C19-C20	6.36	1.61	1.52
38	14	316	A86	C19-C20	6.35	1.61	1.52
38	34	301	A86	C19-C20	6.34	1.61	1.52
38	14	301	A86	C19-C20	6.31	1.61	1.52
38	31	316	A86	C19-C20	6.12	1.60	1.52
38	33	302	A86	C19-C20	6.10	1.60	1.52
38	13	317	A86	C19-C20	6.09	1.60	1.52
38	34	303	A86	C19-C20	6.08	1.60	1.52
38	32	304	A86	C19-C20	6.08	1.60	1.52
38	13	302	A86	C19-C20	6.07	1.60	1.52
38	12	304	A86	C19-C20	6.04	1.60	1.52
38	11	316	A86	C19-C20	6.01	1.60	1.52
36	D	407	PL9	C7-C3	-5.96	1.43	1.51
36	d	407	PL9	C7-C3	-5.87	1.43	1.51
38	12	316	A86	C9-C8	4.87	1.47	1.34
38	13	314	A86	C9-C8	4.86	1.47	1.34
38	34	315	A86	C9-C8	4.85	1.47	1.34
38	32	316	A86	C9-C8	4.84	1.47	1.34
38	11	312	A86	C9-C8	4.82	1.47	1.34
38	33	314	A86	C9-C8	4.82	1.47	1.34
38	14	314	A86	C9-C8	4.82	1.47	1.34
38	31	312	A86	C9-C8	4.81	1.47	1.34
38	13	302	A86	C9-C8	4.79	1.47	1.34
38	34	303	A86	C9-C8	4.77	1.47	1.34
38	11	316	A86	C9-C8	4.76	1.47	1.34
38	32	304	A86	C9-C8	4.76	1.47	1.34
38	33	302	A86	C9-C8	4.76	1.47	1.34
38	13	317	A86	C9-C8	4.75	1.47	1.34
38	31	316	A86	C9-C8	4.74	1.47	1.34
38	12	304	A86	C9-C8	4.74	1.47	1.34
38	12	316	A86	O4-C38	4.68	1.45	1.35
38	11	312	A86	O4-C38	4.68	1.45	1.35
38	13	314	A86	O4-C38	4.68	1.45	1.35
38	14	314	A86	O4-C38	4.67	1.45	1.35
38	31	312	A86	O4-C38	4.66	1.45	1.35
38	32	316	A86	O4-C38	4.66	1.45	1.35
38	34	315	A86	O4-C38	4.65	1.45	1.35
38	33	314	A86	O4-C38	4.64	1.45	1.35
38	32	315	A86	C9-C8	4.64	1.46	1.34
38	33	313	A86	C9-C8	4.63	1.46	1.34
38	31	311	A86	C9-C8	4.62	1.46	1.34
38	14	313	A86	C9-C8	4.62	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	13	313	A86	C9-C8	4.61	1.46	1.34
38	11	311	A86	C9-C8	4.61	1.46	1.34
38	33	316	A86	C9-C8	4.60	1.46	1.34
38	12	315	A86	C9-C8	4.60	1.46	1.34
38	14	301	A86	C9-C8	4.60	1.46	1.34
38	34	314	A86	C9-C8	4.60	1.46	1.34
38	11	310	A86	C9-C8	4.58	1.46	1.34
38	14	312	A86	C9-C8	4.58	1.46	1.34
38	12	314	A86	C9-C8	4.58	1.46	1.34
38	34	313	A86	C9-C8	4.57	1.46	1.34
38	13	312	A86	C9-C8	4.57	1.46	1.34
38	34	301	A86	C9-C8	4.56	1.46	1.34
38	31	314	A86	C9-C8	4.56	1.46	1.34
38	31	310	A86	C9-C8	4.56	1.46	1.34
38	33	315	A86	C9-C8	4.56	1.46	1.34
38	32	318	A86	C9-C8	4.56	1.46	1.34
38	34	316	A86	C9-C8	4.56	1.46	1.34
38	13	316	A86	C9-C8	4.56	1.46	1.34
38	33	312	A86	C9-C8	4.56	1.46	1.34
38	11	314	A86	C9-C8	4.55	1.46	1.34
38	31	313	A86	C9-C8	4.55	1.46	1.34
38	31	311	A86	C17-C18	-4.55	1.45	1.52
38	12	317	A86	C9-C8	4.55	1.46	1.34
38	32	314	A86	C9-C8	4.54	1.46	1.34
38	11	313	A86	C9-C8	4.54	1.46	1.34
38	14	316	A86	C9-C8	4.54	1.46	1.34
38	11	311	A86	C17-C18	-4.53	1.45	1.52
38	12	315	A86	C17-C18	-4.53	1.45	1.52
38	34	314	A86	C17-C18	-4.53	1.45	1.52
38	13	315	A86	C9-C8	4.52	1.46	1.34
38	32	317	A86	C9-C8	4.52	1.46	1.34
38	14	315	A86	C9-C8	4.51	1.46	1.34
38	33	313	A86	C17-C18	-4.50	1.45	1.52
38	32	315	A86	C17-C18	-4.50	1.45	1.52
38	13	313	A86	C17-C18	-4.49	1.45	1.52
38	14	313	A86	C17-C18	-4.48	1.46	1.52
38	13	314	A86	C17-C18	-4.43	1.46	1.52
38	31	312	A86	C17-C18	-4.40	1.46	1.52
36	D	404	PL9	C7-C3	-4.40	1.45	1.51
36	d	404	PL9	C7-C3	-4.39	1.45	1.51
38	11	312	A86	C17-C18	-4.39	1.46	1.52
38	14	314	A86	C17-C18	-4.38	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	33	314	A86	C17-C18	-4.38	1.46	1.52
38	33	315	A86	C7-C6	4.37	1.59	1.50
38	31	313	A86	C7-C6	4.37	1.59	1.50
38	14	301	A86	C21-C20	4.37	1.58	1.51
38	34	315	A86	C17-C18	-4.36	1.46	1.52
38	34	303	A86	C7-C6	4.36	1.59	1.50
38	12	316	A86	C17-C18	-4.35	1.46	1.52
38	13	302	A86	O4-C38	4.35	1.44	1.35
38	32	318	A86	C17-C18	-4.35	1.46	1.52
38	33	315	A86	O4-C38	4.35	1.44	1.35
38	12	317	A86	C7-C6	4.35	1.59	1.50
38	33	316	A86	C17-C18	-4.34	1.46	1.52
38	12	317	A86	O4-C38	4.34	1.44	1.35
38	33	302	A86	O4-C38	4.33	1.44	1.35
38	11	313	A86	O4-C38	4.32	1.44	1.35
38	11	313	A86	C7-C6	4.32	1.59	1.50
38	12	304	A86	C7-C6	4.32	1.59	1.50
38	32	304	A86	O4-C38	4.32	1.44	1.35
38	31	316	A86	C7-C6	4.32	1.59	1.50
38	33	316	A86	C21-C20	4.32	1.58	1.51
38	13	315	A86	C7-C6	4.32	1.59	1.50
38	13	302	A86	C7-C6	4.32	1.59	1.50
38	13	315	A86	O4-C38	4.32	1.44	1.35
38	34	316	A86	C7-C6	4.32	1.59	1.50
38	12	304	A86	O4-C38	4.32	1.44	1.35
38	13	317	A86	C7-C6	4.31	1.59	1.50
38	32	317	A86	O4-C38	4.31	1.44	1.35
38	31	314	A86	C21-C20	4.31	1.58	1.51
38	14	315	A86	O4-C38	4.31	1.44	1.35
38	11	316	A86	C7-C6	4.31	1.59	1.50
38	32	316	A86	C17-C18	-4.31	1.46	1.52
38	11	316	A86	O4-C38	4.31	1.44	1.35
38	32	318	A86	C21-C20	4.31	1.58	1.51
38	32	317	A86	C7-C6	4.31	1.59	1.50
38	13	317	A86	O4-C38	4.31	1.44	1.35
38	32	304	A86	C7-C6	4.30	1.59	1.50
38	34	301	A86	C17-C18	-4.30	1.46	1.52
38	31	313	A86	O4-C38	4.30	1.44	1.35
38	31	316	A86	O4-C38	4.30	1.44	1.35
38	34	303	A86	O4-C38	4.30	1.44	1.35
38	13	316	A86	C17-C18	-4.30	1.46	1.52
38	11	314	A86	C21-C20	4.30	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	34	316	A86	O4-C38	4.30	1.44	1.35
38	13	316	A86	C21-C20	4.30	1.58	1.51
38	33	302	A86	C7-C6	4.30	1.59	1.50
38	13	317	A86	C17-C18	-4.29	1.46	1.52
38	14	316	A86	C21-C20	4.29	1.58	1.51
38	34	303	A86	C17-C18	-4.29	1.46	1.52
38	14	315	A86	C7-C6	4.28	1.59	1.50
38	34	301	A86	C21-C20	4.28	1.58	1.51
38	13	302	A86	C17-C18	-4.28	1.46	1.52
38	33	302	A86	C17-C18	-4.28	1.46	1.52
38	14	316	A86	C17-C18	-4.28	1.46	1.52
38	31	314	A86	C17-C18	-4.28	1.46	1.52
38	32	304	A86	C17-C18	-4.28	1.46	1.52
38	11	314	A86	C17-C18	-4.27	1.46	1.52
38	11	316	A86	C17-C18	-4.27	1.46	1.52
38	34	315	A86	C7-C6	4.27	1.59	1.50
38	11	312	A86	C7-C6	4.26	1.59	1.50
38	31	316	A86	C17-C18	-4.26	1.46	1.52
38	33	314	A86	C7-C6	4.25	1.59	1.50
38	31	313	A86	C21-C20	4.25	1.58	1.51
38	14	301	A86	C17-C18	-4.25	1.46	1.52
38	14	316	A86	C7-C6	4.25	1.59	1.50
38	33	316	A86	C7-C6	4.25	1.59	1.50
38	13	313	A86	O4-C38	4.24	1.44	1.35
38	31	312	A86	C7-C6	4.24	1.59	1.50
38	11	313	A86	C21-C20	4.24	1.58	1.51
38	12	304	A86	C17-C18	-4.24	1.46	1.52
38	32	315	A86	O4-C38	4.24	1.44	1.35
38	34	316	A86	C17-C18	-4.23	1.46	1.52
38	34	301	A86	C7-C6	4.23	1.59	1.50
38	33	312	A86	C21-C20	4.23	1.58	1.51
38	34	313	A86	C21-C20	4.23	1.58	1.51
38	13	316	A86	C7-C6	4.23	1.59	1.50
38	14	313	A86	O4-C38	4.23	1.44	1.35
38	34	314	A86	O4-C38	4.23	1.44	1.35
38	12	315	A86	O4-C38	4.23	1.44	1.35
38	11	314	A86	C7-C6	4.22	1.59	1.50
38	12	316	A86	C7-C6	4.22	1.59	1.50
38	11	316	A86	C21-C20	4.22	1.58	1.51
38	12	317	A86	C21-C20	4.22	1.58	1.51
38	11	311	A86	O4-C38	4.22	1.44	1.35
38	33	315	A86	C21-C20	4.22	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	14	315	A86	C21-C20	4.22	1.58	1.51
38	13	314	A86	C7-C6	4.22	1.59	1.50
38	14	314	A86	C7-C6	4.22	1.59	1.50
38	14	301	A86	C7-C6	4.21	1.59	1.50
38	31	311	A86	O4-C38	4.21	1.44	1.35
38	12	304	A86	C21-C20	4.21	1.58	1.51
38	11	313	A86	C17-C18	-4.21	1.46	1.52
38	32	316	A86	C7-C6	4.20	1.59	1.50
38	32	314	A86	C21-C20	4.20	1.58	1.51
38	33	313	A86	O4-C38	4.20	1.44	1.35
38	13	317	A86	C21-C20	4.20	1.58	1.51
38	31	310	A86	C21-C20	4.20	1.58	1.51
38	31	316	A86	C21-C20	4.20	1.58	1.51
38	13	302	A86	C21-C20	4.20	1.58	1.51
38	33	302	A86	C21-C20	4.20	1.58	1.51
38	14	312	A86	C21-C20	4.19	1.58	1.51
38	12	317	A86	C17-C18	-4.19	1.46	1.52
38	14	313	A86	C7-C6	4.18	1.59	1.50
38	32	304	A86	C21-C20	4.18	1.58	1.51
38	32	317	A86	C21-C20	4.18	1.58	1.51
38	11	310	A86	C21-C20	4.18	1.58	1.51
38	32	318	A86	C7-C6	4.18	1.59	1.50
38	12	314	A86	C21-C20	4.18	1.58	1.51
38	34	303	A86	C21-C20	4.18	1.58	1.51
38	31	314	A86	C7-C6	4.18	1.59	1.50
38	11	311	A86	C7-C6	4.17	1.59	1.50
38	34	314	A86	C7-C6	4.17	1.59	1.50
38	12	314	A86	C17-C18	-4.17	1.46	1.52
38	13	315	A86	C17-C18	-4.16	1.46	1.52
38	14	312	A86	C17-C18	-4.16	1.46	1.52
38	13	315	A86	C21-C20	4.16	1.58	1.51
38	13	312	A86	C21-C20	4.16	1.58	1.51
38	34	301	A86	O4-C38	4.15	1.44	1.35
38	33	313	A86	C7-C6	4.15	1.59	1.50
38	32	315	A86	C7-C6	4.15	1.59	1.50
38	12	315	A86	C7-C6	4.15	1.59	1.50
38	32	314	A86	C17-C18	-4.15	1.46	1.52
38	13	316	A86	O4-C38	4.14	1.44	1.35
38	31	313	A86	C17-C18	-4.14	1.46	1.52
38	14	301	A86	O4-C38	4.14	1.44	1.35
38	14	315	A86	C17-C18	-4.14	1.46	1.52
38	14	316	A86	O4-C38	4.14	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	32	317	A86	C17-C18	-4.14	1.46	1.52
38	31	311	A86	C7-C6	4.14	1.59	1.50
38	13	313	A86	C7-C6	4.13	1.59	1.50
38	12	314	A86	C7-C6	4.13	1.59	1.50
38	31	310	A86	C17-C18	-4.13	1.46	1.52
38	11	314	A86	O4-C38	4.13	1.44	1.35
38	31	310	A86	C7-C6	4.13	1.59	1.50
38	33	316	A86	O4-C38	4.13	1.44	1.35
38	34	313	A86	C7-C6	4.13	1.59	1.50
38	34	316	A86	C21-C20	4.12	1.57	1.51
38	31	314	A86	O4-C38	4.11	1.44	1.35
38	32	318	A86	O4-C38	4.11	1.44	1.35
38	14	312	A86	C7-C6	4.11	1.59	1.50
38	33	312	A86	C17-C18	-4.11	1.46	1.52
38	34	313	A86	C17-C18	-4.11	1.46	1.52
29	M	101	BCR	C30-C25	-4.10	1.48	1.53
38	32	314	A86	C7-C6	4.10	1.59	1.50
38	33	312	A86	C7-C6	4.10	1.59	1.50
38	11	310	A86	C7-C6	4.10	1.59	1.50
38	13	312	A86	C17-C18	-4.09	1.46	1.52
38	33	315	A86	C17-C18	-4.09	1.46	1.52
38	11	310	A86	C17-C18	-4.09	1.46	1.52
38	13	312	A86	C7-C6	4.08	1.59	1.50
29	m	103	BCR	C30-C25	-4.06	1.48	1.53
29	h	101	BCR	C1-C6	-4.05	1.48	1.53
32	l	102	LHG	O7-C5	-4.05	1.37	1.46
38	13	312	A86	O4-C38	4.05	1.44	1.35
38	12	315	A86	C21-C20	4.05	1.57	1.51
38	11	312	A86	C10-C11	4.05	1.45	1.34
38	34	313	A86	O4-C38	4.04	1.44	1.35
38	33	314	A86	C10-C11	4.04	1.45	1.34
38	32	316	A86	C10-C11	4.04	1.45	1.34
38	14	314	A86	C10-C11	4.04	1.45	1.34
38	31	310	A86	O4-C38	4.03	1.44	1.35
38	34	315	A86	C10-C11	4.03	1.45	1.34
38	13	314	A86	C10-C11	4.03	1.45	1.34
38	32	315	A86	C21-C20	4.03	1.57	1.51
38	12	316	A86	C10-C11	4.03	1.45	1.34
32	L	101	LHG	O7-C5	-4.02	1.37	1.46
38	32	314	A86	O4-C38	4.02	1.44	1.35
38	11	310	A86	O4-C38	4.02	1.44	1.35
38	31	312	A86	C10-C11	4.01	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	14	312	A86	O4-C38	4.01	1.44	1.35
38	33	312	A86	O4-C38	4.01	1.44	1.35
29	H	101	BCR	C1-C6	-4.00	1.48	1.53
38	12	314	A86	O4-C38	3.99	1.44	1.35
38	34	314	A86	C21-C20	3.98	1.57	1.51
38	31	311	A86	C21-C20	3.97	1.57	1.51
36	D	407	PL9	C52-C5	-3.96	1.42	1.50
29	C	520	BCR	C30-C25	-3.96	1.48	1.53
38	13	313	A86	C21-C20	3.96	1.57	1.51
38	33	313	A86	C21-C20	3.96	1.57	1.51
38	14	313	A86	C21-C20	3.95	1.57	1.51
38	11	311	A86	C21-C20	3.94	1.57	1.51
38	31	316	A86	C9-C10	3.93	1.55	1.43
38	13	313	A86	C10-C11	3.93	1.45	1.34
38	32	315	A86	C10-C11	3.93	1.45	1.34
38	34	314	A86	C10-C11	3.93	1.45	1.34
38	14	314	A86	C9-C10	3.92	1.55	1.43
36	d	407	PL9	C52-C5	-3.92	1.42	1.50
29	c	515	BCR	C30-C25	-3.92	1.48	1.53
29	c	519	BCR	C30-C25	-3.92	1.48	1.53
38	32	316	A86	C9-C10	3.92	1.55	1.43
38	33	314	A86	C9-C10	3.92	1.55	1.43
38	11	311	A86	C10-C11	3.92	1.45	1.34
38	34	315	A86	C21-C20	3.92	1.57	1.51
29	C	515	BCR	C30-C25	-3.91	1.48	1.53
38	32	304	A86	C9-C10	3.91	1.55	1.43
38	31	312	A86	C9-C10	3.91	1.55	1.43
38	14	313	A86	C10-C11	3.90	1.45	1.34
38	11	316	A86	C9-C10	3.90	1.55	1.43
38	34	315	A86	C9-C10	3.90	1.55	1.43
38	31	311	A86	C10-C11	3.90	1.45	1.34
38	11	312	A86	C9-C10	3.90	1.55	1.43
38	13	302	A86	C9-C10	3.90	1.55	1.43
38	12	315	A86	C10-C11	3.90	1.45	1.34
38	12	304	A86	C9-C10	3.90	1.55	1.43
38	33	302	A86	C9-C10	3.90	1.55	1.43
38	14	314	A86	C21-C20	3.89	1.57	1.51
38	11	312	A86	C21-C20	3.89	1.57	1.51
38	13	314	A86	C9-C10	3.89	1.55	1.43
38	12	316	A86	C9-C10	3.89	1.55	1.43
38	33	313	A86	C10-C11	3.89	1.45	1.34
38	31	312	A86	C21-C20	3.88	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	34	303	A86	C9-C10	3.88	1.55	1.43
38	13	317	A86	C9-C10	3.88	1.55	1.43
38	33	316	A86	C10-C11	3.88	1.45	1.34
38	32	318	A86	C10-C11	3.88	1.45	1.34
38	34	301	A86	C10-C11	3.88	1.45	1.34
38	14	301	A86	C10-C11	3.87	1.45	1.34
38	12	316	A86	C21-C20	3.87	1.57	1.51
38	11	314	A86	C10-C11	3.87	1.45	1.34
38	13	316	A86	C10-C11	3.87	1.45	1.34
38	32	316	A86	C21-C20	3.86	1.57	1.51
38	11	316	A86	C10-C11	3.86	1.45	1.34
38	14	316	A86	C10-C11	3.86	1.45	1.34
38	13	312	A86	C10-C11	3.86	1.45	1.34
38	33	302	A86	C10-C11	3.86	1.45	1.34
38	34	303	A86	C10-C11	3.86	1.45	1.34
38	31	314	A86	C10-C11	3.86	1.45	1.34
38	33	314	A86	C21-C20	3.85	1.57	1.51
38	13	314	A86	C21-C20	3.85	1.57	1.51
38	12	304	A86	C10-C11	3.85	1.45	1.34
38	14	312	A86	C10-C11	3.85	1.45	1.34
29	M	101	BCR	C1-C6	-3.85	1.48	1.53
38	12	314	A86	C10-C11	3.85	1.45	1.34
38	31	310	A86	C10-C11	3.84	1.45	1.34
38	13	317	A86	C10-C11	3.84	1.45	1.34
38	32	314	A86	C10-C11	3.83	1.45	1.34
38	11	310	A86	C10-C11	3.83	1.45	1.34
38	13	302	A86	C10-C11	3.83	1.45	1.34
38	13	316	A86	C9-C10	3.83	1.55	1.43
38	32	318	A86	C9-C10	3.83	1.55	1.43
38	34	313	A86	C10-C11	3.82	1.45	1.34
38	14	301	A86	C9-C10	3.82	1.55	1.43
38	14	316	A86	C9-C10	3.82	1.55	1.43
38	11	314	A86	C9-C10	3.82	1.55	1.43
38	31	316	A86	C10-C11	3.82	1.45	1.34
38	34	314	A86	C9-C10	3.81	1.55	1.43
38	33	312	A86	C10-C11	3.81	1.45	1.34
38	14	313	A86	C9-C10	3.81	1.55	1.43
38	31	313	A86	C10-C11	3.81	1.44	1.34
38	31	311	A86	C9-C10	3.81	1.55	1.43
29	m	103	BCR	C1-C6	-3.81	1.48	1.53
38	34	301	A86	C9-C10	3.81	1.55	1.43
38	32	304	A86	C10-C11	3.80	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	34	316	A86	C9-C10	3.80	1.55	1.43
38	31	314	A86	C9-C10	3.80	1.55	1.43
38	14	315	A86	C10-C11	3.80	1.44	1.34
29	z	101	BCR	C1-C6	-3.80	1.48	1.53
38	33	316	A86	C9-C10	3.80	1.55	1.43
38	32	315	A86	C9-C10	3.80	1.55	1.43
38	12	317	A86	C10-C11	3.80	1.44	1.34
38	33	315	A86	C10-C11	3.80	1.44	1.34
38	11	313	A86	C10-C11	3.79	1.44	1.34
38	32	317	A86	C10-C11	3.79	1.44	1.34
38	11	311	A86	C9-C10	3.79	1.54	1.43
38	11	313	A86	C9-C10	3.79	1.54	1.43
38	33	313	A86	C9-C10	3.78	1.54	1.43
38	13	313	A86	C9-C10	3.78	1.54	1.43
38	13	315	A86	C9-C10	3.78	1.54	1.43
38	34	316	A86	C10-C11	3.78	1.44	1.34
38	12	315	A86	C9-C10	3.78	1.54	1.43
38	13	315	A86	C10-C11	3.78	1.44	1.34
29	Z	101	BCR	C1-C6	-3.77	1.49	1.53
38	32	317	A86	C9-C10	3.77	1.54	1.43
38	14	315	A86	C9-C10	3.76	1.54	1.43
38	31	313	A86	C9-C10	3.76	1.54	1.43
38	33	315	A86	C9-C10	3.76	1.54	1.43
38	12	317	A86	C9-C10	3.76	1.54	1.43
36	d	404	PL9	C3-C4	-3.75	1.43	1.49
29	C	516	BCR	C1-C6	-3.74	1.49	1.53
38	31	310	A86	C9-C10	3.70	1.54	1.43
38	13	312	A86	C9-C10	3.70	1.54	1.43
38	14	312	A86	C9-C10	3.70	1.54	1.43
38	33	312	A86	C9-C10	3.70	1.54	1.43
29	c	516	BCR	C1-C6	-3.69	1.49	1.53
38	11	310	A86	C9-C10	3.69	1.54	1.43
38	12	314	A86	C9-C10	3.69	1.54	1.43
38	32	314	A86	C9-C10	3.69	1.54	1.43
38	34	313	A86	C9-C10	3.68	1.54	1.43
38	12	317	A86	C19-C18	3.68	1.57	1.52
38	13	315	A86	C19-C18	3.68	1.57	1.52
38	14	315	A86	C19-C18	3.68	1.57	1.52
29	a	405	BCR	C1-C6	-3.68	1.49	1.53
29	A	405	BCR	C1-C6	-3.67	1.49	1.53
38	34	316	A86	C19-C18	3.67	1.57	1.52
36	D	404	PL9	C3-C4	-3.66	1.43	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	32	317	A86	C19-C18	3.66	1.57	1.52
38	11	313	A86	C19-C18	3.65	1.57	1.52
38	31	313	A86	C19-C18	3.64	1.57	1.52
29	c	515	BCR	C1-C6	-3.62	1.49	1.53
36	d	407	PL9	C7-C8	-3.61	1.44	1.50
29	C	515	BCR	C1-C6	-3.60	1.49	1.53
38	33	315	A86	C19-C18	3.60	1.57	1.52
27	c	507	CLA	CMB-C2B	-3.59	1.43	1.50
27	b	612	CLA	CMD-C2D	-3.59	1.43	1.50
36	D	407	PL9	C7-C8	-3.59	1.44	1.50
39	12	302	LMU	O5B-C1B	3.58	1.51	1.41
27	C	507	CLA	CMB-C2B	-3.58	1.43	1.50
29	b	623	BCR	C1-C6	-3.58	1.49	1.53
39	32	302	LMU	O5B-C1B	3.58	1.51	1.41
27	B	612	CLA	CMD-C2D	-3.56	1.43	1.50
27	b	611	CLA	CMB-C2B	-3.55	1.43	1.50
27	W	103	CLA	C1D-ND	3.54	1.42	1.37
27	w	103	CLA	C1D-ND	3.53	1.42	1.37
27	B	611	CLA	CMB-C2B	-3.53	1.43	1.50
27	c	509	CLA	CMB-C2B	-3.52	1.43	1.50
29	B	623	BCR	C1-C6	-3.51	1.49	1.53
27	C	509	CLA	CMB-C2B	-3.49	1.43	1.50
29	f	101	BCR	C1-C6	-3.47	1.49	1.53
29	F	101	BCR	C1-C6	-3.46	1.49	1.53
38	12	314	A86	C19-C18	3.45	1.57	1.52
38	13	312	A86	C19-C18	3.45	1.57	1.52
38	32	314	A86	C19-C18	3.43	1.57	1.52
36	D	407	PL9	C53-C6	-3.43	1.43	1.50
29	b	616	BCR	C1-C6	-3.43	1.49	1.53
38	31	310	A86	C19-C18	3.42	1.57	1.52
38	14	312	A86	C19-C18	3.41	1.57	1.52
38	34	313	A86	C19-C18	3.41	1.57	1.52
36	d	407	PL9	C53-C6	-3.39	1.43	1.50
29	B	616	BCR	C1-C6	-3.39	1.49	1.53
38	11	310	A86	C19-C18	3.38	1.57	1.52
38	33	312	A86	C19-C18	3.37	1.57	1.52
29	C	520	BCR	C1-C6	-3.37	1.49	1.53
27	c	511	CLA	CMD-C2D	-3.37	1.43	1.50
29	c	519	BCR	C1-C6	-3.37	1.49	1.53
27	c	511	CLA	MG-NB	-3.36	1.99	2.05
35	c	518	DGD	O2G-C2G	-3.35	1.38	1.46
27	C	511	CLA	MG-NB	-3.35	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	405	BCR	C30-C25	-3.34	1.49	1.53
29	a	405	BCR	C30-C25	-3.33	1.49	1.53
29	B	617	BCR	C1-C6	-3.32	1.49	1.53
27	C	511	CLA	CMD-C2D	-3.32	1.44	1.50
28	A	403	PHO	C4D-ND	-3.31	1.33	1.38
28	a	403	PHO	C4D-ND	-3.31	1.33	1.38
29	b	617	BCR	C1-C6	-3.31	1.49	1.53
35	C	518	DGD	O2G-C2G	-3.31	1.38	1.46
27	B	612	CLA	MG-ND	-3.31	1.99	2.05
27	b	612	CLA	MG-ND	-3.31	1.99	2.05
38	14	313	A86	C19-C18	3.30	1.57	1.52
38	11	311	A86	C19-C18	3.29	1.57	1.52
38	32	315	A86	C19-C18	3.27	1.56	1.52
32	L	102	LHG	O7-C5	-3.27	1.38	1.46
38	34	314	A86	C19-C18	3.26	1.56	1.52
29	B	617	BCR	C30-C25	-3.26	1.49	1.53
38	31	311	A86	C19-C18	3.26	1.56	1.52
32	l	103	LHG	O7-C5	-3.25	1.38	1.46
33	C	519	LMG	O7-C8	-3.25	1.39	1.46
38	12	315	A86	C19-C18	3.24	1.56	1.52
33	q	301	LMG	O7-C8	-3.23	1.39	1.46
38	13	313	A86	C19-C18	3.22	1.56	1.52
35	j	101	DGD	O2G-C2G	-3.22	1.39	1.46
38	33	313	A86	C19-C18	3.22	1.56	1.52
27	b	612	CLA	MG-NB	-3.22	1.99	2.05
27	11	305	CLA	C1D-ND	3.21	1.42	1.37
35	J	101	DGD	O2G-C2G	-3.21	1.39	1.46
28	A	403	PHO	CMC-C2C	-3.21	1.45	1.50
28	a	403	PHO	CMC-C2C	-3.21	1.45	1.50
28	A	403	PHO	CAC-C3C	-3.20	1.46	1.51
28	D	403	PHO	C4D-CHA	3.20	1.44	1.39
29	b	617	BCR	C30-C25	-3.20	1.49	1.53
27	c	509	CLA	MG-NB	-3.19	1.99	2.05
28	d	403	PHO	C4D-CHA	3.19	1.44	1.39
27	33	307	CLA	C1D-ND	3.19	1.42	1.37
28	a	403	PHO	CAC-C3C	-3.18	1.46	1.51
33	D	408	LMG	O7-C8	-3.18	1.39	1.46
33	d	408	LMG	O7-C8	-3.17	1.39	1.46
27	B	612	CLA	MG-NB	-3.17	1.99	2.05
27	31	305	CLA	C1D-ND	3.17	1.42	1.37
27	C	509	CLA	MG-NB	-3.16	1.99	2.05
27	c	503	CLA	MG-NB	-3.16	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	409	BCR	C1-C6	-3.16	1.49	1.53
27	14	307	CLA	C1D-ND	3.16	1.42	1.37
27	D	401	CLA	MG-NB	-3.15	1.99	2.05
28	A	403	PHO	CMD-C2D	-3.15	1.45	1.51
29	b	616	BCR	C30-C25	-3.14	1.49	1.53
29	z	101	BCR	C30-C25	-3.14	1.49	1.53
27	b	602	CLA	C1D-ND	3.13	1.42	1.37
29	A	409	BCR	C1-C6	-3.13	1.49	1.53
27	d	401	CLA	MG-NB	-3.13	1.99	2.05
32	b	621	LHG	O7-C5	-3.12	1.39	1.46
33	C	519	LMG	O1-C7	-3.12	1.38	1.43
27	34	308	CLA	C1D-ND	3.12	1.42	1.37
27	C	503	CLA	MG-NB	-3.12	1.99	2.05
27	32	309	CLA	C1D-ND	3.12	1.42	1.37
33	b	619	LMG	O8-C9	-3.12	1.38	1.45
39	32	302	LMU	O5'-C1'	3.11	1.49	1.41
27	12	309	CLA	C1D-ND	3.11	1.41	1.37
36	D	407	PL9	C36-C34	-3.11	1.44	1.51
28	a	403	PHO	CMD-C2D	-3.11	1.45	1.51
27	z	102	CLA	C1D-ND	3.11	1.41	1.37
28	D	403	PHO	CMC-C2C	-3.11	1.45	1.50
33	q	301	LMG	O1-C7	-3.10	1.38	1.43
27	33	309	CLA	C1D-ND	3.10	1.41	1.37
27	13	307	CLA	C1D-ND	3.10	1.41	1.37
29	B	616	BCR	C30-C25	-3.10	1.49	1.53
36	d	407	PL9	C36-C34	-3.10	1.44	1.51
38	11	311	A86	C25-C24	3.10	1.42	1.34
27	B	602	CLA	C1D-ND	3.10	1.41	1.37
38	31	312	A86	C19-C18	3.09	1.56	1.52
27	Z	102	CLA	C1D-ND	3.09	1.41	1.37
38	32	304	A86	C19-C18	3.09	1.56	1.52
33	B	619	LMG	O8-C9	-3.09	1.38	1.45
39	12	302	LMU	O5'-C1'	3.09	1.49	1.41
29	Z	101	BCR	C30-C25	-3.09	1.49	1.53
38	33	313	A86	C25-C24	3.09	1.42	1.34
27	B	604	CLA	MG-NB	-3.08	1.99	2.05
38	31	311	A86	C25-C24	3.08	1.42	1.34
27	13	309	CLA	C1D-ND	3.08	1.41	1.37
38	32	315	A86	C25-C24	3.08	1.42	1.34
38	11	312	A86	C19-C18	3.08	1.56	1.52
27	c	508	CLA	MG-NB	-3.08	1.99	2.05
32	B	621	LHG	O7-C5	-3.08	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	13	313	A86	C25-C24	3.08	1.42	1.34
38	12	315	A86	C25-C24	3.08	1.42	1.34
27	13	311	CLA	C1D-ND	3.07	1.41	1.37
38	12	316	A86	C19-C18	3.07	1.56	1.52
38	33	314	A86	C19-C18	3.07	1.56	1.52
27	C	510	CLA	MG-NB	-3.07	1.99	2.05
28	D	403	PHO	C4D-ND	-3.07	1.33	1.38
27	31	307	CLA	C1D-ND	3.07	1.41	1.37
38	34	314	A86	C25-C24	3.07	1.42	1.34
38	14	313	A86	C25-C24	3.06	1.42	1.34
35	c	517	DGD	O1G-C1G	-3.06	1.38	1.45
27	c	510	CLA	CMB-C2B	-3.06	1.44	1.50
27	c	510	CLA	MG-NB	-3.06	1.99	2.05
29	a	409	BCR	C30-C25	-3.06	1.49	1.53
27	33	303	CLA	C1D-ND	3.06	1.41	1.37
28	A	403	PHO	C1D-C2D	3.05	1.42	1.39
27	B	615	CLA	C1D-ND	3.05	1.41	1.37
27	11	309	CLA	C1D-ND	3.05	1.41	1.37
35	C	517	DGD	O1G-C1G	-3.05	1.38	1.45
27	C	508	CLA	MG-NB	-3.05	1.99	2.05
27	13	301	CLA	C1D-ND	3.05	1.41	1.37
38	13	314	A86	C19-C18	3.05	1.56	1.52
27	32	311	CLA	C1D-ND	3.05	1.41	1.37
28	d	403	PHO	CMC-C2C	-3.04	1.45	1.50
29	c	516	BCR	C30-C25	-3.04	1.49	1.53
38	12	304	A86	C19-C18	3.04	1.56	1.52
38	32	316	A86	C19-C18	3.04	1.56	1.52
27	C	511	CLA	C1B-NB	-3.04	1.33	1.37
27	31	301	CLA	C1D-ND	3.04	1.41	1.37
27	B	622	CLA	CMD-C2D	-3.04	1.44	1.50
28	a	403	PHO	CBD-CGD	-3.04	1.48	1.52
27	b	615	CLA	C1D-ND	3.04	1.41	1.37
29	A	409	BCR	C30-C25	-3.04	1.49	1.53
27	b	622	CLA	CMD-C2D	-3.04	1.44	1.50
27	b	604	CLA	MG-NB	-3.04	1.99	2.05
27	14	311	CLA	C1D-ND	3.04	1.41	1.37
27	31	309	CLA	C1D-ND	3.04	1.41	1.37
38	34	303	A86	C19-C18	3.04	1.56	1.52
27	14	302	CLA	C1D-ND	3.04	1.41	1.37
30	L	103	SQD	O47-C7	3.04	1.42	1.34
29	H	101	BCR	C30-C25	-3.03	1.49	1.53
27	14	309	CLA	C1D-ND	3.03	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	33	301	CLA	C1D-ND	3.03	1.41	1.37
27	32	313	CLA	C1D-ND	3.03	1.41	1.37
38	33	302	A86	C19-C18	3.03	1.56	1.52
28	d	403	PHO	C4D-ND	-3.03	1.34	1.38
28	A	403	PHO	CBD-CGD	-3.03	1.48	1.52
27	C	510	CLA	CMB-C2B	-3.03	1.44	1.50
27	12	305	CLA	C1D-ND	3.02	1.41	1.37
30	l	101	SQD	O47-C7	3.02	1.42	1.34
27	b	610	CLA	MG-NB	-3.02	1.99	2.05
27	34	312	CLA	C1D-ND	3.02	1.41	1.37
27	33	308	CLA	C4B-NB	3.02	1.41	1.37
27	34	310	CLA	C1D-ND	3.02	1.41	1.37
38	14	314	A86	C19-C18	3.02	1.56	1.52
27	33	306	CLA	C1D-ND	3.02	1.41	1.37
27	33	311	CLA	C1D-ND	3.02	1.41	1.37
27	d	406	CLA	MG-NB	-3.02	1.99	2.05
38	31	312	A86	C25-C24	3.01	1.42	1.34
29	h	101	BCR	C30-C25	-3.01	1.49	1.53
27	12	311	CLA	C1D-ND	3.01	1.41	1.37
27	11	307	CLA	C1D-ND	3.01	1.41	1.37
27	32	305	CLA	C1D-ND	3.01	1.41	1.37
27	14	303	CLA	C1D-ND	3.01	1.41	1.37
27	B	613	CLA	MG-NB	-3.01	1.99	2.05
27	b	613	CLA	MG-NB	-3.01	1.99	2.05
38	13	302	A86	C19-C18	3.01	1.56	1.52
27	13	303	CLA	C1D-ND	3.01	1.41	1.37
38	11	312	A86	C25-C24	3.00	1.42	1.34
27	12	313	CLA	C1D-ND	3.00	1.41	1.37
38	13	317	A86	C19-C18	3.00	1.56	1.52
27	12	303	CLA	C1D-ND	3.00	1.41	1.37
27	b	604	CLA	C1D-ND	3.00	1.41	1.37
27	32	303	CLA	C1D-ND	3.00	1.41	1.37
38	11	316	A86	C19-C18	3.00	1.56	1.52
38	32	316	A86	C25-C24	2.99	1.42	1.34
27	B	610	CLA	MG-NB	-2.99	1.99	2.05
38	31	316	A86	C19-C18	2.99	1.56	1.52
27	c	503	CLA	C1D-ND	2.99	1.41	1.37
38	34	315	A86	C19-C18	2.99	1.56	1.52
38	14	314	A86	C25-C24	2.99	1.42	1.34
27	31	315	CLA	C1D-ND	2.99	1.41	1.37
27	D	406	CLA	MG-NB	-2.99	1.99	2.05
27	b	611	CLA	MG-NB	-2.98	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	516	BCR	C30-C25	-2.98	1.50	1.53
27	34	304	CLA	C1D-ND	2.98	1.41	1.37
38	34	315	A86	C25-C24	2.98	1.42	1.34
27	11	315	CLA	C1D-ND	2.98	1.41	1.37
27	B	611	CLA	MG-NB	-2.98	1.99	2.05
38	13	314	A86	C25-C24	2.98	1.42	1.34
27	11	304	CLA	C1D-ND	2.98	1.41	1.37
27	c	511	CLA	C1B-NB	-2.98	1.34	1.37
38	12	316	A86	C25-C24	2.98	1.42	1.34
27	B	604	CLA	C1D-ND	2.98	1.41	1.37
27	C	503	CLA	C1D-ND	2.97	1.41	1.37
27	14	310	CLA	C1D-ND	2.97	1.41	1.37
27	31	308	CLA	C1D-ND	2.97	1.41	1.37
27	11	301	CLA	C1D-ND	2.97	1.41	1.37
27	D	405	CLA	CMD-C2D	-2.97	1.44	1.50
36	D	404	PL9	C6-C1	-2.97	1.43	1.48
27	31	306	CLA	C4B-NB	2.96	1.41	1.37
27	13	306	CLA	C1D-ND	2.96	1.41	1.37
36	d	404	PL9	C6-C1	-2.96	1.43	1.48
27	b	622	CLA	MG-NB	-2.96	1.99	2.05
27	32	308	CLA	C1D-ND	2.96	1.41	1.37
27	c	507	CLA	MG-NB	-2.96	1.99	2.05
38	33	314	A86	C25-C24	2.96	1.42	1.34
27	W	103	CLA	C4B-NB	2.96	1.41	1.37
27	34	302	CLA	C1D-ND	2.95	1.41	1.37
27	12	310	CLA	C4B-NB	2.95	1.41	1.37
27	c	503	CLA	CMC-C2C	-2.95	1.44	1.50
28	a	403	PHO	C1D-C2D	2.95	1.42	1.39
27	13	308	CLA	C4B-NB	2.95	1.41	1.37
27	C	512	CLA	C1D-ND	2.95	1.41	1.37
27	B	622	CLA	MG-NB	-2.93	2.00	2.05
27	A	404	CLA	MG-NB	-2.93	2.00	2.05
27	31	304	CLA	MG-NB	-2.93	2.00	2.05
27	11	308	CLA	C1D-ND	2.93	1.41	1.37
27	B	611	CLA	CMC-C2C	-2.93	1.44	1.50
27	b	611	CLA	CMC-C2C	-2.93	1.44	1.50
27	c	506	CLA	CMD-C2D	-2.93	1.44	1.50
27	33	306	CLA	MG-NB	-2.93	2.00	2.05
27	34	307	CLA	MG-NB	-2.93	2.00	2.05
27	w	103	CLA	C4B-NB	2.93	1.41	1.37
27	C	507	CLA	MG-NB	-2.93	2.00	2.05
27	c	512	CLA	C1D-ND	2.93	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	32	310	CLA	C4B-NB	2.93	1.41	1.37
27	11	306	CLA	C4B-NB	2.93	1.41	1.37
27	b	606	CLA	CMD-C2D	-2.93	1.44	1.50
27	31	304	CLA	C1D-ND	2.92	1.41	1.37
27	13	310	CLA	C1D-ND	2.92	1.41	1.37
27	14	306	CLA	MG-NB	-2.92	2.00	2.05
27	d	405	CLA	CMD-C2D	-2.92	1.44	1.50
27	a	404	CLA	MG-NB	-2.92	2.00	2.05
38	32	317	A86	C25-C24	2.92	1.42	1.34
30	b	620	SQD	O48-C23	2.92	1.41	1.33
27	14	308	CLA	C4B-NB	2.92	1.41	1.37
27	13	306	CLA	MG-NB	-2.92	2.00	2.05
28	A	403	PHO	CMB-C2B	-2.91	1.45	1.51
27	C	506	CLA	CMD-C2D	-2.91	1.44	1.50
30	B	620	SQD	O48-C23	2.91	1.41	1.33
38	31	316	A86	C25-C24	2.91	1.42	1.34
27	11	304	CLA	MG-NB	-2.91	2.00	2.05
27	C	511	CLA	MG-ND	-2.91	2.00	2.05
27	B	606	CLA	CMD-C2D	-2.91	1.44	1.50
27	32	312	CLA	C1D-ND	2.91	1.41	1.37
27	33	310	CLA	C1D-ND	2.91	1.41	1.37
27	34	309	CLA	C4B-NB	2.91	1.41	1.37
27	C	503	CLA	CMC-C2C	-2.91	1.44	1.50
38	14	315	A86	C25-C24	2.91	1.42	1.34
27	12	308	CLA	C1D-ND	2.91	1.41	1.37
27	14	306	CLA	C1D-ND	2.91	1.41	1.37
38	32	304	A86	C25-C24	2.91	1.42	1.34
27	31	306	CLA	C1D-ND	2.91	1.41	1.37
27	34	305	CLA	C1D-ND	2.91	1.41	1.37
27	12	308	CLA	MG-NB	-2.90	2.00	2.05
28	a	403	PHO	CMB-C2B	-2.90	1.45	1.51
27	34	311	CLA	C1D-ND	2.90	1.41	1.37
27	b	613	CLA	C1B-NB	-2.90	1.34	1.37
27	c	504	CLA	CMD-C2D	-2.90	1.44	1.50
38	13	315	A86	C25-C24	2.90	1.42	1.34
27	D	401	CLA	CMB-C2B	-2.90	1.44	1.50
27	d	401	CLA	CMB-C2B	-2.90	1.44	1.50
28	D	403	PHO	CBD-CGD	-2.90	1.48	1.52
38	12	317	A86	C25-C24	2.90	1.42	1.34
38	31	313	A86	C25-C24	2.90	1.42	1.34
27	33	308	CLA	C1D-ND	2.90	1.41	1.37
38	34	303	A86	C25-C24	2.89	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	11	313	A86	C25-C24	2.89	1.42	1.34
38	34	316	A86	C25-C24	2.89	1.42	1.34
38	13	302	A86	C25-C24	2.89	1.42	1.34
36	d	407	PL9	C26-C24	-2.89	1.45	1.51
27	34	309	CLA	C1D-ND	2.89	1.41	1.37
38	13	317	A86	C25-C24	2.89	1.42	1.34
27	C	503	CLA	MG-ND	-2.89	2.00	2.05
36	d	407	PL9	C11-C9	-2.88	1.45	1.51
38	12	304	A86	C25-C24	2.88	1.42	1.34
38	33	315	A86	C25-C24	2.88	1.42	1.34
27	12	310	CLA	C1D-ND	2.88	1.41	1.37
27	32	308	CLA	MG-NB	-2.88	2.00	2.05
38	33	302	A86	C25-C24	2.88	1.42	1.34
27	Z	102	CLA	MG-NB	-2.88	2.00	2.05
27	c	511	CLA	MG-ND	-2.88	2.00	2.05
27	12	312	CLA	C1D-ND	2.87	1.41	1.37
28	D	403	PHO	CMD-C2D	-2.87	1.45	1.51
28	d	403	PHO	CBD-CGD	-2.87	1.48	1.52
27	32	310	CLA	C1D-ND	2.87	1.41	1.37
35	J	101	DGD	O5D-C6D	-2.87	1.38	1.43
27	z	102	CLA	MG-NB	-2.87	2.00	2.05
27	14	308	CLA	C1D-ND	2.86	1.41	1.37
37	v	201	HEM	CAB-C3B	2.86	1.55	1.47
27	13	308	CLA	C1D-ND	2.86	1.41	1.37
36	D	407	PL9	C11-C9	-2.86	1.45	1.51
27	B	613	CLA	C1B-NB	-2.86	1.34	1.37
38	11	316	A86	C25-C24	2.86	1.42	1.34
27	C	508	CLA	MG-ND	-2.86	2.00	2.05
27	B	607	CLA	MG-NB	-2.86	2.00	2.05
27	D	401	CLA	CMD-C2D	-2.86	1.44	1.50
27	b	607	CLA	MG-NB	-2.86	2.00	2.05
27	11	302	CLA	C1D-ND	2.86	1.41	1.37
27	32	306	CLA	C1D-ND	2.85	1.41	1.37
27	c	503	CLA	MG-ND	-2.85	2.00	2.05
36	D	407	PL9	C26-C24	-2.85	1.45	1.51
27	C	504	CLA	CMD-C2D	-2.85	1.44	1.50
27	b	605	CLA	C1D-ND	2.85	1.41	1.37
27	12	307	CLA	C1D-ND	2.85	1.41	1.37
37	E	101	HEM	CAB-C3B	2.85	1.55	1.47
27	b	603	CLA	MG-NB	-2.84	2.00	2.05
37	f	102	HEM	CAB-C3B	2.84	1.55	1.47
27	31	302	CLA	C1D-ND	2.84	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	11	307	CLA	MG-NB	-2.84	2.00	2.05
27	a	404	CLA	CMD-C2D	-2.84	1.44	1.50
27	B	605	CLA	C1D-ND	2.84	1.41	1.37
35	C	518	DGD	O5D-C6D	-2.84	1.38	1.43
35	c	518	DGD	O5D-C6D	-2.84	1.38	1.43
27	13	309	CLA	MG-NB	-2.84	2.00	2.05
27	B	612	CLA	CMC-C2C	-2.83	1.45	1.50
28	d	403	PHO	CMD-C2D	-2.83	1.46	1.51
27	34	307	CLA	C1D-ND	2.83	1.41	1.37
27	d	401	CLA	CMD-C2D	-2.83	1.45	1.50
27	B	603	CLA	MG-NB	-2.83	2.00	2.05
37	V	201	HEM	CAB-C3B	2.83	1.54	1.47
27	12	306	CLA	C1D-ND	2.83	1.41	1.37
38	13	316	A86	C19-C18	2.83	1.56	1.52
27	C	503	CLA	CMB-C2B	-2.83	1.45	1.50
30	A	406	SQD	O48-C23	2.83	1.41	1.33
27	B	606	CLA	C4B-NB	2.83	1.41	1.37
27	b	612	CLA	CMC-C2C	-2.83	1.45	1.50
27	31	307	CLA	MG-NB	-2.83	2.00	2.05
36	d	404	PL9	C53-C6	-2.82	1.45	1.50
27	A	404	CLA	CMD-C2D	-2.82	1.45	1.50
27	34	310	CLA	MG-NB	-2.82	2.00	2.05
35	j	101	DGD	O5D-C6D	-2.82	1.38	1.43
27	B	604	CLA	CMD-C2D	-2.82	1.45	1.50
27	b	615	CLA	CMC-C2C	-2.82	1.45	1.50
27	b	601	CLA	C1D-ND	2.82	1.41	1.37
27	D	402	CLA	MG-NB	-2.82	2.00	2.05
27	12	311	CLA	MG-NB	-2.82	2.00	2.05
36	D	407	PL9	C5-C4	-2.82	1.37	1.47
27	c	508	CLA	MG-ND	-2.81	2.00	2.05
27	b	604	CLA	MG-ND	-2.81	2.00	2.05
27	14	309	CLA	MG-NB	-2.81	2.00	2.05
27	13	304	CLA	C1D-ND	2.81	1.41	1.37
27	B	601	CLA	MG-NB	-2.81	2.00	2.05
27	B	604	CLA	MG-ND	-2.81	2.00	2.05
27	11	306	CLA	C1D-ND	2.81	1.41	1.37
36	D	404	PL9	C53-C6	-2.81	1.45	1.50
30	a	406	SQD	O48-C23	2.81	1.41	1.33
27	33	309	CLA	MG-NB	-2.81	2.00	2.05
27	b	604	CLA	CMD-C2D	-2.81	1.45	1.50
36	D	407	PL9	C41-C39	-2.81	1.45	1.51
27	C	509	CLA	CMC-C2C	-2.81	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d	405	CLA	MG-NB	-2.81	2.00	2.05
27	32	311	CLA	MG-NB	-2.80	2.00	2.05
36	d	407	PL9	C5-C4	-2.80	1.37	1.47
27	33	309	CLA	O2A-C1	-2.80	1.38	1.46
27	c	509	CLA	CMC-C2C	-2.80	1.45	1.50
37	E	101	HEM	CAC-C3C	2.80	1.54	1.47
38	14	316	A86	C19-C18	2.80	1.56	1.52
38	34	301	A86	C19-C18	2.80	1.56	1.52
38	32	318	A86	C19-C18	2.80	1.56	1.52
27	14	305	CLA	C1D-ND	2.80	1.41	1.37
33	W	101	LMG	O7-C8	-2.79	1.40	1.46
33	w	101	LMG	O7-C8	-2.79	1.40	1.46
27	b	615	CLA	CMD-C2D	-2.79	1.45	1.50
38	11	314	A86	C19-C18	2.79	1.56	1.52
27	B	602	CLA	CMC-C2C	-2.79	1.45	1.50
27	D	405	CLA	MG-NB	-2.79	2.00	2.05
27	d	402	CLA	MG-NB	-2.79	2.00	2.05
27	c	503	CLA	CMB-C2B	-2.79	1.45	1.50
27	32	307	CLA	C1D-ND	2.79	1.41	1.37
27	14	304	CLA	C1D-ND	2.78	1.41	1.37
27	b	601	CLA	MG-NB	-2.78	2.00	2.05
27	b	606	CLA	C4B-NB	2.78	1.41	1.37
33	B	618	LMG	O7-C8	-2.78	1.40	1.46
33	12	301	LMG	O1-C1	2.78	1.44	1.40
27	B	615	CLA	CMC-C2C	-2.78	1.45	1.50
27	B	615	CLA	CMD-C2D	-2.78	1.45	1.50
33	b	618	LMG	O7-C8	-2.78	1.40	1.46
28	D	403	PHO	CAC-C3C	-2.78	1.46	1.51
37	f	102	HEM	CAC-C3C	2.77	1.54	1.47
36	D	407	PL9	C46-C44	-2.77	1.45	1.51
36	d	407	PL9	C46-C44	-2.77	1.45	1.51
27	C	502	CLA	MG-NB	-2.77	2.00	2.05
28	d	403	PHO	CMB-C2B	-2.77	1.46	1.51
38	34	316	A86	C-C1	2.77	1.56	1.50
27	b	602	CLA	CMC-C2C	-2.77	1.45	1.50
27	C	509	CLA	C1B-NB	-2.77	1.34	1.37
38	33	315	A86	C-C1	2.77	1.56	1.50
27	c	505	CLA	MG-NB	-2.77	2.00	2.05
28	D	403	PHO	CMB-C2B	-2.77	1.46	1.51
36	d	407	PL9	C41-C39	-2.77	1.45	1.51
38	31	314	A86	C19-C18	2.77	1.56	1.52
38	11	312	A86	C-C1	2.77	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	13	312	A86	C25-C24	2.77	1.41	1.34
27	B	601	CLA	C1D-ND	2.77	1.41	1.37
27	31	303	CLA	C1D-ND	2.77	1.41	1.37
27	B	603	CLA	CMB-C2B	-2.76	1.45	1.50
27	c	507	CLA	MG-ND	-2.76	2.00	2.05
27	b	604	CLA	CMB-C2B	-2.76	1.45	1.50
38	31	312	A86	C-C1	2.76	1.56	1.50
27	m	101	CLA	CMD-C2D	-2.76	1.45	1.50
38	34	301	A86	C25-C24	2.76	1.41	1.34
38	14	312	A86	C25-C24	2.76	1.41	1.34
38	31	314	A86	C25-C24	2.76	1.41	1.34
27	M	102	CLA	CMD-C2D	-2.76	1.45	1.50
27	13	305	CLA	C1D-ND	2.75	1.41	1.37
27	C	502	CLA	CMD-C2D	-2.75	1.45	1.50
38	32	318	A86	C25-C24	2.75	1.41	1.34
38	34	316	A86	O-C13	-2.75	1.17	1.23
27	B	604	CLA	CMB-C2B	-2.75	1.45	1.50
27	w	103	CLA	CMD-C2D	-2.75	1.45	1.50
38	11	314	A86	C25-C24	2.75	1.41	1.34
27	c	509	CLA	C1B-NB	-2.75	1.34	1.37
27	C	505	CLA	CMB-C2B	-2.75	1.45	1.50
27	b	608	CLA	CMB-C2B	-2.75	1.45	1.50
27	m	101	CLA	MG-NB	-2.75	2.00	2.05
38	32	318	A86	C-C1	2.75	1.56	1.50
27	b	603	CLA	CMB-C2B	-2.75	1.45	1.50
38	12	316	A86	C-C1	2.74	1.56	1.50
38	31	314	A86	C-C1	2.74	1.56	1.50
38	13	316	A86	C-C1	2.74	1.56	1.50
28	d	403	PHO	CAC-C3C	-2.74	1.46	1.51
27	W	103	CLA	CMD-C2D	-2.74	1.45	1.50
38	31	310	A86	C25-C24	2.74	1.41	1.34
27	B	606	CLA	C1D-ND	2.74	1.41	1.37
38	34	313	A86	C25-C24	2.74	1.41	1.34
38	13	316	A86	C25-C24	2.74	1.41	1.34
38	33	312	A86	C25-C24	2.74	1.41	1.34
27	M	102	CLA	MG-NB	-2.74	2.00	2.05
38	32	317	A86	O-C13	-2.74	1.17	1.23
38	32	314	A86	C25-C24	2.74	1.41	1.34
38	11	313	A86	C-C1	2.74	1.56	1.50
38	31	313	A86	C-C1	2.74	1.56	1.50
27	C	507	CLA	MG-ND	-2.74	2.00	2.05
38	14	314	A86	C-C1	2.74	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	608	CLA	CMB-C2B	-2.74	1.45	1.50
38	33	312	A86	O-C13	-2.73	1.17	1.23
27	b	606	CLA	C1D-ND	2.73	1.41	1.37
27	33	304	CLA	C1D-ND	2.73	1.41	1.37
27	c	502	CLA	MG-NB	-2.73	2.00	2.05
38	14	301	A86	C25-C24	2.73	1.41	1.34
27	34	306	CLA	C1D-ND	2.73	1.41	1.37
38	34	315	A86	C-C1	2.73	1.56	1.50
38	13	312	A86	O-C13	-2.73	1.17	1.23
27	c	509	CLA	MG-ND	-2.73	2.00	2.05
35	c	518	DGD	O6D-C5D	-2.73	1.37	1.44
38	14	316	A86	C25-C24	2.73	1.41	1.34
27	C	509	CLA	MG-ND	-2.73	2.00	2.05
35	C	518	DGD	O3G-C3G	-2.73	1.39	1.43
38	14	316	A86	C-C1	2.73	1.56	1.50
38	13	314	A86	C-C1	2.73	1.56	1.50
27	32	305	CLA	MG-NB	-2.72	2.00	2.05
38	12	317	A86	C-C1	2.72	1.56	1.50
38	33	316	A86	C25-C24	2.72	1.41	1.34
38	11	310	A86	C25-C24	2.72	1.41	1.34
38	14	301	A86	C19-C18	2.72	1.56	1.52
27	B	609	CLA	MG-NB	-2.72	2.00	2.05
38	12	317	A86	O-C13	-2.72	1.17	1.23
27	13	303	CLA	MG-NB	-2.72	2.00	2.05
27	B	610	CLA	CMC-C2C	-2.72	1.45	1.50
38	14	301	A86	C-C1	2.72	1.56	1.50
27	12	305	CLA	MG-NB	-2.72	2.00	2.05
38	12	314	A86	O-C13	-2.72	1.17	1.23
38	11	314	A86	C-C1	2.72	1.56	1.50
27	11	303	CLA	C1D-ND	2.72	1.41	1.37
38	33	315	A86	O-C13	-2.72	1.17	1.23
38	32	317	A86	C-C1	2.72	1.56	1.50
27	b	610	CLA	CMC-C2C	-2.72	1.45	1.50
38	32	314	A86	O-C13	-2.71	1.17	1.23
38	14	315	A86	C-C1	2.71	1.56	1.50
30	l	101	SQD	O48-C23	2.71	1.41	1.33
27	b	609	CLA	MG-NB	-2.71	2.00	2.05
38	11	310	A86	O-C13	-2.71	1.17	1.23
27	11	304	CLA	CMD-C2D	-2.71	1.45	1.50
38	13	315	A86	O-C13	-2.71	1.17	1.23
27	B	613	CLA	MG-ND	-2.71	2.00	2.05
27	31	301	CLA	MG-NB	-2.71	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	w	102	CLA	C1D-ND	2.71	1.41	1.37
27	c	502	CLA	CMD-C2D	-2.71	1.45	1.50
27	b	615	CLA	C1B-NB	-2.71	1.34	1.37
38	14	312	A86	O-C13	-2.71	1.17	1.23
38	33	316	A86	C19-C18	2.71	1.56	1.52
38	33	314	A86	C-C1	2.71	1.56	1.50
27	32	308	CLA	CMD-C2D	-2.71	1.45	1.50
38	34	313	A86	O-C13	-2.71	1.17	1.23
35	C	518	DGD	O3G-C1D	-2.71	1.35	1.40
35	c	518	DGD	O3G-C1D	-2.71	1.35	1.40
38	11	313	A86	O-C13	-2.71	1.17	1.23
38	12	314	A86	C25-C24	2.71	1.41	1.34
27	C	506	CLA	C1D-ND	2.71	1.41	1.37
38	32	316	A86	C-C1	2.71	1.56	1.50
37	V	201	HEM	CAC-C3C	2.71	1.54	1.47
27	C	505	CLA	MG-NB	-2.70	2.00	2.05
30	L	103	SQD	O48-C23	2.70	1.41	1.33
27	B	608	CLA	C4B-NB	2.70	1.41	1.37
27	b	603	CLA	CMD-C2D	-2.70	1.45	1.50
27	c	505	CLA	CMB-C2B	-2.70	1.45	1.50
32	A	408	LHG	O7-C5	-2.70	1.40	1.46
27	B	603	CLA	CMD-C2D	-2.70	1.45	1.50
27	33	303	CLA	MG-NB	-2.70	2.00	2.05
27	12	308	CLA	CMD-C2D	-2.70	1.45	1.50
38	14	315	A86	O-C13	-2.70	1.17	1.23
38	33	316	A86	C-C1	2.70	1.56	1.50
27	d	402	CLA	C1D-ND	2.69	1.41	1.37
37	v	201	HEM	CAC-C3C	2.69	1.54	1.47
27	b	608	CLA	C4B-NB	2.69	1.41	1.37
27	13	311	CLA	C4B-NB	2.69	1.41	1.37
38	34	315	A86	C14-C15	2.69	1.58	1.52
38	31	310	A86	O-C13	-2.69	1.17	1.23
32	a	408	LHG	O7-C5	-2.69	1.40	1.46
27	C	512	CLA	MG-NB	-2.69	2.00	2.05
38	34	301	A86	C-C1	2.69	1.56	1.50
27	D	402	CLA	C1D-ND	2.68	1.41	1.37
35	C	518	DGD	O6D-C5D	-2.68	1.37	1.44
35	c	518	DGD	O3G-C3G	-2.68	1.39	1.43
38	31	313	A86	O-C13	-2.68	1.17	1.23
27	33	305	CLA	C1D-ND	2.68	1.41	1.37
27	13	306	CLA	CMD-C2D	-2.68	1.45	1.50
27	11	301	CLA	MG-NB	-2.68	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	13	315	A86	C-C1	2.68	1.56	1.50
27	b	613	CLA	MG-ND	-2.68	2.00	2.05
27	34	306	CLA	MG-NB	-2.68	2.00	2.05
27	14	303	CLA	MG-NB	-2.68	2.00	2.05
38	14	314	A86	C14-C15	2.68	1.57	1.52
38	31	312	A86	C14-C15	2.68	1.57	1.52
27	W	102	CLA	C1D-ND	2.68	1.41	1.37
27	c	506	CLA	C1D-ND	2.68	1.41	1.37
33	D	408	LMG	O1-C7	-2.68	1.39	1.43
27	34	304	CLA	MG-NB	-2.67	2.00	2.05
27	D	401	CLA	CMC-C2C	-2.67	1.45	1.50
27	d	401	CLA	CMC-C2C	-2.67	1.45	1.50
27	12	313	CLA	C4B-NB	2.67	1.41	1.37
27	b	622	CLA	MG-ND	-2.67	2.00	2.05
27	c	512	CLA	MG-NB	-2.67	2.00	2.05
27	34	312	CLA	C4B-NB	2.67	1.41	1.37
27	31	309	CLA	C4B-NB	2.67	1.41	1.37
38	33	315	A86	C14-C15	2.67	1.57	1.52
28	a	403	PHO	C3B-C2B	-2.67	1.36	1.40
27	b	609	CLA	C1D-ND	2.66	1.41	1.37
27	B	612	CLA	CMA-C3A	-2.66	1.47	1.53
27	b	612	CLA	CMA-C3A	-2.66	1.47	1.53
38	32	316	A86	C14-C15	2.66	1.57	1.52
27	b	615	CLA	CMB-C2B	-2.66	1.45	1.50
27	31	304	CLA	CMD-C2D	-2.66	1.45	1.50
27	B	610	CLA	CMD-C2D	-2.66	1.45	1.50
38	14	314	A86	C26-C27	2.66	1.42	1.35
27	c	510	CLA	MG-ND	-2.66	2.00	2.05
27	b	609	CLA	CMD-C2D	-2.66	1.45	1.50
27	33	311	CLA	C4B-NB	2.66	1.41	1.37
38	13	314	A86	C14-C15	2.66	1.57	1.52
38	32	317	A86	C14-C15	2.66	1.57	1.52
27	b	613	CLA	CAA-C2A	-2.66	1.49	1.54
27	33	306	CLA	CMD-C2D	-2.66	1.45	1.50
27	B	605	CLA	CMD-C2D	-2.66	1.45	1.50
27	C	510	CLA	MG-ND	-2.66	2.00	2.05
27	34	307	CLA	CMD-C2D	-2.65	1.45	1.50
27	11	309	CLA	C4B-NB	2.65	1.41	1.37
27	12	307	CLA	MG-NB	-2.65	2.00	2.05
27	B	615	CLA	C1B-NB	-2.65	1.34	1.37
38	33	314	A86	C26-C27	2.65	1.41	1.35
27	C	504	CLA	C1D-ND	2.65	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	33	305	CLA	MG-NB	-2.65	2.00	2.05
27	32	313	CLA	C4B-NB	2.65	1.41	1.37
27	c	510	CLA	C1B-NB	-2.65	1.34	1.37
38	34	316	A86	C14-C15	2.65	1.57	1.52
27	B	606	CLA	C1B-NB	-2.65	1.34	1.37
27	a	402	CLA	MG-NB	-2.65	2.00	2.05
27	13	305	CLA	MG-NB	-2.65	2.00	2.05
27	b	610	CLA	C1B-NB	-2.65	1.34	1.37
38	31	312	A86	C26-C27	2.65	1.41	1.35
27	c	503	CLA	CMD-C2D	-2.65	1.45	1.50
38	13	314	A86	C26-C27	2.65	1.41	1.35
37	v	201	HEM	C2A-C3A	-2.65	1.32	1.38
27	b	605	CLA	CMD-C2D	-2.65	1.45	1.50
38	11	316	A86	C-C1	2.65	1.56	1.50
27	B	613	CLA	CAA-C2A	-2.64	1.49	1.54
27	B	615	CLA	CMB-C2B	-2.64	1.45	1.50
33	d	408	LMG	O1-C7	-2.64	1.39	1.43
38	34	303	A86	C-C1	2.64	1.56	1.50
33	32	301	LMG	O7-C8	-2.64	1.40	1.46
28	A	403	PHO	C3B-C2B	-2.64	1.36	1.40
27	34	311	CLA	CMD-C2D	-2.64	1.45	1.50
27	c	513	CLA	CMD-C2D	-2.64	1.45	1.50
30	A	406	SQD	O47-C7	2.64	1.41	1.34
27	B	609	CLA	CMD-C2D	-2.64	1.45	1.50
38	11	313	A86	C14-C15	2.64	1.57	1.52
38	12	316	A86	C14-C15	2.64	1.57	1.52
33	32	301	LMG	O1-C1	2.64	1.44	1.40
27	B	615	CLA	MG-NB	-2.64	2.00	2.05
27	C	508	CLA	CMD-C2D	-2.64	1.45	1.50
27	14	311	CLA	C4B-NB	2.64	1.41	1.37
27	b	610	CLA	CMD-C2D	-2.64	1.45	1.50
27	A	402	CLA	MG-NB	-2.64	2.00	2.05
27	C	510	CLA	CMC-C2C	-2.63	1.45	1.50
38	12	316	A86	C26-C27	2.63	1.41	1.35
30	a	406	SQD	O47-C7	2.63	1.41	1.34
27	b	606	CLA	CMB-C2B	-2.63	1.45	1.50
27	c	514	CLA	C1B-NB	-2.63	1.34	1.37
33	q	301	LMG	O8-C9	-2.63	1.39	1.45
38	13	317	A86	C-C1	2.63	1.56	1.50
38	31	313	A86	C14-C15	2.63	1.57	1.52
27	C	508	CLA	C1D-ND	2.63	1.41	1.37
27	C	510	CLA	C1B-NB	-2.63	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	33	302	A86	C-C1	2.63	1.56	1.50
27	c	504	CLA	C1D-ND	2.63	1.41	1.37
27	D	401	CLA	MG-ND	-2.63	2.00	2.05
27	d	401	CLA	MG-ND	-2.63	2.00	2.05
38	14	315	A86	C14-C15	2.63	1.57	1.52
38	33	314	A86	C14-C15	2.63	1.57	1.52
37	V	201	HEM	C2A-C3A	-2.63	1.32	1.38
38	12	304	A86	C-C1	2.63	1.56	1.50
27	C	506	CLA	MG-NB	-2.63	2.00	2.05
38	12	317	A86	C14-C15	2.63	1.57	1.52
27	14	302	CLA	CMD-C2D	-2.63	1.45	1.50
27	B	610	CLA	CMB-C2B	-2.62	1.45	1.50
33	C	519	LMG	O8-C9	-2.62	1.39	1.45
27	c	508	CLA	CMD-C2D	-2.62	1.45	1.50
27	31	315	CLA	CMD-C2D	-2.62	1.45	1.50
33	w	101	LMG	O8-C9	-2.62	1.39	1.45
38	31	316	A86	C-C1	2.62	1.56	1.50
27	C	503	CLA	CMD-C2D	-2.62	1.45	1.50
27	31	301	CLA	CMC-C2C	-2.62	1.45	1.50
27	14	306	CLA	CMD-C2D	-2.62	1.45	1.50
27	12	303	CLA	CMD-C2D	-2.62	1.45	1.50
27	32	307	CLA	MG-NB	-2.62	2.00	2.05
38	13	302	A86	C-C1	2.62	1.56	1.50
27	14	305	CLA	MG-NB	-2.62	2.00	2.05
27	D	405	CLA	CMC-C2C	-2.61	1.45	1.50
27	34	304	CLA	CMC-C2C	-2.61	1.45	1.50
27	b	615	CLA	MG-NB	-2.61	2.00	2.05
38	11	311	A86	O-C13	-2.61	1.17	1.23
38	13	314	A86	O-C13	-2.61	1.17	1.23
38	32	304	A86	C-C1	2.61	1.56	1.50
27	c	513	CLA	MG-NB	-2.61	2.00	2.05
38	11	312	A86	C26-C27	2.61	1.41	1.35
27	B	608	CLA	CMD-C2D	-2.61	1.45	1.50
38	11	312	A86	C14-C15	2.61	1.57	1.52
27	C	513	CLA	CMD-C2D	-2.61	1.45	1.50
27	33	303	CLA	CMC-C2C	-2.61	1.45	1.50
38	31	311	A86	O-C13	-2.61	1.17	1.23
38	33	313	A86	O-C13	-2.61	1.17	1.23
38	32	316	A86	C26-C27	2.61	1.41	1.35
27	B	606	CLA	CMB-C2B	-2.61	1.45	1.50
27	b	614	CLA	MG-NB	-2.61	2.00	2.05
27	b	612	CLA	C1B-NB	-2.61	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	13	301	CLA	CMD-C2D	-2.61	1.45	1.50
38	13	313	A86	O-C13	-2.60	1.17	1.23
38	32	315	A86	O-C13	-2.60	1.17	1.23
27	14	310	CLA	CMD-C2D	-2.60	1.45	1.50
27	B	610	CLA	MG-ND	-2.60	2.00	2.05
27	B	606	CLA	CMC-C2C	-2.60	1.45	1.50
27	c	513	CLA	C1D-ND	2.60	1.41	1.37
38	12	315	A86	O-C13	-2.60	1.17	1.23
27	d	405	CLA	CMC-C2C	-2.60	1.45	1.50
27	B	610	CLA	C1B-NB	-2.60	1.34	1.37
27	b	608	CLA	CMD-C2D	-2.60	1.45	1.50
27	b	606	CLA	CMC-C2C	-2.60	1.45	1.50
27	B	622	CLA	MG-ND	-2.60	2.00	2.05
27	b	614	CLA	C1D-ND	2.60	1.41	1.37
38	14	313	A86	O-C13	-2.60	1.17	1.23
38	33	302	A86	C24-C1	2.60	1.51	1.46
27	A	404	CLA	CMB-C2B	-2.60	1.45	1.50
37	V	201	HEM	C3C-C2C	-2.60	1.31	1.37
27	B	605	CLA	CMB-C2B	-2.60	1.45	1.50
27	C	513	CLA	MG-NB	-2.60	2.00	2.05
38	11	316	A86	C24-C1	2.60	1.51	1.46
27	c	510	CLA	CMC-C2C	-2.60	1.45	1.50
33	W	101	LMG	O8-C9	-2.60	1.39	1.45
38	34	315	A86	C26-C27	2.60	1.41	1.35
27	14	303	CLA	CMC-C2C	-2.59	1.45	1.50
38	34	314	A86	O-C13	-2.59	1.17	1.23
27	12	305	CLA	CMC-C2C	-2.59	1.45	1.50
38	13	302	A86	C24-C1	2.59	1.51	1.46
27	b	614	CLA	CMD-C2D	-2.59	1.45	1.50
27	33	301	CLA	CMD-C2D	-2.59	1.45	1.50
37	v	201	HEM	C3C-C2C	-2.59	1.31	1.37
27	B	609	CLA	C1D-ND	2.59	1.41	1.37
27	C	514	CLA	C1B-NB	-2.59	1.34	1.37
27	a	402	CLA	C1D-ND	2.59	1.41	1.37
27	C	505	CLA	C1B-NB	-2.59	1.34	1.37
38	12	314	A86	C-C1	2.59	1.56	1.50
38	12	304	A86	C24-C1	2.59	1.51	1.46
27	a	404	CLA	CMB-C2B	-2.59	1.45	1.50
38	13	315	A86	C14-C15	2.59	1.57	1.52
27	B	612	CLA	C1B-NB	-2.59	1.34	1.37
27	11	301	CLA	CMC-C2C	-2.59	1.45	1.50
27	34	302	CLA	CMD-C2D	-2.59	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	603	CLA	MG-ND	-2.59	2.00	2.05
27	b	603	CLA	MG-ND	-2.59	2.00	2.05
38	14	314	A86	O-C13	-2.59	1.17	1.23
27	31	303	CLA	MG-NB	-2.59	2.00	2.05
27	D	405	CLA	MG-ND	-2.59	2.00	2.05
27	c	512	CLA	MG-ND	-2.59	2.00	2.05
27	11	308	CLA	CMD-C2D	-2.58	1.45	1.50
38	31	312	A86	O-C13	-2.58	1.17	1.23
27	b	606	CLA	C1B-NB	-2.58	1.34	1.37
35	C	517	DGD	O5D-C6D	-2.58	1.39	1.43
27	b	605	CLA	CMB-C2B	-2.58	1.45	1.50
27	b	610	CLA	CMB-C2B	-2.58	1.45	1.50
38	34	315	A86	O-C13	-2.58	1.17	1.23
38	12	316	A86	O-C13	-2.58	1.17	1.23
27	c	508	CLA	C1D-ND	2.58	1.41	1.37
38	12	316	A86	C24-C1	2.58	1.51	1.46
27	32	303	CLA	CMD-C2D	-2.58	1.45	1.50
27	B	604	CLA	CAC-C3C	-2.58	1.44	1.51
27	d	406	CLA	CMD-C2D	-2.58	1.45	1.50
27	13	303	CLA	CMC-C2C	-2.58	1.45	1.50
27	32	312	CLA	CMD-C2D	-2.58	1.45	1.50
27	B	614	CLA	MG-NB	-2.58	2.00	2.05
38	33	314	A86	O-C13	-2.58	1.17	1.23
27	C	514	CLA	C1D-ND	2.58	1.41	1.37
27	a	404	CLA	CMC-C2C	-2.57	1.45	1.50
27	c	505	CLA	C1B-NB	-2.57	1.34	1.37
38	32	316	A86	O-C13	-2.57	1.17	1.23
27	B	614	CLA	CMD-C2D	-2.57	1.45	1.50
29	B	623	BCR	C30-C25	-2.57	1.50	1.53
27	33	308	CLA	MG-NB	-2.57	2.00	2.05
38	33	316	A86	O-C13	-2.57	1.17	1.23
27	11	303	CLA	MG-NB	-2.57	2.00	2.05
27	32	305	CLA	CMC-C2C	-2.57	1.45	1.50
27	32	303	CLA	C4B-NB	2.57	1.41	1.37
27	c	506	CLA	MG-NB	-2.57	2.00	2.05
38	33	314	A86	C24-C1	2.57	1.51	1.46
27	b	609	CLA	CMB-C2B	-2.57	1.45	1.50
27	13	301	CLA	C4B-NB	2.57	1.41	1.37
38	11	312	A86	O-C13	-2.57	1.17	1.23
27	b	607	CLA	CMD-C2D	-2.57	1.45	1.50
27	c	508	CLA	CMC-C2C	-2.57	1.45	1.50
29	b	623	BCR	C30-C25	-2.57	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	14	314	A86	C24-C1	2.57	1.51	1.46
38	31	316	A86	C24-C1	2.57	1.51	1.46
27	C	514	CLA	MG-NB	-2.56	2.00	2.05
27	b	610	CLA	MG-ND	-2.56	2.00	2.05
38	11	310	A86	C-C1	2.56	1.56	1.50
38	34	313	A86	C-C1	2.56	1.56	1.50
27	c	505	CLA	CAC-C3C	-2.56	1.44	1.51
38	13	314	A86	C24-C1	2.56	1.51	1.46
27	C	508	CLA	CMC-C2C	-2.56	1.45	1.50
27	C	508	CLA	C1B-NB	-2.56	1.34	1.37
35	J	101	DGD	O1G-C1G	-2.56	1.39	1.45
38	31	310	A86	C-C1	2.56	1.56	1.50
38	32	304	A86	C24-C1	2.56	1.51	1.46
27	C	513	CLA	C1D-ND	2.56	1.41	1.37
38	13	317	A86	C24-C1	2.56	1.51	1.46
27	c	514	CLA	C1D-ND	2.56	1.41	1.37
27	33	310	CLA	CMD-C2D	-2.56	1.45	1.50
27	13	307	CLA	C4B-NB	2.56	1.41	1.37
27	D	406	CLA	CMD-C2D	-2.56	1.45	1.50
27	b	602	CLA	MG-NB	-2.56	2.00	2.05
27	C	505	CLA	CAC-C3C	-2.56	1.44	1.51
27	11	315	CLA	CMD-C2D	-2.56	1.45	1.50
38	33	312	A86	C-C1	2.56	1.56	1.50
27	b	607	CLA	C1D-ND	2.56	1.41	1.37
38	32	314	A86	C-C1	2.56	1.56	1.50
27	B	613	CLA	CMD-C2D	-2.55	1.45	1.50
27	31	308	CLA	CMD-C2D	-2.55	1.45	1.50
27	A	402	CLA	CMC-C2C	-2.55	1.45	1.50
27	a	402	CLA	CMC-C2C	-2.55	1.45	1.50
27	b	613	CLA	CMD-C2D	-2.55	1.45	1.50
38	34	303	A86	C24-C1	2.55	1.51	1.46
38	32	316	A86	C24-C1	2.55	1.51	1.46
38	14	312	A86	C-C1	2.55	1.56	1.50
27	M	102	CLA	CMB-C2B	-2.55	1.45	1.50
27	C	504	CLA	MG-NB	-2.55	2.00	2.05
38	32	315	A86	C26-C27	2.55	1.41	1.35
27	b	613	CLA	CMC-C2C	-2.55	1.45	1.50
38	13	312	A86	O4-C34	-2.55	1.40	1.46
27	B	605	CLA	MG-NB	-2.55	2.00	2.05
27	c	514	CLA	MG-NB	-2.54	2.00	2.05
27	12	308	CLA	MG-ND	-2.54	2.00	2.05
27	13	310	CLA	CMD-C2D	-2.54	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	34	315	A86	C24-C1	2.54	1.51	1.46
27	B	607	CLA	CMD-C2D	-2.54	1.45	1.50
27	12	312	CLA	CMD-C2D	-2.54	1.45	1.50
27	b	601	CLA	CMB-C2B	-2.54	1.45	1.50
27	C	509	CLA	CMD-C2D	-2.54	1.45	1.50
27	C	514	CLA	CMC-C2C	-2.54	1.45	1.50
35	c	517	DGD	O5D-C6D	-2.54	1.39	1.43
38	31	310	A86	O4-C34	-2.54	1.40	1.46
27	B	614	CLA	C1D-ND	2.54	1.41	1.37
27	a	402	CLA	CMD-C2D	-2.54	1.45	1.50
27	C	507	CLA	CMD-C2D	-2.54	1.45	1.50
38	11	312	A86	C24-C1	2.54	1.51	1.46
27	C	512	CLA	MG-ND	-2.54	2.00	2.05
27	c	503	CLA	CHC-C4B	-2.54	1.33	1.39
30	b	620	SQD	O47-C7	2.54	1.41	1.34
27	d	406	CLA	CMB-C2B	-2.54	1.45	1.50
38	32	318	A86	O-C13	-2.54	1.18	1.23
29	f	101	BCR	C30-C25	-2.54	1.50	1.53
27	b	605	CLA	MG-NB	-2.54	2.00	2.05
27	33	301	CLA	C4B-NB	2.54	1.41	1.37
38	31	312	A86	C24-C1	2.54	1.51	1.46
27	b	604	CLA	CAC-C3C	-2.54	1.44	1.51
27	B	607	CLA	C1D-ND	2.54	1.41	1.37
27	34	302	CLA	C4B-NB	2.54	1.41	1.37
27	A	404	CLA	CMC-C2C	-2.53	1.45	1.50
27	B	609	CLA	CMB-C2B	-2.53	1.45	1.50
27	b	604	CLA	C1B-NB	-2.53	1.34	1.37
27	31	315	CLA	C4B-NB	2.53	1.41	1.37
27	B	611	CLA	C1B-NB	-2.53	1.34	1.37
27	A	402	CLA	CMD-C2D	-2.53	1.45	1.50
27	B	602	CLA	MG-NB	-2.53	2.00	2.05
30	B	620	SQD	O47-C7	2.53	1.41	1.34
27	33	306	CLA	MG-ND	-2.53	2.00	2.05
38	14	313	A86	C26-C27	2.53	1.41	1.35
38	13	312	A86	C-C1	2.53	1.56	1.50
27	B	607	CLA	CMB-C2B	-2.53	1.45	1.50
27	A	402	CLA	C1D-ND	2.53	1.41	1.37
35	C	518	DGD	O4D-C4D	-2.53	1.36	1.43
27	c	514	CLA	CMC-C2C	-2.53	1.45	1.50
27	c	508	CLA	CMB-C2B	-2.53	1.45	1.50
27	c	509	CLA	CMD-C2D	-2.53	1.45	1.50
33	12	301	LMG	O7-C8	-2.53	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	j	101	DGD	O1G-C1G	-2.52	1.39	1.45
27	z	102	CLA	MG-ND	-2.52	2.00	2.05
27	B	601	CLA	CMB-C2B	-2.52	1.45	1.50
27	C	508	CLA	CMB-C2B	-2.52	1.45	1.50
38	14	301	A86	O-C13	-2.52	1.18	1.23
38	32	304	A86	C26-C27	2.52	1.41	1.35
27	c	507	CLA	CMD-C2D	-2.52	1.45	1.50
27	c	504	CLA	MG-NB	-2.52	2.00	2.05
27	d	405	CLA	MG-ND	-2.52	2.00	2.05
38	31	314	A86	O-C13	-2.52	1.18	1.23
38	33	313	A86	C26-C27	2.52	1.41	1.35
27	33	307	CLA	C4B-NB	2.52	1.41	1.37
27	b	603	CLA	C1B-NB	-2.52	1.34	1.37
27	B	613	CLA	CMC-C2C	-2.52	1.45	1.50
27	32	308	CLA	MG-ND	-2.52	2.00	2.05
27	b	622	CLA	CMB-C2B	-2.52	1.45	1.50
27	D	406	CLA	CMB-C2B	-2.51	1.45	1.50
38	31	311	A86	C26-C27	2.51	1.41	1.35
38	33	316	A86	O4-C34	-2.51	1.40	1.46
27	11	315	CLA	C4B-NB	2.51	1.41	1.37
27	12	309	CLA	C4B-NB	2.51	1.41	1.37
27	33	303	CLA	C1B-C2B	2.51	1.49	1.43
27	31	306	CLA	MG-NB	-2.51	2.00	2.05
27	m	101	CLA	CMB-C2B	-2.51	1.45	1.50
27	11	305	CLA	C4B-NB	2.51	1.41	1.37
27	31	305	CLA	C4B-NB	2.51	1.41	1.37
38	32	314	A86	O4-C34	-2.51	1.40	1.46
38	34	313	A86	O4-C34	-2.51	1.40	1.46
35	c	518	DGD	O4D-C4D	-2.51	1.36	1.43
27	Z	102	CLA	MG-ND	-2.51	2.00	2.05
27	14	306	CLA	MG-ND	-2.51	2.00	2.05
27	C	503	CLA	CHC-C4B	-2.51	1.33	1.39
27	c	510	CLA	CMD-C2D	-2.51	1.45	1.50
38	33	312	A86	O4-C34	-2.51	1.40	1.46
27	13	306	CLA	MG-ND	-2.51	2.00	2.05
38	11	314	A86	O4-C34	-2.51	1.40	1.46
27	31	304	CLA	MG-ND	-2.51	2.00	2.05
38	14	312	A86	O4-C34	-2.51	1.40	1.46
27	11	304	CLA	MG-ND	-2.51	2.00	2.05
33	B	619	LMG	O4-C4	-2.51	1.36	1.43
27	c	508	CLA	C1B-NB	-2.51	1.34	1.37
27	34	304	CLA	C1B-C2B	2.51	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	13	316	A86	O-C13	-2.50	1.18	1.23
27	B	611	CLA	CMD-C2D	-2.50	1.45	1.50
27	12	310	CLA	MG-NB	-2.50	2.00	2.05
27	32	305	CLA	C1B-C2B	2.50	1.49	1.43
27	c	507	CLA	C4B-NB	2.50	1.41	1.37
38	11	316	A86	C26-C27	2.50	1.41	1.35
38	12	304	A86	C26-C27	2.50	1.41	1.35
27	C	506	CLA	CMC-C2C	-2.50	1.45	1.50
27	c	506	CLA	CMC-C2C	-2.50	1.45	1.50
38	12	315	A86	C26-C27	2.50	1.41	1.35
27	32	310	CLA	MG-NB	-2.50	2.00	2.05
27	34	305	CLA	MG-NB	-2.50	2.00	2.05
38	33	302	A86	C26-C27	2.50	1.41	1.35
27	34	309	CLA	MG-NB	-2.50	2.00	2.05
27	13	308	CLA	MG-NB	-2.50	2.00	2.05
38	14	316	A86	O-C13	-2.50	1.18	1.23
33	b	619	LMG	O4-C4	-2.50	1.36	1.43
38	13	302	A86	C26-C27	2.50	1.41	1.35
38	14	301	A86	O4-C34	-2.50	1.40	1.46
38	34	303	A86	C26-C27	2.50	1.41	1.35
27	13	303	CLA	C1B-C2B	2.49	1.49	1.43
27	33	307	CLA	MG-NB	-2.49	2.00	2.05
27	11	306	CLA	MG-NB	-2.49	2.00	2.05
35	C	518	DGD	O4E-C4E	-2.49	1.36	1.43
27	B	604	CLA	C1B-NB	-2.49	1.34	1.37
38	34	314	A86	C26-C27	2.49	1.41	1.35
27	11	301	CLA	C1B-C2B	2.49	1.49	1.43
27	13	311	CLA	C1B-C2B	2.49	1.49	1.43
27	31	308	CLA	CMC-C2C	-2.49	1.45	1.50
27	32	309	CLA	C4B-NB	2.49	1.41	1.37
35	c	518	DGD	O4E-C4E	-2.49	1.36	1.43
27	14	302	CLA	C4B-NB	2.49	1.41	1.37
27	b	611	CLA	CMD-C2D	-2.49	1.45	1.50
28	A	403	PHO	CAA-C2A	-2.49	1.49	1.54
27	B	622	CLA	CMB-C2B	-2.49	1.45	1.50
27	13	304	CLA	CMD-C2D	-2.49	1.45	1.50
27	34	311	CLA	MG-ND	-2.49	2.00	2.05
27	b	603	CLA	C1D-ND	2.49	1.41	1.37
27	b	611	CLA	C1B-NB	-2.49	1.34	1.37
38	11	310	A86	O4-C34	-2.49	1.40	1.46
38	34	303	A86	O-C13	-2.49	1.18	1.23
27	31	302	CLA	MG-NB	-2.49	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	33	301	CLA	MG-NB	-2.49	2.00	2.05
27	14	303	CLA	C1B-C2B	2.49	1.49	1.43
27	12	305	CLA	C1B-C2B	2.49	1.49	1.43
38	31	316	A86	C26-C27	2.49	1.41	1.35
27	32	306	CLA	MG-NB	-2.49	2.00	2.05
27	14	310	CLA	MG-ND	-2.49	2.00	2.05
27	34	309	CLA	CMB-C2B	-2.49	1.45	1.50
27	C	511	CLA	CMC-C2C	-2.49	1.45	1.50
38	11	314	A86	O-C13	-2.48	1.18	1.23
38	11	311	A86	C26-C27	2.48	1.41	1.35
38	13	317	A86	C26-C27	2.48	1.41	1.35
27	W	102	CLA	CMC-C2C	-2.48	1.45	1.50
27	13	304	CLA	MG-NB	-2.48	2.00	2.05
38	34	301	A86	O-C13	-2.48	1.18	1.23
27	C	510	CLA	CMD-C2D	-2.48	1.45	1.50
38	12	314	A86	O4-C34	-2.48	1.40	1.46
27	14	307	CLA	C4B-NB	2.48	1.41	1.37
27	13	308	CLA	C1B-C2B	2.48	1.49	1.43
27	c	507	CLA	CMC-C2C	-2.48	1.45	1.50
38	31	314	A86	O4-C34	-2.48	1.40	1.46
38	32	318	A86	O4-C34	-2.48	1.40	1.46
27	w	102	CLA	MG-NB	-2.48	2.00	2.05
27	13	309	CLA	CMD-C2D	-2.48	1.45	1.50
27	34	312	CLA	C1B-C2B	2.48	1.48	1.43
27	31	309	CLA	C1B-C2B	2.48	1.48	1.43
38	32	304	A86	O-C13	-2.48	1.18	1.23
27	c	503	CLA	C1B-NB	-2.48	1.34	1.37
27	B	615	CLA	MG-ND	-2.48	2.00	2.05
27	c	505	CLA	CMD-C2D	-2.48	1.45	1.50
28	a	403	PHO	CAA-C2A	-2.48	1.49	1.54
27	C	505	CLA	CMD-C2D	-2.48	1.45	1.50
27	W	102	CLA	MG-NB	-2.48	2.00	2.05
38	32	316	A86	C2-C1	2.48	1.41	1.35
29	F	101	BCR	C30-C25	-2.48	1.50	1.53
27	31	308	CLA	MG-ND	-2.48	2.00	2.05
27	32	312	CLA	MG-ND	-2.48	2.00	2.05
27	b	611	CLA	C1D-ND	2.47	1.41	1.37
27	34	308	CLA	C4B-NB	2.47	1.41	1.37
38	11	314	A86	C26-C27	2.47	1.41	1.35
38	13	313	A86	C26-C27	2.47	1.41	1.35
27	m	101	CLA	C1D-ND	2.47	1.41	1.37
27	w	102	CLA	CMC-C2C	-2.47	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	12	304	A86	O-C13	-2.47	1.18	1.23
27	33	310	CLA	CMC-C2C	-2.47	1.45	1.50
27	32	303	CLA	MG-NB	-2.47	2.00	2.05
27	34	307	CLA	MG-ND	-2.47	2.00	2.05
27	12	310	CLA	CMB-C2B	-2.47	1.45	1.50
27	c	505	CLA	CMC-C2C	-2.47	1.45	1.50
27	d	402	CLA	CMB-C2B	-2.47	1.45	1.50
28	A	403	PHO	C4D-CHA	2.47	1.43	1.39
27	32	311	CLA	CMD-C2D	-2.47	1.45	1.50
38	13	316	A86	C26-C27	2.47	1.41	1.35
27	31	315	CLA	MG-NB	-2.47	2.00	2.05
38	11	312	A86	C2-C1	2.47	1.41	1.35
38	12	316	A86	C2-C1	2.47	1.41	1.35
27	12	313	CLA	C1B-C2B	2.47	1.48	1.43
28	D	403	PHO	C1D-C2D	2.47	1.42	1.39
27	b	615	CLA	MG-ND	-2.47	2.00	2.05
28	a	403	PHO	C4D-CHA	2.47	1.43	1.39
27	34	310	CLA	CMD-C2D	-2.47	1.45	1.50
27	w	102	CLA	CMB-C2B	-2.47	1.45	1.50
27	13	310	CLA	CMC-C2C	-2.47	1.45	1.50
27	A	404	CLA	MG-ND	-2.47	2.00	2.05
27	12	309	CLA	MG-NB	-2.47	2.00	2.05
27	D	402	CLA	CMB-C2B	-2.47	1.45	1.50
27	33	308	CLA	CMB-C2B	-2.47	1.45	1.50
27	34	311	CLA	CMC-C2C	-2.47	1.45	1.50
27	14	309	CLA	CMD-C2D	-2.47	1.45	1.50
27	33	310	CLA	MG-ND	-2.47	2.00	2.05
27	34	308	CLA	MG-NB	-2.47	2.00	2.05
27	C	503	CLA	C1B-NB	-2.47	1.34	1.37
27	13	308	CLA	CMB-C2B	-2.46	1.45	1.50
27	31	307	CLA	CMD-C2D	-2.46	1.45	1.50
27	32	306	CLA	CMD-C2D	-2.46	1.45	1.50
27	11	302	CLA	MG-NB	-2.46	2.00	2.05
27	14	311	CLA	C1B-C2B	2.46	1.48	1.43
27	12	303	CLA	MG-NB	-2.46	2.00	2.05
27	13	301	CLA	MG-NB	-2.46	2.00	2.05
38	14	313	A86	C14-C15	2.46	1.57	1.52
27	b	614	CLA	CMC-C2C	-2.46	1.45	1.50
38	31	314	A86	C26-C27	2.46	1.41	1.35
27	B	613	CLA	C1D-ND	2.46	1.41	1.37
27	31	301	CLA	C1B-C2B	2.46	1.48	1.43
38	13	317	A86	O-C13	-2.46	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	404	CLA	MG-ND	-2.46	2.00	2.05
27	34	305	CLA	CMD-C2D	-2.46	1.45	1.50
27	32	309	CLA	MG-NB	-2.46	2.00	2.05
38	34	301	A86	O4-C34	-2.46	1.40	1.46
38	14	315	A86	C24-C1	2.46	1.51	1.46
27	B	614	CLA	CMC-C2C	-2.46	1.45	1.50
27	B	609	CLA	C4B-NB	2.46	1.41	1.37
27	34	302	CLA	MG-NB	-2.46	2.00	2.05
36	D	407	PL9	C31-C29	-2.46	1.46	1.51
36	d	407	PL9	C31-C29	-2.46	1.46	1.51
27	13	310	CLA	MG-ND	-2.46	2.00	2.05
38	34	315	A86	C2-C1	2.46	1.41	1.35
27	32	312	CLA	CMC-C2C	-2.46	1.45	1.50
27	31	306	CLA	CMB-C2B	-2.46	1.45	1.50
27	W	102	CLA	CMB-C2B	-2.46	1.45	1.50
27	11	315	CLA	MG-NB	-2.46	2.00	2.05
27	b	607	CLA	CMB-C2B	-2.45	1.45	1.50
38	14	316	A86	C26-C27	2.45	1.41	1.35
27	31	306	CLA	C1B-C2B	2.45	1.48	1.43
27	C	514	CLA	CMD-C2D	-2.45	1.45	1.50
27	C	505	CLA	C1D-ND	2.45	1.41	1.37
27	C	505	CLA	CMC-C2C	-2.45	1.45	1.50
38	13	302	A86	O-C13	-2.45	1.18	1.23
38	34	301	A86	C26-C27	2.45	1.41	1.35
38	13	316	A86	O4-C34	-2.45	1.40	1.46
27	34	309	CLA	C1B-C2B	2.45	1.48	1.43
27	12	306	CLA	MG-NB	-2.45	2.00	2.05
27	33	308	CLA	C1B-C2B	2.45	1.48	1.43
27	14	308	CLA	CMB-C2B	-2.45	1.45	1.50
27	14	308	CLA	MG-NB	-2.45	2.00	2.05
27	c	511	CLA	CMC-C2C	-2.45	1.45	1.50
27	33	309	CLA	CMD-C2D	-2.45	1.45	1.50
27	14	310	CLA	CMC-C2C	-2.45	1.45	1.50
38	11	316	A86	O-C13	-2.45	1.18	1.23
38	33	302	A86	O-C13	-2.45	1.18	1.23
27	B	603	CLA	CMC-C2C	-2.45	1.45	1.50
27	C	504	CLA	MG-ND	-2.45	2.00	2.05
27	11	309	CLA	C1B-C2B	2.45	1.48	1.43
27	12	312	CLA	CMC-C2C	-2.45	1.45	1.50
38	14	314	A86	C2-C1	2.45	1.41	1.35
27	31	302	CLA	CMD-C2D	-2.45	1.45	1.50
38	33	316	A86	C26-C27	2.45	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	613	CLA	C1D-ND	2.45	1.41	1.37
27	11	308	CLA	CMC-C2C	-2.45	1.45	1.50
38	14	315	A86	C26-C27	2.45	1.41	1.35
27	11	306	CLA	CMB-C2B	-2.45	1.45	1.50
27	14	302	CLA	MG-NB	-2.45	2.00	2.05
27	14	304	CLA	MG-NB	-2.45	2.00	2.05
38	14	301	A86	C26-C27	2.45	1.41	1.35
27	12	311	CLA	CMD-C2D	-2.45	1.45	1.50
27	C	503	CLA	CAC-C3C	-2.44	1.44	1.51
27	C	507	CLA	CMC-C2C	-2.44	1.45	1.50
38	32	318	A86	C26-C27	2.44	1.41	1.35
27	32	310	CLA	C1B-C2B	2.44	1.48	1.43
27	32	313	CLA	C1B-C2B	2.44	1.48	1.43
38	31	316	A86	O-C13	-2.44	1.18	1.23
27	12	312	CLA	MG-ND	-2.44	2.00	2.05
27	b	603	CLA	CMC-C2C	-2.44	1.45	1.50
27	12	303	CLA	C4B-NB	2.44	1.41	1.37
27	12	306	CLA	CMD-C2D	-2.44	1.45	1.50
27	32	310	CLA	CMB-C2B	-2.44	1.45	1.50
27	c	504	CLA	MG-ND	-2.44	2.00	2.05
27	14	307	CLA	MG-NB	-2.44	2.01	2.05
27	b	608	CLA	C1D-ND	2.44	1.41	1.37
38	13	315	A86	C24-C1	2.44	1.51	1.46
38	14	316	A86	O4-C34	-2.44	1.40	1.46
38	34	316	A86	C24-C1	2.44	1.51	1.46
27	11	302	CLA	CMD-C2D	-2.44	1.45	1.50
27	13	307	CLA	MG-NB	-2.43	2.01	2.05
27	C	507	CLA	C4B-NB	2.43	1.41	1.37
38	33	313	A86	C14-C15	2.43	1.57	1.52
38	11	311	A86	C-C1	2.43	1.55	1.50
27	12	313	CLA	MG-NB	-2.43	2.01	2.05
37	V	201	HEM	C3D-C2D	-2.43	1.31	1.36
27	31	309	CLA	MG-NB	-2.43	2.01	2.05
27	14	311	CLA	MG-NB	-2.43	2.01	2.05
27	33	304	CLA	C1B-C2B	2.43	1.48	1.43
38	11	311	A86	C14-C15	2.43	1.57	1.52
27	14	308	CLA	C1B-C2B	2.43	1.48	1.43
27	12	310	CLA	C1B-C2B	2.43	1.48	1.43
38	11	313	A86	C24-C1	2.43	1.51	1.46
27	B	601	CLA	CMD-C2D	-2.43	1.45	1.50
27	D	402	CLA	CMD-C2D	-2.43	1.45	1.50
38	31	311	A86	C14-C15	2.43	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	11	309	CLA	MG-NB	-2.43	2.01	2.05
38	13	314	A86	C2-C1	2.43	1.41	1.35
38	31	312	A86	C2-C1	2.43	1.41	1.35
27	11	308	CLA	MG-ND	-2.43	2.01	2.05
27	14	304	CLA	CMD-C2D	-2.43	1.45	1.50
27	33	311	CLA	C1B-C2B	2.43	1.48	1.43
38	13	313	A86	C-C1	2.43	1.55	1.50
38	32	315	A86	C-C1	2.43	1.55	1.50
28	d	403	PHO	C1D-C2D	2.43	1.42	1.39
38	12	317	A86	C26-C27	2.43	1.41	1.35
38	33	315	A86	C24-C1	2.42	1.51	1.46
38	31	313	A86	C26-C27	2.42	1.41	1.35
38	31	311	A86	C-C1	2.42	1.55	1.50
38	34	314	A86	C-C1	2.42	1.55	1.50
38	12	317	A86	C24-C1	2.42	1.51	1.46
39	12	302	LMU	O3'-C3'	2.42	1.49	1.43
27	B	604	CLA	CMC-C2C	-2.42	1.45	1.50
27	B	610	CLA	C1D-ND	2.42	1.41	1.37
27	B	603	CLA	C1B-NB	-2.42	1.34	1.37
27	C	505	CLA	MG-ND	-2.42	2.01	2.05
38	11	313	A86	C26-C27	2.42	1.41	1.35
37	v	201	HEM	C3D-C2D	-2.42	1.31	1.36
27	11	307	CLA	CMD-C2D	-2.42	1.45	1.50
27	C	502	CLA	C1D-ND	2.42	1.41	1.37
27	c	502	CLA	C1D-ND	2.42	1.41	1.37
27	31	305	CLA	MG-NB	-2.42	2.01	2.05
27	b	612	CLA	CMB-C2B	-2.42	1.45	1.50
38	13	317	A86	C2-C1	2.42	1.41	1.35
38	13	313	A86	C14-C15	2.42	1.57	1.52
27	33	304	CLA	MG-NB	-2.42	2.01	2.05
27	11	306	CLA	C1B-C2B	2.42	1.48	1.43
37	E	101	HEM	FE-ND	2.42	2.02	1.94
38	33	314	A86	C2-C1	2.42	1.41	1.35
27	B	603	CLA	C1D-ND	2.42	1.41	1.37
33	B	618	LMG	O1-C7	-2.42	1.39	1.43
38	34	314	A86	C14-C15	2.42	1.57	1.52
27	31	302	CLA	C1B-C2B	2.42	1.48	1.43
27	C	506	CLA	CMB-C2B	-2.42	1.45	1.50
27	11	303	CLA	C1B-C2B	2.42	1.48	1.43
27	32	306	CLA	C1B-C2B	2.42	1.48	1.43
27	B	607	CLA	MG-ND	-2.42	2.01	2.05
27	B	611	CLA	C1D-ND	2.41	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	33	304	CLA	CMD-C2D	-2.41	1.45	1.50
38	12	315	A86	C-C1	2.41	1.55	1.50
27	33	311	CLA	MG-NB	-2.41	2.01	2.05
27	11	303	CLA	CMD-C2D	-2.41	1.45	1.50
27	d	401	CLA	C1D-ND	2.41	1.41	1.37
38	14	313	A86	C-C1	2.41	1.55	1.50
27	b	607	CLA	MG-ND	-2.41	2.01	2.05
38	33	313	A86	C-C1	2.41	1.55	1.50
27	c	512	CLA	CMB-C2B	-2.41	1.45	1.50
27	32	307	CLA	C1B-C2B	2.41	1.48	1.43
27	11	305	CLA	MG-NB	-2.41	2.01	2.05
27	31	309	CLA	CMD-C2D	-2.41	1.45	1.50
37	f	102	HEM	FE-ND	2.41	2.02	1.94
27	12	306	CLA	C1B-C2B	2.41	1.48	1.43
27	11	308	CLA	MG-NB	-2.41	2.01	2.05
27	c	503	CLA	CAC-C3C	-2.41	1.44	1.51
27	13	311	CLA	MG-NB	-2.41	2.01	2.05
27	B	612	CLA	CMB-C2B	-2.41	1.45	1.50
30	A	406	SQD	O2-C2	-2.41	1.37	1.43
27	C	502	CLA	CMC-C2C	-2.41	1.45	1.50
38	32	317	A86	C26-C27	2.41	1.41	1.35
27	31	303	CLA	C1B-C2B	2.41	1.48	1.43
27	c	506	CLA	CMB-C2B	-2.41	1.45	1.50
38	12	315	A86	C14-C15	2.41	1.57	1.52
38	31	313	A86	C24-C1	2.41	1.51	1.46
27	W	102	CLA	CMD-C2D	-2.41	1.45	1.50
38	13	315	A86	C26-C27	2.41	1.41	1.35
27	11	302	CLA	C1B-C2B	2.41	1.48	1.43
27	B	607	CLA	CMC-C2C	-2.40	1.45	1.50
27	34	306	CLA	CMD-C2D	-2.40	1.45	1.50
27	C	512	CLA	CMB-C2B	-2.40	1.45	1.50
27	b	607	CLA	CMC-C2C	-2.40	1.45	1.50
27	c	502	CLA	CMC-C2C	-2.40	1.45	1.50
27	c	504	CLA	CMC-C2C	-2.40	1.45	1.50
27	32	313	CLA	MG-NB	-2.40	2.01	2.05
38	32	315	A86	C14-C15	2.40	1.57	1.52
27	14	311	CLA	CMD-C2D	-2.40	1.45	1.50
27	33	305	CLA	CMD-C2D	-2.40	1.45	1.50
27	d	402	CLA	MG-ND	-2.40	2.01	2.05
27	14	304	CLA	C1B-C2B	2.40	1.48	1.43
27	14	310	CLA	MG-NB	-2.40	2.01	2.05
27	B	608	CLA	C1D-ND	2.40	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	11	309	CLA	CMD-C2D	-2.40	1.45	1.50
27	12	307	CLA	CMD-C2D	-2.40	1.45	1.50
27	c	514	CLA	MG-ND	-2.40	2.01	2.05
27	C	512	CLA	CMC-C2C	-2.40	1.45	1.50
35	c	518	DGD	O1G-C1G	-2.40	1.39	1.45
27	32	313	CLA	CMD-C2D	-2.40	1.45	1.50
27	34	312	CLA	MG-NB	-2.40	2.01	2.05
38	12	304	A86	C2-C1	2.40	1.41	1.35
38	32	317	A86	C24-C1	2.40	1.51	1.46
27	w	102	CLA	CMD-C2D	-2.40	1.45	1.50
27	D	402	CLA	MG-ND	-2.40	2.01	2.05
27	14	305	CLA	C1B-C2B	2.40	1.48	1.43
27	z	102	CLA	C1B-C2B	2.40	1.48	1.43
27	12	313	CLA	CMD-C2D	-2.39	1.45	1.50
27	C	514	CLA	MG-ND	-2.39	2.01	2.05
38	32	304	A86	C2-C1	2.39	1.41	1.35
27	C	504	CLA	C1B-C2B	2.39	1.48	1.43
27	34	306	CLA	C1B-C2B	2.39	1.48	1.43
35	C	518	DGD	O1G-C1G	-2.39	1.39	1.45
38	33	315	A86	C26-C27	2.39	1.41	1.35
27	B	614	CLA	C1B-C2B	2.39	1.48	1.43
27	b	604	CLA	CHC-C4B	-2.39	1.34	1.39
27	c	514	CLA	CMD-C2D	-2.39	1.45	1.50
27	d	402	CLA	CMD-C2D	-2.39	1.45	1.50
27	33	310	CLA	MG-NB	-2.39	2.01	2.05
33	12	301	LMG	O4-C4	-2.39	1.37	1.43
38	14	313	A86	O4-C34	-2.39	1.41	1.46
27	12	307	CLA	C1B-C2B	2.39	1.48	1.43
27	M	102	CLA	CMC-C2C	-2.39	1.45	1.50
27	Z	102	CLA	C1B-C2B	2.39	1.48	1.43
38	32	314	A86	C14-C15	2.39	1.57	1.52
38	11	316	A86	C2-C1	2.39	1.41	1.35
27	b	604	CLA	CMC-C2C	-2.39	1.45	1.50
27	31	303	CLA	CMD-C2D	-2.39	1.45	1.50
27	b	610	CLA	C1D-ND	2.39	1.41	1.37
27	B	604	CLA	CHC-C4B	-2.39	1.34	1.39
27	33	311	CLA	CMD-C2D	-2.39	1.45	1.50
38	31	310	A86	C14-C15	2.39	1.57	1.52
38	34	316	A86	C26-C27	2.39	1.41	1.35
27	B	602	CLA	CMB-C2B	-2.39	1.45	1.50
27	32	312	CLA	MG-NB	-2.39	2.01	2.05
38	34	303	A86	C2-C1	2.39	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	33	316	A86	C14-C15	2.38	1.57	1.52
27	33	305	CLA	C1B-C2B	2.38	1.48	1.43
27	D	406	CLA	MG-ND	-2.38	2.01	2.05
27	b	611	CLA	MG-ND	-2.38	2.01	2.05
27	13	305	CLA	C1B-C2B	2.38	1.48	1.43
27	13	304	CLA	C1B-C2B	2.38	1.48	1.43
38	12	315	A86	O4-C34	-2.38	1.41	1.46
27	M	102	CLA	C1D-ND	2.38	1.41	1.37
27	A	402	CLA	CMB-C2B	-2.38	1.45	1.50
38	13	302	A86	C2-C1	2.38	1.41	1.35
30	a	406	SQD	O2-C2	-2.38	1.37	1.43
27	c	512	CLA	CMC-C2C	-2.38	1.45	1.50
27	c	507	CLA	C1B-NB	-2.38	1.34	1.37
38	13	313	A86	O4-C34	-2.38	1.41	1.46
27	C	504	CLA	CMC-C2C	-2.38	1.45	1.50
27	D	406	CLA	CMC-C2C	-2.38	1.45	1.50
27	12	310	CLA	CMD-C2D	-2.38	1.45	1.50
38	31	316	A86	C2-C1	2.37	1.41	1.35
38	32	315	A86	O4-C34	-2.37	1.41	1.46
27	b	602	CLA	CMB-C2B	-2.37	1.45	1.50
33	b	618	LMG	O1-C7	-2.37	1.39	1.43
27	12	312	CLA	MG-NB	-2.37	2.01	2.05
27	13	309	CLA	CMC-C2C	-2.37	1.45	1.50
27	14	305	CLA	CMD-C2D	-2.37	1.45	1.50
38	33	312	A86	C14-C15	2.37	1.57	1.52
27	m	101	CLA	CMC-C2C	-2.37	1.45	1.50
27	11	306	CLA	CMD-C2D	-2.37	1.45	1.50
27	Z	102	CLA	C4B-NB	2.37	1.41	1.37
27	c	504	CLA	C1B-C2B	2.37	1.48	1.43
27	b	601	CLA	CMD-C2D	-2.37	1.45	1.50
27	32	307	CLA	CMD-C2D	-2.37	1.45	1.50
27	33	306	CLA	C1B-NB	-2.37	1.34	1.37
27	B	614	CLA	CMB-C2B	-2.37	1.45	1.50
27	b	602	CLA	CMD-C2D	-2.37	1.45	1.50
27	B	608	CLA	MG-NB	-2.37	2.01	2.05
38	14	316	A86	C24-C1	2.37	1.51	1.46
27	13	310	CLA	C1B-C2B	2.36	1.48	1.43
27	33	309	CLA	CMC-C2C	-2.36	1.45	1.50
27	B	602	CLA	CMD-C2D	-2.36	1.45	1.50
27	W	103	CLA	C1B-C2B	2.36	1.48	1.43
27	c	502	CLA	C1B-C2B	2.36	1.48	1.43
27	b	609	CLA	C4B-NB	2.36	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	13	311	CLA	CMD-C2D	-2.36	1.45	1.50
27	34	310	CLA	CMC-C2C	-2.36	1.45	1.50
27	12	312	CLA	C1B-C2B	2.36	1.48	1.43
27	c	502	CLA	MG-ND	-2.36	2.01	2.05
27	13	310	CLA	MG-NB	-2.36	2.01	2.05
38	33	313	A86	O4-C34	-2.36	1.41	1.46
27	32	308	CLA	C1B-NB	-2.36	1.34	1.37
38	13	316	A86	C14-C15	2.36	1.57	1.52
27	31	306	CLA	CMD-C2D	-2.36	1.45	1.50
27	34	311	CLA	C1B-C2B	2.36	1.48	1.43
27	B	611	CLA	MG-ND	-2.36	2.01	2.05
27	b	607	CLA	C1B-NB	-2.36	1.34	1.37
38	34	313	A86	C14-C15	2.36	1.57	1.52
37	f	102	HEM	C2A-C3A	-2.36	1.32	1.38
27	34	310	CLA	MG-ND	-2.36	2.01	2.05
27	14	310	CLA	C1B-C2B	2.36	1.48	1.43
27	a	402	CLA	CMB-C2B	-2.36	1.45	1.50
27	31	307	CLA	CMB-C2B	-2.36	1.45	1.50
27	33	308	CLA	CMD-C2D	-2.36	1.45	1.50
38	34	314	A86	O4-C34	-2.36	1.41	1.46
27	b	601	CLA	CMC-C2C	-2.35	1.45	1.50
38	13	312	A86	C14-C15	2.35	1.57	1.52
27	34	311	CLA	MG-NB	-2.35	2.01	2.05
27	12	308	CLA	C1B-NB	-2.35	1.34	1.37
27	34	312	CLA	CMD-C2D	-2.35	1.45	1.50
38	33	302	A86	C2-C1	2.35	1.41	1.35
27	31	308	CLA	MG-NB	-2.35	2.01	2.05
27	34	305	CLA	C1B-C2B	2.35	1.48	1.43
27	12	311	CLA	CMC-C2C	-2.35	1.45	1.50
27	d	406	CLA	CMC-C2C	-2.35	1.45	1.50
27	13	308	CLA	CMD-C2D	-2.35	1.45	1.50
27	c	505	CLA	C1D-ND	2.35	1.41	1.37
38	11	311	A86	O4-C34	-2.35	1.41	1.46
27	d	406	CLA	MG-ND	-2.35	2.01	2.05
27	33	306	CLA	C4B-NB	2.35	1.40	1.37
38	34	301	A86	C24-C1	2.35	1.51	1.46
38	14	312	A86	C14-C15	2.35	1.57	1.52
27	31	308	CLA	C1B-C2B	2.35	1.48	1.43
27	B	608	CLA	CMC-C2C	-2.35	1.46	1.50
27	11	304	CLA	C1B-NB	-2.35	1.34	1.37
27	b	614	CLA	CMB-C2B	-2.35	1.46	1.50
38	12	314	A86	C14-C15	2.35	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	601	CLA	CMC-C2C	-2.35	1.46	1.50
27	14	309	CLA	CMC-C2C	-2.35	1.46	1.50
27	31	305	CLA	C1B-C2B	2.35	1.48	1.43
27	W	102	CLA	C4B-NB	2.35	1.40	1.37
27	13	305	CLA	CMD-C2D	-2.35	1.46	1.50
38	32	318	A86	C14-C15	2.35	1.57	1.52
27	d	401	CLA	C1B-NB	-2.35	1.34	1.37
27	32	312	CLA	C1B-C2B	2.35	1.48	1.43
27	33	307	CLA	C1B-C2B	2.35	1.48	1.43
27	B	605	CLA	CMC-C2C	-2.35	1.46	1.50
27	C	504	CLA	CMB-C2B	-2.35	1.46	1.50
27	C	513	CLA	CMB-C2B	-2.35	1.46	1.50
27	32	311	CLA	CMC-C2C	-2.35	1.46	1.50
38	31	311	A86	O4-C34	-2.35	1.41	1.46
27	14	308	CLA	CMD-C2D	-2.35	1.46	1.50
27	z	102	CLA	C4B-NB	2.35	1.40	1.37
27	D	401	CLA	C1D-ND	2.34	1.40	1.37
27	D	406	CLA	C1B-NB	-2.34	1.34	1.37
38	32	318	A86	C2-C1	2.34	1.41	1.35
38	14	301	A86	C24-C1	2.34	1.51	1.46
27	11	307	CLA	CMC-C2C	-2.34	1.46	1.50
27	14	309	CLA	CMB-C2B	-2.34	1.46	1.50
27	C	502	CLA	MG-ND	-2.34	2.01	2.05
27	31	307	CLA	MG-ND	-2.34	2.01	2.05
27	c	513	CLA	CMB-C2B	-2.34	1.46	1.50
33	m	102	LMG	O4-C4	-2.34	1.37	1.43
37	E	101	HEM	C2A-C3A	-2.34	1.32	1.38
27	B	607	CLA	C1B-NB	-2.34	1.34	1.37
38	33	316	A86	C2-C1	2.34	1.41	1.35
27	11	315	CLA	C1B-C2B	2.34	1.48	1.43
27	D	401	CLA	C1B-NB	-2.34	1.34	1.37
27	31	304	CLA	C4B-NB	2.34	1.40	1.37
27	C	511	CLA	CAA-C2A	-2.34	1.49	1.54
27	b	608	CLA	MG-NB	-2.34	2.01	2.05
27	c	505	CLA	MG-ND	-2.34	2.01	2.05
27	34	306	CLA	CMC-C2C	-2.34	1.46	1.50
27	34	309	CLA	CMD-C2D	-2.34	1.46	1.50
27	34	310	CLA	CMB-C2B	-2.34	1.46	1.50
38	11	310	A86	C14-C15	2.34	1.57	1.52
27	34	308	CLA	C1B-C2B	2.34	1.48	1.43
27	w	103	CLA	C1B-C2B	2.34	1.48	1.43
27	D	405	CLA	CMB-C2B	-2.34	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d	406	CLA	C1B-NB	-2.34	1.34	1.37
27	32	309	CLA	C1B-C2B	2.34	1.48	1.43
27	14	302	CLA	C1B-C2B	2.34	1.48	1.43
38	11	314	A86	C14-C15	2.34	1.57	1.52
27	32	312	CLA	C4B-NB	2.33	1.40	1.37
38	33	316	A86	C24-C1	2.33	1.50	1.46
27	31	304	CLA	C1B-NB	-2.33	1.34	1.37
27	c	513	CLA	CMC-C2C	-2.33	1.46	1.50
27	33	309	CLA	CMB-C2B	-2.33	1.46	1.50
27	13	309	CLA	CMB-C2B	-2.33	1.46	1.50
27	32	311	CLA	CMB-C2B	-2.33	1.46	1.50
38	34	301	A86	C14-C15	2.33	1.57	1.52
27	13	309	CLA	MG-ND	-2.33	2.01	2.05
27	b	622	CLA	C4B-NB	2.33	1.40	1.37
27	11	307	CLA	CMB-C2B	-2.33	1.46	1.50
27	11	305	CLA	C1B-C2B	2.33	1.48	1.43
27	32	303	CLA	C1B-C2B	2.33	1.48	1.43
38	14	301	A86	C14-C15	2.33	1.57	1.52
27	32	310	CLA	CMD-C2D	-2.33	1.46	1.50
33	b	618	LMG	O8-C9	-2.33	1.40	1.45
27	12	311	CLA	MG-ND	-2.33	2.01	2.05
27	B	614	CLA	C1B-NB	-2.33	1.34	1.37
27	B	622	CLA	C4B-NB	2.33	1.40	1.37
27	12	309	CLA	C1B-C2B	2.33	1.48	1.43
33	12	301	LMG	O6-C5	-2.33	1.38	1.44
38	31	314	A86	C24-C1	2.33	1.50	1.46
38	13	316	A86	C2-C1	2.33	1.41	1.35
27	32	311	CLA	MG-ND	-2.33	2.01	2.05
27	w	103	CLA	MG-NB	-2.33	2.01	2.05
27	13	306	CLA	C4B-NB	2.32	1.40	1.37
27	13	307	CLA	C1B-C2B	2.32	1.48	1.43
27	b	608	CLA	CMC-C2C	-2.32	1.46	1.50
27	c	510	CLA	C1D-ND	2.32	1.40	1.37
27	A	402	CLA	MG-ND	-2.32	2.01	2.05
27	a	402	CLA	MG-ND	-2.32	2.01	2.05
27	32	308	CLA	C4B-NB	2.32	1.40	1.37
27	33	309	CLA	MG-ND	-2.32	2.01	2.05
27	b	614	CLA	C1B-C2B	2.32	1.48	1.43
27	11	308	CLA	C1B-C2B	2.32	1.48	1.43
27	c	512	CLA	CMD-C2D	-2.32	1.46	1.50
27	12	311	CLA	CMB-C2B	-2.32	1.46	1.50
27	31	307	CLA	CMC-C2C	-2.32	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	622	CLA	C1B-NB	-2.32	1.34	1.37
27	C	502	CLA	C1B-C2B	2.32	1.48	1.43
27	c	506	CLA	MG-ND	-2.32	2.01	2.05
27	c	502	CLA	CMB-C2B	-2.32	1.46	1.50
27	14	307	CLA	C1B-C2B	2.32	1.48	1.43
38	12	315	A86	C24-C1	2.32	1.50	1.46
27	b	606	CLA	CAC-C3C	-2.32	1.45	1.51
38	32	318	A86	C24-C1	2.32	1.50	1.46
27	13	310	CLA	C4B-NB	2.32	1.40	1.37
27	B	606	CLA	CAC-C3C	-2.32	1.45	1.51
27	b	605	CLA	CMC-C2C	-2.32	1.46	1.50
38	13	315	A86	C2-C1	2.32	1.41	1.35
27	33	301	CLA	C1B-C2B	2.32	1.48	1.43
38	11	314	A86	C2-C1	2.32	1.41	1.35
38	31	314	A86	C2-C1	2.32	1.41	1.35
27	c	504	CLA	CMB-C2B	-2.32	1.46	1.50
27	33	310	CLA	C1B-C2B	2.32	1.48	1.43
27	B	609	CLA	CMC-C2C	-2.31	1.46	1.50
27	C	507	CLA	C1B-NB	-2.31	1.34	1.37
27	c	512	CLA	C1B-NB	-2.31	1.34	1.37
27	C	512	CLA	CMD-C2D	-2.31	1.46	1.50
38	11	313	A86	C2-C1	2.31	1.41	1.35
27	c	511	CLA	CAA-C2A	-2.31	1.49	1.54
38	33	315	A86	C2-C1	2.31	1.41	1.35
27	C	510	CLA	C1D-ND	2.31	1.40	1.37
35	c	517	DGD	O2G-C2G	-2.31	1.41	1.46
27	d	406	CLA	C1D-ND	2.31	1.40	1.37
27	13	306	CLA	C1B-NB	-2.31	1.34	1.37
27	B	608	CLA	C3B-C4B	2.31	1.49	1.42
27	C	513	CLA	CMC-C2C	-2.31	1.46	1.50
27	W	103	CLA	MG-NB	-2.31	2.01	2.05
27	34	302	CLA	C1B-C2B	2.31	1.48	1.43
38	11	311	A86	C24-C1	2.31	1.50	1.46
27	b	601	CLA	MG-ND	-2.31	2.01	2.05
38	14	316	A86	C14-C15	2.31	1.57	1.52
38	14	313	A86	C24-C1	2.31	1.50	1.46
33	M	103	LMG	O4-C4	-2.31	1.37	1.43
27	12	303	CLA	C1B-C2B	2.31	1.48	1.43
27	b	614	CLA	C1B-NB	-2.31	1.34	1.37
27	C	508	CLA	CHC-C4B	-2.30	1.34	1.39
38	13	316	A86	C24-C1	2.30	1.50	1.46
27	b	609	CLA	CMC-C2C	-2.30	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	406	CLA	C1D-ND	2.30	1.40	1.37
27	12	303	CLA	CMB-C2B	-2.30	1.46	1.50
35	C	517	DGD	O2G-C2G	-2.30	1.41	1.46
38	13	315	A86	O4-C34	-2.30	1.41	1.46
27	b	605	CLA	C4B-NB	2.30	1.40	1.37
27	11	308	CLA	C4B-NB	2.30	1.40	1.37
27	C	512	CLA	C1B-NB	-2.30	1.34	1.37
38	34	314	A86	C24-C1	2.30	1.50	1.46
38	13	302	A86	C14-C15	2.30	1.57	1.52
38	11	314	A86	C24-C1	2.30	1.50	1.46
38	32	304	A86	C14-C15	2.30	1.57	1.52
27	14	306	CLA	C1B-NB	-2.30	1.34	1.37
27	b	622	CLA	C1B-NB	-2.30	1.34	1.37
27	34	307	CLA	C1B-NB	-2.30	1.34	1.37
27	14	303	CLA	CMD-C2D	-2.30	1.46	1.50
27	11	303	CLA	CMC-C2C	-2.30	1.46	1.50
38	33	313	A86	C24-C1	2.30	1.50	1.46
27	C	506	CLA	MG-ND	-2.30	2.01	2.05
27	b	608	CLA	C3B-C4B	2.30	1.49	1.42
27	c	508	CLA	CHC-C4B	-2.30	1.34	1.39
27	C	502	CLA	C1B-NB	-2.30	1.34	1.37
27	31	315	CLA	C1B-C2B	2.29	1.48	1.43
38	14	301	A86	C2-C1	2.29	1.41	1.35
38	33	315	A86	O4-C34	-2.29	1.41	1.46
27	12	307	CLA	C4B-NB	2.29	1.40	1.37
27	12	308	CLA	C4B-NB	2.29	1.40	1.37
38	32	317	A86	O4-C34	-2.29	1.41	1.46
38	11	316	A86	C14-C15	2.29	1.57	1.52
27	12	305	CLA	C4B-NB	2.29	1.40	1.37
38	31	311	A86	C2-C1	2.29	1.41	1.35
27	34	305	CLA	C4B-NB	2.29	1.40	1.37
27	B	622	CLA	CMC-C2C	-2.29	1.46	1.50
27	33	305	CLA	C4B-NB	2.29	1.40	1.37
38	32	317	A86	C2-C1	2.29	1.41	1.35
33	B	618	LMG	O8-C9	-2.29	1.40	1.45
38	14	315	A86	C2-C1	2.29	1.41	1.35
27	14	304	CLA	C4B-NB	2.29	1.40	1.37
38	13	317	A86	O4-C34	-2.29	1.41	1.46
27	C	502	CLA	CMB-C2B	-2.29	1.46	1.50
27	11	301	CLA	CMD-C2D	-2.29	1.46	1.50
27	13	305	CLA	CMC-C2C	-2.29	1.46	1.50
36	d	404	PL9	C36-C34	-2.29	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	34	301	A86	C2-C1	2.29	1.41	1.35
38	31	314	A86	C14-C15	2.29	1.57	1.52
27	w	102	CLA	C4B-NB	2.29	1.40	1.37
27	31	308	CLA	C4B-NB	2.29	1.40	1.37
27	13	303	CLA	CMD-C2D	-2.29	1.46	1.50
38	31	313	A86	O4-C34	-2.28	1.41	1.46
27	d	405	CLA	CMB-C2B	-2.28	1.46	1.50
27	31	303	CLA	CMC-C2C	-2.28	1.46	1.50
27	31	307	CLA	C4B-NB	2.28	1.40	1.37
27	33	303	CLA	C4B-NB	2.28	1.40	1.37
27	14	309	CLA	MG-ND	-2.28	2.01	2.05
27	13	301	CLA	C1B-C2B	2.28	1.48	1.43
27	12	307	CLA	CMC-C2C	-2.28	1.46	1.50
27	12	305	CLA	CMD-C2D	-2.28	1.46	1.50
27	c	502	CLA	C1B-NB	-2.28	1.34	1.37
27	W	102	CLA	MG-ND	-2.28	2.01	2.05
27	c	505	CLA	CHC-C4B	-2.28	1.34	1.39
27	11	315	CLA	CMB-C2B	-2.28	1.46	1.50
27	32	306	CLA	C4B-NB	2.28	1.40	1.37
27	w	102	CLA	MG-ND	-2.28	2.01	2.05
27	c	508	CLA	CAC-C3C	-2.28	1.45	1.51
38	33	302	A86	C14-C15	2.28	1.57	1.52
38	32	315	A86	C24-C1	2.28	1.50	1.46
27	A	402	CLA	C1B-C2B	2.28	1.48	1.43
38	13	317	A86	C14-C15	2.28	1.57	1.52
27	32	311	CLA	C4B-NB	2.27	1.40	1.37
38	12	317	A86	C2-C1	2.27	1.41	1.35
30	b	620	SQD	O47-C45	-2.27	1.41	1.46
38	31	316	A86	O4-C34	-2.27	1.41	1.46
27	33	303	CLA	CMD-C2D	-2.27	1.46	1.50
27	34	311	CLA	CMB-C2B	-2.27	1.46	1.50
27	11	307	CLA	MG-ND	-2.27	2.01	2.05
27	12	312	CLA	C4B-NB	2.27	1.40	1.37
33	B	619	LMG	O7-C8	-2.27	1.41	1.46
27	11	307	CLA	C4B-NB	2.27	1.40	1.37
38	14	312	A86	C26-C27	2.27	1.41	1.35
27	14	305	CLA	CMC-C2C	-2.27	1.46	1.50
27	14	310	CLA	CMB-C2B	-2.27	1.46	1.50
27	32	312	CLA	CMB-C2B	-2.27	1.46	1.50
27	D	405	CLA	C1B-NB	-2.27	1.34	1.37
27	34	307	CLA	C4B-NB	2.27	1.40	1.37
27	c	513	CLA	MG-ND	-2.27	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	13	313	A86	C2-C1	2.27	1.41	1.35
27	33	305	CLA	CMC-C2C	-2.27	1.46	1.50
38	31	313	A86	C2-C1	2.27	1.41	1.35
38	34	316	A86	C2-C1	2.27	1.41	1.35
27	33	301	CLA	CMB-C2B	-2.27	1.46	1.50
38	34	303	A86	O4-C34	-2.27	1.41	1.46
27	33	310	CLA	C4B-NB	2.27	1.40	1.37
38	14	316	A86	C2-C1	2.27	1.41	1.35
38	12	304	A86	C14-C15	2.27	1.57	1.52
38	11	313	A86	O4-C34	-2.27	1.41	1.46
27	32	305	CLA	CMD-C2D	-2.27	1.46	1.50
38	31	316	A86	C14-C15	2.27	1.57	1.52
38	32	315	A86	C2-C1	2.27	1.41	1.35
27	31	302	CLA	C4B-NB	2.27	1.40	1.37
27	B	601	CLA	MG-ND	-2.27	2.01	2.05
27	11	304	CLA	C4B-NB	2.27	1.40	1.37
38	31	311	A86	C24-C1	2.27	1.50	1.46
27	12	311	CLA	C4B-NB	2.26	1.40	1.37
27	13	301	CLA	CMB-C2B	-2.26	1.46	1.50
27	B	615	CLA	C3B-C4B	2.26	1.49	1.42
38	11	311	A86	C2-C1	2.26	1.41	1.35
38	14	313	A86	C2-C1	2.26	1.41	1.35
38	12	317	A86	O4-C34	-2.26	1.41	1.46
27	d	405	CLA	CAA-C2A	-2.26	1.50	1.54
27	b	615	CLA	C3B-C4B	2.26	1.49	1.42
27	32	306	CLA	CMC-C2C	-2.26	1.46	1.50
38	32	304	A86	O4-C34	-2.26	1.41	1.46
38	13	313	A86	C24-C1	2.26	1.50	1.46
27	w	102	CLA	C3B-C4B	2.26	1.49	1.42
35	J	101	DGD	O3G-C3G	-2.26	1.39	1.43
38	14	315	A86	O4-C34	-2.26	1.41	1.46
27	B	602	CLA	C4B-NB	2.26	1.40	1.37
33	d	408	LMG	O4-C4	-2.26	1.37	1.43
27	C	508	CLA	CAC-C3C	-2.26	1.45	1.51
27	12	306	CLA	C4B-NB	2.26	1.40	1.37
38	13	312	A86	C26-C27	2.26	1.41	1.35
27	32	303	CLA	CMB-C2B	-2.26	1.46	1.50
27	a	402	CLA	C1B-C2B	2.26	1.48	1.43
38	34	314	A86	C2-C1	2.26	1.41	1.35
29	F	101	BCR	C33-C5	-2.26	1.47	1.50
27	b	622	CLA	CMC-C2C	-2.26	1.46	1.50
27	C	513	CLA	MG-ND	-2.26	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	b	619	LMG	O7-C8	-2.26	1.41	1.46
27	D	405	CLA	CAA-C2A	-2.26	1.50	1.54
27	c	513	CLA	C4B-NB	2.26	1.40	1.37
27	34	304	CLA	CMD-C2D	-2.26	1.46	1.50
27	a	404	CLA	CAB-C3B	-2.26	1.41	1.47
27	b	602	CLA	C4B-NB	2.26	1.40	1.37
27	31	301	CLA	C4B-NB	2.26	1.40	1.37
27	31	301	CLA	CMD-C2D	-2.26	1.46	1.50
27	b	606	CLA	C3B-C4B	2.26	1.49	1.42
27	14	302	CLA	CMB-C2B	-2.25	1.46	1.50
27	14	309	CLA	C4B-NB	2.25	1.40	1.37
27	m	101	CLA	MG-ND	-2.25	2.01	2.05
27	12	303	CLA	C3B-C4B	2.25	1.49	1.42
27	13	305	CLA	C4B-NB	2.25	1.40	1.37
35	j	101	DGD	O3G-C3G	-2.25	1.39	1.43
27	32	307	CLA	CMC-C2C	-2.25	1.46	1.50
27	13	304	CLA	C4B-NB	2.25	1.40	1.37
27	D	402	CLA	CMC-C2C	-2.25	1.46	1.50
38	12	314	A86	C24-C1	2.25	1.50	1.46
27	32	305	CLA	C4B-NB	2.25	1.40	1.37
27	33	309	CLA	C4B-NB	2.25	1.40	1.37
38	12	314	A86	C26-C27	2.25	1.41	1.35
27	34	302	CLA	CMB-C2B	-2.25	1.46	1.50
27	14	305	CLA	C4B-NB	2.25	1.40	1.37
27	14	306	CLA	C4B-NB	2.25	1.40	1.37
38	33	312	A86	C24-C1	2.25	1.50	1.46
27	11	303	CLA	C4B-NB	2.25	1.40	1.37
27	31	303	CLA	C4B-NB	2.25	1.40	1.37
38	11	310	A86	C2-C1	2.25	1.41	1.35
27	d	402	CLA	CMC-C2C	-2.25	1.46	1.50
27	32	303	CLA	CMC-C2C	-2.25	1.46	1.50
27	d	405	CLA	C1B-NB	-2.25	1.34	1.37
27	14	310	CLA	C4B-NB	2.25	1.40	1.37
27	33	301	CLA	CMC-C2C	-2.25	1.46	1.50
30	B	620	SQD	O3-C3	-2.25	1.37	1.43
27	B	605	CLA	C4B-NB	2.25	1.40	1.37
27	A	404	CLA	CAB-C3B	-2.25	1.41	1.47
27	14	302	CLA	CMC-C2C	-2.25	1.46	1.50
38	12	315	A86	C2-C1	2.25	1.41	1.35
27	11	315	CLA	C3B-C4B	2.25	1.49	1.42
27	32	303	CLA	C3B-C4B	2.25	1.49	1.42
27	11	302	CLA	C4B-NB	2.25	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	34	316	A86	O4-C34	-2.25	1.41	1.46
38	34	313	A86	C24-C1	2.24	1.50	1.46
38	32	314	A86	C26-C27	2.24	1.41	1.35
27	32	307	CLA	C4B-NB	2.24	1.40	1.37
27	w	103	CLA	C3B-C4B	2.24	1.49	1.42
27	31	315	CLA	C3B-C4B	2.24	1.49	1.42
27	11	315	CLA	CMC-C2C	-2.24	1.46	1.50
38	34	303	A86	C14-C15	2.24	1.57	1.52
27	11	303	CLA	MG-ND	-2.24	2.01	2.05
28	d	403	PHO	C3B-C2B	-2.24	1.37	1.40
38	32	314	A86	C24-C1	2.24	1.50	1.46
38	32	314	A86	C2-C1	2.24	1.41	1.35
27	C	507	CLA	C1D-ND	2.24	1.40	1.37
27	c	507	CLA	C1D-ND	2.24	1.40	1.37
27	31	315	CLA	CMB-C2B	-2.24	1.46	1.50
27	C	505	CLA	CHC-C4B	-2.24	1.34	1.39
30	B	620	SQD	O47-C45	-2.24	1.41	1.46
27	12	312	CLA	CMB-C2B	-2.24	1.46	1.50
27	13	301	CLA	C3B-C4B	2.24	1.49	1.42
27	14	302	CLA	C3B-C4B	2.24	1.49	1.42
29	f	101	BCR	C33-C5	-2.24	1.47	1.50
38	13	302	A86	O4-C34	-2.24	1.41	1.46
27	34	305	CLA	CMC-C2C	-2.24	1.46	1.50
27	b	609	CLA	C1B-C2B	2.24	1.48	1.43
27	M	102	CLA	MG-ND	-2.24	2.01	2.05
27	31	315	CLA	CMC-C2C	-2.24	1.46	1.50
27	13	309	CLA	C4B-NB	2.24	1.40	1.37
38	11	310	A86	C24-C1	2.23	1.50	1.46
27	13	301	CLA	CMC-C2C	-2.23	1.46	1.50
28	D	403	PHO	C3D-CAD	-2.23	1.43	1.47
38	31	310	A86	C26-C27	2.23	1.41	1.35
27	33	301	CLA	C3B-C4B	2.23	1.49	1.42
27	11	308	CLA	CMB-C2B	-2.23	1.46	1.50
27	31	308	CLA	CMB-C2B	-2.23	1.46	1.50
38	33	312	A86	C2-C1	2.23	1.41	1.35
27	12	303	CLA	CMC-C2C	-2.23	1.46	1.50
27	W	102	CLA	C3B-C4B	2.23	1.49	1.42
38	34	313	A86	C2-C1	2.23	1.41	1.35
27	14	304	CLA	CMC-C2C	-2.23	1.46	1.50
38	13	312	A86	C2-C1	2.23	1.41	1.35
38	33	313	A86	C2-C1	2.23	1.41	1.35
38	12	304	A86	O4-C34	-2.23	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	11	310	A86	C26-C27	2.23	1.41	1.35
27	12	305	CLA	CMB-C2B	-2.23	1.46	1.50
27	13	310	CLA	CMB-C2B	-2.23	1.46	1.50
27	31	302	CLA	CMC-C2C	-2.23	1.46	1.50
38	34	313	A86	C26-C27	2.23	1.41	1.35
27	B	606	CLA	C3B-C4B	2.23	1.49	1.42
29	z	101	BCR	C33-C5	-2.23	1.47	1.50
27	34	308	CLA	CMB-C2B	-2.23	1.46	1.50
36	D	404	PL9	C36-C34	-2.23	1.46	1.51
27	c	514	CLA	CMB-C2B	-2.23	1.46	1.50
38	11	316	A86	O4-C34	-2.23	1.41	1.46
27	12	307	CLA	CMB-C2B	-2.23	1.46	1.50
27	B	609	CLA	C1B-C2B	2.23	1.48	1.43
27	34	306	CLA	C4B-NB	2.23	1.40	1.37
27	31	301	CLA	CMB-C2B	-2.23	1.46	1.50
30	B	620	SQD	O2-C2	-2.22	1.37	1.43
27	31	303	CLA	CMB-C2B	-2.22	1.46	1.50
36	D	407	PL9	C15-C14	-2.22	1.45	1.50
27	14	303	CLA	C4B-NB	2.22	1.40	1.37
27	b	614	CLA	MG-ND	-2.22	2.01	2.05
27	11	304	CLA	C3B-C4B	2.22	1.49	1.42
27	31	304	CLA	C3B-C4B	2.22	1.49	1.42
27	13	305	CLA	CMB-C2B	-2.22	1.46	1.50
27	31	305	CLA	CMD-C2D	-2.22	1.46	1.50
27	B	609	CLA	MG-ND	-2.22	2.01	2.05
27	32	305	CLA	CMB-C2B	-2.22	1.46	1.50
27	14	305	CLA	MG-ND	-2.22	2.01	2.05
27	b	613	CLA	CMB-C2B	-2.22	1.46	1.50
33	32	301	LMG	O4-C4	-2.22	1.37	1.43
27	b	606	CLA	MG-ND	-2.22	2.01	2.05
30	b	620	SQD	O3-C3	-2.22	1.37	1.43
28	D	403	PHO	C3B-C2B	-2.22	1.37	1.40
27	z	102	CLA	CMB-C2B	-2.22	1.46	1.50
27	12	306	CLA	CMC-C2C	-2.22	1.46	1.50
27	14	303	CLA	CMB-C2B	-2.22	1.46	1.50
27	33	307	CLA	CMD-C2D	-2.22	1.46	1.50
27	13	307	CLA	CMD-C2D	-2.22	1.46	1.50
27	11	303	CLA	CMB-C2B	-2.22	1.46	1.50
27	13	305	CLA	MG-ND	-2.22	2.01	2.05
27	11	301	CLA	C4B-NB	2.22	1.40	1.37
27	B	613	CLA	CMB-C2B	-2.22	1.46	1.50
33	D	408	LMG	O4-C4	-2.22	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	11	301	CLA	CMB-C2B	-2.22	1.46	1.50
27	13	304	CLA	CMC-C2C	-2.22	1.46	1.50
27	34	302	CLA	C3B-C4B	2.22	1.49	1.42
27	c	512	CLA	C4B-NB	2.22	1.40	1.37
27	C	504	CLA	C4B-NB	2.22	1.40	1.37
38	33	302	A86	O4-C34	-2.22	1.41	1.46
27	B	606	CLA	MG-ND	-2.22	2.01	2.05
27	11	302	CLA	CMC-C2C	-2.22	1.46	1.50
27	12	308	CLA	C3B-C4B	2.22	1.49	1.42
27	12	307	CLA	MG-ND	-2.21	2.01	2.05
27	Z	102	CLA	CMB-C2B	-2.21	1.46	1.50
27	b	609	CLA	MG-ND	-2.21	2.01	2.05
27	W	103	CLA	C3B-C4B	2.21	1.49	1.42
38	13	312	A86	C24-C1	2.21	1.50	1.46
27	C	509	CLA	C1D-ND	2.21	1.40	1.37
27	B	611	CLA	CAC-C3C	-2.21	1.45	1.51
27	D	405	CLA	C1B-C2B	2.21	1.48	1.43
38	31	310	A86	C2-C1	2.21	1.40	1.35
38	33	312	A86	C26-C27	2.21	1.40	1.35
27	b	611	CLA	CAC-C3C	-2.21	1.45	1.51
27	32	307	CLA	CMB-C2B	-2.21	1.46	1.50
27	14	302	CLA	MG-ND	-2.21	2.01	2.05
27	33	306	CLA	C3B-C4B	2.21	1.49	1.42
38	31	310	A86	C24-C1	2.21	1.50	1.46
35	C	517	DGD	O2E-C2E	-2.21	1.37	1.43
36	d	407	PL9	C15-C14	-2.21	1.45	1.50
27	14	306	CLA	C3B-C4B	2.21	1.49	1.42
27	32	307	CLA	MG-ND	-2.21	2.01	2.05
27	13	306	CLA	CMB-C2B	-2.21	1.46	1.50
27	33	303	CLA	CMB-C2B	-2.21	1.46	1.50
30	b	620	SQD	O4-C4	-2.21	1.37	1.43
27	11	302	CLA	MG-ND	-2.21	2.01	2.05
28	d	403	PHO	C3D-CAD	-2.21	1.43	1.47
30	b	620	SQD	O2-C2	-2.21	1.37	1.43
27	33	307	CLA	CMB-C2B	-2.20	1.46	1.50
27	34	304	CLA	C4B-NB	2.20	1.40	1.37
27	34	311	CLA	C4B-NB	2.20	1.40	1.37
27	c	514	CLA	C1B-C2B	2.20	1.48	1.43
27	z	102	CLA	CMC-C2C	-2.20	1.46	1.50
27	34	302	CLA	CMC-C2C	-2.20	1.46	1.50
27	M	102	CLA	C1B-NB	-2.20	1.35	1.37
27	31	303	CLA	MG-ND	-2.20	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	14	312	A86	C2-C1	2.20	1.40	1.35
27	14	305	CLA	CMB-C2B	-2.20	1.46	1.50
29	Z	101	BCR	C33-C5	-2.20	1.47	1.50
27	32	309	CLA	CMD-C2D	-2.20	1.46	1.50
35	c	517	DGD	O2E-C2E	-2.20	1.37	1.43
27	B	614	CLA	MG-ND	-2.20	2.01	2.05
27	33	304	CLA	MG-ND	-2.20	2.01	2.05
27	34	306	CLA	CMB-C2B	-2.20	1.46	1.50
27	34	307	CLA	C3B-C4B	2.20	1.49	1.42
27	13	303	CLA	C4B-NB	2.20	1.40	1.37
29	B	623	BCR	C33-C5	-2.20	1.47	1.50
27	32	308	CLA	C3B-C4B	2.20	1.49	1.42
27	34	310	CLA	C4B-NB	2.20	1.40	1.37
27	12	313	CLA	CMB-C2B	-2.20	1.46	1.50
27	c	504	CLA	C4B-NB	2.20	1.40	1.37
27	13	303	CLA	CMB-C2B	-2.20	1.46	1.50
27	34	307	CLA	CMB-C2B	-2.19	1.46	1.50
27	32	303	CLA	MG-ND	-2.19	2.01	2.05
27	32	309	CLA	CMC-C2C	-2.19	1.46	1.50
27	14	304	CLA	MG-ND	-2.19	2.01	2.05
35	J	101	DGD	O3D-C3D	-2.19	1.37	1.43
29	c	516	BCR	C38-C26	-2.19	1.47	1.50
30	B	620	SQD	O4-C4	-2.19	1.37	1.43
27	13	304	CLA	MG-ND	-2.19	2.01	2.05
27	31	304	CLA	CMB-C2B	-2.19	1.46	1.50
35	j	101	DGD	O6D-C5D	-2.19	1.39	1.44
27	34	304	CLA	CMB-C2B	-2.19	1.46	1.50
27	C	510	CLA	CMA-C3A	-2.19	1.48	1.53
38	14	312	A86	C24-C1	2.19	1.50	1.46
27	33	307	CLA	CMC-C2C	-2.19	1.46	1.50
27	34	312	CLA	CMB-C2B	-2.19	1.46	1.50
27	12	308	CLA	CMB-C2B	-2.19	1.46	1.50
27	11	305	CLA	CMB-C2B	-2.18	1.46	1.50
27	13	307	CLA	CMC-C2C	-2.18	1.46	1.50
39	32	302	LMU	O3'-C3'	2.18	1.48	1.43
27	32	306	CLA	MG-ND	-2.18	2.01	2.05
30	a	406	SQD	O3-C3	-2.18	1.37	1.43
27	C	512	CLA	C4B-NB	2.18	1.40	1.37
27	c	511	CLA	CMB-C2B	-2.18	1.46	1.50
27	11	305	CLA	CMC-C2C	-2.18	1.46	1.50
27	14	306	CLA	CMB-C2B	-2.18	1.46	1.50
27	31	302	CLA	MG-ND	-2.18	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	406	SQD	O3-C3	-2.18	1.37	1.43
27	14	307	CLA	CMD-C2D	-2.18	1.46	1.50
27	31	315	CLA	MG-ND	-2.18	2.01	2.05
30	A	406	SQD	O47-C45	-2.18	1.41	1.46
27	32	306	CLA	CMB-C2B	-2.18	1.46	1.50
27	C	511	CLA	CMB-C2B	-2.18	1.46	1.50
27	32	313	CLA	CMB-C2B	-2.18	1.46	1.50
27	34	308	CLA	CMD-C2D	-2.18	1.46	1.50
27	C	503	CLA	C1B-C2B	2.18	1.48	1.43
38	12	314	A86	C2-C1	2.18	1.40	1.35
27	C	514	CLA	CMB-C2B	-2.18	1.46	1.50
27	31	309	CLA	CMB-C2B	-2.18	1.46	1.50
27	11	304	CLA	CMB-C2B	-2.18	1.46	1.50
27	c	509	CLA	C1D-ND	2.18	1.40	1.37
27	32	313	CLA	C3B-C4B	2.18	1.49	1.42
28	a	403	PHO	CMA-C3A	-2.18	1.49	1.53
27	Z	102	CLA	CMD-C2D	-2.18	1.46	1.50
35	j	101	DGD	O2E-C2E	-2.18	1.37	1.43
27	13	306	CLA	C3B-C4B	2.18	1.49	1.42
27	33	310	CLA	CMB-C2B	-2.18	1.46	1.50
35	J	101	DGD	O2E-C2E	-2.18	1.37	1.43
27	C	513	CLA	C4B-NB	2.18	1.40	1.37
27	12	306	CLA	MG-ND	-2.18	2.01	2.05
27	34	306	CLA	MG-ND	-2.18	2.01	2.05
27	13	301	CLA	MG-ND	-2.17	2.01	2.05
28	A	403	PHO	CMA-C3A	-2.17	1.49	1.53
27	33	304	CLA	CMC-C2C	-2.17	1.46	1.50
27	Z	102	CLA	CMC-C2C	-2.17	1.46	1.50
27	13	311	CLA	CMB-C2B	-2.17	1.46	1.50
27	12	309	CLA	CMD-C2D	-2.17	1.46	1.50
27	33	305	CLA	CMB-C2B	-2.17	1.46	1.50
27	32	309	CLA	CMB-C2B	-2.17	1.46	1.50
27	b	601	CLA	C1B-NB	-2.17	1.35	1.37
35	H	102	DGD	O4D-C4D	-2.17	1.37	1.43
27	34	305	CLA	MG-ND	-2.17	2.01	2.05
35	J	101	DGD	O6D-C5D	-2.17	1.39	1.44
27	33	311	CLA	CMB-C2B	-2.17	1.46	1.50
27	c	510	CLA	CMA-C3A	-2.17	1.48	1.53
27	33	304	CLA	CMB-C2B	-2.17	1.46	1.50
27	31	309	CLA	C3B-C4B	2.17	1.49	1.42
27	34	312	CLA	C3B-C4B	2.17	1.49	1.42
30	A	406	SQD	O4-C4	-2.17	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	13	311	CLA	C3B-C4B	2.17	1.49	1.42
35	j	101	DGD	O3D-C3D	-2.17	1.37	1.43
27	12	309	CLA	CMB-C2B	-2.17	1.46	1.50
27	d	405	CLA	C1B-C2B	2.17	1.48	1.43
27	11	305	CLA	CMD-C2D	-2.17	1.46	1.50
27	31	305	CLA	CMB-C2B	-2.16	1.46	1.50
27	33	305	CLA	MG-ND	-2.16	2.01	2.05
35	C	517	DGD	O4D-C4D	-2.16	1.37	1.43
27	11	309	CLA	CMB-C2B	-2.16	1.46	1.50
27	12	306	CLA	CMB-C2B	-2.16	1.46	1.50
27	C	514	CLA	C1B-C2B	2.16	1.48	1.43
29	C	516	BCR	C33-C5	-2.16	1.47	1.50
27	14	307	CLA	CMB-C2B	-2.16	1.46	1.50
27	32	308	CLA	CMB-C2B	-2.16	1.46	1.50
27	14	311	CLA	C3B-C4B	2.16	1.49	1.42
27	34	308	CLA	CMC-C2C	-2.16	1.46	1.50
30	l	101	SQD	O2-C2	-2.16	1.37	1.43
27	C	502	CLA	CAC-C3C	-2.16	1.45	1.51
27	12	313	CLA	C3B-C4B	2.16	1.49	1.42
27	B	606	CLA	MG-NB	-2.16	2.01	2.05
35	c	517	DGD	O4D-C4D	-2.16	1.37	1.43
27	33	311	CLA	C3B-C4B	2.16	1.49	1.42
27	31	305	CLA	CMC-C2C	-2.16	1.46	1.50
27	12	303	CLA	MG-ND	-2.16	2.01	2.05
29	C	516	BCR	C38-C26	-2.16	1.47	1.50
27	33	306	CLA	CMB-C2B	-2.16	1.46	1.50
33	C	519	LMG	O4-C4	-2.16	1.37	1.43
27	14	311	CLA	CMB-C2B	-2.16	1.46	1.50
27	13	307	CLA	CMB-C2B	-2.16	1.46	1.50
27	33	304	CLA	C4B-NB	2.16	1.40	1.37
27	11	315	CLA	MG-ND	-2.15	2.01	2.05
33	m	102	LMG	O8-C9	-2.15	1.40	1.45
27	z	102	CLA	CMD-C2D	-2.15	1.46	1.50
27	33	304	CLA	C1B-NB	-2.15	1.35	1.37
30	a	406	SQD	O4-C4	-2.15	1.37	1.43
27	m	101	CLA	C1B-NB	-2.15	1.35	1.37
27	34	305	CLA	CMB-C2B	-2.15	1.46	1.50
27	33	301	CLA	MG-ND	-2.15	2.01	2.05
27	b	606	CLA	MG-NB	-2.15	2.01	2.05
27	34	307	CLA	CMC-C2C	-2.15	1.46	1.50
35	J	101	DGD	O2D-C2D	-2.15	1.37	1.43
27	14	306	CLA	CMC-C2C	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	515	BCR	C33-C5	-2.15	1.47	1.50
30	a	406	SQD	O47-C45	-2.14	1.41	1.46
27	31	302	CLA	CMB-C2B	-2.14	1.46	1.50
33	32	301	LMG	O6-C5	-2.14	1.39	1.44
27	11	309	CLA	C3B-C4B	2.14	1.49	1.42
27	c	502	CLA	CAC-C3C	-2.14	1.45	1.51
27	12	309	CLA	CMC-C2C	-2.14	1.46	1.50
27	B	606	CLA	C5-C3	-2.14	1.46	1.51
33	B	619	LMG	O3-C3	-2.14	1.37	1.43
35	h	102	DGD	O4D-C4D	-2.13	1.37	1.43
33	b	618	LMG	O4-C4	-2.13	1.37	1.43
27	14	307	CLA	CMC-C2C	-2.13	1.46	1.50
27	34	302	CLA	MG-ND	-2.13	2.01	2.05
27	14	304	CLA	CMB-C2B	-2.13	1.46	1.50
27	B	603	CLA	CHC-C4B	-2.13	1.34	1.39
33	q	301	LMG	O4-C4	-2.13	1.37	1.43
27	B	622	CLA	C1B-C2B	2.13	1.48	1.43
29	c	516	BCR	C33-C5	-2.13	1.47	1.50
35	j	101	DGD	O2D-C2D	-2.13	1.37	1.43
33	B	619	LMG	O2-C2	-2.13	1.37	1.43
27	w	102	CLA	C1B-C2B	2.13	1.48	1.43
33	b	619	LMG	O2-C2	-2.13	1.37	1.43
29	b	623	BCR	C33-C5	-2.13	1.47	1.50
27	11	302	CLA	CMB-C2B	-2.12	1.46	1.50
35	c	517	DGD	O3G-C1D	-2.12	1.36	1.40
27	13	311	CLA	MG-ND	-2.12	2.01	2.05
27	D	405	CLA	C4B-NB	2.12	1.40	1.37
27	d	405	CLA	C4B-NB	2.12	1.40	1.37
38	32	316	A86	C5-C6	2.12	1.40	1.35
27	14	307	CLA	C3B-C4B	2.12	1.48	1.42
27	13	304	CLA	CMB-C2B	-2.12	1.46	1.50
27	31	305	CLA	C3B-C4B	2.12	1.48	1.42
27	32	309	CLA	C3B-C4B	2.12	1.48	1.42
27	32	313	CLA	MG-ND	-2.12	2.01	2.05
29	C	516	BCR	C27-C26	-2.12	1.47	1.51
33	M	103	LMG	O8-C9	-2.12	1.40	1.45
27	b	605	CLA	C1B-NB	-2.12	1.35	1.37
27	C	511	CLA	CHC-C1C	2.12	1.42	1.38
27	A	402	CLA	C1B-NB	-2.12	1.35	1.37
29	C	515	BCR	C33-C5	-2.11	1.47	1.50
27	33	307	CLA	C3B-C4B	2.11	1.48	1.42
38	34	315	A86	C5-C6	2.11	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	514	CLA	C3B-C4B	2.11	1.48	1.42
27	C	511	CLA	CAC-C3C	-2.11	1.45	1.51
27	12	308	CLA	CMC-C2C	-2.11	1.46	1.50
27	b	603	CLA	CHC-C4B	-2.11	1.34	1.39
35	c	518	DGD	O2E-C2E	-2.11	1.37	1.43
27	b	605	CLA	CAC-C3C	-2.11	1.45	1.51
27	34	308	CLA	C3B-C4B	2.11	1.48	1.42
27	c	503	CLA	C1B-C2B	2.11	1.48	1.43
29	H	101	BCR	C38-C26	-2.11	1.47	1.50
30	L	103	SQD	O2-C2	-2.11	1.37	1.43
29	c	516	BCR	C27-C26	-2.11	1.47	1.51
27	11	302	CLA	C1B-NB	-2.11	1.35	1.37
33	b	619	LMG	O3-C3	-2.11	1.37	1.43
27	c	512	CLA	CHC-C1C	2.11	1.42	1.38
27	d	401	CLA	CAC-C3C	-2.11	1.45	1.51
38	14	314	A86	C5-C6	2.11	1.40	1.35
27	b	612	CLA	C1B-C2B	2.11	1.48	1.43
27	c	511	CLA	CHC-C1C	2.11	1.42	1.38
27	W	102	CLA	C1B-C2B	2.11	1.48	1.43
27	D	401	CLA	CAC-C3C	-2.11	1.45	1.51
27	31	304	CLA	CMC-C2C	-2.11	1.46	1.50
27	33	311	CLA	CMC-C2C	-2.11	1.46	1.50
38	12	316	A86	C5-C6	2.10	1.40	1.35
27	34	312	CLA	MG-ND	-2.10	2.01	2.05
27	b	622	CLA	C1B-C2B	2.10	1.48	1.43
38	33	314	A86	C5-C6	2.10	1.40	1.35
27	13	306	CLA	CMC-C2C	-2.10	1.46	1.50
27	13	307	CLA	C3B-C4B	2.10	1.48	1.42
27	12	309	CLA	C3B-C4B	2.10	1.48	1.42
27	14	311	CLA	CMC-C2C	-2.10	1.46	1.50
27	b	606	CLA	C5-C3	-2.10	1.47	1.51
27	c	511	CLA	CAC-C3C	-2.10	1.45	1.51
27	b	602	CLA	CAC-C3C	-2.10	1.45	1.51
27	13	311	CLA	CMC-C2C	-2.10	1.46	1.50
27	B	605	CLA	CAC-C3C	-2.10	1.45	1.51
27	B	601	CLA	C1B-NB	-2.10	1.35	1.37
27	B	605	CLA	C1B-NB	-2.10	1.35	1.37
29	H	101	BCR	C33-C5	-2.10	1.47	1.50
29	h	101	BCR	C33-C5	-2.10	1.47	1.50
27	B	615	CLA	C4B-NB	2.10	1.40	1.37
27	11	305	CLA	C3B-C4B	2.10	1.48	1.42
35	C	518	DGD	O2E-C2E	-2.10	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	B	618	LMG	O4-C4	-2.10	1.37	1.43
27	C	514	CLA	C3B-C4B	2.09	1.48	1.42
27	31	309	CLA	MG-ND	-2.09	2.01	2.05
38	13	314	A86	C5-C6	2.09	1.40	1.35
27	C	511	CLA	C1D-ND	2.09	1.40	1.37
27	11	309	CLA	MG-ND	-2.09	2.01	2.05
27	b	601	CLA	C4B-NB	2.09	1.40	1.37
27	31	309	CLA	CMC-C2C	-2.09	1.46	1.50
27	33	311	CLA	MG-ND	-2.09	2.01	2.05
27	D	406	CLA	C1B-C2B	2.09	1.48	1.43
27	33	303	CLA	CHC-C1C	2.09	1.42	1.38
36	d	407	PL9	C10-C9	-2.09	1.45	1.50
36	d	407	PL9	C35-C34	-2.09	1.45	1.50
29	h	101	BCR	C38-C26	-2.09	1.47	1.50
27	11	309	CLA	CMC-C2C	-2.09	1.46	1.50
27	b	610	CLA	CAC-C3C	-2.09	1.45	1.51
27	12	306	CLA	C1B-NB	-2.09	1.35	1.37
27	11	304	CLA	CMC-C2C	-2.09	1.46	1.50
27	34	312	CLA	CMC-C2C	-2.08	1.46	1.50
27	C	513	CLA	C3B-C4B	2.08	1.48	1.42
27	d	402	CLA	C1B-NB	-2.08	1.35	1.37
27	32	308	CLA	CMC-C2C	-2.08	1.46	1.50
27	B	610	CLA	CAC-C3C	-2.08	1.45	1.51
38	11	312	A86	C5-C6	2.08	1.40	1.35
27	C	513	CLA	C1B-C2B	2.08	1.48	1.43
27	W	103	CLA	CMB-C2B	-2.08	1.46	1.50
27	C	506	CLA	C4B-NB	2.08	1.40	1.37
27	31	302	CLA	C1B-NB	-2.08	1.35	1.37
27	12	313	CLA	MG-ND	-2.08	2.01	2.05
27	d	406	CLA	C1B-C2B	2.08	1.48	1.43
27	c	509	CLA	CHC-C4B	-2.08	1.34	1.39
35	C	517	DGD	O3D-C3D	-2.08	1.37	1.43
27	32	306	CLA	C1B-NB	-2.08	1.35	1.37
27	w	103	CLA	CMB-C2B	-2.08	1.46	1.50
27	33	306	CLA	CMC-C2C	-2.08	1.46	1.50
27	12	313	CLA	CMC-C2C	-2.07	1.46	1.50
27	14	303	CLA	CHC-C1C	2.07	1.42	1.38
27	c	502	CLA	CHC-C4B	-2.07	1.34	1.39
35	c	517	DGD	O3D-C3D	-2.07	1.37	1.43
27	12	305	CLA	CHC-C1C	2.07	1.42	1.38
27	W	103	CLA	CHC-C1C	2.07	1.42	1.38
27	B	607	CLA	C1B-C2B	2.07	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	504	CLA	C1B-NB	-2.07	1.35	1.37
27	c	504	CLA	C1B-NB	-2.07	1.35	1.37
27	31	301	CLA	CHC-C1C	2.07	1.42	1.38
36	D	407	PL9	C10-C9	-2.07	1.45	1.50
36	d	404	PL9	C41-C39	-2.07	1.47	1.51
27	32	313	CLA	CMC-C2C	-2.07	1.46	1.50
38	13	317	A86	C5-C6	2.07	1.40	1.35
27	c	513	CLA	C3B-C4B	2.07	1.48	1.42
27	z	102	CLA	C1B-NB	-2.07	1.35	1.37
27	13	304	CLA	C1B-NB	-2.07	1.35	1.37
27	34	310	CLA	C1B-C2B	2.07	1.48	1.43
27	b	608	CLA	MG-ND	-2.07	2.01	2.05
27	11	307	CLA	C1B-NB	-2.07	1.35	1.37
27	11	301	CLA	CHC-C1C	2.07	1.42	1.38
27	Z	102	CLA	C1B-NB	-2.07	1.35	1.37
38	31	312	A86	C5-C6	2.06	1.40	1.35
27	c	513	CLA	C1B-NB	-2.06	1.35	1.37
27	14	304	CLA	C1B-NB	-2.06	1.35	1.37
27	13	310	CLA	C1B-NB	-2.06	1.35	1.37
27	11	303	CLA	C1B-NB	-2.06	1.35	1.37
27	w	103	CLA	CHC-C1C	2.06	1.42	1.38
27	c	506	CLA	C4B-NB	2.06	1.40	1.37
27	C	509	CLA	CHC-C4B	-2.06	1.34	1.39
27	c	513	CLA	C1B-C2B	2.06	1.48	1.43
35	C	517	DGD	O3G-C1D	-2.06	1.36	1.40
27	a	402	CLA	C1B-NB	-2.06	1.35	1.37
27	11	305	CLA	MG-ND	-2.06	2.01	2.05
27	C	512	CLA	CHC-C1C	2.06	1.42	1.38
27	13	303	CLA	CHC-C1C	2.06	1.42	1.38
38	33	302	A86	C5-C6	2.06	1.40	1.35
27	B	606	CLA	C1B-C2B	2.05	1.48	1.43
27	B	601	CLA	C1B-C2B	2.05	1.47	1.43
27	B	612	CLA	C1B-C2B	2.05	1.47	1.43
27	B	602	CLA	C1B-C2B	2.05	1.47	1.43
27	C	513	CLA	C1B-NB	-2.05	1.35	1.37
27	13	305	CLA	C1B-NB	-2.05	1.35	1.37
27	14	309	CLA	C1B-NB	-2.05	1.35	1.37
36	D	407	PL9	C35-C34	-2.05	1.45	1.50
36	D	404	PL9	C41-C39	-2.05	1.47	1.51
27	b	615	CLA	CAC-C3C	-2.05	1.45	1.51
27	31	307	CLA	C1B-NB	-2.05	1.35	1.37
28	A	403	PHO	C3D-CAD	-2.05	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	32	311	CLA	C1B-C2B	2.05	1.47	1.43
27	32	305	CLA	MG-ND	-2.05	2.01	2.05
28	a	403	PHO	C3D-CAD	-2.05	1.43	1.47
27	12	311	CLA	C1B-NB	-2.05	1.35	1.37
36	d	407	PL9	C25-C24	-2.05	1.45	1.50
29	A	409	BCR	C33-C5	-2.05	1.47	1.50
27	14	311	CLA	MG-ND	-2.05	2.01	2.05
27	34	304	CLA	CHC-C1C	2.05	1.42	1.38
27	33	305	CLA	C1B-NB	-2.05	1.35	1.37
27	32	305	CLA	CHC-C1C	2.05	1.42	1.38
27	c	508	CLA	C1B-C2B	2.05	1.47	1.43
27	b	615	CLA	C4B-NB	2.04	1.40	1.37
27	B	602	CLA	CAC-C3C	-2.04	1.45	1.51
27	B	608	CLA	MG-ND	-2.04	2.01	2.05
32	A	408	LHG	C8-C7	-2.04	1.44	1.50
27	D	402	CLA	C1B-NB	-2.04	1.35	1.37
27	13	309	CLA	C1B-NB	-2.04	1.35	1.37
27	33	309	CLA	C1B-NB	-2.04	1.35	1.37
27	34	311	CLA	C1B-NB	-2.04	1.35	1.37
38	12	304	A86	C5-C6	2.04	1.40	1.35
36	D	407	PL9	C16-C14	-2.04	1.47	1.51
38	11	316	A86	C5-C6	2.04	1.40	1.35
27	b	601	CLA	C1B-C2B	2.04	1.47	1.43
27	34	310	CLA	O2A-C1	-2.04	1.40	1.46
27	34	304	CLA	MG-ND	-2.04	2.01	2.05
27	b	614	CLA	CHC-C4B	-2.04	1.34	1.39
27	B	615	CLA	CAC-C3C	-2.04	1.45	1.51
27	32	311	CLA	C1B-NB	-2.04	1.35	1.37
27	b	602	CLA	C1B-C2B	2.04	1.47	1.43
27	C	512	CLA	C3B-C4B	2.04	1.48	1.42
27	31	301	CLA	MG-ND	-2.04	2.01	2.05
27	D	402	CLA	C1B-C2B	2.03	1.47	1.43
38	34	303	A86	C5-C6	2.03	1.40	1.35
29	Z	101	BCR	C34-C9	-2.03	1.46	1.50
27	M	102	CLA	C1B-C2B	2.03	1.47	1.43
27	C	508	CLA	C1B-C2B	2.03	1.47	1.43
27	b	607	CLA	C1B-C2B	2.03	1.47	1.43
27	12	311	CLA	C1B-C2B	2.03	1.47	1.43
27	B	601	CLA	C4B-NB	2.03	1.40	1.37
27	b	606	CLA	C1B-C2B	2.03	1.47	1.43
29	a	405	BCR	C33-C5	-2.03	1.47	1.50
38	31	316	A86	C5-C6	2.03	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	32	307	CLA	C1B-NB	-2.03	1.35	1.37
27	B	614	CLA	CHC-C4B	-2.03	1.34	1.39
29	A	405	BCR	C33-C5	-2.03	1.47	1.50
27	14	303	CLA	MG-ND	-2.03	2.01	2.05
29	a	409	BCR	C33-C5	-2.03	1.47	1.50
27	13	309	CLA	C1B-C2B	2.03	1.47	1.43
38	13	302	A86	C5-C6	2.02	1.40	1.35
27	c	511	CLA	C1D-ND	2.02	1.40	1.37
36	D	407	PL9	C25-C24	-2.02	1.45	1.50
27	C	502	CLA	CHC-C4B	-2.02	1.34	1.39
27	33	303	CLA	MG-ND	-2.02	2.01	2.05
27	32	312	CLA	C1B-NB	-2.02	1.35	1.37
27	14	307	CLA	MG-ND	-2.02	2.01	2.05
27	d	402	CLA	C1B-C2B	2.02	1.47	1.43
35	c	517	DGD	O4E-C4E	-2.02	1.38	1.43
32	a	408	LHG	C8-C7	-2.02	1.44	1.50
27	m	101	CLA	C1B-C2B	2.02	1.47	1.43
27	12	312	CLA	C1B-NB	-2.02	1.35	1.37
27	33	309	CLA	C1B-C2B	2.02	1.47	1.43
27	11	301	CLA	MG-ND	-2.02	2.01	2.05
27	31	303	CLA	C1B-NB	-2.02	1.35	1.37
27	34	310	CLA	C1B-NB	-2.02	1.35	1.37
27	11	307	CLA	C1B-C2B	2.02	1.47	1.43
27	12	305	CLA	MG-ND	-2.02	2.01	2.05
27	M	102	CLA	C4B-NB	2.01	1.40	1.37
27	c	512	CLA	C3B-C4B	2.01	1.48	1.42
27	B	604	CLA	C1B-C2B	2.01	1.47	1.43
35	j	101	DGD	O4D-C4D	-2.01	1.38	1.43
27	m	101	CLA	C3B-C4B	2.01	1.48	1.42
27	14	305	CLA	C1B-NB	-2.01	1.35	1.37
38	32	318	A86	C5-C6	2.01	1.40	1.35
27	31	305	CLA	MG-ND	-2.01	2.01	2.05
27	M	102	CLA	CHC-C1C	2.01	1.42	1.38
27	13	307	CLA	MG-ND	-2.01	2.01	2.05
27	C	512	CLA	C1B-C2B	2.01	1.47	1.43
36	d	407	PL9	C16-C14	-2.01	1.47	1.51
27	b	604	CLA	C1B-C2B	2.01	1.47	1.43
38	33	314	A86	C39-C38	2.01	1.56	1.49
27	32	310	CLA	C1B-NB	-2.01	1.35	1.37
27	14	309	CLA	C1B-C2B	2.01	1.47	1.43
27	B	622	CLA	C3B-C4B	2.01	1.48	1.42
35	j	101	DGD	O4E-C4E	-2.01	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	512	CLA	C1B-C2B	2.01	1.47	1.43
38	14	314	A86	C39-C38	2.01	1.56	1.49
27	31	307	CLA	C1B-C2B	2.01	1.47	1.43
38	32	304	A86	C5-C6	2.00	1.40	1.35
27	C	506	CLA	CHC-C4B	-2.00	1.34	1.39
27	11	308	CLA	C1B-NB	-2.00	1.35	1.37
27	31	308	CLA	C1B-NB	-2.00	1.35	1.37
30	L	103	SQD	O3-C3	-2.00	1.38	1.43
27	12	307	CLA	C1B-NB	-2.00	1.35	1.37

All (2815) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	33	312	A86	O1-C20-C19	44.00	154.72	113.49
38	34	313	A86	O1-C20-C19	43.99	154.72	113.49
38	12	314	A86	O1-C20-C19	43.99	154.72	113.49
38	14	312	A86	O1-C20-C19	43.98	154.71	113.49
38	13	312	A86	O1-C20-C19	43.97	154.71	113.49
38	11	310	A86	O1-C20-C19	43.97	154.70	113.49
38	32	314	A86	O1-C20-C19	43.96	154.69	113.49
38	31	310	A86	O1-C20-C19	43.94	154.67	113.49
38	31	313	A86	O1-C20-C19	43.38	154.14	113.49
38	14	315	A86	O1-C20-C19	43.36	154.12	113.49
38	11	313	A86	O1-C20-C19	43.35	154.12	113.49
38	13	315	A86	O1-C20-C19	43.34	154.11	113.49
38	32	317	A86	O1-C20-C19	43.34	154.11	113.49
38	12	317	A86	O1-C20-C19	43.32	154.09	113.49
38	33	315	A86	O1-C20-C19	43.32	154.09	113.49
38	34	316	A86	O1-C20-C19	43.27	154.04	113.49
38	13	316	A86	O1-C20-C19	42.02	152.87	113.49
38	31	314	A86	O1-C20-C19	42.01	152.87	113.49
38	11	314	A86	O1-C20-C19	42.00	152.85	113.49
38	14	301	A86	O1-C20-C19	42.00	152.85	113.49
38	33	316	A86	O1-C20-C19	42.00	152.85	113.49
38	14	316	A86	O1-C20-C19	41.99	152.85	113.49
38	32	318	A86	O1-C20-C19	41.98	152.84	113.49
38	34	301	A86	O1-C20-C19	41.97	152.82	113.49
38	14	313	A86	O1-C20-C19	41.53	152.41	113.49
38	12	315	A86	O1-C20-C19	41.52	152.40	113.49
38	34	314	A86	O1-C20-C19	41.52	152.40	113.49
38	13	313	A86	O1-C20-C19	41.51	152.40	113.49
38	31	311	A86	O1-C20-C19	41.48	152.37	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	32	315	A86	O1-C20-C19	41.48	152.37	113.49
38	11	311	A86	O1-C20-C19	41.47	152.35	113.49
38	33	313	A86	O1-C20-C19	41.45	152.34	113.49
38	11	312	A86	O1-C20-C19	40.48	151.43	113.49
38	34	315	A86	O1-C20-C19	40.44	151.40	113.49
38	31	312	A86	O1-C20-C19	40.43	151.39	113.49
38	12	316	A86	O1-C20-C19	40.43	151.38	113.49
38	13	314	A86	O1-C20-C19	40.42	151.37	113.49
38	32	316	A86	O1-C20-C19	40.41	151.37	113.49
38	33	314	A86	O1-C20-C19	40.41	151.37	113.49
38	14	314	A86	O1-C20-C19	40.40	151.35	113.49
38	33	302	A86	O1-C20-C19	38.35	149.44	113.49
38	13	302	A86	O1-C20-C19	38.35	149.43	113.49
38	13	317	A86	O1-C20-C19	38.33	149.42	113.49
38	32	304	A86	O1-C20-C19	38.33	149.41	113.49
38	31	316	A86	O1-C20-C19	38.32	149.40	113.49
38	12	304	A86	O1-C20-C19	38.31	149.40	113.49
38	34	303	A86	O1-C20-C19	38.30	149.39	113.49
38	11	316	A86	O1-C20-C19	38.30	149.39	113.49
38	31	313	A86	O1-C20-C21	-12.07	101.56	115.05
38	33	315	A86	O1-C20-C21	-12.06	101.57	115.05
38	11	313	A86	O1-C20-C21	-12.05	101.58	115.05
38	32	317	A86	O1-C20-C21	-12.05	101.58	115.05
38	14	315	A86	O1-C20-C21	-12.04	101.59	115.05
38	13	315	A86	O1-C20-C21	-12.03	101.61	115.05
38	12	317	A86	O1-C20-C21	-12.02	101.62	115.05
38	34	316	A86	O1-C20-C21	-12.00	101.64	115.05
38	12	314	A86	O1-C20-C21	-11.70	101.97	115.05
38	33	312	A86	O1-C20-C21	-11.69	101.98	115.05
38	11	310	A86	O1-C20-C21	-11.68	102.00	115.05
38	14	312	A86	O1-C20-C21	-11.67	102.00	115.05
38	32	314	A86	O1-C20-C21	-11.67	102.00	115.05
38	34	313	A86	O1-C20-C21	-11.66	102.01	115.05
38	13	312	A86	O1-C20-C21	-11.66	102.02	115.05
38	31	310	A86	O1-C20-C21	-11.66	102.02	115.05
38	11	314	A86	C21-C20-C19	-10.86	102.04	114.24
38	13	316	A86	C21-C20-C19	-10.86	102.04	114.24
38	14	313	A86	O1-C20-C21	-10.84	102.93	115.05
38	31	314	A86	C21-C20-C19	-10.84	102.06	114.24
38	13	313	A86	O1-C20-C21	-10.84	102.94	115.05
38	14	316	A86	C21-C20-C19	-10.83	102.07	114.24
38	32	318	A86	C21-C20-C19	-10.83	102.08	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	14	301	A86	C21-C20-C19	-10.82	102.08	114.24
38	34	301	A86	C21-C20-C19	-10.82	102.08	114.24
38	12	315	A86	O1-C20-C21	-10.82	102.95	115.05
38	34	314	A86	O1-C20-C21	-10.81	102.97	115.05
38	33	316	A86	C21-C20-C19	-10.80	102.11	114.24
38	31	311	A86	O1-C20-C21	-10.80	102.98	115.05
38	33	313	A86	O1-C20-C21	-10.79	102.98	115.05
38	11	311	A86	O1-C20-C21	-10.78	103.00	115.05
38	32	315	A86	O1-C20-C21	-10.78	103.00	115.05
38	34	313	A86	C21-C20-C19	-10.61	102.33	114.24
38	13	312	A86	C21-C20-C19	-10.58	102.36	114.24
38	33	312	A86	C21-C20-C19	-10.58	102.36	114.24
38	11	310	A86	C21-C20-C19	-10.57	102.37	114.24
38	14	312	A86	C21-C20-C19	-10.57	102.37	114.24
38	32	314	A86	C21-C20-C19	-10.56	102.38	114.24
38	12	314	A86	C21-C20-C19	-10.56	102.38	114.24
38	31	310	A86	C21-C20-C19	-10.55	102.39	114.24
38	11	312	A86	C21-C20-C19	-10.52	102.43	114.24
38	13	314	A86	C21-C20-C19	-10.51	102.44	114.24
38	33	314	A86	C21-C20-C19	-10.51	102.44	114.24
38	12	316	A86	C21-C20-C19	-10.49	102.46	114.24
38	31	312	A86	C21-C20-C19	-10.49	102.46	114.24
38	34	315	A86	C21-C20-C19	-10.49	102.46	114.24
38	14	314	A86	C21-C20-C19	-10.46	102.49	114.24
38	32	316	A86	C21-C20-C19	-10.44	102.51	114.24
38	33	302	A86	C21-C20-C19	-10.15	102.84	114.24
38	31	316	A86	C21-C20-C19	-10.14	102.85	114.24
38	32	304	A86	C21-C20-C19	-10.12	102.87	114.24
38	12	304	A86	C21-C20-C19	-10.12	102.87	114.24
38	13	317	A86	C21-C20-C19	-10.11	102.89	114.24
38	13	302	A86	C21-C20-C19	-10.11	102.89	114.24
38	34	303	A86	C21-C20-C19	-10.09	102.91	114.24
38	11	316	A86	C21-C20-C19	-10.09	102.91	114.24
38	14	301	A86	O1-C20-C21	-10.07	103.80	115.05
38	33	316	A86	O1-C20-C21	-10.06	103.80	115.05
38	31	314	A86	O1-C20-C21	-10.05	103.82	115.05
38	14	316	A86	O1-C20-C21	-10.04	103.83	115.05
38	32	318	A86	O1-C20-C21	-10.03	103.83	115.05
38	34	301	A86	O1-C20-C21	-10.03	103.84	115.05
38	11	314	A86	O1-C20-C21	-10.02	103.84	115.05
38	13	316	A86	O1-C20-C21	-10.02	103.85	115.05
27	B	612	CLA	C4A-NA-C1A	9.91	111.20	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	12	317	A86	C21-C20-C19	-9.85	103.18	114.24
27	b	612	CLA	C4A-NA-C1A	9.84	111.17	106.68
38	32	315	A86	C21-C20-C19	-9.84	103.19	114.24
38	13	315	A86	C21-C20-C19	-9.84	103.19	114.24
38	14	315	A86	C21-C20-C19	-9.83	103.19	114.24
38	34	314	A86	C21-C20-C19	-9.83	103.19	114.24
38	11	313	A86	C21-C20-C19	-9.83	103.20	114.24
38	31	313	A86	C21-C20-C19	-9.83	103.20	114.24
38	12	315	A86	C21-C20-C19	-9.82	103.21	114.24
38	11	311	A86	C21-C20-C19	-9.82	103.21	114.24
38	32	317	A86	C21-C20-C19	-9.82	103.21	114.24
38	34	316	A86	C21-C20-C19	-9.81	103.22	114.24
38	14	313	A86	C21-C20-C19	-9.81	103.22	114.24
38	13	313	A86	C21-C20-C19	-9.81	103.23	114.24
38	31	311	A86	C21-C20-C19	-9.80	103.23	114.24
38	33	313	A86	C21-C20-C19	-9.78	103.25	114.24
38	33	315	A86	C21-C20-C19	-9.77	103.26	114.24
38	32	316	A86	O1-C20-C21	-9.50	104.43	115.05
38	11	312	A86	O1-C20-C21	-9.49	104.44	115.05
38	34	315	A86	O1-C20-C21	-9.48	104.45	115.05
38	12	316	A86	O1-C20-C21	-9.48	104.45	115.05
38	31	312	A86	O1-C20-C21	-9.48	104.45	115.05
38	14	314	A86	O1-C20-C21	-9.47	104.46	115.05
38	13	314	A86	O1-C20-C21	-9.45	104.49	115.05
38	33	314	A86	O1-C20-C21	-9.44	104.50	115.05
38	12	304	A86	C33-C32-C31	9.02	117.98	109.21
27	11	301	CLA	C4A-NA-C1A	9.02	110.79	106.68
38	31	316	A86	C33-C32-C31	9.01	117.97	109.21
38	34	303	A86	C33-C32-C31	9.01	117.96	109.21
38	13	302	A86	C33-C32-C31	9.00	117.96	109.21
38	13	317	A86	C33-C32-C31	9.00	117.96	109.21
38	33	302	A86	C33-C32-C31	8.99	117.95	109.21
38	11	316	A86	C33-C32-C31	8.99	117.94	109.21
38	32	304	A86	C33-C32-C31	8.98	117.94	109.21
27	13	303	CLA	C4A-NA-C1A	8.97	110.77	106.68
27	c	510	CLA	C4A-NA-C1A	8.95	110.76	106.68
27	33	303	CLA	C4A-NA-C1A	8.95	110.76	106.68
27	32	305	CLA	C4A-NA-C1A	8.94	110.76	106.68
27	12	305	CLA	C4A-NA-C1A	8.92	110.75	106.68
27	31	301	CLA	C4A-NA-C1A	8.89	110.74	106.68
27	34	304	CLA	C4A-NA-C1A	8.87	110.73	106.68
27	14	303	CLA	C4A-NA-C1A	8.87	110.72	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	510	CLA	C4A-NA-C1A	8.85	110.72	106.68
38	13	314	A86	C33-C32-C31	8.54	117.51	109.21
38	14	314	A86	C33-C32-C31	8.52	117.49	109.21
38	13	317	A86	C4-C5-C6	-8.50	115.36	127.28
38	33	302	A86	C4-C5-C6	-8.49	115.37	127.28
38	12	316	A86	C33-C32-C31	8.49	117.46	109.21
38	12	304	A86	C4-C5-C6	-8.48	115.38	127.28
38	11	316	A86	C4-C5-C6	-8.48	115.39	127.28
38	32	304	A86	C4-C5-C6	-8.47	115.39	127.28
38	34	315	A86	C33-C32-C31	8.47	117.44	109.21
38	11	312	A86	C33-C32-C31	8.46	117.44	109.21
38	32	316	A86	C33-C32-C31	8.46	117.44	109.21
38	33	314	A86	C33-C32-C31	8.46	117.43	109.21
38	34	303	A86	C4-C5-C6	-8.45	115.42	127.28
38	31	316	A86	C4-C5-C6	-8.45	115.42	127.28
38	13	302	A86	C4-C5-C6	-8.45	115.43	127.28
38	31	312	A86	C33-C32-C31	8.44	117.41	109.21
27	c	505	CLA	C4A-NA-C1A	8.26	110.45	106.68
27	C	505	CLA	C4A-NA-C1A	8.20	110.42	106.68
28	a	403	PHO	C4D-CHA-CBD	-8.18	104.53	108.45
27	d	406	CLA	C4A-NA-C1A	8.11	110.38	106.68
27	11	306	CLA	C4A-NA-C1A	8.10	110.37	106.68
27	33	308	CLA	C4A-NA-C1A	8.09	110.37	106.68
27	13	308	CLA	C4A-NA-C1A	8.09	110.37	106.68
27	b	609	CLA	C4A-NA-C1A	8.08	110.36	106.68
28	A	403	PHO	C4D-CHA-CBD	-8.07	104.59	108.45
27	A	402	CLA	C4A-NA-C1A	8.06	110.36	106.68
27	B	609	CLA	C4A-NA-C1A	8.06	110.35	106.68
27	D	406	CLA	C4A-NA-C1A	8.04	110.35	106.68
27	12	310	CLA	C4A-NA-C1A	8.02	110.34	106.68
27	C	502	CLA	C4A-NA-C1A	8.01	110.33	106.68
27	a	402	CLA	C4A-NA-C1A	7.99	110.32	106.68
27	31	306	CLA	C4A-NA-C1A	7.98	110.32	106.68
27	14	308	CLA	C4A-NA-C1A	7.96	110.31	106.68
27	c	502	CLA	C4A-NA-C1A	7.96	110.31	106.68
27	34	309	CLA	C4A-NA-C1A	7.95	110.31	106.68
27	32	310	CLA	C4A-NA-C1A	7.94	110.30	106.68
38	13	312	A86	C33-C32-C31	7.91	116.90	109.21
38	11	310	A86	C33-C32-C31	7.89	116.88	109.21
38	34	313	A86	C33-C32-C31	7.88	116.87	109.21
38	31	310	A86	C33-C32-C31	7.88	116.87	109.21
38	32	314	A86	C33-C32-C31	7.87	116.86	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	13	302	A86	O1-C20-C21	-7.84	106.28	115.05
38	12	314	A86	C33-C32-C31	7.83	116.83	109.21
38	32	304	A86	O1-C20-C21	-7.83	106.29	115.05
38	13	317	A86	O1-C20-C21	-7.83	106.30	115.05
38	11	316	A86	O1-C20-C21	-7.83	106.30	115.05
38	14	312	A86	C33-C32-C31	7.82	116.81	109.21
38	34	303	A86	O1-C20-C21	-7.82	106.31	115.05
38	33	312	A86	C33-C32-C31	7.82	116.81	109.21
38	12	304	A86	O1-C20-C21	-7.81	106.31	115.05
38	33	302	A86	O1-C20-C21	-7.80	106.33	115.05
38	31	316	A86	O1-C20-C21	-7.78	106.35	115.05
27	C	514	CLA	C4A-NA-C1A	7.78	110.23	106.68
27	c	514	CLA	C4A-NA-C1A	7.77	110.22	106.68
27	B	601	CLA	C4A-NA-C1A	7.66	110.17	106.68
27	34	306	CLA	C4A-NA-C1A	7.65	110.17	106.68
27	C	504	CLA	C4A-NA-C1A	7.63	110.16	106.68
28	d	403	PHO	C4D-CHA-CBD	-7.62	104.80	108.45
27	32	307	CLA	C4A-NA-C1A	7.61	110.15	106.68
28	D	403	PHO	C4D-CHA-CBD	-7.60	104.81	108.45
27	12	307	CLA	C4A-NA-C1A	7.59	110.14	106.68
27	14	305	CLA	C4A-NA-C1A	7.59	110.14	106.68
27	11	303	CLA	C4A-NA-C1A	7.59	110.14	106.68
27	13	305	CLA	C4A-NA-C1A	7.57	110.13	106.68
27	b	601	CLA	C4A-NA-C1A	7.56	110.13	106.68
27	b	608	CLA	C4A-NA-C1A	7.54	110.12	106.68
27	31	303	CLA	C4A-NA-C1A	7.53	110.11	106.68
27	33	305	CLA	C4A-NA-C1A	7.52	110.11	106.68
27	c	504	CLA	C4A-NA-C1A	7.52	110.11	106.68
27	B	608	CLA	C4A-NA-C1A	7.48	110.09	106.68
27	13	304	CLA	C4A-NA-C1A	7.46	110.08	106.68
27	32	306	CLA	C4A-NA-C1A	7.43	110.07	106.68
27	14	304	CLA	C4A-NA-C1A	7.40	110.06	106.68
27	b	603	CLA	C4A-NA-C1A	7.40	110.05	106.68
27	b	613	CLA	C4A-NA-C1A	7.40	110.05	106.68
27	34	307	CLA	C4A-NA-C1A	7.37	110.04	106.68
27	33	304	CLA	C4A-NA-C1A	7.37	110.04	106.68
27	34	305	CLA	C4A-NA-C1A	7.36	110.04	106.68
27	B	603	CLA	C4A-NA-C1A	7.36	110.04	106.68
27	11	302	CLA	C4A-NA-C1A	7.32	110.02	106.68
27	12	306	CLA	C4A-NA-C1A	7.31	110.01	106.68
27	c	509	CLA	C4A-NA-C1A	7.30	110.01	106.68
27	33	306	CLA	C4A-NA-C1A	7.30	110.01	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	611	CLA	C4A-NA-C1A	7.29	110.00	106.68
27	14	306	CLA	C4A-NA-C1A	7.29	110.00	106.68
27	31	302	CLA	C4A-NA-C1A	7.29	110.00	106.68
27	B	611	CLA	C4A-NA-C1A	7.27	110.00	106.68
27	31	304	CLA	C4A-NA-C1A	7.27	110.00	106.68
27	C	509	CLA	C4A-NA-C1A	7.26	109.99	106.68
27	C	512	CLA	C4A-NA-C1A	7.25	109.99	106.68
38	33	313	A86	C33-C32-C31	7.25	116.25	109.21
38	31	311	A86	C33-C32-C31	7.24	116.25	109.21
38	14	313	A86	C33-C32-C31	7.24	116.25	109.21
38	32	315	A86	C33-C32-C31	7.24	116.25	109.21
27	32	308	CLA	C4A-NA-C1A	7.23	109.98	106.68
27	C	513	CLA	C4A-NA-C1A	7.23	109.98	106.68
38	11	311	A86	C33-C32-C31	7.23	116.23	109.21
38	13	313	A86	C33-C32-C31	7.23	116.23	109.21
38	32	317	A86	C33-C32-C31	7.22	116.23	109.21
38	13	315	A86	C33-C32-C31	7.22	116.23	109.21
27	C	508	CLA	C4A-NA-C1A	7.22	109.97	106.68
27	B	613	CLA	C4A-NA-C1A	7.21	109.97	106.68
38	12	315	A86	C33-C32-C31	7.21	116.22	109.21
38	11	313	A86	C33-C32-C31	7.21	116.22	109.21
38	34	314	A86	C33-C32-C31	7.21	116.22	109.21
27	Z	102	CLA	C4A-NA-C1A	7.21	109.97	106.68
27	13	307	CLA	C4A-NA-C1A	7.20	109.96	106.68
38	12	317	A86	C33-C32-C31	7.19	116.20	109.21
27	z	102	CLA	C4A-NA-C1A	7.18	109.96	106.68
27	12	308	CLA	C4A-NA-C1A	7.18	109.95	106.68
38	31	313	A86	C33-C32-C31	7.17	116.18	109.21
38	14	315	A86	C33-C32-C31	7.17	116.18	109.21
27	11	305	CLA	C4A-NA-C1A	7.16	109.95	106.68
27	D	402	CLA	C4A-NA-C1A	7.15	109.94	106.68
27	12	309	CLA	C4A-NA-C1A	7.15	109.94	106.68
27	c	513	CLA	C4A-NA-C1A	7.15	109.94	106.68
38	33	315	A86	C33-C32-C31	7.15	116.16	109.21
27	B	607	CLA	C4A-NA-C1A	7.14	109.94	106.68
27	b	614	CLA	C4A-NA-C1A	7.13	109.93	106.68
38	34	316	A86	C33-C32-C31	7.13	116.14	109.21
27	11	304	CLA	C4A-NA-C1A	7.12	109.93	106.68
27	D	405	CLA	C4A-NA-C1A	7.10	109.92	106.68
27	b	607	CLA	C4A-NA-C1A	7.10	109.92	106.68
27	A	404	CLA	C4A-NA-C1A	7.10	109.92	106.68
27	d	405	CLA	C4A-NA-C1A	7.09	109.91	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	13	306	CLA	C4A-NA-C1A	7.09	109.91	106.68
27	d	402	CLA	C4A-NA-C1A	7.08	109.91	106.68
27	a	404	CLA	C4A-NA-C1A	7.08	109.91	106.68
27	c	512	CLA	C4A-NA-C1A	7.08	109.91	106.68
27	B	606	CLA	C4A-NA-C1A	7.07	109.90	106.68
27	B	614	CLA	C4A-NA-C1A	7.06	109.90	106.68
27	14	307	CLA	C4A-NA-C1A	7.06	109.90	106.68
27	33	307	CLA	C4A-NA-C1A	7.03	109.89	106.68
27	31	305	CLA	C4A-NA-C1A	7.03	109.89	106.68
27	32	309	CLA	C4A-NA-C1A	7.03	109.89	106.68
27	34	308	CLA	C4A-NA-C1A	7.02	109.88	106.68
27	11	315	CLA	C4A-NA-C1A	7.01	109.88	106.68
27	B	622	CLA	C4A-NA-C1A	7.00	109.87	106.68
27	c	508	CLA	C4A-NA-C1A	6.99	109.87	106.68
27	33	301	CLA	C4A-NA-C1A	6.99	109.87	106.68
27	14	302	CLA	C4A-NA-C1A	6.99	109.87	106.68
27	32	303	CLA	C4A-NA-C1A	6.98	109.86	106.68
27	12	303	CLA	C4A-NA-C1A	6.95	109.85	106.68
27	31	315	CLA	C4A-NA-C1A	6.95	109.85	106.68
27	13	301	CLA	C4A-NA-C1A	6.94	109.85	106.68
27	b	606	CLA	C4A-NA-C1A	6.90	109.83	106.68
27	34	302	CLA	C4A-NA-C1A	6.88	109.82	106.68
27	B	610	CLA	C4A-NA-C1A	6.88	109.82	106.68
27	C	503	CLA	C4A-NA-C1A	6.88	109.82	106.68
27	b	622	CLA	C4A-NA-C1A	6.84	109.80	106.68
27	c	503	CLA	C4A-NA-C1A	6.83	109.80	106.68
27	b	610	CLA	C4A-NA-C1A	6.82	109.79	106.68
27	B	605	CLA	C4A-NA-C1A	6.77	109.77	106.68
27	b	604	CLA	C4A-NA-C1A	6.74	109.76	106.68
27	d	401	CLA	C4A-NA-C1A	6.74	109.76	106.68
27	D	401	CLA	C4A-NA-C1A	6.74	109.75	106.68
27	b	605	CLA	C4A-NA-C1A	6.71	109.74	106.68
27	B	604	CLA	C4A-NA-C1A	6.70	109.74	106.68
27	B	602	CLA	C4A-NA-C1A	6.69	109.73	106.68
27	c	506	CLA	C4A-NA-C1A	6.69	109.73	106.68
27	b	602	CLA	C4A-NA-C1A	6.65	109.71	106.68
27	C	506	CLA	C4A-NA-C1A	6.65	109.71	106.68
27	12	312	CLA	C4A-NA-C1A	6.49	109.64	106.68
27	11	308	CLA	C4A-NA-C1A	6.48	109.63	106.68
38	13	314	A86	C4-C5-C6	-6.48	118.19	127.28
38	32	316	A86	C4-C5-C6	-6.47	118.20	127.28
38	14	314	A86	C4-C5-C6	-6.47	118.21	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	32	311	CLA	C4A-NA-C1A	6.46	109.63	106.68
27	33	309	CLA	C4A-NA-C1A	6.46	109.62	106.68
27	14	310	CLA	C4A-NA-C1A	6.46	109.62	106.68
27	13	310	CLA	C4A-NA-C1A	6.45	109.62	106.68
38	34	315	A86	C4-C5-C6	-6.45	118.23	127.28
38	12	316	A86	C4-C5-C6	-6.45	118.24	127.28
38	11	312	A86	C4-C5-C6	-6.44	118.25	127.28
38	33	314	A86	C4-C5-C6	-6.43	118.25	127.28
27	33	310	CLA	C4A-NA-C1A	6.43	109.61	106.68
38	31	312	A86	C4-C5-C6	-6.43	118.26	127.28
27	31	308	CLA	C4A-NA-C1A	6.42	109.61	106.68
27	14	309	CLA	C4A-NA-C1A	6.42	109.61	106.68
27	w	103	CLA	C4A-NA-C1A	6.39	109.60	106.68
27	32	312	CLA	C4A-NA-C1A	6.37	109.58	106.68
27	11	307	CLA	C4A-NA-C1A	6.36	109.58	106.68
27	W	103	CLA	C4A-NA-C1A	6.36	109.58	106.68
27	34	311	CLA	C4A-NA-C1A	6.35	109.58	106.68
27	13	309	CLA	C4A-NA-C1A	6.33	109.57	106.68
27	31	307	CLA	C4A-NA-C1A	6.32	109.56	106.68
27	12	311	CLA	C4A-NA-C1A	6.29	109.55	106.68
27	34	310	CLA	C4A-NA-C1A	6.22	109.52	106.68
38	12	315	A86	C3-C2-C1	-6.16	118.63	127.28
38	11	311	A86	C3-C2-C1	-6.16	118.64	127.28
38	34	314	A86	C3-C2-C1	-6.15	118.65	127.28
38	14	313	A86	C3-C2-C1	-6.13	118.67	127.28
38	31	311	A86	C3-C2-C1	-6.13	118.68	127.28
38	33	313	A86	C3-C2-C1	-6.13	118.68	127.28
38	32	315	A86	C3-C2-C1	-6.12	118.69	127.28
38	13	313	A86	C3-C2-C1	-6.12	118.70	127.28
27	11	309	CLA	C4A-NA-C1A	6.08	109.45	106.68
27	34	312	CLA	C4A-NA-C1A	6.08	109.45	106.68
27	14	311	CLA	C4A-NA-C1A	6.07	109.45	106.68
27	13	311	CLA	C4A-NA-C1A	6.05	109.44	106.68
27	33	311	CLA	C4A-NA-C1A	6.05	109.44	106.68
27	31	309	CLA	C4A-NA-C1A	6.03	109.43	106.68
27	32	313	CLA	C4A-NA-C1A	6.01	109.42	106.68
27	w	102	CLA	C4A-NA-C1A	6.01	109.42	106.68
27	W	102	CLA	C4A-NA-C1A	6.00	109.42	106.68
27	12	313	CLA	C4A-NA-C1A	6.00	109.42	106.68
38	33	316	A86	C3-C2-C1	-5.86	119.06	127.28
38	14	301	A86	C3-C2-C1	-5.82	119.12	127.28
38	32	318	A86	C3-C2-C1	-5.81	119.13	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	14	316	A86	C3-C2-C1	-5.80	119.14	127.28
38	34	301	A86	C3-C2-C1	-5.80	119.14	127.28
38	31	314	A86	C3-C2-C1	-5.78	119.17	127.28
38	13	316	A86	C3-C2-C1	-5.78	119.17	127.28
38	11	314	A86	C3-C2-C1	-5.77	119.18	127.28
27	M	102	CLA	C4A-NA-C1A	5.65	109.25	106.68
27	m	101	CLA	C4A-NA-C1A	5.58	109.23	106.68
38	12	315	A86	C4-C5-C6	-5.51	119.54	127.28
38	32	315	A86	C4-C5-C6	-5.50	119.57	127.28
38	11	311	A86	C4-C5-C6	-5.50	119.57	127.28
38	13	313	A86	C4-C5-C6	-5.49	119.57	127.28
38	33	302	A86	C25-C26-C27	-5.49	119.58	127.28
38	14	313	A86	C4-C5-C6	-5.48	119.59	127.28
38	31	311	A86	C4-C5-C6	-5.48	119.59	127.28
38	33	313	A86	C4-C5-C6	-5.48	119.59	127.28
38	34	303	A86	C25-C26-C27	-5.48	119.60	127.28
38	34	314	A86	C4-C5-C6	-5.48	119.60	127.28
38	31	316	A86	C25-C26-C27	-5.46	119.62	127.28
38	13	302	A86	C25-C26-C27	-5.46	119.62	127.28
38	32	304	A86	C25-C26-C27	-5.46	119.62	127.28
38	13	317	A86	C25-C26-C27	-5.46	119.63	127.28
38	11	316	A86	C25-C26-C27	-5.45	119.64	127.28
38	12	304	A86	C25-C26-C27	-5.44	119.64	127.28
27	c	507	CLA	CAA-C2A-C3A	-5.37	98.49	113.00
27	C	507	CLA	CAA-C2A-C3A	-5.36	98.50	113.00
38	11	314	A86	C33-C32-C31	5.33	114.39	109.21
38	34	313	A86	C3-C2-C1	-5.32	119.81	127.28
38	33	312	A86	C3-C2-C1	-5.32	119.82	127.28
38	31	314	A86	C33-C32-C31	5.32	114.38	109.21
38	32	314	A86	C3-C2-C1	-5.31	119.83	127.28
38	34	301	A86	C33-C32-C31	5.30	114.36	109.21
38	14	301	A86	C33-C32-C31	5.30	114.36	109.21
38	32	318	A86	C33-C32-C31	5.30	114.36	109.21
38	13	316	A86	C33-C32-C31	5.30	114.36	109.21
38	14	316	A86	C33-C32-C31	5.30	114.36	109.21
38	31	310	A86	C3-C2-C1	-5.30	119.85	127.28
38	13	315	A86	C3-C2-C1	-5.29	119.86	127.28
38	11	310	A86	C3-C2-C1	-5.29	119.87	127.28
38	13	312	A86	C3-C2-C1	-5.28	119.87	127.28
38	12	314	A86	C3-C2-C1	-5.26	119.90	127.28
38	14	315	A86	C3-C2-C1	-5.26	119.90	127.28
38	14	313	A86	O4-C38-C39	5.25	120.46	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	14	312	A86	C3-C2-C1	-5.25	119.92	127.28
38	34	314	A86	O4-C38-C39	5.25	120.45	111.09
38	12	317	A86	C3-C2-C1	-5.25	119.92	127.28
38	33	315	A86	C3-C2-C1	-5.25	119.92	127.28
38	13	313	A86	O4-C38-C39	5.24	120.44	111.09
38	11	313	A86	C3-C2-C1	-5.24	119.93	127.28
38	12	315	A86	O4-C38-C39	5.24	120.43	111.09
38	31	311	A86	O4-C38-C39	5.24	120.43	111.09
38	33	316	A86	C33-C32-C31	5.24	114.30	109.21
38	34	316	A86	C3-C2-C1	-5.23	119.94	127.28
38	33	313	A86	O4-C38-C39	5.23	120.41	111.09
38	32	315	A86	O4-C38-C39	5.23	120.41	111.09
38	11	311	A86	O4-C38-C39	5.22	120.40	111.09
38	32	317	A86	C3-C2-C1	-5.21	119.97	127.28
38	31	313	A86	C3-C2-C1	-5.20	119.99	127.28
30	L	103	SQD	O6-C1-C2	5.16	116.11	108.27
38	32	304	A86	O4-C38-C39	5.16	120.29	111.09
38	34	303	A86	O4-C38-C39	5.15	120.27	111.09
38	13	302	A86	O4-C38-C39	5.14	120.26	111.09
38	11	316	A86	O4-C38-C39	5.14	120.26	111.09
38	13	317	A86	O4-C38-C39	5.14	120.25	111.09
38	31	316	A86	O4-C38-C39	5.13	120.24	111.09
38	12	304	A86	O4-C38-C39	5.13	120.24	111.09
38	33	302	A86	O4-C38-C39	5.12	120.23	111.09
30	l	101	SQD	O6-C1-C2	5.12	116.05	108.27
27	B	615	CLA	C4A-NA-C1A	5.05	108.98	106.68
27	c	511	CLA	C4A-NA-C1A	5.03	108.97	106.68
27	C	511	CLA	C4A-NA-C1A	5.02	108.97	106.68
27	b	615	CLA	C4A-NA-C1A	5.00	108.96	106.68
38	33	314	A86	O4-C38-C39	4.99	119.98	111.09
38	12	316	A86	O4-C38-C39	4.98	119.97	111.09
38	31	312	A86	O4-C38-C39	4.98	119.96	111.09
38	32	316	A86	O4-C38-C39	4.98	119.96	111.09
38	11	312	A86	O4-C38-C39	4.97	119.95	111.09
38	14	314	A86	O4-C38-C39	4.97	119.95	111.09
38	13	314	A86	O4-C38-C39	4.96	119.94	111.09
38	32	317	A86	O4-C38-C39	4.95	119.92	111.09
38	34	315	A86	O4-C38-C39	4.95	119.91	111.09
38	34	316	A86	O4-C38-C39	4.94	119.90	111.09
38	14	315	A86	O4-C38-C39	4.94	119.90	111.09
38	31	313	A86	O4-C38-C39	4.94	119.90	111.09
38	11	313	A86	O4-C38-C39	4.94	119.89	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	33	315	A86	O4-C38-C39	4.93	119.89	111.09
38	13	315	A86	O4-C38-C39	4.93	119.89	111.09
38	12	317	A86	O4-C38-C39	4.93	119.88	111.09
38	13	316	A86	O4-C38-C39	4.91	119.84	111.09
38	32	318	A86	O4-C38-C39	4.90	119.83	111.09
38	33	316	A86	O4-C38-C39	4.90	119.83	111.09
38	11	314	A86	O4-C38-C39	4.90	119.83	111.09
38	14	316	A86	O4-C38-C39	4.90	119.82	111.09
38	31	314	A86	O4-C38-C39	4.89	119.81	111.09
27	c	507	CLA	C4A-NA-C1A	4.88	108.91	106.68
38	14	301	A86	O4-C38-C39	4.88	119.80	111.09
38	34	301	A86	O4-C38-C39	4.87	119.77	111.09
27	C	507	CLA	C4A-NA-C1A	4.83	108.88	106.68
38	32	315	A86	C25-C26-C27	-4.72	120.66	127.28
38	33	313	A86	C25-C26-C27	-4.72	120.66	127.28
38	34	314	A86	C25-C26-C27	-4.72	120.66	127.28
31	a	407	BCT	O2-C-O1	4.71	131.73	119.68
38	31	311	A86	C25-C26-C27	-4.71	120.67	127.28
38	14	313	A86	C25-C26-C27	-4.70	120.68	127.28
38	11	311	A86	C25-C26-C27	-4.69	120.69	127.28
38	13	313	A86	C25-C26-C27	-4.69	120.70	127.28
38	12	315	A86	C25-C26-C27	-4.69	120.70	127.28
31	A	407	BCT	O2-C-O1	4.69	131.67	119.68
35	C	517	DGD	O3G-C3G-C2G	-4.66	99.48	110.82
35	c	517	DGD	O3G-C3G-C2G	-4.66	99.48	110.82
38	12	314	A86	O4-C38-C39	4.66	119.40	111.09
38	11	310	A86	O4-C38-C39	4.65	119.39	111.09
38	13	312	A86	O4-C38-C39	4.63	119.34	111.09
38	32	314	A86	O4-C38-C39	4.63	119.34	111.09
38	11	312	A86	C41-C32-C31	-4.62	106.33	110.47
38	34	315	A86	C41-C32-C31	-4.62	106.34	110.47
38	34	313	A86	O4-C38-C39	4.62	119.33	111.09
38	33	312	A86	O4-C38-C39	4.62	119.32	111.09
38	14	312	A86	O4-C38-C39	4.61	119.32	111.09
38	12	316	A86	C41-C32-C31	-4.60	106.35	110.47
38	31	310	A86	O4-C38-C39	4.60	119.29	111.09
27	b	603	CLA	O2D-CGD-O1D	-4.59	114.91	123.85
38	33	315	A86	C25-C26-C27	-4.58	120.85	127.28
38	13	314	A86	C41-C32-C31	-4.58	106.37	110.47
38	12	317	A86	C25-C26-C27	-4.58	120.86	127.28
38	31	312	A86	C41-C32-C31	-4.57	106.38	110.47
38	32	316	A86	C41-C32-C31	-4.57	106.38	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	14	314	A86	C41-C32-C31	-4.56	106.39	110.47
38	14	315	A86	C25-C26-C27	-4.56	120.88	127.28
27	B	603	CLA	O2D-CGD-O1D	-4.56	114.97	123.85
38	33	314	A86	C41-C32-C31	-4.56	106.39	110.47
38	13	315	A86	C25-C26-C27	-4.55	120.90	127.28
38	31	313	A86	C25-C26-C27	-4.54	120.91	127.28
32	B	621	LHG	O4-P-O5	4.54	133.58	112.44
38	11	313	A86	C25-C26-C27	-4.54	120.92	127.28
32	b	621	LHG	O4-P-O5	4.54	133.54	112.44
38	34	316	A86	C25-C26-C27	-4.53	120.93	127.28
38	32	317	A86	C25-C26-C27	-4.52	120.93	127.28
32	a	408	LHG	O4-P-O5	4.51	133.44	112.44
32	A	408	LHG	O4-P-O5	4.51	133.43	112.44
36	d	404	PL9	C7-C3-C4	4.44	120.57	116.91
27	a	404	CLA	C3B-C4B-NB	-4.40	106.61	110.53
27	A	404	CLA	C3B-C4B-NB	-4.39	106.61	110.53
32	l	102	LHG	O4-P-O5	4.39	132.88	112.44
38	11	310	A86	C4-C5-C6	-4.39	121.12	127.28
32	L	101	LHG	O4-P-O5	4.39	132.85	112.44
38	13	312	A86	C4-C5-C6	-4.38	121.13	127.28
38	34	313	A86	C4-C5-C6	-4.37	121.14	127.28
38	33	312	A86	C4-C5-C6	-4.36	121.16	127.28
38	31	310	A86	C4-C5-C6	-4.36	121.17	127.28
38	32	314	A86	C4-C5-C6	-4.35	121.18	127.28
36	D	404	PL9	C7-C3-C4	4.33	120.48	116.91
38	12	314	A86	C4-C5-C6	-4.33	121.20	127.28
38	14	312	A86	C4-C5-C6	-4.33	121.21	127.28
30	l	101	SQD	O7-S-C6	4.31	113.18	106.76
32	l	103	LHG	O4-P-O5	4.29	132.42	112.44
32	L	102	LHG	O4-P-O5	4.29	132.40	112.44
30	L	103	SQD	O7-S-C6	4.25	113.11	106.76
29	B	617	BCR	C2-C1-C6	4.24	116.60	110.44
28	D	403	PHO	C2B-C1B-NB	-4.19	106.40	109.43
29	b	617	BCR	C2-C1-C6	4.19	116.52	110.44
28	d	403	PHO	C2B-C1B-NB	-4.19	106.41	109.43
39	32	302	LMU	C1B-O1B-C4'	-4.14	108.16	117.98
28	a	403	PHO	C2B-C1B-NB	-4.14	106.44	109.43
28	A	403	PHO	C2B-C1B-NB	-4.13	106.45	109.43
38	13	315	A86	C41-C32-C31	-4.13	106.78	110.47
38	13	312	A86	C25-C26-C27	-4.12	121.49	127.28
38	32	314	A86	C25-C26-C27	-4.11	121.51	127.28
29	c	519	BCR	C24-C23-C22	-4.11	120.15	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	520	BCR	C24-C23-C22	-4.11	120.15	126.23
38	14	312	A86	C25-C26-C27	-4.11	121.51	127.28
38	31	310	A86	C25-C26-C27	-4.11	121.51	127.28
38	11	310	A86	C25-C26-C27	-4.11	121.52	127.28
38	33	312	A86	C25-C26-C27	-4.11	121.52	127.28
38	34	313	A86	C25-C26-C27	-4.10	121.53	127.28
39	32	302	LMU	O1'-C1'-C2'	4.10	114.49	108.27
38	32	318	A86	C25-C24-C1	-4.09	115.14	126.36
38	13	316	A86	C25-C24-C1	-4.09	115.14	126.36
38	34	301	A86	C25-C24-C1	-4.09	115.16	126.36
38	12	314	A86	C25-C26-C27	-4.09	121.55	127.28
38	14	316	A86	C25-C24-C1	-4.08	115.17	126.36
38	33	316	A86	C25-C24-C1	-4.08	115.17	126.36
38	31	314	A86	C25-C24-C1	-4.08	115.18	126.36
38	34	316	A86	C41-C32-C31	-4.08	106.82	110.47
38	11	313	A86	C41-C32-C31	-4.08	106.83	110.47
38	14	301	A86	C25-C24-C1	-4.07	115.19	126.36
38	11	314	A86	C25-C24-C1	-4.07	115.20	126.36
38	33	315	A86	C41-C32-C31	-4.07	106.83	110.47
38	12	317	A86	C41-C32-C31	-4.07	106.83	110.47
38	14	315	A86	C41-C32-C31	-4.06	106.84	110.47
38	31	313	A86	C41-C32-C31	-4.06	106.84	110.47
38	32	317	A86	C41-C32-C31	-4.02	106.87	110.47
27	33	310	CLA	C2A-C1A-CHA	4.01	130.82	123.87
27	32	312	CLA	C2A-C1A-CHA	4.00	130.80	123.87
39	12	302	LMU	O1'-C1'-C2'	3.99	114.33	108.27
27	13	310	CLA	C2A-C1A-CHA	3.98	130.77	123.87
27	31	308	CLA	C2A-C1A-CHA	3.97	130.76	123.87
27	12	312	CLA	C2A-C1A-CHA	3.97	130.76	123.87
27	14	310	CLA	C2A-C1A-CHA	3.97	130.76	123.87
27	b	622	CLA	CBA-CAA-C2A	3.97	125.60	113.79
27	11	308	CLA	C2A-C1A-CHA	3.96	130.75	123.87
27	34	311	CLA	C2A-C1A-CHA	3.96	130.74	123.87
30	B	620	SQD	O9-S-O7	-3.96	100.95	113.82
30	b	620	SQD	O9-S-O7	-3.96	100.96	113.82
39	12	302	LMU	C1B-O1B-C4'	-3.95	108.62	117.98
29	M	101	BCR	C15-C16-C17	-3.92	115.49	123.52
27	B	622	CLA	CBA-CAA-C2A	3.92	125.46	113.79
38	13	312	A86	C12-C11-C13	3.91	122.35	116.00
38	33	312	A86	C41-C32-C31	-3.91	106.97	110.47
38	13	312	A86	C41-C32-C31	-3.90	106.98	110.47
35	C	518	DGD	O6D-C1D-O3G	-3.90	100.82	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	m	103	BCR	C15-C16-C17	-3.90	115.54	123.52
38	12	314	A86	C12-C11-C13	3.90	122.32	116.00
38	31	310	A86	C12-C11-C13	3.89	122.31	116.00
38	33	312	A86	C12-C11-C13	3.89	122.31	116.00
38	14	312	A86	C12-C11-C13	3.89	122.31	116.00
38	11	310	A86	C12-C11-C13	3.89	122.30	116.00
38	32	314	A86	C41-C32-C31	-3.89	107.00	110.47
38	34	313	A86	C12-C11-C13	3.88	122.30	116.00
35	c	518	DGD	O6D-C1D-O3G	-3.88	100.87	110.04
38	31	310	A86	C41-C32-C31	-3.88	107.00	110.47
38	34	313	A86	C41-C32-C31	-3.87	107.00	110.47
38	32	314	A86	C12-C11-C13	3.87	122.28	116.00
30	a	406	SQD	O47-C7-C8	3.85	119.80	111.48
38	14	312	A86	C41-C32-C31	-3.84	107.03	110.47
30	A	406	SQD	O47-C7-C8	3.84	119.79	111.48
38	12	314	A86	C41-C32-C31	-3.84	107.04	110.47
30	A	406	SQD	O9-S-O7	-3.82	101.39	113.82
30	a	406	SQD	O9-S-O7	-3.82	101.39	113.82
38	11	310	A86	C41-C32-C31	-3.82	107.06	110.47
27	b	622	CLA	CAA-C2A-C3A	-3.81	102.71	113.00
30	l	101	SQD	C4-C3-C2	3.81	117.51	110.83
36	d	404	PL9	C7-C3-C2	-3.80	118.91	123.39
35	h	102	DGD	C1D-C2D-C3D	-3.79	102.03	110.01
38	14	301	A86	C4-C5-C6	-3.79	121.97	127.28
38	11	314	A86	C4-C5-C6	-3.78	121.98	127.28
27	C	509	CLA	CMB-C2B-C1B	-3.78	119.67	125.42
35	H	102	DGD	C1D-C2D-C3D	-3.77	102.07	110.01
38	32	318	A86	C4-C5-C6	-3.77	121.99	127.28
27	C	511	CLA	CMB-C2B-C1B	-3.77	119.67	125.42
30	L	103	SQD	C4-C3-C2	3.77	117.45	110.83
27	33	306	CLA	CMB-C2B-C1B	-3.77	119.68	125.42
27	c	509	CLA	CMB-C2B-C1B	-3.77	119.69	125.42
27	B	622	CLA	CAA-C2A-C3A	-3.76	102.83	113.00
28	D	403	PHO	O1D-CGD-CBD	3.76	130.43	124.72
36	D	404	PL9	C7-C3-C2	-3.76	118.95	123.39
38	31	314	A86	C4-C5-C6	-3.76	122.00	127.28
27	c	511	CLA	CMB-C2B-C1B	-3.76	119.69	125.42
27	32	308	CLA	CMB-C2B-C1B	-3.76	119.69	125.42
38	33	316	A86	C4-C5-C6	-3.76	122.01	127.28
27	12	308	CLA	CMB-C2B-C1B	-3.75	119.70	125.42
38	33	314	A86	C25-C26-C27	-3.75	122.02	127.28
27	14	306	CLA	CMB-C2B-C1B	-3.75	119.71	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	13	306	CLA	CMB-C2B-C1B	-3.75	119.71	125.42
38	32	318	A86	C12-C11-C13	3.75	122.08	116.00
38	34	301	A86	C4-C5-C6	-3.74	122.03	127.28
30	a	406	SQD	O6-C1-C2	3.74	113.96	108.27
38	14	316	A86	C4-C5-C6	-3.74	122.03	127.28
38	11	314	A86	C12-C11-C13	3.74	122.06	116.00
38	14	301	A86	C12-C11-C13	3.74	122.06	116.00
38	31	314	A86	C12-C11-C13	3.74	122.06	116.00
38	12	316	A86	C25-C26-C27	-3.73	122.04	127.28
38	13	314	A86	C25-C26-C27	-3.73	122.05	127.28
30	b	620	SQD	O47-C7-C8	3.73	119.54	111.48
27	11	304	CLA	CMB-C2B-C1B	-3.73	119.75	125.42
27	31	304	CLA	CMB-C2B-C1B	-3.73	119.75	125.42
38	34	315	A86	C25-C26-C27	-3.73	122.05	127.28
38	34	301	A86	C12-C11-C13	3.72	122.04	116.00
38	32	316	A86	C25-C26-C27	-3.72	122.06	127.28
38	13	316	A86	C4-C5-C6	-3.72	122.06	127.28
38	33	316	A86	C12-C11-C13	3.72	122.03	116.00
28	d	403	PHO	O1D-CGD-CBD	3.72	130.37	124.72
27	A	404	CLA	O2D-CGD-O1D	-3.72	116.61	123.85
27	34	307	CLA	CMB-C2B-C1B	-3.72	119.76	125.42
38	11	312	A86	C25-C26-C27	-3.72	122.06	127.28
38	31	311	A86	C41-C32-C31	-3.72	107.14	110.47
38	13	316	A86	C12-C11-C13	3.72	122.03	116.00
27	a	404	CLA	O2D-CGD-O1D	-3.72	116.61	123.85
38	14	316	A86	C12-C11-C13	3.71	122.02	116.00
27	12	313	CLA	CAA-C2A-C3A	-3.71	102.97	113.00
30	L	103	SQD	O9-S-O7	-3.71	101.75	113.82
27	13	311	CLA	CAA-C2A-C3A	-3.71	102.97	113.00
38	14	314	A86	C25-C26-C27	-3.71	122.08	127.28
38	31	312	A86	C25-C26-C27	-3.71	122.08	127.28
38	32	315	A86	C41-C32-C31	-3.71	107.15	110.47
30	A	406	SQD	O6-C1-C2	3.71	113.90	108.27
38	34	314	A86	C41-C32-C31	-3.71	107.16	110.47
27	C	511	CLA	C3B-C4B-NB	-3.70	107.22	110.53
30	B	620	SQD	O47-C7-C8	3.70	119.49	111.48
38	12	315	A86	C41-C32-C31	-3.70	107.16	110.47
27	34	312	CLA	CAA-C2A-C3A	-3.70	103.00	113.00
30	l	101	SQD	O9-S-O7	-3.70	101.79	113.82
30	L	103	SQD	O47-C7-C8	3.70	119.48	111.48
27	c	511	CLA	C3B-C4B-NB	-3.69	107.23	110.53
38	33	313	A86	C41-C32-C31	-3.69	107.17	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	L	103	SQD	O5-C5-C4	3.69	116.35	109.70
27	31	309	CLA	CAA-C2A-C3A	-3.69	103.02	113.00
27	33	311	CLA	CAA-C2A-C3A	-3.69	103.02	113.00
27	11	309	CLA	CAA-C2A-C3A	-3.69	103.03	113.00
27	14	311	CLA	CAA-C2A-C3A	-3.69	103.03	113.00
38	14	313	A86	C41-C32-C31	-3.69	107.17	110.47
27	32	313	CLA	CAA-C2A-C3A	-3.69	103.04	113.00
38	11	311	A86	C41-C32-C31	-3.68	107.17	110.47
27	34	304	CLA	C1-C2-C3	-3.68	120.17	126.20
27	32	305	CLA	C1-C2-C3	-3.67	120.18	126.20
27	31	301	CLA	C1-C2-C3	-3.67	120.18	126.20
27	14	303	CLA	C1-C2-C3	-3.67	120.19	126.20
30	l	101	SQD	O47-C7-C8	3.67	119.42	111.48
27	13	303	CLA	C1-C2-C3	-3.67	120.19	126.20
38	13	313	A86	C41-C32-C31	-3.66	107.20	110.47
27	33	303	CLA	C1-C2-C3	-3.66	120.20	126.20
27	12	305	CLA	C1-C2-C3	-3.66	120.20	126.20
38	14	314	A86	C26-C25-C24	-3.66	112.60	123.20
30	A	406	SQD	O5-C5-C4	3.65	116.28	109.70
30	l	101	SQD	O5-C5-C4	3.65	116.28	109.70
38	31	312	A86	C26-C25-C24	-3.65	112.62	123.20
38	12	316	A86	C26-C25-C24	-3.65	112.62	123.20
38	32	316	A86	C26-C25-C24	-3.65	112.62	123.20
38	13	314	A86	C26-C25-C24	-3.65	112.63	123.20
38	34	315	A86	C26-C25-C24	-3.65	112.64	123.20
38	33	314	A86	C26-C25-C24	-3.64	112.65	123.20
30	a	406	SQD	O5-C5-C4	3.64	116.26	109.70
38	11	312	A86	C26-C25-C24	-3.64	112.65	123.20
27	11	301	CLA	C1-C2-C3	-3.64	120.23	126.20
38	11	310	A86	C34-O4-C38	-3.64	111.42	117.85
38	34	313	A86	C34-O4-C38	-3.63	111.43	117.85
38	13	312	A86	C34-O4-C38	-3.63	111.44	117.85
38	31	310	A86	C34-O4-C38	-3.63	111.44	117.85
38	32	314	A86	C34-O4-C38	-3.62	111.45	117.85
38	12	314	A86	C34-O4-C38	-3.62	111.46	117.85
35	J	101	DGD	O6D-C1D-O3G	-3.61	101.50	110.04
38	14	312	A86	C34-O4-C38	-3.61	111.47	117.85
38	33	312	A86	C34-O4-C38	-3.61	111.47	117.85
35	j	101	DGD	O6D-C1D-O3G	-3.59	101.56	110.04
28	D	403	PHO	CMB-C2B-C3B	3.57	131.82	124.68
28	d	403	PHO	CMB-C2B-C3B	3.57	131.82	124.68
35	J	101	DGD	O3G-C3G-C2G	-3.57	102.15	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	14	301	A86	C36-C31-C32	-3.56	116.16	119.70
35	j	101	DGD	O3G-C3G-C2G	-3.55	102.19	110.82
38	34	301	A86	C36-C31-C32	-3.55	116.18	119.70
38	32	318	A86	C36-C31-C32	-3.54	116.18	119.70
38	13	316	A86	C36-C31-C32	-3.54	116.18	119.70
29	c	515	BCR	C15-C16-C17	-3.54	116.28	123.52
38	14	316	A86	C36-C31-C32	-3.54	116.19	119.70
29	C	515	BCR	C15-C16-C17	-3.53	116.29	123.52
27	d	401	CLA	C3B-C4B-NB	-3.53	107.38	110.53
38	31	314	A86	C36-C31-C32	-3.53	116.19	119.70
29	C	515	BCR	C11-C10-C9	-3.52	122.33	127.28
38	12	316	A86	C3-C2-C1	-3.52	122.34	127.28
27	d	406	CLA	O2D-CGD-O1D	-3.52	116.99	123.85
38	33	314	A86	C3-C2-C1	-3.52	122.34	127.28
38	11	316	A86	C4-C3-C2	-3.52	116.32	123.52
38	33	316	A86	C36-C31-C32	-3.52	116.20	119.70
38	13	317	A86	C4-C3-C2	-3.52	116.32	123.52
38	11	314	A86	C36-C31-C32	-3.51	116.21	119.70
29	c	515	BCR	C11-C10-C9	-3.51	122.35	127.28
38	13	314	A86	C3-C2-C1	-3.51	122.35	127.28
27	D	401	CLA	C3B-C4B-NB	-3.51	107.40	110.53
33	d	408	LMG	C1-C2-C3	-3.51	102.63	110.01
38	31	316	A86	C4-C3-C2	-3.51	116.34	123.52
38	11	312	A86	C3-C2-C1	-3.51	122.36	127.28
29	b	617	BCR	C24-C23-C22	-3.51	121.05	126.23
27	D	406	CLA	O2D-CGD-O1D	-3.50	117.03	123.85
38	14	314	A86	C36-C31-C32	-3.50	116.22	119.70
38	34	303	A86	C4-C3-C2	-3.50	116.35	123.52
38	12	304	A86	C4-C3-C2	-3.50	116.35	123.52
38	32	304	A86	C4-C3-C2	-3.50	116.35	123.52
38	33	302	A86	C4-C3-C2	-3.50	116.35	123.52
29	C	520	BCR	C15-C16-C17	-3.50	116.36	123.52
38	13	314	A86	C36-C31-C32	-3.50	116.22	119.70
29	B	617	BCR	C24-C23-C22	-3.50	121.06	126.23
38	14	314	A86	C3-C2-C1	-3.50	122.37	127.28
33	D	408	LMG	C1-C2-C3	-3.50	102.65	110.01
38	32	316	A86	C3-C2-C1	-3.50	122.37	127.28
29	a	405	BCR	C15-C16-C17	-3.50	116.37	123.52
38	34	315	A86	C36-C31-C32	-3.50	116.23	119.70
27	33	303	CLA	CHB-C4A-NA	3.50	129.44	124.40
29	c	519	BCR	C15-C16-C17	-3.50	116.37	123.52
27	12	305	CLA	CHB-C4A-NA	3.49	129.44	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	32	305	CLA	CHB-C4A-NA	3.49	129.44	124.40
27	c	505	CLA	CHB-C4A-NA	3.49	129.44	124.40
29	A	405	BCR	C15-C16-C17	-3.49	116.38	123.52
38	11	312	A86	C36-C31-C32	-3.49	116.23	119.70
38	33	314	A86	C36-C31-C32	-3.49	116.24	119.70
27	C	511	CLA	CMB-C2B-C3B	3.49	134.75	126.55
38	31	312	A86	C36-C31-C32	-3.48	116.24	119.70
38	34	315	A86	C3-C2-C1	-3.48	122.39	127.28
27	13	303	CLA	CHB-C4A-NA	3.48	129.42	124.40
38	13	302	A86	C4-C3-C2	-3.48	116.40	123.52
38	34	316	A86	C10-C9-C8	-3.48	113.13	123.20
38	11	316	A86	C3-C2-C1	-3.48	122.40	127.28
38	31	316	A86	C3-C2-C1	-3.48	122.40	127.28
38	31	313	A86	C10-C9-C8	-3.47	113.14	123.20
27	c	511	CLA	CMB-C2B-C3B	3.47	134.72	126.55
38	31	312	A86	C3-C2-C1	-3.47	122.41	127.28
38	11	313	A86	C10-C9-C8	-3.47	113.14	123.20
27	C	505	CLA	CHB-C4A-NA	3.47	129.41	124.40
38	14	315	A86	C10-C9-C8	-3.47	113.15	123.20
27	11	301	CLA	CHB-C4A-NA	3.47	129.41	124.40
38	12	304	A86	C3-C2-C1	-3.47	122.42	127.28
38	34	303	A86	C3-C2-C1	-3.47	122.42	127.28
38	13	317	A86	C3-C2-C1	-3.46	122.42	127.28
27	31	301	CLA	CHB-C4A-NA	3.46	129.40	124.40
38	32	317	A86	C10-C9-C8	-3.46	113.17	123.20
38	33	315	A86	C10-C9-C8	-3.46	113.17	123.20
27	C	512	CLA	C3B-C4B-NB	-3.46	107.44	110.53
38	33	302	A86	C3-C2-C1	-3.46	122.43	127.28
38	32	316	A86	C36-C31-C32	-3.46	116.26	119.70
38	13	302	A86	C3-C2-C1	-3.46	122.43	127.28
38	31	311	A86	C36-C31-C32	-3.45	116.27	119.70
27	14	303	CLA	CHB-C4A-NA	3.45	129.38	124.40
38	12	317	A86	C10-C9-C8	-3.45	113.20	123.20
27	34	304	CLA	CHB-C4A-NA	3.45	129.38	124.40
38	13	315	A86	C10-C9-C8	-3.44	113.22	123.20
38	12	316	A86	C36-C31-C32	-3.44	116.28	119.70
27	c	512	CLA	C3B-C4B-NB	-3.44	107.46	110.53
38	32	304	A86	C3-C2-C1	-3.43	122.47	127.28
35	c	518	DGD	O3G-C3G-C2G	-3.42	102.49	110.82
38	32	315	A86	C36-C31-C32	-3.42	116.30	119.70
38	33	313	A86	C36-C31-C32	-3.42	116.30	119.70
35	C	518	DGD	O3G-C3G-C2G	-3.42	102.50	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	14	313	A86	C36-C31-C32	-3.42	116.30	119.70
38	12	315	A86	C36-C31-C32	-3.41	116.31	119.70
27	b	610	CLA	O2D-CGD-O1D	-3.41	117.22	123.85
38	11	316	A86	C40-C32-C31	-3.40	107.42	110.47
27	B	610	CLA	O2D-CGD-O1D	-3.40	117.22	123.85
38	34	314	A86	C36-C31-C32	-3.40	116.32	119.70
38	11	311	A86	C36-C31-C32	-3.39	116.33	119.70
38	13	313	A86	C36-C31-C32	-3.39	116.33	119.70
38	11	313	A86	C12-C11-C13	3.39	121.49	116.00
38	33	316	A86	C10-C9-C8	-3.39	113.39	123.20
38	31	313	A86	C12-C11-C13	3.39	121.49	116.00
38	34	301	A86	C10-C9-C8	-3.38	113.39	123.20
38	13	315	A86	C12-C11-C13	3.38	121.48	116.00
38	13	316	A86	C10-C9-C8	-3.38	113.40	123.20
27	b	614	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
38	14	315	A86	C12-C11-C13	3.38	121.48	116.00
38	14	301	A86	C10-C9-C8	-3.38	113.41	123.20
27	B	614	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
38	32	318	A86	C10-C9-C8	-3.38	113.41	123.20
38	14	316	A86	C10-C9-C8	-3.38	113.42	123.20
38	12	317	A86	C12-C11-C13	3.38	121.47	116.00
38	32	304	A86	C40-C32-C31	-3.37	107.45	110.47
38	34	316	A86	C12-C11-C13	3.37	121.47	116.00
38	11	314	A86	C10-C9-C8	-3.37	113.43	123.20
38	33	315	A86	C12-C11-C13	3.37	121.46	116.00
38	13	315	A86	C3-C4-C5	-3.37	116.63	123.52
30	l	101	SQD	O9-S-C6	3.37	111.78	106.76
27	b	613	CLA	CMB-C2B-C1B	-3.37	120.30	125.42
38	32	317	A86	C12-C11-C13	3.36	121.46	116.00
38	31	316	A86	C40-C32-C31	-3.36	107.46	110.47
38	31	314	A86	C10-C9-C8	-3.36	113.46	123.20
29	a	405	BCR	C15-C14-C13	-3.36	122.57	127.28
38	12	317	A86	C3-C4-C5	-3.35	116.66	123.52
38	32	317	A86	C3-C4-C5	-3.35	116.66	123.52
38	14	315	A86	C3-C4-C5	-3.35	116.66	123.52
38	13	313	A86	C12-C11-C13	3.35	121.43	116.00
38	34	316	A86	C3-C4-C5	-3.35	116.67	123.52
38	34	314	A86	C12-C11-C13	3.35	121.43	116.00
38	33	302	A86	C40-C32-C31	-3.35	107.48	110.47
27	c	514	CLA	CHB-C4A-NA	3.34	129.22	124.40
38	33	315	A86	C3-C4-C5	-3.34	116.68	123.52
27	B	613	CLA	CMB-C2B-C1B	-3.34	120.33	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	405	BCR	C15-C14-C13	-3.34	122.60	127.28
38	11	313	A86	C3-C4-C5	-3.34	116.69	123.52
38	13	317	A86	C40-C32-C31	-3.34	107.49	110.47
38	13	302	A86	C40-C32-C31	-3.33	107.49	110.47
30	L	103	SQD	O9-S-C6	3.33	111.73	106.76
38	12	304	A86	C40-C32-C31	-3.33	107.49	110.47
38	11	311	A86	C12-C11-C13	3.33	121.40	116.00
38	31	313	A86	C3-C4-C5	-3.33	116.71	123.52
27	C	514	CLA	CHB-C4A-NA	3.33	129.21	124.40
38	32	315	A86	C12-C11-C13	3.33	121.40	116.00
38	34	303	A86	C40-C32-C31	-3.33	107.50	110.47
38	31	311	A86	C12-C11-C13	3.32	121.39	116.00
27	13	305	CLA	CAA-C2A-C3A	-3.32	104.03	113.00
38	14	313	A86	C12-C11-C13	3.31	121.37	116.00
38	12	315	A86	C12-C11-C13	3.31	121.37	116.00
27	11	303	CLA	CAA-C2A-C3A	-3.31	104.06	113.00
27	12	307	CLA	CAA-C2A-C3A	-3.31	104.07	113.00
27	32	307	CLA	CAA-C2A-C3A	-3.30	104.08	113.00
27	14	305	CLA	CAA-C2A-C3A	-3.30	104.08	113.00
27	31	303	CLA	CAA-C2A-C3A	-3.30	104.08	113.00
30	B	620	SQD	O7-S-C6	3.30	111.68	106.76
38	33	313	A86	C12-C11-C13	3.29	121.34	116.00
27	33	305	CLA	CAA-C2A-C3A	-3.29	104.11	113.00
30	l	101	SQD	C1-O5-C5	3.29	120.14	113.72
29	a	405	BCR	C24-C23-C22	-3.29	121.37	126.23
35	H	102	DGD	O3G-C3G-C2G	-3.29	102.82	110.82
27	34	306	CLA	CAA-C2A-C3A	-3.29	104.12	113.00
35	h	102	DGD	O3G-C3G-C2G	-3.28	102.84	110.82
29	A	405	BCR	C24-C23-C22	-3.28	121.38	126.23
30	L	103	SQD	C1-O5-C5	3.28	120.12	113.72
27	B	612	CLA	CHB-C4A-NA	3.28	129.13	124.40
30	b	620	SQD	O7-S-C6	3.27	111.64	106.76
27	M	102	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
27	14	304	CLA	CHB-C4A-NA	3.27	129.12	124.40
27	b	601	CLA	CHB-C4A-NA	3.27	129.12	124.40
39	12	302	LMU	C3'-C4'-C5'	3.27	118.18	110.93
27	b	612	CLA	CHB-C4A-NA	3.27	129.12	124.40
27	13	304	CLA	CHB-C4A-NA	3.27	129.12	124.40
27	33	304	CLA	CHB-C4A-NA	3.27	129.12	124.40
39	32	302	LMU	O5B-C5B-C4B	3.27	115.59	109.70
27	B	601	CLA	CHB-C4A-NA	3.26	129.11	124.40
27	33	303	CLA	C3B-C4B-NB	-3.26	107.62	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	14	309	CLA	CHB-C4A-NA	3.26	129.11	124.40
27	34	305	CLA	CHB-C4A-NA	3.26	129.11	124.40
27	32	311	CLA	CHB-C4A-NA	3.26	129.10	124.40
27	B	604	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
27	m	101	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
27	11	307	CLA	CHB-C4A-NA	3.25	129.09	124.40
27	b	604	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
27	D	405	CLA	CAA-C2A-C3A	-3.25	104.22	113.00
27	d	402	CLA	C3B-C4B-NB	-3.25	107.63	110.53
27	12	306	CLA	CHB-C4A-NA	3.24	129.08	124.40
27	13	309	CLA	CHB-C4A-NA	3.24	129.08	124.40
27	B	608	CLA	O2D-CGD-O1D	-3.24	117.53	123.85
27	C	506	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
27	31	302	CLA	CHB-C4A-NA	3.24	129.08	124.40
27	d	405	CLA	CAA-C2A-C3A	-3.24	104.24	113.00
27	c	506	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
39	32	302	LMU	C3'-C4'-C5'	3.24	118.11	110.93
27	31	307	CLA	CHB-C4A-NA	3.24	129.07	124.40
27	32	306	CLA	CHB-C4A-NA	3.24	129.07	124.40
27	34	310	CLA	CHB-C4A-NA	3.24	129.07	124.40
28	a	403	PHO	O1D-CGD-CBD	3.24	129.63	124.72
35	C	517	DGD	O6D-C1D-O3G	-3.24	102.39	110.04
27	14	303	CLA	C3B-C4B-NB	-3.24	107.64	110.53
38	34	303	A86	C36-C31-C32	-3.23	116.49	119.70
27	C	507	CLA	CMB-C2B-C1B	-3.23	120.50	125.42
27	33	309	CLA	CHB-C4A-NA	3.23	129.06	124.40
27	b	608	CLA	O2D-CGD-O1D	-3.22	117.57	123.85
27	11	302	CLA	CHB-C4A-NA	3.22	129.05	124.40
27	C	512	CLA	CHB-C4A-NA	3.22	129.05	124.40
27	a	404	CLA	CHB-C4A-NA	3.21	129.04	124.40
27	12	312	CLA	CHB-C4A-NA	3.21	129.04	124.40
27	12	305	CLA	C3B-C4B-NB	-3.21	107.67	110.53
28	A	403	PHO	O1D-CGD-CBD	3.21	129.59	124.72
39	12	302	LMU	O5B-C5B-C4B	3.21	115.48	109.70
27	A	404	CLA	CHB-C4A-NA	3.21	129.03	124.40
27	11	301	CLA	C3B-C4B-NB	-3.20	107.67	110.53
27	34	304	CLA	C3B-C4B-NB	-3.20	107.67	110.53
38	13	302	A86	C36-C31-C32	-3.20	116.52	119.70
27	C	508	CLA	CHB-C4A-NA	3.20	129.02	124.40
27	b	610	CLA	C3B-C4B-NB	-3.20	107.67	110.53
27	c	507	CLA	CMB-C2B-C1B	-3.20	120.54	125.42
35	c	517	DGD	O6D-C1D-O3G	-3.20	102.48	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	12	311	CLA	CHB-C4A-NA	3.20	129.02	124.40
27	32	305	CLA	C3B-C4B-NB	-3.20	107.67	110.53
38	11	316	A86	C36-C31-C32	-3.20	116.52	119.70
27	D	402	CLA	C3B-C4B-NB	-3.20	107.68	110.53
27	13	310	CLA	CHB-C4A-NA	3.20	129.01	124.40
27	c	514	CLA	CMB-C2B-C1B	-3.20	120.55	125.42
27	31	308	CLA	CHB-C4A-NA	3.19	129.01	124.40
27	12	311	CLA	C1-C2-C3	-3.19	120.97	126.20
36	D	407	PL9	C7-C8-C9	-3.19	121.34	126.83
27	33	309	CLA	C1-C2-C3	-3.19	120.97	126.20
38	12	304	A86	C36-C31-C32	-3.19	116.53	119.70
38	31	316	A86	C36-C31-C32	-3.19	116.53	119.70
27	C	514	CLA	CMB-C2B-C1B	-3.19	120.57	125.42
27	31	307	CLA	C1-C2-C3	-3.18	120.98	126.20
29	B	623	BCR	C7-C8-C9	-3.18	121.52	126.23
27	b	607	CLA	CMB-C2B-C1B	-3.18	120.57	125.42
27	c	512	CLA	CHB-C4A-NA	3.18	128.99	124.40
36	d	407	PL9	C7-C8-C9	-3.18	121.35	126.83
38	33	302	A86	C36-C31-C32	-3.18	116.54	119.70
27	32	312	CLA	CHB-C4A-NA	3.18	128.99	124.40
38	32	304	A86	C36-C31-C32	-3.18	116.54	119.70
27	11	308	CLA	CHB-C4A-NA	3.18	128.99	124.40
27	14	309	CLA	C3B-C4B-NB	-3.18	107.69	110.53
27	w	103	CLA	O2D-CGD-O1D	-3.18	117.67	123.85
27	31	301	CLA	C3B-C4B-NB	-3.17	107.70	110.53
27	B	609	CLA	CHB-C4A-NA	3.17	128.98	124.40
38	13	317	A86	C36-C31-C32	-3.17	116.55	119.70
27	33	309	CLA	C3B-C4B-NB	-3.17	107.70	110.53
27	14	310	CLA	CHB-C4A-NA	3.17	128.97	124.40
27	13	303	CLA	C3B-C4B-NB	-3.17	107.70	110.53
27	c	508	CLA	CHB-C4A-NA	3.16	128.97	124.40
27	W	103	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
27	33	310	CLA	CHB-C4A-NA	3.16	128.97	124.40
32	A	408	LHG	O8-C23-C24	3.16	121.47	111.83
32	a	408	LHG	O8-C23-C24	3.16	121.46	111.83
27	b	608	CLA	CHB-C4A-NA	3.16	128.96	124.40
27	34	310	CLA	C1-C2-C3	-3.16	121.03	126.20
27	11	307	CLA	C1-C2-C3	-3.16	121.03	126.20
27	B	608	CLA	C3B-C4B-NB	-3.16	107.71	110.53
27	b	609	CLA	CHB-C4A-NA	3.15	128.95	124.40
37	v	201	HEM	CAC-C3C-C4C	3.15	132.35	124.82
27	B	608	CLA	CHB-C4A-NA	3.15	128.95	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	31	307	CLA	C3B-C4B-NB	-3.15	107.72	110.53
27	32	311	CLA	C1-C2-C3	-3.15	121.04	126.20
27	34	311	CLA	CHB-C4A-NA	3.15	128.94	124.40
29	A	409	BCR	C11-C10-C9	-3.15	122.86	127.28
39	32	302	LMU	O5'-C5'-C4'	3.14	116.22	109.72
27	14	309	CLA	C1-C2-C3	-3.14	121.05	126.20
27	13	309	CLA	C1-C2-C3	-3.14	121.05	126.20
27	11	307	CLA	C3B-C4B-NB	-3.14	107.72	110.53
27	32	311	CLA	C3B-C4B-NB	-3.14	107.73	110.53
29	a	409	BCR	C11-C10-C9	-3.14	122.87	127.28
37	V	201	HEM	CAC-C3C-C4C	3.14	132.31	124.82
27	B	605	CLA	CHB-C4A-NA	3.14	128.93	124.40
27	B	607	CLA	CMB-C2B-C1B	-3.14	120.64	125.42
27	B	610	CLA	C3B-C4B-NB	-3.13	107.74	110.53
27	b	601	CLA	C3B-C4B-NB	-3.13	107.74	110.53
27	13	309	CLA	C3B-C4B-NB	-3.13	107.74	110.53
27	b	608	CLA	C3B-C4B-NB	-3.12	107.75	110.53
27	Z	102	CLA	C3B-C4B-NB	-3.12	107.75	110.53
27	B	612	CLA	C3B-C4B-NB	-3.11	107.75	110.53
27	b	605	CLA	CHB-C4A-NA	3.11	128.89	124.40
31	a	407	BCT	O3-C-O1	-3.11	111.72	119.68
27	12	311	CLA	C3B-C4B-NB	-3.11	107.75	110.53
27	34	310	CLA	C3B-C4B-NB	-3.11	107.76	110.53
27	14	310	CLA	CAA-C2A-C1A	3.11	122.15	111.97
27	D	406	CLA	C3B-C4B-NB	-3.11	107.76	110.53
27	13	310	CLA	CAA-C2A-C1A	3.10	122.14	111.97
31	A	407	BCT	O3-C-O1	-3.10	111.74	119.68
27	34	311	CLA	CAA-C2A-C1A	3.10	122.13	111.97
27	11	308	CLA	CAA-C2A-C1A	3.10	122.13	111.97
29	c	515	BCR	C24-C23-C22	-3.10	121.65	126.23
27	32	312	CLA	CAA-C2A-C1A	3.10	122.12	111.97
30	A	406	SQD	O48-C23-C24	3.09	121.27	111.83
27	33	310	CLA	CAA-C2A-C1A	3.09	122.11	111.97
27	12	312	CLA	CAA-C2A-C1A	3.09	122.11	111.97
30	a	406	SQD	O48-C23-C24	3.09	121.26	111.83
27	b	622	CLA	CAA-C2A-C1A	3.09	122.11	111.97
27	C	510	CLA	CMB-C2B-C1B	-3.09	120.71	125.42
27	31	308	CLA	CAA-C2A-C1A	3.09	122.10	111.97
27	c	505	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
27	c	508	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
29	b	616	BCR	C15-C14-C13	-3.08	122.95	127.28
32	B	621	LHG	O8-C23-C24	3.08	121.24	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	b	621	LHG	O8-C23-C24	3.08	121.23	111.83
27	z	102	CLA	C3B-C4B-NB	-3.08	107.78	110.53
27	C	512	CLA	CAA-CBA-CGA	-3.08	104.47	113.21
27	c	512	CLA	CAA-CBA-CGA	-3.08	104.47	113.21
27	33	306	CLA	CHB-C4A-NA	3.08	128.84	124.40
38	33	314	A86	C12-C11-C13	3.08	120.99	116.00
27	31	307	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
27	33	305	CLA	CBA-CAA-C2A	3.07	122.93	113.79
27	c	507	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
39	12	302	LMU	O5'-C5'-C4'	3.07	116.07	109.72
29	B	616	BCR	C15-C14-C13	-3.07	122.97	127.28
27	c	510	CLA	CMB-C2B-C1B	-3.07	120.75	125.42
27	d	406	CLA	C3B-C4B-NB	-3.06	107.80	110.53
29	C	515	BCR	C24-C23-C22	-3.06	121.70	126.23
38	12	316	A86	C12-C11-C13	3.06	120.96	116.00
27	C	505	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
27	C	508	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
27	11	307	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
27	31	304	CLA	CHB-C4A-NA	3.05	128.81	124.40
27	12	307	CLA	CBA-CAA-C2A	3.05	122.88	113.79
27	34	306	CLA	CBA-CAA-C2A	3.05	122.88	113.79
27	14	305	CLA	CBA-CAA-C2A	3.05	122.87	113.79
27	C	507	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
27	11	304	CLA	C2A-C1A-CHA	3.05	129.16	123.87
27	W	102	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
27	32	307	CLA	CBA-CAA-C2A	3.05	122.86	113.79
27	33	309	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
27	13	305	CLA	CBA-CAA-C2A	3.05	122.86	113.79
27	b	612	CLA	C3B-C4B-NB	-3.05	107.81	110.53
38	34	315	A86	C12-C11-C13	3.05	120.94	116.00
38	32	316	A86	C12-C11-C13	3.05	120.94	116.00
38	11	312	A86	C12-C11-C13	3.04	120.94	116.00
29	c	516	BCR	C11-C10-C9	-3.04	123.01	127.28
27	11	303	CLA	CBA-CAA-C2A	3.04	122.85	113.79
27	12	308	CLA	CHB-C4A-NA	3.04	128.79	124.40
29	C	516	BCR	C11-C10-C9	-3.04	123.01	127.28
27	b	613	CLA	CMB-C2B-C3B	3.04	133.71	126.55
38	13	314	A86	C12-C11-C13	3.04	120.93	116.00
27	b	614	CLA	O2D-CGD-CBD	3.04	116.55	111.23
27	B	614	CLA	O2D-CGD-CBD	3.04	116.55	111.23
27	12	308	CLA	CMB-C2B-C3B	3.04	133.70	126.55
30	A	406	SQD	O9-S-C6	3.04	111.30	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	12	311	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
27	B	601	CLA	C3B-C4B-NB	-3.04	107.82	110.53
27	31	303	CLA	CBA-CAA-C2A	3.04	122.83	113.79
38	14	314	A86	C12-C11-C13	3.04	120.93	116.00
27	B	622	CLA	CAA-C2A-C1A	3.04	121.93	111.97
27	14	306	CLA	CHB-C4A-NA	3.04	128.78	124.40
27	32	311	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
27	w	102	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
38	11	313	A86	C25-C24-C1	-3.03	118.04	126.36
27	13	309	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
27	13	311	CLA	C3B-C4B-NB	-3.03	107.82	110.53
30	a	406	SQD	O9-S-C6	3.03	111.28	106.76
38	12	317	A86	C25-C24-C1	-3.03	118.05	126.36
38	31	312	A86	C12-C11-C13	3.03	120.92	116.00
27	b	606	CLA	C1-C2-C3	-3.03	121.23	126.20
38	14	313	A86	C34-O4-C38	-3.03	112.49	117.85
28	D	403	PHO	C3B-C4B-NB	-3.03	105.49	107.46
27	34	310	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
27	14	306	CLA	CMB-C2B-C3B	3.03	133.67	126.55
38	33	315	A86	C25-C24-C1	-3.03	118.06	126.36
38	33	313	A86	C34-O4-C38	-3.03	112.50	117.85
38	13	315	A86	C25-C24-C1	-3.03	118.06	126.36
38	34	314	A86	C34-O4-C38	-3.03	112.50	117.85
27	32	308	CLA	CMB-C2B-C3B	3.03	133.67	126.55
29	b	623	BCR	C7-C8-C9	-3.03	121.76	126.23
30	l	101	SQD	C3-C4-C5	3.03	115.72	110.23
38	11	311	A86	C34-O4-C38	-3.03	112.50	117.85
38	14	315	A86	C25-C24-C1	-3.02	118.07	126.36
27	13	306	CLA	CMB-C2B-C3B	3.02	133.66	126.55
38	31	311	A86	C34-O4-C38	-3.02	112.51	117.85
35	C	517	DGD	C1D-C2D-C3D	-3.02	103.65	110.01
27	32	308	CLA	CHB-C4A-NA	3.02	128.76	124.40
38	31	313	A86	C25-C24-C1	-3.02	118.08	126.36
27	32	308	CLA	C2A-C1A-CHA	3.02	129.11	123.87
27	33	306	CLA	CMB-C2B-C3B	3.02	133.66	126.55
38	32	317	A86	C25-C24-C1	-3.02	118.08	126.36
27	12	308	CLA	C2A-C1A-CHA	3.02	129.11	123.87
27	11	304	CLA	CHB-C4A-NA	3.02	128.76	124.40
38	34	316	A86	C25-C24-C1	-3.02	118.08	126.36
38	12	317	A86	C36-C31-C32	-3.02	116.70	119.70
38	13	313	A86	C34-O4-C38	-3.02	112.52	117.85
27	14	309	CLA	O2D-CGD-O1D	-3.02	117.97	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	11	304	CLA	CMB-C2B-C3B	3.02	133.65	126.55
27	33	306	CLA	C2A-C1A-CHA	3.02	129.10	123.87
27	34	307	CLA	CMB-C2B-C3B	3.02	133.64	126.55
38	12	315	A86	C34-O4-C38	-3.02	112.52	117.85
27	34	307	CLA	CHB-C4A-NA	3.02	128.75	124.40
35	C	518	DGD	CDB-CCB-CBB	-3.01	99.13	114.37
30	L	103	SQD	C3-C4-C5	3.01	115.70	110.23
38	32	315	A86	C34-O4-C38	-3.01	112.52	117.85
27	B	613	CLA	CMB-C2B-C3B	3.01	133.64	126.55
35	c	518	DGD	CDB-CCB-CBB	-3.01	99.14	114.37
38	33	315	A86	C7-C6-C8	3.01	122.69	118.09
27	14	306	CLA	C2A-C1A-CHA	3.01	129.10	123.87
29	B	623	BCR	C11-C10-C9	-3.01	123.05	127.28
38	13	315	A86	C36-C31-C32	-3.01	116.71	119.70
27	13	306	CLA	C2A-C1A-CHA	3.01	129.09	123.87
27	34	307	CLA	C2A-C1A-CHA	3.01	129.09	123.87
27	c	508	CLA	C2A-C1A-CHA	3.01	129.09	123.87
38	14	315	A86	C7-C6-C8	3.01	122.69	118.09
27	C	502	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
27	31	304	CLA	C2A-C1A-CHA	3.01	129.09	123.87
29	C	516	BCR	C15-C16-C17	-3.01	117.37	123.52
27	31	304	CLA	CMB-C2B-C3B	3.01	133.62	126.55
35	c	517	DGD	O5D-C6D-C5D	-3.00	102.65	109.42
35	c	517	DGD	C1D-C2D-C3D	-3.00	103.69	110.01
29	A	405	BCR	C11-C10-C9	-3.00	123.07	127.28
38	31	313	A86	C7-C6-C8	3.00	122.67	118.09
38	32	317	A86	C36-C31-C32	-3.00	116.72	119.70
27	13	306	CLA	CHB-C4A-NA	3.00	128.73	124.40
38	11	313	A86	C36-C31-C32	-3.00	116.72	119.70
38	14	313	A86	C3-C4-C5	-2.99	117.40	123.52
38	13	313	A86	C3-C4-C5	-2.99	117.40	123.52
38	11	311	A86	C3-C4-C5	-2.99	117.40	123.52
27	B	622	CLA	C3B-C4B-NB	-2.99	107.86	110.53
29	c	516	BCR	C15-C16-C17	-2.99	117.41	123.52
38	32	315	A86	C3-C4-C5	-2.99	117.41	123.52
33	b	619	LMG	O6-C1-O1	-2.99	102.99	110.04
38	32	317	A86	C7-C6-C8	2.98	122.65	118.09
33	B	619	LMG	O6-C1-O1	-2.98	102.99	110.04
27	B	606	CLA	C1-C2-C3	-2.98	121.31	126.20
38	12	317	A86	C7-C6-C8	2.98	122.64	118.09
38	33	313	A86	C3-C4-C5	-2.98	117.42	123.52
38	31	311	A86	C3-C4-C5	-2.98	117.42	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	13	315	A86	C7-C6-C8	2.98	122.64	118.09
38	14	315	A86	C36-C31-C32	-2.98	116.74	119.70
27	34	312	CLA	C3B-C4B-NB	-2.98	107.87	110.53
38	34	314	A86	C3-C4-C5	-2.98	117.42	123.52
27	C	508	CLA	C2A-C1A-CHA	2.98	129.03	123.87
38	11	313	A86	C7-C6-C8	2.98	122.64	118.09
38	12	315	A86	C3-C4-C5	-2.98	117.43	123.52
27	32	313	CLA	C3B-C4B-NB	-2.98	107.87	110.53
38	34	316	A86	C36-C31-C32	-2.97	116.75	119.70
27	c	502	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
27	d	402	CLA	CHB-C4A-NA	2.96	128.68	124.40
35	C	517	DGD	O5D-C6D-C5D	-2.96	102.74	109.42
27	12	313	CLA	C3B-C4B-NB	-2.96	107.89	110.53
35	J	101	DGD	O2D-C2D-C1D	-2.96	103.03	110.08
27	33	311	CLA	C3B-C4B-NB	-2.96	107.89	110.53
27	d	406	CLA	CHB-C4A-NA	2.96	128.67	124.40
38	31	313	A86	C36-C31-C32	-2.95	116.77	119.70
27	b	614	CLA	CHB-C4A-NA	2.95	128.66	124.40
38	34	316	A86	C7-C6-C8	2.95	122.60	118.09
27	14	311	CLA	C3B-C4B-NB	-2.95	107.90	110.53
28	d	403	PHO	C3B-C4B-NB	-2.95	105.54	107.46
29	z	101	BCR	C24-C23-C22	-2.94	121.88	126.23
35	j	101	DGD	O2D-C2D-C1D	-2.94	103.07	110.08
29	a	405	BCR	C11-C10-C9	-2.94	123.15	127.28
27	D	402	CLA	CHB-C4A-NA	2.94	128.64	124.40
27	31	309	CLA	C3B-C4B-NB	-2.94	107.91	110.53
38	31	314	A86	C41-C32-C31	-2.94	107.84	110.47
27	D	406	CLA	CHB-C4A-NA	2.93	128.63	124.40
38	34	303	A86	C21-C20-C15	-2.93	113.88	123.35
27	c	510	CLA	O2D-CGD-CBD	2.93	116.36	111.23
38	11	312	A86	C21-C20-C15	-2.93	113.89	123.35
27	b	604	CLA	C1-C2-C3	-2.93	121.40	126.20
38	33	316	A86	C41-C32-C31	-2.93	107.85	110.47
27	32	303	CLA	CAA-C2A-C3A	-2.93	105.08	113.00
27	b	604	CLA	CHB-C4A-NA	2.93	128.63	124.40
27	b	622	CLA	C3B-C4B-NB	-2.93	107.92	110.53
27	11	309	CLA	C3B-C4B-NB	-2.93	107.92	110.53
38	11	316	A86	C21-C20-C15	-2.93	113.91	123.35
38	13	302	A86	C21-C20-C15	-2.93	113.91	123.35
38	13	315	A86	C4-C5-C6	-2.92	123.18	127.28
38	14	301	A86	C41-C32-C31	-2.92	107.86	110.47
27	C	510	CLA	O2D-CGD-CBD	2.92	116.34	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	31	316	A86	C21-C20-C15	-2.92	113.92	123.35
38	33	314	A86	C35-C34-C33	2.92	115.13	109.89
38	12	304	A86	C21-C20-C15	-2.92	113.92	123.35
38	33	302	A86	C21-C20-C15	-2.92	113.92	123.35
38	13	317	A86	C21-C20-C15	-2.92	113.93	123.35
27	12	303	CLA	CAA-C2A-C3A	-2.92	105.11	113.00
38	33	315	A86	C36-C31-C32	-2.92	116.80	119.70
29	Z	101	BCR	C24-C23-C22	-2.92	121.92	126.23
27	31	315	CLA	CAA-C2A-C3A	-2.92	105.12	113.00
38	14	314	A86	C21-C20-C15	-2.92	113.94	123.35
27	13	301	CLA	CAA-C2A-C3A	-2.91	105.12	113.00
38	31	312	A86	C21-C20-C15	-2.91	113.95	123.35
38	32	316	A86	C21-C20-C15	-2.91	113.95	123.35
27	11	315	CLA	CAA-C2A-C3A	-2.91	105.13	113.00
27	B	604	CLA	C1-C2-C3	-2.91	121.43	126.20
38	12	316	A86	C21-C20-C15	-2.91	113.95	123.35
38	32	304	A86	C21-C20-C15	-2.91	113.95	123.35
38	12	316	A86	C35-C34-C33	2.91	115.11	109.89
27	B	602	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
38	13	314	A86	C35-C34-C33	2.91	115.11	109.89
38	11	314	A86	C41-C32-C31	-2.91	107.87	110.47
38	13	316	A86	C41-C32-C31	-2.91	107.87	110.47
27	B	612	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
27	34	309	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
38	11	313	A86	C4-C5-C6	-2.91	123.20	127.28
27	A	402	CLA	C7-C6-C5	-2.91	105.52	113.26
27	33	301	CLA	CAA-C2A-C3A	-2.91	105.15	113.00
38	32	318	A86	C41-C32-C31	-2.91	107.87	110.47
29	b	623	BCR	C11-C10-C9	-2.90	123.20	127.28
38	34	315	A86	C21-C20-C15	-2.90	113.97	123.35
27	34	302	CLA	CAA-C2A-C3A	-2.90	105.15	113.00
38	33	314	A86	C21-C20-C15	-2.90	113.98	123.35
27	14	302	CLA	CAA-C2A-C3A	-2.90	105.15	113.00
38	32	316	A86	C35-C34-C33	2.90	115.10	109.89
29	z	101	BCR	C16-C15-C14	-2.90	117.58	123.52
38	32	317	A86	C4-C5-C6	-2.90	123.21	127.28
29	Z	101	BCR	C16-C15-C14	-2.90	117.58	123.52
27	B	604	CLA	CHB-C4A-NA	2.90	128.58	124.40
38	13	314	A86	C21-C20-C15	-2.90	114.00	123.35
27	B	614	CLA	CHB-C4A-NA	2.90	128.58	124.40
27	C	513	CLA	CHB-C4A-NA	2.90	128.58	124.40
27	33	308	CLA	CHB-C4A-NA	2.90	128.58	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	14	314	A86	C35-C34-C33	2.89	115.08	109.89
27	a	402	CLA	C7-C6-C5	-2.89	105.55	113.26
27	33	304	CLA	C2A-C1A-CHA	2.89	128.88	123.87
27	b	602	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
27	33	308	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
27	12	309	CLA	CHB-C4A-NA	2.89	128.57	124.40
27	c	512	CLA	C2A-C1A-CHA	2.89	128.88	123.87
27	b	612	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
27	32	310	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
27	C	512	CLA	C2A-C1A-CHA	2.89	128.88	123.87
27	33	301	CLA	CHB-C4A-NA	2.89	128.57	124.40
38	31	312	A86	C35-C34-C33	2.89	115.07	109.89
38	34	301	A86	C41-C32-C31	-2.89	107.89	110.47
38	34	316	A86	C4-C5-C6	-2.88	123.23	127.28
27	12	310	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
27	14	304	CLA	C2A-C1A-CHA	2.88	128.87	123.87
29	Z	101	BCR	C11-C10-C9	-2.88	123.23	127.28
27	11	305	CLA	CHB-C4A-NA	2.88	128.56	124.40
29	c	516	BCR	C15-C14-C13	-2.88	123.24	127.28
38	14	315	A86	C4-C5-C6	-2.88	123.24	127.28
27	31	302	CLA	C2A-C1A-CHA	2.88	128.86	123.87
27	13	308	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
27	34	308	CLA	CHB-C4A-NA	2.88	128.55	124.40
29	C	516	BCR	C15-C14-C13	-2.87	123.25	127.28
38	14	316	A86	C41-C32-C31	-2.87	107.90	110.47
27	13	307	CLA	CHB-C4A-NA	2.87	128.55	124.40
27	31	306	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
38	31	310	A86	C3-C4-C5	-2.87	117.64	123.52
27	32	306	CLA	C2A-C1A-CHA	2.87	128.85	123.87
38	34	315	A86	C35-C34-C33	2.87	115.05	109.89
38	34	313	A86	C3-C4-C5	-2.87	117.64	123.52
38	11	312	A86	C35-C34-C33	2.87	115.04	109.89
27	b	615	CLA	C3B-C4B-NB	-2.87	107.97	110.53
38	13	312	A86	C3-C4-C5	-2.87	117.65	123.52
38	14	313	A86	C21-C20-C15	-2.87	114.10	123.35
27	34	305	CLA	C2A-C1A-CHA	2.87	128.84	123.87
38	31	311	A86	C21-C20-C15	-2.87	114.10	123.35
38	34	314	A86	C21-C20-C15	-2.87	114.10	123.35
27	14	308	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
38	13	313	A86	C21-C20-C15	-2.86	114.10	123.35
27	12	307	CLA	CHB-C4A-NA	2.86	128.53	124.40
27	31	303	CLA	CHB-C4A-NA	2.86	128.53	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	32	315	A86	C21-C20-C15	-2.86	114.11	123.35
38	33	315	A86	C4-C5-C6	-2.86	123.26	127.28
27	33	311	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
27	D	405	CLA	CMB-C2B-C1B	-2.86	121.06	125.42
38	12	315	A86	C21-C20-C15	-2.86	114.11	123.35
27	11	315	CLA	CHB-C4A-NA	2.86	128.53	124.40
38	11	310	A86	C3-C4-C5	-2.86	117.67	123.52
27	c	513	CLA	CHB-C4A-NA	2.86	128.53	124.40
27	12	303	CLA	CHB-C4A-NA	2.86	128.53	124.40
27	c	510	CLA	CHB-C4A-NA	2.86	128.52	124.40
27	34	312	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
27	11	306	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
27	13	304	CLA	C2A-C1A-CHA	2.86	128.82	123.87
38	11	311	A86	C21-C20-C15	-2.86	114.13	123.35
29	M	101	BCR	C7-C8-C9	-2.86	122.01	126.23
27	32	303	CLA	CHB-C4A-NA	2.85	128.52	124.40
27	34	309	CLA	CHB-C4A-NA	2.85	128.52	124.40
38	33	313	A86	C21-C20-C15	-2.85	114.14	123.35
29	z	101	BCR	C11-C10-C9	-2.85	123.28	127.28
27	31	305	CLA	C3B-C4B-NB	-2.85	107.98	110.53
27	32	307	CLA	CHB-C4A-NA	2.85	128.51	124.40
27	33	305	CLA	CHB-C4A-NA	2.85	128.51	124.40
27	11	302	CLA	C2A-C1A-CHA	2.85	128.81	123.87
38	32	314	A86	C3-C4-C5	-2.85	117.69	123.52
38	12	317	A86	C4-C5-C6	-2.85	123.28	127.28
33	b	619	LMG	O3-C3-C2	-2.85	103.66	110.38
27	b	603	CLA	O2D-CGD-CBD	2.85	116.21	111.23
27	b	611	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
27	B	603	CLA	O2D-CGD-CBD	2.85	116.21	111.23
27	B	611	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
27	14	307	CLA	CHB-C4A-NA	2.85	128.51	124.40
27	b	601	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
27	b	613	CLA	CHB-C4A-NA	2.85	128.51	124.40
27	11	306	CLA	CHB-C4A-NA	2.85	128.51	124.40
38	33	312	A86	C3-C4-C5	-2.85	117.69	123.52
27	12	306	CLA	C2A-C1A-CHA	2.85	128.81	123.87
27	33	307	CLA	CHB-C4A-NA	2.85	128.51	124.40
27	14	305	CLA	CHB-C4A-NA	2.85	128.51	124.40
27	31	315	CLA	CHB-C4A-NA	2.85	128.51	124.40
27	d	405	CLA	CMB-C2B-C1B	-2.85	121.09	125.42
38	14	312	A86	C3-C4-C5	-2.84	117.70	123.52
27	c	514	CLA	CMB-C2B-C3B	2.84	133.24	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	m	103	BCR	C7-C8-C9	-2.84	122.03	126.23
33	B	619	LMG	O3-C3-C2	-2.84	103.67	110.38
27	14	311	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
29	c	519	BCR	C27-C26-C25	2.84	126.54	122.70
35	j	101	DGD	C3G-C2G-C1G	-2.84	105.16	111.78
27	13	311	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
27	C	510	CLA	CHB-C4A-NA	2.84	128.50	124.40
27	13	305	CLA	CHB-C4A-NA	2.84	128.50	124.40
35	J	101	DGD	C3G-C2G-C1G	-2.84	105.17	111.78
27	11	303	CLA	CHB-C4A-NA	2.84	128.49	124.40
27	31	305	CLA	CHB-C4A-NA	2.84	128.49	124.40
38	12	314	A86	C3-C4-C5	-2.84	117.72	123.52
27	34	306	CLA	CHB-C4A-NA	2.83	128.49	124.40
38	31	313	A86	C4-C5-C6	-2.83	123.30	127.28
27	12	313	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
27	32	309	CLA	CHB-C4A-NA	2.83	128.49	124.40
27	11	309	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
27	B	607	CLA	CHB-C4A-NA	2.83	128.48	124.40
27	d	402	CLA	O2D-CGD-CBD	2.83	116.18	111.23
27	31	309	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
27	14	308	CLA	CHB-C4A-NA	2.83	128.48	124.40
27	b	607	CLA	CHB-C4A-NA	2.83	128.48	124.40
29	A	409	BCR	C15-C16-C17	-2.83	117.73	123.52
35	h	102	DGD	CDB-CCB-CBB	-2.83	100.08	114.37
27	B	613	CLA	CHB-C4A-NA	2.83	128.48	124.40
27	C	514	CLA	CMB-C2B-C3B	2.83	133.20	126.55
27	13	301	CLA	CHB-C4A-NA	2.83	128.48	124.40
35	H	102	DGD	CDB-CCB-CBB	-2.83	100.09	114.37
33	q	301	LMG	O6-C1-O1	-2.82	103.37	110.04
27	B	601	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
27	11	305	CLA	C3B-C4B-NB	-2.82	108.01	110.53
27	b	607	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
27	m	101	CLA	C3B-C4B-NB	-2.82	108.01	110.53
33	C	519	LMG	O6-C1-O1	-2.82	103.38	110.04
27	32	310	CLA	CHB-C4A-NA	2.82	128.47	124.40
27	14	302	CLA	CHB-C4A-NA	2.82	128.47	124.40
27	B	615	CLA	C3B-C4B-NB	-2.82	108.01	110.53
27	12	309	CLA	C3B-C4B-NB	-2.82	108.01	110.53
27	B	607	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
27	13	308	CLA	CHB-C4A-NA	2.82	128.47	124.40
29	a	409	BCR	C15-C16-C17	-2.82	117.76	123.52
27	32	313	CLA	O2D-CGD-O1D	-2.82	118.37	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	520	BCR	C27-C26-C25	2.82	126.51	122.70
27	34	302	CLA	CHB-C4A-NA	2.81	128.46	124.40
27	31	306	CLA	CHB-C4A-NA	2.81	128.46	124.40
27	D	402	CLA	O2D-CGD-CBD	2.81	116.14	111.23
27	c	502	CLA	CAA-C2A-C3A	-2.81	105.41	113.00
27	M	102	CLA	C3B-C4B-NB	-2.80	108.03	110.53
27	14	307	CLA	C3B-C4B-NB	-2.80	108.03	110.53
27	12	310	CLA	CHB-C4A-NA	2.80	128.44	124.40
36	d	407	PL9	C22-C23-C24	-2.80	121.22	127.62
27	32	309	CLA	C3B-C4B-NB	-2.80	108.03	110.53
36	D	407	PL9	C22-C23-C24	-2.80	121.22	127.62
27	C	502	CLA	CAA-C2A-C3A	-2.80	105.44	113.00
27	34	308	CLA	C3B-C4B-NB	-2.79	108.03	110.53
27	34	306	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
27	b	622	CLA	CMD-C2D-C1D	-2.79	119.82	124.73
27	b	615	CLA	O2D-CGD-O1D	-2.79	118.43	123.85
35	C	517	DGD	C3G-C2G-C1G	-2.78	105.29	111.78
27	13	307	CLA	C3B-C4B-NB	-2.78	108.05	110.53
27	c	508	CLA	O1D-CGD-CBD	2.78	130.00	124.52
35	c	517	DGD	C3G-C2G-C1G	-2.78	105.31	111.78
27	C	509	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
27	12	307	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
27	13	305	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
35	J	101	DGD	CDB-CCB-CBB	-2.77	100.34	114.37
30	a	406	SQD	C1-O5-C5	2.77	119.14	113.72
27	C	508	CLA	O1D-CGD-CBD	2.77	129.99	124.52
27	B	605	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
30	b	620	SQD	O8-S-C6	2.77	111.33	105.97
27	b	604	CLA	CAA-C2A-C3A	-2.77	105.51	113.00
27	a	402	CLA	CMB-C2B-C1B	-2.77	121.20	125.42
29	b	616	BCR	C11-C10-C9	-2.77	123.39	127.28
27	c	509	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
35	j	101	DGD	CDB-CCB-CBB	-2.77	100.36	114.37
27	11	303	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
29	B	616	BCR	C27-C26-C25	2.77	126.44	122.70
27	c	502	CLA	CMB-C2B-C1B	-2.77	121.20	125.42
27	B	615	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
27	C	502	CLA	CMB-C2B-C1B	-2.77	121.21	125.42
30	A	406	SQD	C1-O5-C5	2.76	119.12	113.72
27	c	504	CLA	C3B-C4B-NB	-2.76	108.06	110.53
27	b	602	CLA	CHB-C4A-NA	2.76	128.39	124.40
29	b	616	BCR	C27-C26-C25	2.76	126.44	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	620	SQD	O8-S-C6	2.76	111.30	105.97
29	B	616	BCR	C11-C10-C9	-2.76	123.41	127.28
27	32	307	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
27	33	305	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
27	B	610	CLA	CHB-C4A-NA	2.76	128.38	124.40
35	j	101	DGD	O3G-C1D-C2D	-2.76	104.09	108.27
27	14	305	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
27	B	604	CLA	CAA-C2A-C3A	-2.75	105.56	113.00
27	31	303	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
27	b	605	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
27	C	504	CLA	CAA-CBA-CGA	-2.75	105.40	113.21
27	B	602	CLA	CHB-C4A-NA	2.75	128.37	124.40
27	C	504	CLA	C3B-C4B-NB	-2.74	108.08	110.53
27	c	509	CLA	CHB-C4A-NA	2.74	128.36	124.40
27	A	402	CLA	CMB-C2B-C1B	-2.74	121.24	125.42
27	b	609	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
27	c	502	CLA	CHB-C4A-NA	2.74	128.36	124.40
27	C	505	CLA	C3C-C4C-NC	-2.74	106.92	110.43
27	C	509	CLA	CHB-C4A-NA	2.74	128.35	124.40
27	B	609	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
27	C	502	CLA	CHB-C4A-NA	2.74	128.35	124.40
36	D	404	PL9	C40-C39-C41	2.74	119.98	115.23
36	D	407	PL9	C40-C39-C41	2.74	119.98	115.23
27	c	504	CLA	CAA-CBA-CGA	-2.74	105.44	113.21
27	b	610	CLA	CHB-C4A-NA	2.73	128.35	124.40
35	J	101	DGD	O3G-C1D-C2D	-2.73	104.12	108.27
36	d	407	PL9	C40-C39-C41	2.73	119.97	115.23
27	d	402	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
27	33	307	CLA	C3B-C4B-NB	-2.73	108.09	110.53
29	C	516	BCR	C28-C27-C26	-2.72	109.20	114.06
27	c	507	CLA	C2A-C1A-CHA	2.72	128.59	123.87
27	12	308	CLA	CHB-C1B-NB	2.72	128.13	124.05
27	31	304	CLA	CHB-C1B-NB	2.72	128.13	124.05
36	d	404	PL9	C40-C39-C41	2.72	119.95	115.23
27	33	306	CLA	CHB-C1B-NB	2.72	128.13	124.05
27	W	102	CLA	C3B-C4B-NB	-2.72	108.10	110.53
27	B	603	CLA	CHB-C4A-NA	2.72	128.32	124.40
27	b	613	CLA	C3B-C4B-NB	-2.72	108.10	110.53
27	w	102	CLA	C3B-C4B-NB	-2.71	108.11	110.53
27	w	102	CLA	CHB-C4A-NA	2.71	128.31	124.40
27	13	306	CLA	CHB-C1B-NB	2.71	128.12	124.05
38	14	314	A86	C3-C4-C5	-2.71	117.97	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	516	BCR	C29-C30-C25	2.71	114.37	110.44
27	11	304	CLA	CHB-C1B-NB	2.71	128.11	124.05
29	c	519	BCR	C11-C10-C9	-2.71	123.48	127.28
36	D	404	PL9	C41-C39-C38	-2.71	115.09	121.17
38	32	316	A86	C3-C4-C5	-2.71	117.98	123.52
27	c	509	CLA	C3B-C4B-NB	-2.71	108.11	110.53
27	c	505	CLA	C3C-C4C-NC	-2.70	106.97	110.43
27	D	402	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
27	C	507	CLA	C2A-C1A-CHA	2.70	128.56	123.87
36	d	404	PL9	C41-C39-C38	-2.70	115.10	121.17
27	b	610	CLA	O2D-CGD-CBD	2.70	115.95	111.23
27	b	606	CLA	CAA-CBA-CGA	-2.70	105.53	113.21
27	B	610	CLA	O2D-CGD-CBD	2.70	115.95	111.23
27	C	509	CLA	C3B-C4B-NB	-2.70	108.12	110.53
27	34	307	CLA	C3A-C2A-C1A	2.70	105.38	101.34
38	34	315	A86	C3-C4-C5	-2.70	118.00	123.52
27	12	303	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
27	11	304	CLA	C3A-C2A-C1A	2.70	105.38	101.34
33	b	618	LMG	C1-C2-C3	-2.70	104.34	110.01
27	11	315	CLA	C3B-C4B-NB	-2.70	108.12	110.53
38	11	312	A86	C3-C4-C5	-2.69	118.00	123.52
38	14	315	A86	C21-C20-C15	-2.69	114.65	123.35
38	12	316	A86	C3-C4-C5	-2.69	118.01	123.52
33	B	618	LMG	C1-C2-C3	-2.69	104.34	110.01
27	B	606	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
38	31	313	A86	C21-C20-C15	-2.69	114.66	123.35
27	14	302	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
27	12	308	CLA	C3A-C2A-C1A	2.69	105.37	101.34
35	C	518	DGD	O2D-C2D-C1D	-2.69	103.66	110.08
27	34	307	CLA	CHB-C1B-NB	2.69	128.08	124.05
27	W	102	CLA	CHB-C4A-NA	2.69	128.28	124.40
27	b	603	CLA	CHB-C4A-NA	2.69	128.28	124.40
29	c	516	BCR	C28-C27-C26	-2.69	109.26	114.06
29	C	520	BCR	C11-C10-C9	-2.69	123.51	127.28
27	B	606	CLA	CHB-C4A-NA	2.69	128.28	124.40
38	13	314	A86	C3-C4-C5	-2.69	118.02	123.52
38	33	314	A86	C3-C4-C5	-2.69	118.02	123.52
27	32	308	CLA	CHB-C1B-NB	2.69	128.08	124.05
29	m	103	BCR	C11-C10-C9	-2.69	123.51	127.28
27	B	606	CLA	CAA-CBA-CGA	-2.69	105.58	113.21
27	c	506	CLA	CHB-C4A-NA	2.68	128.27	124.40
38	31	312	A86	C3-C4-C5	-2.68	118.03	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	d	405	CLA	CAA-CBA-CGA	-2.68	105.59	113.21
38	33	315	A86	C21-C20-C15	-2.68	114.69	123.35
27	32	303	CLA	C3B-C4B-NB	-2.68	108.14	110.53
38	32	318	A86	C7-C6-C8	2.68	122.19	118.09
27	b	614	CLA	O2A-CGA-O1A	-2.68	116.92	123.63
27	33	301	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
27	b	606	CLA	CHB-C4A-NA	2.68	128.27	124.40
35	c	518	DGD	O2D-C2D-C1D	-2.68	103.69	110.08
38	13	315	A86	C21-C20-C15	-2.68	114.70	123.35
33	C	519	LMG	O2-C2-C1	-2.68	103.69	110.08
27	C	503	CLA	CHB-C4A-NA	2.68	128.27	124.40
27	B	613	CLA	C3B-C4B-NB	-2.68	108.14	110.53
27	11	315	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
27	C	506	CLA	CHB-C4A-NA	2.68	128.27	124.40
27	14	306	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
27	c	503	CLA	CHB-C4A-NA	2.68	128.26	124.40
27	b	610	CLA	CAA-C2A-C3A	-2.68	105.76	113.00
27	Z	102	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
29	M	101	BCR	C24-C23-C22	-2.68	122.28	126.23
27	C	510	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
27	b	606	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
27	c	510	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
38	31	314	A86	C7-C6-C8	2.68	122.18	118.09
33	12	301	LMG	O3-C3-C2	-2.68	104.07	110.38
33	q	301	LMG	O2-C2-C1	-2.68	103.70	110.08
27	31	304	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
27	32	303	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
27	D	405	CLA	CAA-CBA-CGA	-2.67	105.61	113.21
27	B	610	CLA	CAA-C2A-C3A	-2.67	105.78	113.00
27	13	301	CLA	C3B-C4B-NB	-2.67	108.14	110.53
27	z	102	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
29	C	516	BCR	C29-C30-C25	2.67	114.32	110.44
27	14	306	CLA	CHB-C1B-NB	2.67	128.06	124.05
38	12	317	A86	C21-C20-C15	-2.67	114.73	123.35
35	H	102	DGD	O6D-C1D-O3G	-2.67	103.73	110.04
27	B	614	CLA	O2A-CGA-O1A	-2.67	116.95	123.63
38	32	317	A86	C21-C20-C15	-2.67	114.73	123.35
32	l	103	LHG	O8-C23-C24	2.67	119.97	111.83
29	M	101	BCR	C11-C10-C9	-2.67	123.53	127.28
38	11	313	A86	C21-C20-C15	-2.67	114.73	123.35
38	34	316	A86	C21-C20-C15	-2.67	114.74	123.35
29	M	101	BCR	C27-C26-C25	2.67	126.31	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	13	316	A86	C7-C6-C8	2.67	122.16	118.09
35	H	102	DGD	C3G-C2G-C1G	-2.67	105.57	111.78
27	b	612	CLA	CMB-C2B-C1B	-2.67	121.36	125.42
27	13	301	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
32	L	102	LHG	O8-C23-C24	2.66	119.96	111.83
27	33	306	CLA	C3A-C2A-C1A	2.66	105.33	101.34
27	c	514	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
27	c	510	CLA	C3B-C4B-NB	-2.66	108.15	110.53
27	B	611	CLA	C3B-C4B-NB	-2.66	108.15	110.53
27	b	611	CLA	C3B-C4B-NB	-2.66	108.15	110.53
27	13	306	CLA	C3A-C2A-C1A	2.66	105.33	101.34
27	W	103	CLA	C3B-C4B-NB	-2.66	108.16	110.53
27	34	302	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
27	33	301	CLA	C3B-C4B-NB	-2.66	108.16	110.53
28	a	403	PHO	O2D-CGD-O1D	-2.66	118.67	123.85
27	14	302	CLA	C3B-C4B-NB	-2.66	108.16	110.53
29	m	103	BCR	C27-C26-C25	2.66	126.30	122.70
27	B	622	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
27	31	315	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
35	h	102	DGD	C3G-C2G-C1G	-2.66	105.59	111.78
29	B	616	BCR	C40-C30-C25	2.65	114.41	110.24
27	B	612	CLA	CMB-C2B-C1B	-2.65	121.38	125.42
29	m	103	BCR	C24-C23-C22	-2.65	122.31	126.23
27	C	509	CLA	O2D-CGD-CBD	2.65	115.87	111.23
35	h	102	DGD	O6D-C1D-O3G	-2.65	103.77	110.04
27	w	103	CLA	C3B-C4B-NB	-2.65	108.16	110.53
38	34	301	A86	C7-C6-C8	2.65	122.14	118.09
27	Z	102	CLA	CHB-C4A-NA	2.65	128.23	124.40
27	34	307	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
27	31	304	CLA	C3A-C2A-C1A	2.65	105.31	101.34
38	14	301	A86	C7-C6-C8	2.65	122.14	118.09
38	11	314	A86	C7-C6-C8	2.65	122.14	118.09
38	14	316	A86	C7-C6-C8	2.65	122.14	118.09
27	b	622	CLA	CHB-C4A-NA	2.65	128.22	124.40
27	31	315	CLA	C3B-C4B-NB	-2.65	108.17	110.53
27	C	514	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
27	32	308	CLA	C3A-C2A-C1A	2.65	105.30	101.34
38	33	316	A86	C7-C6-C8	2.64	122.12	118.09
33	32	301	LMG	O3-C3-C2	-2.64	104.15	110.38
27	b	622	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
27	33	306	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
27	B	622	CLA	CHB-C4A-NA	2.64	128.21	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	13	312	A86	C10-C9-C8	-2.64	115.56	123.20
27	14	306	CLA	C3A-C2A-C1A	2.64	105.29	101.34
38	31	310	A86	C10-C9-C8	-2.64	115.56	123.20
38	14	312	A86	C10-C9-C8	-2.64	115.56	123.20
27	32	308	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
38	12	314	A86	C10-C9-C8	-2.64	115.56	123.20
29	b	616	BCR	C40-C30-C25	2.64	114.38	110.24
27	11	304	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
27	13	305	CLA	C3B-C4B-NB	-2.64	108.18	110.53
32	L	102	LHG	C20-C19-C18	-2.63	101.05	114.37
27	12	308	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
27	c	507	CLA	C3B-C4B-NB	-2.63	108.18	110.53
35	C	518	DGD	CBB-CAB-C9B	-2.63	101.06	114.37
27	C	512	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
27	c	509	CLA	O2D-CGD-CBD	2.63	115.83	111.23
27	B	604	CLA	CAA-CBA-CGA	-2.63	105.73	113.21
38	11	310	A86	C10-C9-C8	-2.63	115.57	123.20
27	13	306	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
38	34	313	A86	C10-C9-C8	-2.63	115.58	123.20
35	c	518	DGD	CBB-CAB-C9B	-2.63	101.08	114.37
28	A	403	PHO	C2D-C1D-ND	-2.63	107.53	109.43
32	l	103	LHG	C20-C19-C18	-2.63	101.09	114.37
38	32	314	A86	C10-C9-C8	-2.63	115.59	123.20
28	A	403	PHO	O2D-CGD-O1D	-2.63	118.74	123.85
35	c	517	DGD	C1E-O6E-C5E	2.62	118.85	113.72
27	z	102	CLA	CHB-C4A-NA	2.62	128.19	124.40
28	A	403	PHO	CMB-C2B-C3B	2.62	129.93	124.68
38	33	312	A86	C10-C9-C8	-2.62	115.59	123.20
27	b	604	CLA	CAA-CBA-CGA	-2.62	105.76	113.21
27	34	302	CLA	C3B-C4B-NB	-2.62	108.19	110.53
33	D	408	LMG	O1-C7-C8	-2.62	104.44	110.82
33	d	408	LMG	O1-C7-C8	-2.62	104.44	110.82
38	14	315	A86	C8-C6-C5	-2.62	114.89	119.01
27	d	401	CLA	CHB-C4A-NA	2.62	128.18	124.40
27	C	507	CLA	C3B-C4B-NB	-2.62	108.19	110.53
27	12	303	CLA	C3B-C4B-NB	-2.62	108.19	110.53
27	31	303	CLA	C3B-C4B-NB	-2.61	108.20	110.53
27	32	307	CLA	C3B-C4B-NB	-2.61	108.20	110.53
27	14	306	CLA	O2D-CGD-CBD	2.61	115.80	111.23
38	13	315	A86	C8-C6-C5	-2.61	114.90	119.01
27	11	303	CLA	C3B-C4B-NB	-2.61	108.20	110.53
27	33	305	CLA	C3B-C4B-NB	-2.61	108.20	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	403	PHO	CMB-C2B-C3B	2.61	129.90	124.68
28	a	403	PHO	C2D-C1D-ND	-2.61	107.54	109.43
38	11	313	A86	C8-C6-C5	-2.61	114.91	119.01
37	f	102	HEM	CMB-C2B-C1B	-2.61	120.96	125.03
27	C	506	CLA	O2D-CGD-CBD	2.61	115.79	111.23
27	c	512	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
38	33	315	A86	C8-C6-C5	-2.61	114.91	119.01
35	C	517	DGD	C1E-O6E-C5E	2.61	118.81	113.72
27	D	406	CLA	O2D-CGD-CBD	2.61	115.78	111.23
27	C	504	CLA	CHB-C4A-NA	2.60	128.16	124.40
38	32	317	A86	C8-C6-C5	-2.60	114.91	119.01
39	32	302	LMU	O5B-C1B-C2B	2.60	115.72	110.37
27	C	510	CLA	C3B-C4B-NB	-2.60	108.21	110.53
27	D	401	CLA	CHB-C4A-NA	2.60	128.15	124.40
27	c	504	CLA	C2A-C1A-CHA	2.60	128.38	123.87
27	12	308	CLA	O2D-CGD-CBD	2.60	115.77	111.23
27	d	406	CLA	O2D-CGD-CBD	2.60	115.77	111.23
27	14	305	CLA	C3B-C4B-NB	-2.59	108.21	110.53
27	31	304	CLA	O2D-CGD-CBD	2.59	115.77	111.23
27	13	306	CLA	O2D-CGD-CBD	2.59	115.76	111.23
27	c	508	CLA	CMB-C2B-C1B	-2.59	121.47	125.42
27	B	607	CLA	CMB-C2B-C3B	2.59	132.65	126.55
27	12	307	CLA	C3B-C4B-NB	-2.59	108.22	110.53
29	B	617	BCR	C3-C4-C5	-2.59	109.44	114.06
27	33	307	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
27	b	612	CLA	CMB-C2B-C3B	2.59	132.64	126.55
35	c	518	DGD	O6D-C5D-C6D	-2.59	101.56	106.69
27	c	510	CLA	CAA-C2A-C3A	-2.59	106.00	113.00
27	c	506	CLA	O2D-CGD-CBD	2.59	115.75	111.23
37	E	101	HEM	CMB-C2B-C1B	-2.59	120.99	125.03
29	z	101	BCR	C28-C27-C26	-2.59	109.44	114.06
27	A	404	CLA	CAA-C2A-C3A	-2.59	106.01	113.00
27	a	404	CLA	CAA-C2A-C3A	-2.59	106.01	113.00
27	11	304	CLA	O2D-CGD-CBD	2.59	115.75	111.23
27	34	307	CLA	O2D-CGD-CBD	2.59	115.75	111.23
33	M	103	LMG	O2-C2-C1	-2.58	103.92	110.08
38	34	316	A86	C8-C6-C5	-2.58	114.94	119.01
27	C	504	CLA	C2A-C1A-CHA	2.58	128.35	123.87
35	C	518	DGD	O6D-C5D-C6D	-2.58	101.58	106.69
38	13	312	A86	C7-C6-C8	2.58	122.03	118.09
38	34	313	A86	C25-C24-C1	-2.58	119.29	126.36
27	32	308	CLA	O2D-CGD-CBD	2.58	115.74	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	607	CLA	CMB-C2B-C3B	2.58	132.62	126.55
27	33	306	CLA	O2D-CGD-CBD	2.58	115.74	111.23
27	M	102	CLA	CHB-C4A-NA	2.58	128.12	124.40
27	C	510	CLA	CAA-C2A-C3A	-2.58	106.03	113.00
27	33	309	CLA	CMB-C2B-C1B	-2.58	121.50	125.42
27	32	313	CLA	CHB-C4A-NA	2.57	128.12	124.40
29	F	101	BCR	C7-C8-C9	-2.57	122.43	126.23
29	b	617	BCR	C3-C4-C5	-2.57	109.47	114.06
29	B	623	BCR	C15-C14-C13	-2.57	123.67	127.28
38	13	312	A86	C25-C24-C1	-2.57	119.31	126.36
27	B	612	CLA	CMB-C2B-C3B	2.57	132.60	126.55
38	31	310	A86	C25-C24-C1	-2.57	119.31	126.36
38	34	313	A86	C7-C6-C8	2.57	122.02	118.09
38	32	314	A86	C25-C24-C1	-2.57	119.31	126.36
27	11	305	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
38	11	310	A86	C25-C24-C1	-2.57	119.32	126.36
27	C	508	CLA	CMB-C2B-C1B	-2.57	121.51	125.42
27	C	514	CLA	CAA-C2A-C3A	-2.57	106.06	113.00
29	Z	101	BCR	C28-C27-C26	-2.57	109.48	114.06
27	33	311	CLA	CHB-C4A-NA	2.57	128.10	124.40
38	31	313	A86	C8-C6-C5	-2.57	114.97	119.01
38	33	312	A86	C7-C6-C8	2.57	122.01	118.09
27	13	311	CLA	CHB-C4A-NA	2.57	128.10	124.40
27	32	309	CLA	O2D-CGD-O1D	-2.57	118.86	123.85
29	A	409	BCR	C15-C14-C13	-2.56	123.68	127.28
27	C	513	CLA	C3B-C4B-NB	-2.56	108.24	110.53
30	A	406	SQD	O8-S-C6	2.56	110.92	105.97
38	12	317	A86	C8-C6-C5	-2.56	114.98	119.01
27	12	309	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
27	13	307	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
27	11	301	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
38	14	312	A86	C7-C6-C8	2.56	122.00	118.09
33	m	102	LMG	O2-C2-C1	-2.56	103.97	110.08
27	34	308	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
33	W	101	LMG	O1-C1-C2	-2.56	104.39	108.27
27	34	310	CLA	CMB-C2B-C1B	-2.56	121.52	125.42
38	32	318	A86	C3-C4-C5	-2.56	118.28	123.52
33	W	101	LMG	C38-C37-C36	-2.56	101.44	114.37
38	33	312	A86	C25-C24-C1	-2.56	119.35	126.36
29	f	101	BCR	C7-C8-C9	-2.56	122.45	126.23
38	33	316	A86	C3-C4-C5	-2.56	118.29	123.52
27	14	311	CLA	CHB-C4A-NA	2.55	128.09	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	c	504	CLA	CHB-C4A-NA	2.55	128.09	124.40
29	M	101	BCR	C15-C14-C13	-2.55	123.70	127.28
33	w	101	LMG	C38-C37-C36	-2.55	101.46	114.37
28	A	403	PHO	C3B-C4B-NB	-2.55	105.80	107.46
30	a	406	SQD	O8-S-C6	2.55	110.90	105.97
27	31	305	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
27	D	405	CLA	CMB-C2B-C3B	2.55	132.55	126.55
27	14	307	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
27	11	309	CLA	CHB-C4A-NA	2.55	128.08	124.40
27	12	305	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
27	m	101	CLA	CHB-C4A-NA	2.55	128.08	124.40
33	w	101	LMG	C1-C2-C3	-2.55	104.65	110.01
38	14	312	A86	C25-C24-C1	-2.55	119.37	126.36
29	F	101	BCR	C11-C10-C9	-2.55	123.70	127.28
27	c	514	CLA	CAA-C2A-C3A	-2.55	106.11	113.00
27	c	513	CLA	C3B-C4B-NB	-2.55	108.25	110.53
38	11	310	A86	C7-C6-C8	2.55	121.98	118.09
33	W	101	LMG	O3-C3-C2	-2.55	104.37	110.38
35	J	101	DGD	O5D-C6D-C5D	-2.55	103.68	109.42
27	33	303	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
38	33	302	A86	C12-C11-C13	2.55	120.13	116.00
38	14	301	A86	C3-C4-C5	-2.55	118.31	123.52
29	b	623	BCR	C15-C14-C13	-2.55	123.71	127.28
27	B	604	CLA	C2A-C1A-CHA	2.55	128.29	123.87
33	W	101	LMG	C1-C2-C3	-2.55	104.65	110.01
27	14	303	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
33	M	103	LMG	O3-C3-C2	-2.55	104.38	110.38
27	31	309	CLA	CHB-C4A-NA	2.55	128.07	124.40
38	14	313	A86	C10-C9-C8	-2.54	115.83	123.20
27	C	503	CLA	O2A-CGA-O1A	-2.54	117.26	123.63
27	d	401	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
38	12	314	A86	C7-C6-C8	2.54	121.97	118.09
27	13	303	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
38	13	317	A86	C12-C11-C13	2.54	120.12	116.00
33	w	101	LMG	O1-C1-C2	-2.54	104.41	108.27
27	b	604	CLA	C2A-C1A-CHA	2.54	128.28	123.87
27	34	304	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
38	13	302	A86	C12-C11-C13	2.54	120.12	116.00
38	34	303	A86	C12-C11-C13	2.54	120.12	116.00
27	13	309	CLA	C2A-C1A-CHA	2.54	128.28	123.87
27	11	307	CLA	CMB-C2B-C1B	-2.54	121.55	125.42
38	33	313	A86	C10-C9-C8	-2.54	115.84	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	32	314	A86	C7-C6-C8	2.54	121.97	118.09
38	12	314	A86	C25-C24-C1	-2.54	119.40	126.36
27	c	511	CLA	CHB-C4A-NA	2.54	128.06	124.40
27	c	503	CLA	O2A-CGA-O1A	-2.54	117.28	123.63
27	13	309	CLA	CMB-C2B-C1B	-2.54	121.55	125.42
38	11	314	A86	C3-C4-C5	-2.54	118.32	123.52
27	32	311	CLA	C2A-C1A-CHA	2.54	128.27	123.87
38	13	313	A86	C10-C9-C8	-2.54	115.84	123.20
33	w	101	LMG	O3-C3-C2	-2.54	104.39	110.38
27	34	310	CLA	C2A-C1A-CHA	2.54	128.27	123.87
38	31	314	A86	C3-C4-C5	-2.54	118.33	123.52
27	b	622	CLA	CMD-C2D-C3D	2.54	133.51	127.69
37	v	201	HEM	C4A-CHB-C1B	-2.54	120.28	126.25
38	34	314	A86	C10-C9-C8	-2.54	115.85	123.20
27	C	511	CLA	CHB-C4A-NA	2.54	128.06	124.40
33	m	102	LMG	O3-C3-C2	-2.54	104.40	110.38
27	12	311	CLA	CMB-C2B-C1B	-2.54	121.56	125.42
38	11	316	A86	C12-C11-C13	2.54	120.11	116.00
27	b	611	CLA	C1-C2-C3	-2.53	122.04	126.20
38	31	310	A86	C7-C6-C8	2.53	121.96	118.09
38	32	315	A86	C10-C9-C8	-2.53	115.86	123.20
27	B	611	CLA	C1-C2-C3	-2.53	122.05	126.20
27	34	312	CLA	CHB-C4A-NA	2.53	128.06	124.40
29	m	103	BCR	C15-C14-C13	-2.53	123.72	127.28
27	D	401	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
36	D	404	PL9	C7-C8-C9	-2.53	122.47	126.83
30	B	620	SQD	O9-S-C6	2.53	110.54	106.76
29	b	616	BCR	C15-C16-C17	-2.53	118.34	123.52
38	11	311	A86	C10-C9-C8	-2.53	115.86	123.20
27	14	309	CLA	CMB-C2B-C1B	-2.53	121.56	125.42
27	31	307	CLA	CMB-C2B-C1B	-2.53	121.56	125.42
27	31	301	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
29	c	515	BCR	C7-C8-C9	-2.53	122.49	126.23
38	31	311	A86	C10-C9-C8	-2.53	115.87	123.20
38	34	301	A86	C3-C4-C5	-2.53	118.34	123.52
38	11	312	A86	C9-C10-C11	-2.53	119.48	126.64
29	B	616	BCR	C15-C16-C17	-2.53	118.34	123.52
38	12	304	A86	C12-C11-C13	2.53	120.10	116.00
38	12	314	A86	C21-C20-C15	-2.53	115.19	123.35
38	13	314	A86	C9-C10-C11	-2.53	119.49	126.64
38	14	314	A86	C9-C10-C11	-2.53	119.49	126.64
33	d	408	LMG	O6-C1-O1	-2.53	104.07	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	403	PHO	C3B-C4B-NB	-2.53	105.82	107.46
38	34	315	A86	C9-C10-C11	-2.53	119.50	126.64
35	j	101	DGD	O5D-C6D-C5D	-2.53	103.72	109.42
27	34	306	CLA	C3B-C4B-NB	-2.53	108.28	110.53
27	32	305	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
32	B	621	LHG	C11-C10-C9	-2.53	101.60	114.37
29	C	515	BCR	C7-C8-C9	-2.53	122.50	126.23
38	13	302	A86	C41-C32-C31	-2.53	108.21	110.47
38	12	315	A86	C10-C9-C8	-2.53	115.88	123.20
37	V	201	HEM	C4A-CHB-C1B	-2.53	120.31	126.25
27	12	313	CLA	CHB-C4A-NA	2.53	128.04	124.40
38	14	316	A86	C3-C4-C5	-2.52	118.35	123.52
27	d	405	CLA	CMB-C2B-C3B	2.52	132.49	126.55
36	d	404	PL9	C7-C8-C9	-2.52	122.48	126.83
38	13	316	A86	C3-C4-C5	-2.52	118.35	123.52
29	a	409	BCR	C15-C14-C13	-2.52	123.74	127.28
29	f	101	BCR	C11-C10-C9	-2.52	123.74	127.28
28	a	403	PHO	CAA-CBA-CGA	-2.52	106.04	113.21
39	12	302	LMU	O5B-C1B-C2B	2.52	115.56	110.37
33	D	408	LMG	O6-C1-O1	-2.52	104.08	110.04
27	31	307	CLA	C2A-C1A-CHA	2.52	128.25	123.87
38	13	312	A86	C21-C20-C15	-2.52	115.21	123.35
32	b	621	LHG	C11-C10-C9	-2.52	101.62	114.37
28	A	403	PHO	CAA-CBA-CGA	-2.52	106.05	113.21
27	c	503	CLA	C1D-ND-C4D	2.52	108.08	106.31
32	l	102	LHG	C20-C19-C18	-2.52	101.63	114.37
32	L	101	LHG	C20-C19-C18	-2.52	101.63	114.37
38	31	310	A86	C21-C20-C15	-2.52	115.22	123.35
27	12	311	CLA	C2A-C1A-CHA	2.52	128.24	123.87
27	14	309	CLA	C2A-C1A-CHA	2.52	128.24	123.87
38	31	316	A86	C12-C11-C13	2.52	120.08	116.00
38	14	313	A86	C25-C24-C1	-2.52	119.46	126.36
38	14	312	A86	C21-C20-C15	-2.52	115.22	123.35
27	b	605	CLA	C3B-C4B-NB	-2.52	108.28	110.53
27	w	103	CLA	CHB-C4A-NA	2.52	128.03	124.40
38	32	314	A86	C21-C20-C15	-2.52	115.23	123.35
38	33	312	A86	C21-C20-C15	-2.52	115.23	123.35
38	11	310	A86	C21-C20-C15	-2.51	115.23	123.35
38	12	316	A86	C9-C10-C11	-2.51	119.53	126.64
38	32	316	A86	C9-C10-C11	-2.51	119.53	126.64
27	11	302	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
38	11	311	A86	C25-C24-C1	-2.51	119.47	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	32	304	A86	C12-C11-C13	2.51	120.08	116.00
33	b	618	LMG	O6-C1-O1	-2.51	104.11	110.04
32	A	408	LHG	C20-C19-C18	-2.51	101.67	114.37
27	11	307	CLA	C2A-C1A-CHA	2.51	128.23	123.87
38	34	313	A86	C21-C20-C15	-2.51	115.24	123.35
27	33	309	CLA	C2A-C1A-CHA	2.51	128.22	123.87
27	32	311	CLA	CMB-C2B-C1B	-2.51	121.60	125.42
38	33	313	A86	C25-C24-C1	-2.51	119.48	126.36
38	33	315	A86	C40-C32-C31	-2.51	108.23	110.47
29	C	515	BCR	C27-C26-C25	2.51	126.09	122.70
32	a	408	LHG	C20-C19-C18	-2.51	101.70	114.37
38	13	302	A86	C7-C6-C5	-2.51	118.75	122.82
33	B	618	LMG	O6-C1-O1	-2.51	104.12	110.04
38	34	303	A86	C7-C6-C5	-2.50	118.76	122.82
27	c	513	CLA	O2D-CGD-O1D	-2.50	118.97	123.85
30	b	620	SQD	O9-S-C6	2.50	110.50	106.76
38	34	303	A86	C41-C32-C31	-2.50	108.23	110.47
38	12	315	A86	C25-C24-C1	-2.50	119.50	126.36
38	31	312	A86	C9-C10-C11	-2.50	119.56	126.64
27	12	306	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
27	b	622	CLA	C1-C2-C3	-2.50	122.10	126.20
27	C	513	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
38	13	313	A86	C25-C24-C1	-2.50	119.50	126.36
38	31	311	A86	C25-C24-C1	-2.50	119.50	126.36
29	c	515	BCR	C27-C26-C25	2.50	126.08	122.70
38	33	314	A86	C9-C10-C11	-2.50	119.57	126.64
27	c	502	CLA	CMB-C2B-C3B	2.50	132.43	126.55
32	L	101	LHG	O8-C23-C24	2.50	119.45	111.83
38	34	314	A86	C25-C24-C1	-2.50	119.51	126.36
27	c	503	CLA	C2A-C1A-CHA	2.50	128.20	123.87
38	11	316	A86	C41-C32-C31	-2.50	108.24	110.47
32	l	102	LHG	O8-C23-C24	2.50	119.44	111.83
38	31	313	A86	C40-C32-C31	-2.49	108.24	110.47
27	c	504	CLA	O2A-CGA-O1A	-2.49	117.39	123.63
27	W	103	CLA	CHB-C4A-NA	2.49	128.00	124.40
38	32	315	A86	C25-C24-C1	-2.49	119.53	126.36
38	11	316	A86	C7-C6-C5	-2.49	118.78	122.82
38	11	313	A86	C40-C32-C31	-2.49	108.24	110.47
27	D	405	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
27	B	615	CLA	CHB-C4A-NA	2.49	128.00	124.40
38	12	304	A86	C7-C6-C5	-2.49	118.78	122.82
38	13	315	A86	C40-C32-C31	-2.49	108.25	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	615	CLA	CHB-C4A-NA	2.49	127.99	124.40
38	31	316	A86	C7-C6-C5	-2.49	118.78	122.82
27	13	304	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
29	h	101	BCR	C27-C26-C25	2.49	126.06	122.70
27	C	504	CLA	O2A-CGA-O1A	-2.49	117.41	123.63
27	C	502	CLA	CMB-C2B-C3B	2.49	132.40	126.55
30	b	620	SQD	O48-C23-O10	-2.49	117.41	123.63
38	14	315	A86	C40-C32-C31	-2.49	108.25	110.47
27	B	605	CLA	C3B-C4B-NB	-2.48	108.31	110.53
27	14	304	CLA	O2D-CGD-O1D	-2.48	119.01	123.85
38	34	316	A86	C40-C32-C31	-2.48	108.25	110.47
38	12	304	A86	C41-C32-C31	-2.48	108.25	110.47
33	q	301	LMG	C9-C8-C7	-2.48	106.00	111.78
27	34	305	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
33	C	519	LMG	C9-C8-C7	-2.48	106.00	111.78
38	32	317	A86	C40-C32-C31	-2.48	108.25	110.47
27	31	302	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
27	d	405	CLA	CHB-C4A-NA	2.48	127.98	124.40
27	33	304	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
33	B	619	LMG	O1-C1-C2	-2.48	104.51	108.27
30	B	620	SQD	O48-C23-O10	-2.48	117.43	123.63
27	C	503	CLA	C2A-C1A-CHA	2.48	128.17	123.87
29	H	101	BCR	C11-C10-C9	-2.48	123.80	127.28
38	31	316	A86	C41-C32-C31	-2.48	108.26	110.47
38	32	304	A86	C41-C32-C31	-2.47	108.26	110.47
38	13	317	A86	C7-C6-C5	-2.47	118.81	122.82
38	12	317	A86	C40-C32-C31	-2.47	108.26	110.47
29	C	520	BCR	C15-C14-C13	-2.47	123.81	127.28
38	13	317	A86	C41-C32-C31	-2.47	108.26	110.47
38	33	302	A86	C7-C6-C5	-2.47	118.81	122.82
27	d	401	CLA	CHB-C1B-NB	2.47	127.75	124.05
29	Z	101	BCR	C7-C8-C9	-2.47	122.58	126.23
38	34	313	A86	C23-C16-C22	-2.47	103.78	107.37
27	B	606	CLA	CHC-C1C-NC	2.47	128.03	124.31
27	d	405	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
35	J	101	DGD	O3D-C3D-C4D	-2.47	104.56	110.38
29	h	101	BCR	C11-C10-C9	-2.46	123.82	127.28
27	b	611	CLA	CMB-C2B-C1B	-2.46	121.67	125.42
27	b	615	CLA	CHA-C1A-NA	-2.46	120.81	126.39
29	c	519	BCR	C15-C14-C13	-2.46	123.83	127.28
38	33	302	A86	C41-C32-C31	-2.46	108.27	110.47
27	D	401	CLA	CHB-C1B-NB	2.46	127.74	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	32	306	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
35	j	101	DGD	O3D-C3D-C4D	-2.46	104.58	110.38
27	B	611	CLA	CMB-C2B-C1B	-2.46	121.67	125.42
38	32	314	A86	C23-C16-C22	-2.46	103.80	107.37
32	L	102	LHG	C11-C10-C9	-2.46	101.95	114.37
28	D	403	PHO	O2D-CGD-O1D	-2.46	119.07	123.85
27	c	509	CLA	CMB-C2B-C3B	2.46	132.33	126.55
36	D	407	PL9	C7-C3-C4	2.46	118.93	116.91
27	C	509	CLA	CMB-C2B-C3B	2.45	132.32	126.55
38	32	304	A86	C7-C6-C5	-2.45	118.84	122.82
32	l	103	LHG	C11-C10-C9	-2.45	101.97	114.37
27	14	306	CLA	CBA-CAA-C2A	-2.45	106.50	113.79
38	31	310	A86	C23-C16-C22	-2.45	103.81	107.37
37	V	201	HEM	CAC-C3C-C2C	-2.45	120.46	128.43
36	d	407	PL9	C42-C43-C44	-2.45	122.02	127.62
33	b	619	LMG	O1-C1-C2	-2.45	104.55	108.27
38	33	312	A86	C23-C16-C22	-2.45	103.81	107.37
38	14	312	A86	C23-C16-C22	-2.45	103.81	107.37
27	D	401	CLA	CMB-C2B-C1B	-2.45	121.69	125.42
27	34	310	CLA	CHA-C1A-NA	-2.45	120.85	126.39
38	11	316	A86	C9-C10-C11	-2.45	119.72	126.64
36	D	407	PL9	O1-C4-C3	-2.45	118.15	120.73
27	b	609	CLA	C2A-C1A-CHA	2.45	128.11	123.87
27	34	309	CLA	C2A-C1A-CHA	2.44	128.11	123.87
27	D	405	CLA	CHB-C4A-NA	2.44	127.93	124.40
27	b	612	CLA	CMD-C2D-C1D	-2.44	120.42	124.73
27	11	306	CLA	C2A-C1A-CHA	2.44	128.11	123.87
38	31	316	A86	C9-C10-C11	-2.44	119.73	126.64
27	32	308	CLA	CBA-CAA-C2A	-2.44	106.52	113.79
27	12	308	CLA	CBA-CAA-C2A	-2.44	106.53	113.79
27	B	609	CLA	C2A-C1A-CHA	2.44	128.10	123.87
27	13	306	CLA	CBA-CAA-C2A	-2.44	106.53	113.79
27	13	309	CLA	CHA-C1A-NA	-2.44	120.87	126.39
28	d	403	PHO	O2D-CGD-O1D	-2.44	119.10	123.85
27	31	304	CLA	CBA-CAA-C2A	-2.44	106.53	113.79
38	12	304	A86	C9-C10-C11	-2.44	119.74	126.64
38	13	302	A86	C9-C10-C11	-2.44	119.75	126.64
27	c	511	CLA	CAA-C2A-C3A	-2.44	106.41	113.00
35	C	517	DGD	O3D-C3D-C4D	-2.44	104.63	110.38
37	v	201	HEM	CAC-C3C-C2C	-2.44	120.51	128.43
28	D	403	PHO	C1-C2-C3	-2.44	122.20	126.20
27	31	307	CLA	CHA-C1A-NA	-2.44	120.88	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	d	407	PL9	C7-C3-C4	2.44	118.92	116.91
27	12	310	CLA	C2A-C1A-CHA	2.43	128.09	123.87
36	d	407	PL9	O1-C4-C3	-2.43	118.16	120.73
35	c	517	DGD	O3D-C3D-C4D	-2.43	104.64	110.38
38	34	303	A86	C9-C10-C11	-2.43	119.76	126.64
27	32	310	CLA	C2A-C1A-CHA	2.43	128.09	123.87
38	33	302	A86	C9-C10-C11	-2.43	119.76	126.64
28	d	403	PHO	C1-C2-C3	-2.43	122.21	126.20
33	b	619	LMG	O7-C10-O9	-2.43	118.02	123.70
27	B	615	CLA	CHA-C1A-NA	-2.43	120.88	126.39
33	W	101	LMG	O2-C2-C1	-2.43	104.28	110.08
27	b	604	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
36	d	404	PL9	O2-C1-C6	2.43	124.35	120.48
29	H	101	BCR	C27-C26-C25	2.43	125.99	122.70
27	14	308	CLA	C2A-C1A-CHA	2.43	128.08	123.87
27	11	304	CLA	CBA-CAA-C2A	-2.43	106.56	113.79
38	32	304	A86	C9-C10-C11	-2.43	119.77	126.64
27	33	306	CLA	CBA-CAA-C2A	-2.43	106.57	113.79
29	b	623	BCR	C27-C26-C25	2.43	125.99	122.70
29	B	623	BCR	C33-C5-C6	-2.43	121.83	124.48
27	C	503	CLA	C1D-ND-C4D	2.43	108.02	106.31
27	13	308	CLA	C2A-C1A-CHA	2.43	128.08	123.87
27	c	508	CLA	CHA-C1A-NA	-2.43	120.89	126.39
38	13	317	A86	C9-C10-C11	-2.43	119.78	126.64
29	z	101	BCR	C7-C8-C9	-2.43	122.65	126.23
33	q	301	LMG	C40-C39-C38	-2.42	102.11	114.37
38	32	315	A86	C40-C32-C31	-2.42	108.30	110.47
38	12	314	A86	C23-C16-C22	-2.42	103.85	107.37
29	b	616	BCR	C30-C25-C26	-2.42	119.32	122.64
27	C	511	CLA	CAA-C2A-C3A	-2.42	106.45	113.00
27	34	307	CLA	CBA-CAA-C2A	-2.42	106.58	113.79
33	C	519	LMG	C40-C39-C38	-2.42	102.12	114.37
32	A	408	LHG	C11-C10-C9	-2.42	102.13	114.37
29	c	516	BCR	C7-C8-C9	-2.42	122.66	126.23
27	12	311	CLA	CHA-C1A-NA	-2.42	120.91	126.39
38	13	312	A86	C23-C16-C22	-2.42	103.86	107.37
36	D	407	PL9	C42-C43-C44	-2.42	122.09	127.62
27	B	612	CLA	CMD-C2D-C1D	-2.42	120.47	124.73
27	b	607	CLA	CAA-C2A-C3A	-2.42	106.47	113.00
29	C	516	BCR	C7-C8-C9	-2.42	122.66	126.23
33	w	101	LMG	O2-C2-C1	-2.42	104.32	110.08
33	B	619	LMG	O7-C10-O9	-2.42	118.06	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	b	619	LMG	O2-C2-C1	-2.42	104.32	110.08
29	b	616	BCR	C24-C23-C22	-2.42	122.66	126.23
38	13	313	A86	C40-C32-C31	-2.42	108.31	110.47
37	f	102	HEM	CAC-C3C-C4C	-2.42	119.05	124.82
27	14	309	CLA	CHA-C1A-NA	-2.42	120.92	126.39
27	b	615	CLA	O2A-CGA-O1A	-2.42	117.59	123.63
38	11	310	A86	C23-C16-C22	-2.41	103.86	107.37
27	C	509	CLA	CHB-C1B-NB	2.41	127.67	124.05
27	11	307	CLA	CHA-C1A-NA	-2.41	120.92	126.39
37	E	101	HEM	CAC-C3C-C4C	-2.41	119.06	124.82
33	q	301	LMG	C38-C37-C36	-2.41	102.17	114.37
27	C	510	CLA	O2A-CGA-O1A	-2.41	117.59	123.63
33	C	519	LMG	C38-C37-C36	-2.41	102.18	114.37
33	B	619	LMG	O2-C2-C1	-2.41	104.33	110.08
27	b	606	CLA	CHC-C1C-NC	2.41	127.94	124.31
27	32	311	CLA	CHA-C1A-NA	-2.41	120.93	126.39
27	c	509	CLA	CHB-C1B-NB	2.41	127.67	124.05
27	31	306	CLA	C2A-C1A-CHA	2.41	128.05	123.87
29	h	101	BCR	C15-C14-C13	-2.41	123.90	127.28
32	a	408	LHG	C11-C10-C9	-2.41	102.21	114.37
27	B	615	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
27	c	510	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
30	A	406	SQD	C1-C2-C3	-2.40	104.95	110.01
35	c	517	DGD	O6E-C5E-C6E	-2.40	100.49	106.44
36	D	404	PL9	O2-C1-C6	2.40	124.30	120.48
27	33	308	CLA	C2A-C1A-CHA	2.40	128.04	123.87
27	B	607	CLA	CAA-C2A-C3A	-2.40	106.51	113.00
37	V	201	HEM	CHD-C4C-C3C	2.40	129.26	125.21
33	B	618	LMG	O3-C3-C2	-2.40	104.72	110.38
27	c	507	CLA	O1D-CGD-CBD	2.40	129.25	124.52
38	33	313	A86	C40-C32-C31	-2.40	108.32	110.47
27	B	604	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
29	B	616	BCR	C24-C23-C22	-2.40	122.69	126.23
35	j	101	DGD	O3E-C3E-C2E	-2.40	104.73	110.38
27	d	401	CLA	CMB-C2B-C1B	-2.40	121.77	125.42
37	v	201	HEM	CHD-C4C-C3C	2.39	129.25	125.21
35	J	101	DGD	O3E-C3E-C2E	-2.39	104.73	110.38
29	B	616	BCR	C30-C25-C26	-2.39	119.37	122.64
27	C	504	CLA	CAA-C2A-C3A	-2.39	106.54	113.00
38	31	311	A86	C40-C32-C31	-2.39	108.33	110.47
36	d	404	PL9	C20-C19-C21	2.39	119.38	115.23
29	H	101	BCR	C15-C14-C13	-2.39	123.93	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	622	CLA	C1-C2-C3	-2.39	122.29	126.20
27	c	504	CLA	CAA-C2A-C3A	-2.39	106.55	113.00
33	m	102	LMG	O6-C1-O1	-2.39	104.41	110.04
35	C	517	DGD	CDB-CCB-CBB	-2.39	102.31	114.37
27	33	309	CLA	CHA-C1A-NA	-2.39	120.99	126.39
30	a	406	SQD	C1-C2-C3	-2.39	104.99	110.01
35	c	517	DGD	CDB-CCB-CBB	-2.39	102.31	114.37
35	C	517	DGD	O6E-C5E-C6E	-2.38	100.53	106.44
33	D	408	LMG	C40-C39-C38	-2.38	102.32	114.37
29	B	623	BCR	C27-C26-C25	2.38	125.92	122.70
33	b	618	LMG	O3-C3-C2	-2.38	104.76	110.38
27	B	613	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
33	M	103	LMG	O6-C1-O1	-2.38	104.42	110.04
27	C	507	CLA	O1D-CGD-CBD	2.38	129.22	124.52
36	D	404	PL9	C20-C19-C21	2.38	119.36	115.23
27	32	312	CLA	CHA-C1A-NA	-2.38	121.00	126.39
29	z	101	BCR	C29-C30-C25	2.38	113.90	110.44
27	C	510	CLA	CMB-C2B-C3B	2.38	132.15	126.55
35	c	517	DGD	O5E-C6E-C5E	-2.38	103.23	111.33
27	C	508	CLA	CHA-C1A-NA	-2.38	121.00	126.39
33	32	301	LMG	C1-C2-C3	-2.38	105.01	110.01
33	d	408	LMG	C40-C39-C38	-2.38	102.36	114.37
29	f	101	BCR	C27-C26-C25	2.38	125.91	122.70
29	B	617	BCR	C15-C16-C17	-2.38	118.66	123.52
27	33	310	CLA	CHA-C1A-NA	-2.37	121.01	126.39
38	14	313	A86	C40-C32-C31	-2.37	108.35	110.47
33	d	408	LMG	O3-C3-C2	-2.37	104.78	110.38
35	c	518	DGD	O3E-C3E-C2E	-2.37	104.78	110.38
29	F	101	BCR	C16-C15-C14	-2.37	118.67	123.52
35	C	518	DGD	O3E-C3E-C2E	-2.37	104.79	110.38
29	f	101	BCR	C16-C15-C14	-2.37	118.67	123.52
32	a	408	LHG	C18-C17-C16	-2.37	102.39	114.37
32	A	408	LHG	C18-C17-C16	-2.37	102.39	114.37
27	b	613	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
27	c	510	CLA	CMB-C2B-C3B	2.37	132.12	126.55
29	F	101	BCR	C27-C26-C25	2.37	125.91	122.70
33	b	618	LMG	O1-C1-C2	-2.37	104.68	108.27
38	34	314	A86	C40-C32-C31	-2.37	108.35	110.47
27	m	101	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
27	31	308	CLA	CHA-C1A-NA	-2.37	121.03	126.39
30	b	620	SQD	C1-O5-C5	2.37	118.34	113.72
33	W	101	LMG	C40-C39-C38	-2.37	102.41	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	D	408	LMG	O3-C3-C2	-2.37	104.80	110.38
33	B	618	LMG	O1-C1-C2	-2.36	104.68	108.27
29	c	515	BCR	C33-C5-C6	-2.36	121.91	124.48
35	C	517	DGD	O2D-C2D-C1D	-2.36	104.44	110.08
33	w	101	LMG	C40-C39-C38	-2.36	102.42	114.37
27	b	607	CLA	C3B-C4B-NB	-2.36	108.42	110.53
27	11	306	CLA	C3B-C4B-NB	-2.36	108.42	110.53
27	13	308	CLA	C3B-C4B-NB	-2.36	108.42	110.53
27	32	310	CLA	C3B-C4B-NB	-2.36	108.42	110.53
27	13	310	CLA	CHA-C1A-NA	-2.36	121.05	126.39
35	c	517	DGD	O2D-C2D-C1D	-2.36	104.45	110.08
27	W	103	CLA	CMB-C2B-C1B	-2.36	121.83	125.42
35	C	517	DGD	O5E-C6E-C5E	-2.36	103.31	111.33
30	B	620	SQD	C4-C3-C2	2.36	114.97	110.83
27	b	614	CLA	C2A-C1A-CHA	2.36	127.95	123.87
38	11	311	A86	C40-C32-C31	-2.35	108.36	110.47
27	c	505	CLA	O2A-CGA-O1A	-2.35	117.74	123.63
27	b	612	CLA	CMD-C2D-C3D	2.35	133.09	127.69
38	12	315	A86	C40-C32-C31	-2.35	108.37	110.47
30	B	620	SQD	C1-O5-C5	2.35	118.31	113.72
27	c	509	CLA	CGD-CBD-CAD	-2.35	103.23	110.85
29	b	617	BCR	C15-C16-C17	-2.35	118.71	123.52
29	C	515	BCR	C33-C5-C6	-2.35	121.92	124.48
27	B	603	CLA	CMB-C2B-C1B	-2.35	121.84	125.42
30	b	620	SQD	C4-C3-C2	2.35	114.95	110.83
27	12	312	CLA	CHA-C1A-NA	-2.35	121.07	126.39
29	b	617	BCR	C27-C26-C25	2.35	125.88	122.70
27	c	511	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
27	C	511	CLA	C1-C2-C3	-2.35	122.35	126.20
27	12	308	CLA	CHB-C1B-C2B	-2.34	120.62	127.43
27	14	310	CLA	CHA-C1A-NA	-2.34	121.08	126.39
27	34	311	CLA	CHA-C1A-NA	-2.34	121.08	126.39
27	B	614	CLA	C2A-C1A-CHA	2.34	127.94	123.87
27	11	308	CLA	CHA-C1A-NA	-2.34	121.09	126.39
27	C	509	CLA	CGD-CBD-CAD	-2.34	103.26	110.85
38	33	316	A86	C-C1-C24	2.34	121.67	118.09
29	Z	101	BCR	C29-C30-C25	2.34	113.84	110.44
38	11	314	A86	C-C1-C24	2.34	121.66	118.09
27	C	505	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
27	11	304	CLA	CHB-C1B-C2B	-2.34	120.63	127.43
35	c	518	DGD	C3D-C4D-C5D	-2.34	105.99	110.23
27	B	607	CLA	C3B-C4B-NB	-2.34	108.44	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	31	304	CLA	CHB-C1B-C2B	-2.34	120.64	127.43
27	M	102	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
27	A	402	CLA	CHB-C4A-NA	2.34	127.77	124.40
35	j	101	DGD	CAB-C9B-C8B	-2.34	102.56	114.37
38	31	314	A86	C-C1-C24	2.34	121.66	118.09
27	b	611	CLA	CHB-C4A-NA	2.33	127.77	124.40
27	b	602	CLA	C3B-C4B-NB	-2.33	108.45	110.53
27	c	504	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
29	h	101	BCR	C24-C23-C22	-2.33	122.78	126.23
36	D	404	PL9	C37-C38-C39	-2.33	122.29	127.62
33	b	618	LMG	C40-C39-C38	-2.33	102.58	114.37
27	c	511	CLA	C1-C2-C3	-2.33	122.38	126.20
33	B	618	LMG	C40-C39-C38	-2.33	102.59	114.37
27	w	103	CLA	CMB-C2B-C1B	-2.33	121.87	125.42
29	F	101	BCR	C15-C16-C17	-2.33	118.75	123.52
35	J	101	DGD	CAB-C9B-C8B	-2.33	102.59	114.37
27	C	511	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
38	12	316	A86	C7-C6-C8	2.33	121.65	118.09
27	13	306	CLA	CHB-C1B-C2B	-2.33	120.66	127.43
33	12	301	LMG	C1-C2-C3	-2.33	105.11	110.01
29	B	617	BCR	C27-C26-C25	2.33	125.85	122.70
27	34	307	CLA	CHB-C1B-C2B	-2.33	120.67	127.43
29	f	101	BCR	C15-C16-C17	-2.33	118.76	123.52
27	B	612	CLA	CMD-C2D-C3D	2.33	133.03	127.69
35	C	518	DGD	C3D-C4D-C5D	-2.33	106.02	110.23
38	13	314	A86	C7-C6-C8	2.32	121.64	118.09
29	a	409	BCR	C27-C26-C25	2.32	125.84	122.70
27	b	603	CLA	CMB-C2B-C1B	-2.32	121.88	125.42
27	33	306	CLA	CHB-C1B-C2B	-2.32	120.68	127.43
27	c	505	CLA	C3B-C4B-NB	-2.32	108.46	110.53
27	B	611	CLA	C7-C6-C5	-2.32	107.08	113.26
27	32	308	CLA	CHB-C1B-C2B	-2.32	120.69	127.43
27	c	507	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
27	B	611	CLA	CHB-C1B-NB	2.32	127.53	124.05
38	14	301	A86	C-C1-C24	2.32	121.63	118.09
38	13	316	A86	C-C1-C24	2.32	121.63	118.09
27	C	506	CLA	CMC-C2C-C1C	-2.32	121.42	125.03
27	B	603	CLA	O2A-CGA-O1A	-2.32	117.84	123.63
38	32	318	A86	C-C1-C24	2.31	121.62	118.09
27	14	306	CLA	CHB-C1B-C2B	-2.31	120.71	127.43
33	d	408	LMG	C6-C5-C4	-2.31	107.34	113.02
27	33	308	CLA	C3B-C4B-NB	-2.31	108.47	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	623	BCR	C33-C5-C6	-2.31	121.96	124.48
38	14	316	A86	C-C1-C24	2.31	121.62	118.09
27	31	306	CLA	C3B-C4B-NB	-2.31	108.47	110.53
27	b	609	CLA	CHC-C4B-NB	2.31	127.52	124.05
27	B	611	CLA	CHB-C4A-NA	2.31	127.73	124.40
38	34	301	A86	C-C1-C24	2.31	121.62	118.09
27	B	613	CLA	C2A-C1A-CHA	2.31	127.88	123.87
27	14	308	CLA	C3B-C4B-NB	-2.31	108.47	110.53
38	14	301	A86	C21-C20-C15	-2.31	115.89	123.35
27	b	611	CLA	C7-C6-C5	-2.31	107.11	113.26
38	31	314	A86	C21-C20-C15	-2.31	115.90	123.35
27	a	402	CLA	CMB-C2B-C3B	2.31	131.98	126.55
36	d	404	PL9	C37-C38-C39	-2.31	122.34	127.62
27	W	102	CLA	CAA-C2A-C3A	-2.31	106.76	113.00
27	b	611	CLA	CHB-C1B-NB	2.31	127.51	124.05
27	c	506	CLA	CMC-C2C-C1C	-2.31	121.43	125.03
27	w	102	CLA	CAA-C2A-C3A	-2.31	106.77	113.00
27	D	405	CLA	C3B-C4B-NB	-2.31	108.47	110.53
27	a	402	CLA	CHB-C4A-NA	2.31	127.73	124.40
27	C	505	CLA	C3B-C4B-NB	-2.31	108.47	110.53
27	c	506	CLA	C3B-C4B-NB	-2.31	108.47	110.53
27	C	504	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
38	13	316	A86	C21-C20-C15	-2.30	115.91	123.35
27	Z	102	CLA	C2A-C1A-CHA	2.30	127.87	123.87
27	b	603	CLA	O2A-CGA-O1A	-2.30	117.86	123.63
38	32	318	A86	C21-C20-C15	-2.30	115.91	123.35
38	14	316	A86	C21-C20-C15	-2.30	115.92	123.35
27	d	405	CLA	C3B-C4B-NB	-2.30	108.47	110.53
27	34	309	CLA	C3B-C4B-NB	-2.30	108.47	110.53
27	C	502	CLA	C1-C2-C3	-2.30	122.42	126.20
27	B	612	CLA	CHC-C4B-NB	2.30	127.50	124.05
38	34	301	A86	C21-C20-C15	-2.30	115.92	123.35
32	L	101	LHG	C18-C17-C16	-2.30	102.74	114.37
38	33	316	A86	C21-C20-C15	-2.30	115.92	123.35
33	D	408	LMG	C6-C5-C4	-2.30	107.37	113.02
29	H	101	BCR	C24-C23-C22	-2.30	122.83	126.23
33	d	408	LMG	C38-C37-C36	-2.30	102.74	114.37
38	32	316	A86	C7-C6-C8	2.30	121.60	118.09
27	14	307	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
33	D	408	LMG	C38-C37-C36	-2.30	102.75	114.37
27	B	602	CLA	C3B-C4B-NB	-2.30	108.48	110.53
27	A	402	CLA	CMB-C2B-C3B	2.30	131.95	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	h	101	BCR	C40-C30-C25	2.30	113.84	110.24
32	l	102	LHG	C18-C17-C16	-2.30	102.76	114.37
29	A	409	BCR	C27-C26-C25	2.30	125.81	122.70
27	c	503	CLA	CHA-C1A-NA	-2.30	121.19	126.39
33	B	618	LMG	O1-C7-C8	-2.29	105.24	110.82
27	b	609	CLA	O1D-CGD-CBD	2.29	129.04	124.52
27	12	310	CLA	C3B-C4B-NB	-2.29	108.48	110.53
27	B	602	CLA	O2D-CGD-CBD	2.29	115.24	111.23
27	31	305	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
27	33	307	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
27	W	102	CLA	CAA-CBA-CGA	-2.29	106.70	113.21
27	B	609	CLA	C3B-C4B-NB	-2.29	108.48	110.53
27	b	601	CLA	C2A-C1A-CHA	2.29	127.84	123.87
38	11	314	A86	C21-C20-C15	-2.29	115.96	123.35
38	33	314	A86	C7-C6-C8	2.29	121.59	118.09
35	H	102	DGD	CBB-CAB-C9B	-2.29	102.80	114.37
33	q	301	LMG	O3-C3-C2	-2.29	104.98	110.38
27	B	601	CLA	C2A-C1A-CHA	2.29	127.84	123.87
27	c	508	CLA	CAA-C2A-C3A	-2.29	106.82	113.00
35	h	102	DGD	CBB-CAB-C9B	-2.29	102.80	114.37
33	b	618	LMG	O1-C7-C8	-2.29	105.25	110.82
27	z	102	CLA	C2A-C1A-CHA	2.29	127.84	123.87
38	14	314	A86	C7-C6-C8	2.29	121.58	118.09
38	31	312	A86	C7-C6-C8	2.29	121.58	118.09
27	C	507	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
27	b	613	CLA	C2A-C1A-CHA	2.28	127.83	123.87
38	34	315	A86	C7-C6-C8	2.28	121.58	118.09
27	C	506	CLA	C3B-C4B-NB	-2.28	108.49	110.53
27	c	502	CLA	C1-C2-C3	-2.28	122.46	126.20
27	C	508	CLA	CAA-C2A-C3A	-2.28	106.83	113.00
27	C	503	CLA	CHA-C1A-NA	-2.28	121.23	126.39
27	w	102	CLA	CAA-CBA-CGA	-2.28	106.73	113.21
27	13	304	CLA	CAA-C2A-C3A	-2.28	106.84	113.00
27	b	602	CLA	O2D-CGD-CBD	2.28	115.21	111.23
32	l	103	LHG	C18-C17-C16	-2.28	102.85	114.37
38	11	312	A86	C7-C6-C8	2.28	121.57	118.09
27	B	605	CLA	C1-C2-C3	-2.28	122.47	126.20
27	d	401	CLA	CAA-C2A-C3A	-2.28	106.85	113.00
27	D	401	CLA	CAA-C2A-C3A	-2.28	106.85	113.00
27	11	302	CLA	CAA-C2A-C3A	-2.28	106.85	113.00
27	14	304	CLA	CAA-C2A-C3A	-2.28	106.85	113.00
27	33	304	CLA	CAA-C2A-C3A	-2.28	106.85	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	13	307	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
27	b	613	CLA	C4-C3-C5	2.27	119.17	115.23
27	B	609	CLA	O1D-CGD-CBD	2.27	129.00	124.52
33	C	519	LMG	O3-C3-C2	-2.27	105.02	110.38
27	32	306	CLA	CAA-C2A-C3A	-2.27	106.86	113.00
27	12	306	CLA	CAA-C2A-C3A	-2.27	106.86	113.00
29	H	101	BCR	C40-C30-C25	2.27	113.81	110.24
27	B	609	CLA	CHC-C4B-NB	2.27	127.46	124.05
36	D	407	PL9	C7-C3-C2	-2.27	120.71	123.39
27	34	305	CLA	CAA-C2A-C3A	-2.27	106.87	113.00
27	31	307	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
27	B	622	CLA	CMD-C2D-C1D	-2.27	120.73	124.73
27	31	302	CLA	CAA-C2A-C3A	-2.27	106.87	113.00
32	L	102	LHG	C18-C17-C16	-2.27	102.90	114.37
27	34	308	CLA	CMB-C2B-C1B	-2.27	121.97	125.42
27	b	608	CLA	O2D-CGD-CBD	2.27	115.19	111.23
27	b	609	CLA	C3B-C4B-NB	-2.27	108.51	110.53
27	14	309	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
27	B	608	CLA	O2D-CGD-CBD	2.27	115.19	111.23
27	b	612	CLA	CHC-C4B-NB	2.26	127.45	124.05
35	c	518	DGD	O6E-C1E-O5D	-2.26	104.69	110.04
27	11	307	CLA	O2A-CGA-O1A	-2.26	117.96	123.63
27	34	311	CLA	O2D-CGD-O1D	-2.26	119.44	123.85
36	d	407	PL9	C7-C3-C2	-2.26	120.72	123.39
27	B	613	CLA	C4-C3-C5	2.26	119.15	115.23
27	32	311	CLA	CHB-C1B-NB	2.26	127.44	124.05
27	b	613	CLA	CAA-C2A-C3A	-2.26	106.89	113.00
27	11	306	CLA	CHC-C4B-NB	2.26	127.44	124.05
27	13	308	CLA	CHC-C4B-NB	2.26	127.44	124.05
27	c	513	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
27	13	309	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
27	B	613	CLA	CAA-C2A-C3A	-2.26	106.90	113.00
30	b	620	SQD	O48-C23-C24	2.26	118.71	111.83
27	11	305	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
35	C	518	DGD	O6E-C1E-O5D	-2.25	104.72	110.04
28	D	403	PHO	C2D-C1D-ND	-2.25	107.80	109.43
27	b	615	CLA	C2A-C1A-CHA	2.25	127.77	123.87
27	34	309	CLA	CHC-C4B-NB	2.25	127.43	124.05
33	w	101	LMG	C6-C5-C4	-2.25	107.49	113.02
27	32	309	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
30	B	620	SQD	O48-C23-C24	2.25	118.69	111.83
33	b	618	LMG	C38-C37-C36	-2.25	103.00	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	d	401	CLA	O2D-CGD-CBD	2.25	115.16	111.23
33	W	101	LMG	C6-C5-C4	-2.25	107.50	113.02
28	A	403	PHO	CBA-CAA-C2A	-2.25	107.16	113.78
27	B	615	CLA	C2A-C1A-CHA	2.24	127.76	123.87
27	33	309	CLA	O2A-CGA-O1A	-2.24	118.01	123.63
32	b	621	LHG	C18-C17-C16	-2.24	103.02	114.37
27	b	605	CLA	C1-C2-C3	-2.24	122.52	126.20
27	B	609	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
27	12	309	CLA	CMB-C2B-C1B	-2.24	122.00	125.42
27	C	513	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
32	B	621	LHG	C18-C17-C16	-2.24	103.04	114.37
28	d	403	PHO	C2D-C1D-ND	-2.24	107.81	109.43
27	34	310	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
27	b	604	CLA	CHA-C1A-NA	-2.24	121.32	126.39
27	33	304	CLA	CHA-C1A-NA	-2.24	121.32	126.39
33	B	618	LMG	C38-C37-C36	-2.24	103.05	114.37
28	a	403	PHO	CBA-CAA-C2A	-2.24	107.18	113.78
27	b	609	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
27	32	310	CLA	CHC-C4B-NB	2.24	127.41	124.05
27	32	311	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
35	C	518	DGD	C3G-C2G-C1G	-2.24	106.57	111.78
39	32	302	LMU	C1B-O5B-C5B	2.24	118.09	113.72
27	34	310	CLA	CHB-C1B-NB	2.24	127.41	124.05
27	b	602	CLA	CAA-C2A-C3A	-2.24	106.95	113.00
27	B	606	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
27	b	606	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
27	d	405	CLA	C1-C2-C3	-2.24	122.53	126.20
27	14	304	CLA	CHA-C1A-NA	-2.23	121.33	126.39
30	a	406	SQD	O48-C23-O10	-2.23	118.04	123.63
29	B	617	BCR	C11-C10-C9	-2.23	124.15	127.28
27	12	312	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
29	B	617	BCR	C40-C30-C25	2.23	113.75	110.24
38	33	315	A86	C-C1-C24	2.23	121.50	118.09
27	12	306	CLA	CHA-C1A-NA	-2.23	121.33	126.39
27	31	302	CLA	CHA-C1A-NA	-2.23	121.33	126.39
27	31	308	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
32	a	408	LHG	C5-O7-C7	-2.23	112.46	117.80
27	b	622	CLA	CHA-C1A-NA	-2.23	121.34	126.39
27	B	604	CLA	CHA-C1A-NA	-2.23	121.34	126.39
29	b	617	BCR	C11-C10-C9	-2.23	124.15	127.28
27	c	505	CLA	CAA-C2A-C3A	-2.23	106.98	113.00
27	12	311	CLA	O2A-CGA-O1A	-2.23	118.06	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	406	SQD	O48-C23-O10	-2.23	118.06	123.63
37	E	101	HEM	C1C-CHC-C4B	-2.23	121.29	126.02
27	13	310	CLA	O2D-CGD-O1D	-2.23	119.52	123.85
27	B	611	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
27	13	309	CLA	CHB-C1B-NB	2.22	127.39	124.05
27	11	308	CLA	O2D-CGD-O1D	-2.22	119.52	123.85
27	32	312	CLA	O2D-CGD-O1D	-2.22	119.52	123.85
27	c	508	CLA	CMB-C2B-C3B	2.22	131.78	126.55
37	V	201	HEM	C3B-C4B-NB	2.22	111.06	109.47
37	f	102	HEM	C1C-CHC-C4B	-2.22	121.30	126.02
29	B	617	BCR	C16-C15-C14	-2.22	118.98	123.52
33	12	301	LMG	O2-C2-C3	-2.22	105.14	110.38
32	A	408	LHG	C5-O7-C7	-2.22	112.48	117.80
35	c	518	DGD	C3G-C2G-C1G	-2.22	106.61	111.78
27	34	305	CLA	CHA-C1A-NA	-2.22	121.37	126.39
27	B	615	CLA	CHB-C1B-NB	2.22	127.38	124.05
27	33	310	CLA	O2D-CGD-O1D	-2.22	119.53	123.85
27	11	302	CLA	CHA-C1A-NA	-2.22	121.37	126.39
27	14	308	CLA	CHC-C4B-NB	2.22	127.38	124.05
27	31	304	CLA	C3B-C4B-NB	-2.22	108.55	110.53
27	C	505	CLA	CAA-C2A-C3A	-2.22	107.01	113.00
29	m	103	BCR	C33-C5-C6	-2.22	122.07	124.48
27	C	510	CLA	C16-C15-C13	-2.21	108.61	115.97
27	D	401	CLA	O2D-CGD-CBD	2.21	115.10	111.23
37	v	201	HEM	C3B-C4B-NB	2.21	111.06	109.47
27	12	310	CLA	CHC-C4B-NB	2.21	127.37	124.05
27	12	311	CLA	CHB-C1B-NB	2.21	127.37	124.05
27	b	603	CLA	O1D-CGD-CBD	2.21	128.88	124.52
29	c	515	BCR	C15-C14-C13	-2.21	124.17	127.28
27	11	304	CLA	C3B-C4B-NB	-2.21	108.56	110.53
38	11	313	A86	C34-O4-C38	-2.21	113.94	117.85
38	32	316	A86	C-C1-C24	2.21	121.47	118.09
27	b	615	CLA	CHB-C1B-NB	2.21	127.37	124.05
35	C	518	DGD	CAB-C9B-C8B	-2.21	103.19	114.37
29	b	617	BCR	C40-C30-C25	2.21	113.71	110.24
38	14	315	A86	C-C1-C24	2.21	121.47	118.09
27	B	602	CLA	CAA-C2A-C3A	-2.21	107.03	113.00
33	B	619	LMG	C38-C37-C36	-2.21	103.20	114.37
28	a	403	PHO	CMA-C3A-C4A	-2.21	109.85	114.61
38	32	317	A86	C-C1-C24	2.21	121.46	118.09
27	13	304	CLA	CHA-C1A-NA	-2.21	121.39	126.39
27	32	306	CLA	CHA-C1A-NA	-2.21	121.39	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	31	306	CLA	CHC-C4B-NB	2.21	127.36	124.05
29	f	101	BCR	C24-C23-C22	-2.21	122.97	126.23
38	12	304	A86	C35-C34-C33	2.21	113.85	109.89
38	12	317	A86	C34-O4-C38	-2.21	113.95	117.85
27	33	306	CLA	C3B-C4B-NB	-2.21	108.56	110.53
29	B	617	BCR	C15-C14-C13	-2.21	124.18	127.28
27	d	405	CLA	CAC-C3C-C4C	2.21	127.66	124.79
27	C	506	CLA	C2D-C1D-ND	-2.21	107.94	110.13
38	12	317	A86	C-C1-C24	2.21	121.46	118.09
33	b	619	LMG	C38-C37-C36	-2.21	103.21	114.37
29	M	101	BCR	C33-C5-C6	-2.21	122.08	124.48
28	A	403	PHO	CMA-C3A-C4A	-2.21	109.86	114.61
38	13	315	A86	C-C1-C24	2.20	121.46	118.09
27	c	502	CLA	C7-C6-C5	-2.20	107.39	113.26
27	11	307	CLA	CHB-C1B-NB	2.20	127.36	124.05
27	C	508	CLA	CMB-C2B-C3B	2.20	131.73	126.55
38	34	316	A86	C34-O4-C38	-2.20	113.95	117.85
38	14	314	A86	C-C1-C24	2.20	121.45	118.09
27	b	611	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
38	11	313	A86	C-C1-C24	2.20	121.45	118.09
38	13	315	A86	C34-O4-C38	-2.20	113.96	117.85
27	14	310	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
27	32	308	CLA	C3B-C4B-NB	-2.20	108.57	110.53
27	c	510	CLA	C16-C15-C13	-2.20	108.65	115.97
27	14	309	CLA	CHB-C1B-NB	2.20	127.35	124.05
27	33	309	CLA	CHB-C1B-NB	2.20	127.34	124.05
35	c	518	DGD	CAB-C9B-C8B	-2.20	103.27	114.37
27	C	502	CLA	C7-C6-C5	-2.20	107.41	113.26
29	b	617	BCR	C15-C14-C13	-2.19	124.20	127.28
39	12	302	LMU	C1B-O5B-C5B	2.19	118.00	113.72
35	j	101	DGD	CBB-CAB-C9B	-2.19	103.28	114.37
29	b	617	BCR	C16-C15-C14	-2.19	119.03	123.52
27	c	503	CLA	C3B-C4B-NB	-2.19	108.57	110.53
27	D	405	CLA	C1-C2-C3	-2.19	122.60	126.20
38	31	313	A86	C-C1-C24	2.19	121.44	118.09
36	d	407	PL9	C27-C28-C29	-2.19	122.61	127.62
27	c	506	CLA	C2D-C1D-ND	-2.19	107.96	110.13
27	B	622	CLA	CMD-C2D-C3D	2.19	132.72	127.69
35	c	518	DGD	O5E-C6E-C5E	-2.19	103.87	111.33
27	D	405	CLA	CAC-C3C-C4C	2.19	127.64	124.79
33	b	619	LMG	C6-C5-C4	-2.19	107.64	113.02
29	F	101	BCR	C24-C23-C22	-2.19	123.00	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	32	317	A86	C34-O4-C38	-2.19	113.98	117.85
36	D	407	PL9	C27-C28-C29	-2.19	122.61	127.62
27	b	603	CLA	CAA-CBA-CGA	-2.19	107.00	113.21
38	31	313	A86	C34-O4-C38	-2.19	113.98	117.85
33	M	103	LMG	C9-C8-C7	-2.19	106.69	111.78
29	c	516	BCR	C30-C25-C26	-2.19	119.65	122.64
27	c	514	CLA	C2A-C1A-CHA	2.19	127.66	123.87
38	34	316	A86	C-C1-C24	2.19	121.43	118.09
29	z	101	BCR	C34-C9-C10	-2.19	119.28	122.82
38	14	315	A86	C34-O4-C38	-2.18	113.99	117.85
38	13	302	A86	C35-C34-C33	2.18	113.81	109.89
27	b	610	CLA	CHB-C1B-NB	2.18	127.32	124.05
27	B	603	CLA	CAA-CBA-CGA	-2.18	107.01	113.21
29	Z	101	BCR	C34-C9-C10	-2.18	119.28	122.82
35	J	101	DGD	CBB-CAB-C9B	-2.18	103.34	114.37
27	A	402	CLA	CAA-C2A-C3A	-2.18	107.10	113.00
29	C	516	BCR	C30-C25-C26	-2.18	119.65	122.64
38	34	315	A86	C-C1-C24	2.18	121.42	118.09
27	B	603	CLA	O1D-CGD-CBD	2.18	128.82	124.52
38	33	315	A86	C34-O4-C38	-2.18	113.99	117.85
29	C	515	BCR	C15-C14-C13	-2.18	124.22	127.28
35	C	518	DGD	O5E-C6E-C5E	-2.18	103.91	111.33
38	31	316	A86	C35-C34-C33	2.18	113.80	109.89
27	34	310	CLA	CMB-C2B-C3B	2.18	131.68	126.55
33	b	618	LMG	O2-C2-C1	-2.18	104.88	110.08
38	32	304	A86	C35-C34-C33	2.18	113.80	109.89
27	a	402	CLA	O2D-CGD-O1D	-2.18	119.61	123.85
27	12	308	CLA	C3B-C4B-NB	-2.18	108.59	110.53
27	B	622	CLA	CHA-C1A-NA	-2.18	121.46	126.39
38	33	302	A86	C35-C34-C33	2.18	113.80	109.89
27	c	512	CLA	CHA-C1A-NA	-2.18	121.46	126.39
38	13	314	A86	C-C1-C24	2.18	121.41	118.09
38	31	312	A86	C-C1-C24	2.18	121.41	118.09
27	A	404	CLA	CHB-C1B-NB	2.18	127.31	124.05
27	C	502	CLA	CHC-C4B-NB	2.18	127.31	124.05
29	c	519	BCR	C20-C21-C22	-2.18	124.23	127.28
27	B	610	CLA	CHB-C1B-NB	2.18	127.31	124.05
27	a	404	CLA	CHB-C1B-NB	2.18	127.31	124.05
36	d	407	PL9	C36-C34-C33	-2.17	116.28	121.17
35	j	101	DGD	O6E-C1E-O5D	-2.17	104.91	110.04
27	31	307	CLA	CHB-C1B-NB	2.17	127.31	124.05
32	b	621	LHG	C20-C19-C18	-2.17	103.38	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	b	619	LMG	C40-C39-C38	-2.17	103.38	114.37
27	C	512	CLA	CHA-C4D-ND	2.17	137.03	132.55
37	v	201	HEM	CHC-C1C-NC	2.17	126.82	124.45
38	12	316	A86	C-C1-C24	2.17	121.41	118.09
27	c	502	CLA	CHC-C4B-NB	2.17	127.31	124.05
29	C	515	BCR	C16-C15-C14	-2.17	119.07	123.52
33	m	102	LMG	C9-C8-C7	-2.17	106.72	111.78
36	D	407	PL9	C36-C34-C33	-2.17	116.29	121.17
38	11	316	A86	C35-C34-C33	2.17	113.79	109.89
27	c	512	CLA	CHA-C4D-ND	2.17	137.03	132.55
27	13	310	CLA	C3B-C4B-NB	-2.17	108.59	110.53
38	33	314	A86	C-C1-C24	2.17	121.40	118.09
33	B	619	LMG	C6-C5-C4	-2.17	107.69	113.02
27	33	309	CLA	CMB-C2B-C3B	2.17	131.65	126.55
35	J	101	DGD	C3D-C4D-C5D	-2.17	106.30	110.23
29	C	516	BCR	C21-C20-C19	-2.17	116.92	123.20
32	B	621	LHG	C20-C19-C18	-2.17	103.41	114.37
38	11	312	A86	C-C1-C24	2.17	121.40	118.09
27	C	514	CLA	C2A-C1A-CHA	2.17	127.63	123.87
27	14	306	CLA	C3B-C4B-NB	-2.17	108.60	110.53
27	c	505	CLA	CHC-C1C-NC	2.17	127.57	124.31
27	a	402	CLA	CAA-C2A-C3A	-2.17	107.14	113.00
27	33	308	CLA	CHC-C4B-NB	2.17	127.30	124.05
33	B	618	LMG	O2-C2-C1	-2.16	104.92	110.08
38	13	317	A86	C35-C34-C33	2.16	113.77	109.89
27	34	307	CLA	C3B-C4B-NB	-2.16	108.60	110.53
27	C	505	CLA	CHC-C1C-NC	2.16	127.57	124.31
35	H	102	DGD	C5B-C4B-C3B	-2.16	103.44	114.37
33	B	619	LMG	C40-C39-C38	-2.16	103.44	114.37
27	C	507	CLA	CHB-C1B-NB	2.16	127.29	124.05
35	j	101	DGD	C3D-C4D-C5D	-2.16	106.31	110.23
36	D	404	PL9	C22-C23-C24	-2.16	122.68	127.62
35	h	102	DGD	C5B-C4B-C3B	-2.16	103.45	114.37
38	34	303	A86	C35-C34-C33	2.16	113.77	109.89
27	c	507	CLA	CHB-C1B-NB	2.16	127.29	124.05
27	32	312	CLA	C3B-C4B-NB	-2.16	108.60	110.53
27	11	307	CLA	CMB-C2B-C3B	2.16	131.63	126.55
27	C	511	CLA	C2D-C1D-ND	-2.16	107.99	110.13
27	B	604	CLA	C1D-ND-C4D	2.16	107.83	106.31
29	c	515	BCR	C16-C15-C14	-2.16	119.10	123.52
36	d	404	PL9	C22-C23-C24	-2.16	122.69	127.62
27	A	404	CLA	O2A-CGA-O1A	-2.16	118.24	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	d	404	PL9	O1-C4-C3	-2.15	118.46	120.73
27	C	512	CLA	CHA-C1A-NA	-2.15	121.51	126.39
27	A	402	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
33	M	103	LMG	C1-O6-C5	-2.15	109.51	113.72
27	a	404	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
27	c	511	CLA	C2D-C1D-ND	-2.15	108.00	110.13
33	m	102	LMG	C1-C2-C3	-2.15	105.49	110.01
29	c	516	BCR	C21-C20-C19	-2.15	116.97	123.20
33	M	103	LMG	C1-C2-C3	-2.15	105.49	110.01
27	13	306	CLA	C3B-C4B-NB	-2.15	108.61	110.53
27	C	511	CLA	CHB-C1B-NB	2.15	127.27	124.05
29	C	520	BCR	C20-C21-C22	-2.15	124.27	127.28
33	C	519	LMG	C3-C4-C5	-2.15	106.34	110.23
33	m	102	LMG	C1-O6-C5	-2.15	109.53	113.72
33	q	301	LMG	C3-C4-C5	-2.14	106.34	110.23
27	31	308	CLA	C3B-C4B-NB	-2.14	108.62	110.53
27	14	307	CLA	C2A-C1A-CHA	2.14	127.59	123.87
29	M	101	BCR	C21-C20-C19	-2.14	116.99	123.20
27	31	307	CLA	CMB-C2B-C3B	2.14	131.59	126.55
27	B	606	CLA	C3B-C4B-NB	-2.14	108.62	110.53
36	d	404	PL9	O2-C1-C2	-2.14	116.96	121.83
27	W	102	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
27	b	604	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
27	13	309	CLA	CMB-C2B-C3B	2.14	131.58	126.55
27	34	308	CLA	C2A-C1A-CHA	2.14	127.58	123.87
37	V	201	HEM	CHC-C1C-NC	2.14	126.78	124.45
27	32	311	CLA	CMB-C2B-C3B	2.14	131.58	126.55
35	C	518	DGD	C8B-C7B-C6B	-2.14	103.55	114.37
27	12	311	CLA	CMB-C2B-C3B	2.14	131.58	126.55
27	c	511	CLA	C2A-C1A-CHA	2.14	127.58	123.87
27	c	508	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
27	34	304	CLA	CAA-CBA-CGA	-2.14	107.14	113.21
29	m	103	BCR	C21-C20-C19	-2.14	117.01	123.20
29	z	101	BCR	C16-C17-C18	-2.13	124.28	127.28
33	q	301	LMG	C1-C2-C3	-2.13	105.52	110.01
27	C	511	CLA	C2A-C1A-CHA	2.13	127.57	123.87
32	l	102	LHG	C5-O7-C7	-2.13	112.69	117.80
27	34	311	CLA	C3B-C4B-NB	-2.13	108.62	110.53
27	14	309	CLA	CMB-C2B-C3B	2.13	131.57	126.55
27	b	608	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
27	C	503	CLA	CHC-C1C-NC	2.13	127.52	124.31
36	D	404	PL9	O2-C1-C2	-2.13	116.98	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	622	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
29	F	101	BCR	C40-C30-C25	2.13	113.58	110.24
27	12	312	CLA	C3B-C4B-NB	-2.13	108.63	110.53
35	J	101	DGD	O6E-C1E-O5D	-2.13	105.01	110.04
35	c	518	DGD	C8B-C7B-C6B	-2.13	103.60	114.37
36	D	404	PL9	O1-C4-C3	-2.13	118.48	120.73
27	B	603	CLA	C3B-C4B-NB	-2.13	108.63	110.53
27	33	310	CLA	C3B-C4B-NB	-2.13	108.63	110.53
32	L	101	LHG	C5-O7-C7	-2.13	112.70	117.80
27	33	307	CLA	C2A-C1A-CHA	2.13	127.56	123.87
27	B	606	CLA	C6-C7-C8	-2.13	108.89	115.97
29	f	101	BCR	C40-C30-C25	2.13	113.58	110.24
27	33	303	CLA	CAA-CBA-CGA	-2.13	107.17	113.21
27	b	603	CLA	C3B-C4B-NB	-2.13	108.63	110.53
27	c	502	CLA	C3B-C4B-NB	-2.13	108.63	110.53
27	C	508	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
27	13	303	CLA	CAA-CBA-CGA	-2.13	107.17	113.21
29	a	405	BCR	C7-C8-C9	-2.13	123.09	126.23
27	B	608	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
27	C	503	CLA	C3B-C4B-NB	-2.12	108.63	110.53
27	32	305	CLA	CAA-CBA-CGA	-2.12	107.18	113.21
27	13	307	CLA	C2A-C1A-CHA	2.12	127.55	123.87
39	32	302	LMU	C2'-C3'-C4'	2.12	114.50	109.68
27	31	301	CLA	CAA-CBA-CGA	-2.12	107.18	113.21
27	b	606	CLA	C6-C7-C8	-2.12	108.92	115.97
36	d	407	PL9	C11-C9-C8	-2.12	116.41	121.17
27	B	615	CLA	CMA-C3A-C4A	-2.12	106.08	111.77
27	b	606	CLA	C3B-C4B-NB	-2.12	108.64	110.53
27	32	309	CLA	C2A-C1A-CHA	2.12	127.55	123.87
27	b	615	CLA	O2D-CGD-CBD	2.12	114.94	111.23
29	z	101	BCR	C15-C16-C17	-2.12	119.18	123.52
27	A	402	CLA	C3B-C4B-NB	-2.12	108.64	110.53
27	11	308	CLA	C3B-C4B-NB	-2.12	108.64	110.53
38	14	316	A86	C19-C18-C17	-2.12	106.83	110.79
27	b	615	CLA	CMA-C3A-C4A	-2.12	106.08	111.77
27	B	604	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
29	Z	101	BCR	C15-C16-C17	-2.12	119.19	123.52
27	B	607	CLA	CHB-C1B-NB	2.12	127.22	124.05
29	B	617	BCR	C1-C6-C5	-2.12	119.75	122.64
27	12	309	CLA	C2A-C1A-CHA	2.11	127.54	123.87
27	w	102	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
27	12	305	CLA	CAA-CBA-CGA	-2.11	107.21	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	D	407	PL9	C50-C49-C48	-2.11	116.31	122.66
27	11	305	CLA	C2A-C1A-CHA	2.11	127.53	123.87
27	31	305	CLA	C2A-C1A-CHA	2.11	127.53	123.87
27	c	506	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
32	l	103	LHG	C27-C26-C25	-2.11	103.69	114.37
32	L	102	LHG	C27-C26-C25	-2.11	103.69	114.37
27	c	512	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
27	C	507	CLA	CHA-C1A-NA	-2.11	121.61	126.39
27	11	301	CLA	CAA-CBA-CGA	-2.11	107.21	113.21
27	C	506	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
27	D	401	CLA	CMB-C2B-C3B	2.11	131.52	126.55
27	B	614	CLA	C3A-C2A-C1A	2.11	104.50	101.34
27	b	604	CLA	C1D-ND-C4D	2.11	107.79	106.31
27	b	622	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
27	c	511	CLA	CHB-C1B-NB	2.11	127.21	124.05
27	C	512	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
37	f	102	HEM	CAA-C2A-C1A	2.11	129.06	124.94
27	14	303	CLA	CAA-CBA-CGA	-2.11	107.22	113.21
27	c	507	CLA	CHA-C1A-NA	-2.11	121.62	126.39
29	a	409	BCR	C24-C23-C22	-2.11	123.12	126.23
27	34	306	CLA	CAA-C2A-C1A	2.10	118.87	111.97
38	34	301	A86	C19-C18-C17	-2.10	106.85	110.79
36	D	407	PL9	C11-C9-C8	-2.10	116.44	121.17
33	C	519	LMG	C1-C2-C3	-2.10	105.58	110.01
33	12	301	LMG	O7-C10-O9	-2.10	118.79	123.70
27	d	401	CLA	CMB-C2B-C3B	2.10	131.49	126.55
29	b	617	BCR	C1-C6-C5	-2.10	119.76	122.64
38	13	316	A86	C19-C18-C17	-2.10	106.86	110.79
35	J	101	DGD	C7B-C6B-C5B	-2.10	103.75	114.37
35	j	101	DGD	C7B-C6B-C5B	-2.10	103.75	114.37
29	Z	101	BCR	C16-C17-C18	-2.10	124.33	127.28
27	C	506	CLA	CMC-C2C-C3C	2.10	131.83	126.15
27	33	305	CLA	CAA-C2A-C1A	2.10	118.85	111.97
27	12	308	CLA	CAA-C2A-C3A	-2.10	107.33	113.00
37	E	101	HEM	CAA-C2A-C1A	2.10	129.04	124.94
27	13	306	CLA	CAA-C2A-C3A	-2.10	107.33	113.00
33	m	102	LMG	O1-C7-C8	-2.10	105.72	110.82
27	14	305	CLA	CAA-C2A-C1A	2.10	118.85	111.97
27	31	303	CLA	CAA-C2A-C1A	2.10	118.85	111.97
29	B	616	BCR	C16-C15-C14	-2.10	119.23	123.52
30	a	406	SQD	O7-S-C6	2.10	109.89	106.76
27	31	304	CLA	CAA-C2A-C3A	-2.10	107.34	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	607	CLA	CHB-C1B-NB	2.10	127.19	124.05
27	b	614	CLA	C3A-C2A-C1A	2.10	104.48	101.34
27	b	615	CLA	CHB-C1B-C2B	-2.09	121.34	127.43
29	B	623	BCR	C15-C16-C17	-2.09	119.23	123.52
38	11	314	A86	C19-C18-C17	-2.09	106.87	110.79
27	c	503	CLA	CHC-C1C-NC	2.09	127.47	124.31
27	C	513	CLA	C2A-C1A-CHA	2.09	127.50	123.87
27	c	511	CLA	CHA-C4D-ND	2.09	136.87	132.55
27	32	307	CLA	CAA-C2A-C1A	2.09	118.83	111.97
36	d	407	PL9	C50-C49-C48	-2.09	116.38	122.66
27	13	305	CLA	CAA-C2A-C1A	2.09	118.83	111.97
33	12	301	LMG	O6-C1-O1	-2.09	105.10	110.04
27	11	303	CLA	CAA-C2A-C1A	2.09	118.83	111.97
27	32	308	CLA	CAA-C2A-C3A	-2.09	107.35	113.00
27	B	615	CLA	O2D-CGD-CBD	2.09	114.89	111.23
27	33	306	CLA	CAA-C2A-C3A	-2.09	107.35	113.00
27	B	612	CLA	C2A-C1A-CHA	2.09	127.49	123.87
27	14	306	CLA	CAA-C2A-C3A	-2.09	107.35	113.00
27	12	307	CLA	CAA-C2A-C1A	2.09	118.82	111.97
33	M	103	LMG	O1-C7-C8	-2.09	105.74	110.82
27	34	307	CLA	CAA-C2A-C3A	-2.09	107.36	113.00
27	W	103	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
38	14	301	A86	C19-C18-C17	-2.09	106.88	110.79
29	A	405	BCR	C7-C8-C9	-2.09	123.15	126.23
29	b	616	BCR	C16-C15-C14	-2.09	119.25	123.52
38	32	318	A86	C19-C18-C17	-2.09	106.89	110.79
27	b	602	CLA	CAA-CBA-CGA	-2.09	107.28	113.21
27	c	506	CLA	CMC-C2C-C3C	2.09	131.79	126.15
29	A	409	BCR	C24-C23-C22	-2.09	123.15	126.23
27	c	506	CLA	CHB-C1B-NB	2.09	127.18	124.05
29	H	101	BCR	C37-C22-C21	-2.08	119.44	122.82
27	B	615	CLA	CHB-C1B-C2B	-2.08	121.38	127.43
30	L	103	SQD	O48-C23-O10	-2.08	118.42	123.63
27	14	310	CLA	C3B-C4B-NB	-2.08	108.67	110.53
29	C	516	BCR	C24-C23-C22	-2.08	123.16	126.23
27	11	304	CLA	CAA-C2A-C3A	-2.08	107.37	113.00
27	B	602	CLA	CAA-CBA-CGA	-2.08	107.30	113.21
33	32	301	LMG	O7-C10-O9	-2.08	118.84	123.70
27	13	305	CLA	C2A-C1A-CHA	2.08	127.47	123.87
29	A	405	BCR	C27-C26-C25	2.08	125.51	122.70
27	c	513	CLA	C2A-C1A-CHA	2.08	127.47	123.87
27	13	301	CLA	C2A-C1A-CHA	2.08	127.47	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	14	302	CLA	C2A-C1A-CHA	2.08	127.47	123.87
27	b	612	CLA	C2A-C1A-CHA	2.08	127.47	123.87
38	31	314	A86	C19-C18-C17	-2.08	106.91	110.79
30	l	101	SQD	O48-C23-O10	-2.07	118.44	123.63
27	B	603	CLA	C4-C3-C5	2.07	118.83	115.23
27	31	303	CLA	C2A-C1A-CHA	2.07	127.46	123.87
27	34	306	CLA	C2A-C1A-CHA	2.07	127.46	123.87
36	d	407	PL9	C37-C38-C39	-2.07	122.88	127.62
27	A	404	CLA	O2D-CGD-CBD	2.07	114.85	111.23
33	32	301	LMG	O2-C2-C3	-2.07	105.49	110.38
27	34	308	CLA	CMB-C2B-C3B	2.07	131.42	126.55
27	c	502	CLA	C11-C12-C13	-2.07	109.08	115.97
30	A	406	SQD	O7-S-C6	2.07	109.85	106.76
27	a	402	CLA	C3B-C4B-NB	-2.07	108.68	110.53
32	b	621	LHG	C27-C26-C25	-2.07	103.91	114.37
27	12	303	CLA	C2A-C1A-CHA	2.07	127.46	123.87
27	32	303	CLA	C2A-C1A-CHA	2.07	127.46	123.87
27	C	502	CLA	C3B-C4B-NB	-2.07	108.68	110.53
27	B	612	CLA	CMA-C3A-C4A	-2.07	106.22	111.77
27	34	302	CLA	C2A-C1A-CHA	2.07	127.45	123.87
27	b	603	CLA	C4-C3-C5	2.07	118.82	115.23
27	32	307	CLA	C2A-C1A-CHA	2.07	127.45	123.87
36	d	404	PL9	C36-C34-C33	-2.07	116.53	121.17
27	A	402	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
27	C	502	CLA	C11-C12-C13	-2.06	109.10	115.97
32	B	621	LHG	C27-C26-C25	-2.06	103.94	114.37
36	D	404	PL9	C36-C34-C33	-2.06	116.53	121.17
27	34	310	CLA	CAA-C2A-C3A	-2.06	107.42	113.00
27	a	404	CLA	O2D-CGD-CBD	2.06	114.84	111.23
27	C	506	CLA	CHB-C1B-NB	2.06	127.14	124.05
27	33	301	CLA	C2A-C1A-CHA	2.06	127.44	123.87
38	33	316	A86	C19-C18-C17	-2.06	106.93	110.79
27	C	511	CLA	CHA-C4D-ND	2.06	136.80	132.55
27	w	103	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
36	D	404	PL9	C27-C28-C29	-2.06	122.91	127.62
27	33	307	CLA	CMB-C2B-C3B	2.06	131.39	126.55
27	B	613	CLA	O1D-CGD-CBD	2.06	128.58	124.52
27	c	514	CLA	C3B-C4B-NB	-2.06	108.69	110.53
27	31	307	CLA	CAA-C2A-C3A	-2.06	107.44	113.00
27	11	307	CLA	CAA-C2A-C3A	-2.06	107.44	113.00
27	C	512	CLA	O2D-CGD-CBD	2.06	114.83	111.23
36	d	404	PL9	C27-C28-C29	-2.06	122.91	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	32	308	CLA	C1D-ND-C4D	2.06	107.75	106.31
27	14	305	CLA	C2A-C1A-CHA	2.06	127.44	123.87
27	33	309	CLA	CAA-C2A-C3A	-2.06	107.44	113.00
27	14	309	CLA	CAA-C2A-C3A	-2.06	107.44	113.00
27	b	612	CLA	CMA-C3A-C4A	-2.06	106.25	111.77
27	11	315	CLA	C2A-C1A-CHA	2.05	127.43	123.87
27	11	305	CLA	CMB-C2B-C3B	2.05	131.38	126.55
27	31	305	CLA	CMB-C2B-C3B	2.05	131.38	126.55
27	12	307	CLA	C2A-C1A-CHA	2.05	127.43	123.87
35	H	102	DGD	O6E-C1E-O5D	-2.05	105.20	110.04
27	14	307	CLA	CMB-C2B-C3B	2.05	131.37	126.55
27	31	315	CLA	C2A-C1A-CHA	2.05	127.42	123.87
27	32	311	CLA	CAA-C2A-C3A	-2.05	107.46	113.00
27	12	306	CLA	CMB-C2B-C3B	2.05	131.37	126.55
29	f	101	BCR	C35-C13-C14	-2.05	119.50	122.82
27	c	512	CLA	O2D-CGD-CBD	2.05	114.81	111.23
27	b	604	CLA	C3C-C4C-NC	-2.05	107.81	110.43
35	c	517	DGD	C4E-C3E-C2E	-2.05	107.23	110.83
36	D	407	PL9	C37-C38-C39	-2.05	122.94	127.62
27	c	514	CLA	O1D-CGD-CBD	2.05	128.56	124.52
35	h	102	DGD	O6E-C1E-O5D	-2.05	105.21	110.04
27	C	512	CLA	CAA-C2A-C3A	-2.05	107.47	113.00
27	32	309	CLA	CMB-C2B-C3B	2.05	131.36	126.55
29	C	516	BCR	C16-C15-C14	-2.05	119.33	123.52
27	13	309	CLA	CAA-C2A-C3A	-2.05	107.47	113.00
27	12	311	CLA	CAA-C2A-C3A	-2.04	107.47	113.00
27	a	404	CLA	O1D-CGD-CBD	2.04	128.55	124.52
27	C	512	CLA	C7-C6-C5	-2.04	107.82	113.26
29	F	101	BCR	C35-C13-C14	-2.04	119.51	122.82
27	14	304	CLA	CMB-C2B-C3B	2.04	131.35	126.55
29	a	405	BCR	C27-C26-C25	2.04	125.46	122.70
29	M	101	BCR	C16-C15-C14	-2.04	119.34	123.52
27	A	404	CLA	O1D-CGD-CBD	2.04	128.54	124.52
27	32	306	CLA	CMB-C2B-C3B	2.04	131.35	126.55
29	h	101	BCR	C37-C22-C21	-2.04	119.51	122.82
38	13	312	A86	C26-C25-C24	-2.04	117.29	123.20
27	14	308	CLA	CHA-C1A-NA	-2.04	121.77	126.39
27	12	309	CLA	CMB-C2B-C3B	2.04	131.34	126.55
27	11	303	CLA	C2A-C1A-CHA	2.04	127.40	123.87
29	c	516	BCR	C16-C15-C14	-2.04	119.35	123.52
35	C	517	DGD	CBB-CAB-C9B	-2.04	104.07	114.37
35	C	517	DGD	C4E-C3E-C2E	-2.04	107.25	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	c	512	CLA	C7-C6-C5	-2.04	107.84	113.26
32	a	408	LHG	O8-C23-O10	-2.03	118.54	123.63
35	c	517	DGD	CBB-CAB-C9B	-2.03	104.08	114.37
38	32	314	A86	C26-C25-C24	-2.03	117.31	123.20
38	11	310	A86	C26-C25-C24	-2.03	117.31	123.20
27	D	401	CLA	C3A-C2A-C1A	2.03	104.39	101.34
29	b	623	BCR	C15-C16-C17	-2.03	119.36	123.52
27	c	512	CLA	CAA-C2A-C3A	-2.03	107.51	113.00
38	33	314	A86	C23-C16-C22	-2.03	104.42	107.37
27	34	307	CLA	C1D-ND-C4D	2.03	107.74	106.31
29	h	101	BCR	C20-C21-C22	-2.03	124.43	127.28
27	C	514	CLA	O1D-CGD-CBD	2.03	128.53	124.52
27	C	514	CLA	C3B-C4B-NB	-2.03	108.72	110.53
29	m	103	BCR	C16-C15-C14	-2.03	119.36	123.52
27	b	613	CLA	O1D-CGD-CBD	2.03	128.52	124.52
33	D	408	LMG	O6-C1-C2	-2.03	106.20	110.37
29	f	101	BCR	C33-C5-C6	-2.03	122.27	124.48
29	H	101	BCR	C7-C8-C9	-2.03	123.23	126.23
27	34	309	CLA	CHA-C1A-NA	-2.03	121.80	126.39
29	c	519	BCR	C21-C20-C19	-2.03	117.33	123.20
27	32	310	CLA	CHA-C1A-NA	-2.03	121.80	126.39
27	13	307	CLA	CMB-C2B-C3B	2.03	131.31	126.55
27	33	305	CLA	C2A-C1A-CHA	2.02	127.38	123.87
38	31	310	A86	C26-C25-C24	-2.02	117.33	123.20
38	34	303	A86	C8-C6-C5	2.02	122.19	119.01
29	c	516	BCR	C24-C23-C22	-2.02	123.24	126.23
27	33	304	CLA	CMB-C2B-C3B	2.02	131.31	126.55
29	h	101	BCR	C7-C8-C9	-2.02	123.24	126.23
38	33	312	A86	C26-C25-C24	-2.02	117.34	123.20
35	j	101	DGD	C5B-C4B-C3B	-2.02	104.15	114.37
27	c	512	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
29	b	616	BCR	C7-C8-C9	-2.02	123.25	126.23
38	14	301	A86	C8-C6-C5	-2.02	115.83	119.01
38	34	313	A86	C26-C25-C24	-2.02	117.34	123.20
27	d	401	CLA	C3A-C2A-C1A	2.02	104.37	101.34
27	z	102	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
27	a	402	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
27	11	302	CLA	CMB-C2B-C3B	2.02	131.30	126.55
27	B	604	CLA	C3C-C4C-NC	-2.02	107.84	110.43
28	A	403	PHO	CAA-C2A-C3A	-2.02	107.54	113.00
35	c	517	DGD	C7A-C6A-C5A	-2.02	104.16	114.37
32	A	408	LHG	O8-C23-O10	-2.02	118.58	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	d	408	LMG	O6-C1-C2	-2.02	106.22	110.37
27	32	305	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
29	C	520	BCR	C21-C20-C19	-2.02	117.35	123.20
38	31	314	A86	C8-C6-C5	-2.02	115.83	119.01
27	12	305	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
27	13	304	CLA	CMB-C2B-C3B	2.02	131.30	126.55
27	14	303	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
27	11	301	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
27	B	604	CLA	CHA-C4D-ND	2.02	136.71	132.55
29	F	101	BCR	C33-C5-C6	-2.02	122.28	124.48
38	12	314	A86	C26-C25-C24	-2.02	117.36	123.20
27	31	302	CLA	CMB-C2B-C3B	2.02	131.29	126.55
38	33	316	A86	C4-C3-C2	-2.02	119.39	123.52
27	33	303	CLA	O2A-CGA-O1A	-2.02	118.59	123.63
35	C	517	DGD	C7A-C6A-C5A	-2.02	104.18	114.37
38	14	312	A86	C26-C25-C24	-2.01	117.36	123.20
27	34	305	CLA	CMB-C2B-C3B	2.01	131.29	126.55
27	14	308	CLA	CAA-C2A-C3A	-2.01	107.56	113.00
27	B	609	CLA	CHA-C1A-NA	-2.01	121.83	126.39
27	13	308	CLA	CHA-C1A-NA	-2.01	121.83	126.39
27	B	605	CLA	C3C-C4C-NC	-2.01	107.85	110.43
27	Z	102	CLA	CHC-C4B-NB	2.01	127.07	124.05
27	b	601	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
33	q	301	LMG	C22-C21-C20	-2.01	104.20	114.37
38	11	314	A86	C8-C6-C5	-2.01	115.84	119.01
27	b	609	CLA	CHA-C1A-NA	-2.01	121.84	126.39
35	J	101	DGD	C5B-C4B-C3B	-2.01	104.20	114.37
27	34	304	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
27	b	610	CLA	C2A-C1A-CHA	2.01	127.36	123.87
29	z	101	BCR	C2-C1-C6	2.01	113.36	110.44
38	32	318	A86	C8-C6-C5	-2.01	115.85	119.01
27	31	301	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
27	11	306	CLA	CHA-C1A-NA	-2.01	121.84	126.39
35	c	518	DGD	C7B-C6B-C5B	-2.01	104.22	114.37
27	D	401	CLA	C2A-C1A-CHA	2.01	127.35	123.87
27	B	601	CLA	C3A-C2A-C1A	2.01	104.35	101.34
27	12	310	CLA	CHA-C1A-NA	-2.01	121.85	126.39
29	H	101	BCR	C20-C21-C22	-2.01	124.46	127.28
27	B	610	CLA	C2A-C1A-CHA	2.01	127.35	123.87
35	C	517	DGD	O3E-C3E-C2E	-2.01	105.65	110.38
27	31	306	CLA	CAA-C2A-C3A	-2.01	107.58	113.00
28	a	403	PHO	CAA-C2A-C3A	-2.00	107.58	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	604	CLA	C2D-C1D-ND	-2.00	108.14	110.13
38	13	302	A86	C8-C6-C5	2.00	122.16	119.01
33	b	619	LMG	C9-C8-C7	-2.00	107.11	111.78
27	b	604	CLA	CHA-C4D-ND	2.00	136.68	132.55
38	11	312	A86	C23-C16-C22	-2.00	104.46	107.37
27	Z	102	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
35	C	518	DGD	C7B-C6B-C5B	-2.00	104.24	114.37
38	12	304	A86	C8-C6-C5	2.00	122.16	119.01
27	33	308	CLA	CHA-C1A-NA	-2.00	121.86	126.39
38	31	316	A86	C8-C6-C5	2.00	122.16	119.01
27	b	606	CLA	C2A-C1A-CHA	2.00	127.34	123.87
27	31	306	CLA	CHA-C1A-NA	-2.00	121.86	126.39
27	b	602	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
27	C	504	CLA	C3A-C2A-C1A	2.00	104.33	101.34

All (146) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	A	402	CLA	ND
27	A	404	CLA	ND
27	B	601	CLA	ND
27	B	602	CLA	ND
27	B	603	CLA	ND
27	B	604	CLA	ND
27	B	605	CLA	ND
27	B	606	CLA	ND
27	B	607	CLA	ND
27	B	608	CLA	ND
27	B	609	CLA	ND
27	B	610	CLA	ND
27	B	611	CLA	ND
27	B	612	CLA	ND
27	B	613	CLA	ND
27	B	614	CLA	ND
27	B	615	CLA	ND
27	B	622	CLA	ND
27	C	502	CLA	ND
27	C	503	CLA	ND
27	C	504	CLA	ND
27	C	505	CLA	ND
27	C	506	CLA	ND
27	C	507	CLA	ND

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Mol	Chain	Res	Type	Atom
27	C	508	CLA	ND
27	C	509	CLA	ND
27	C	510	CLA	ND
27	C	511	CLA	ND
27	C	512	CLA	ND
27	C	513	CLA	ND
27	C	514	CLA	ND
27	D	401	CLA	ND
27	D	402	CLA	ND
27	D	405	CLA	ND
27	D	406	CLA	ND
27	M	102	CLA	ND
27	W	102	CLA	ND
27	a	402	CLA	ND
27	a	404	CLA	ND
27	b	601	CLA	ND
27	b	602	CLA	ND
27	b	603	CLA	ND
27	b	604	CLA	ND
27	b	605	CLA	ND
27	b	606	CLA	ND
27	b	607	CLA	ND
27	b	608	CLA	ND
27	b	609	CLA	ND
27	b	610	CLA	ND
27	b	611	CLA	ND
27	b	612	CLA	ND
27	b	613	CLA	ND
27	b	614	CLA	ND
27	b	615	CLA	ND
27	b	622	CLA	ND
27	c	502	CLA	ND
27	c	503	CLA	ND
27	c	504	CLA	ND
27	c	505	CLA	ND
27	c	506	CLA	ND
27	c	507	CLA	ND
27	c	508	CLA	ND
27	c	509	CLA	ND
27	c	510	CLA	ND
27	c	511	CLA	ND
27	c	512	CLA	ND

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Mol	Chain	Res	Type	Atom
27	c	513	CLA	ND
27	c	514	CLA	ND
27	d	401	CLA	ND
27	d	402	CLA	ND
27	d	405	CLA	ND
27	d	406	CLA	ND
27	m	101	CLA	ND
27	w	102	CLA	ND
27	11	301	CLA	ND
27	11	302	CLA	ND
27	11	303	CLA	ND
27	11	304	CLA	ND
27	11	305	CLA	ND
27	11	306	CLA	ND
27	11	307	CLA	ND
27	11	309	CLA	ND
27	11	315	CLA	ND
27	12	303	CLA	ND
27	12	305	CLA	ND
27	12	306	CLA	ND
27	12	307	CLA	ND
27	12	308	CLA	ND
27	12	309	CLA	ND
27	12	310	CLA	ND
27	12	311	CLA	ND
27	12	313	CLA	ND
27	13	301	CLA	ND
27	13	303	CLA	ND
27	13	304	CLA	ND
27	13	305	CLA	ND
27	13	306	CLA	ND
27	13	307	CLA	ND
27	13	308	CLA	ND
27	13	309	CLA	ND
27	13	311	CLA	ND
27	14	302	CLA	ND
27	14	303	CLA	ND
27	14	304	CLA	ND
27	14	305	CLA	ND
27	14	306	CLA	ND
27	14	307	CLA	ND
27	14	308	CLA	ND

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Mol	Chain	Res	Type	Atom
27	14	309	CLA	ND
27	14	311	CLA	ND
27	31	301	CLA	ND
27	31	302	CLA	ND
27	31	303	CLA	ND
27	31	304	CLA	ND
27	31	305	CLA	ND
27	31	306	CLA	ND
27	31	307	CLA	ND
27	31	309	CLA	ND
27	31	315	CLA	ND
27	32	303	CLA	ND
27	32	305	CLA	ND
27	32	306	CLA	ND
27	32	307	CLA	ND
27	32	308	CLA	ND
27	32	309	CLA	ND
27	32	310	CLA	ND
27	32	311	CLA	ND
27	32	313	CLA	ND
27	33	301	CLA	ND
27	33	303	CLA	ND
27	33	304	CLA	ND
27	33	305	CLA	ND
27	33	306	CLA	ND
27	33	307	CLA	ND
27	33	308	CLA	ND
27	33	309	CLA	ND
27	33	311	CLA	ND
27	34	302	CLA	ND
27	34	304	CLA	ND
27	34	305	CLA	ND
27	34	306	CLA	ND
27	34	307	CLA	ND
27	34	308	CLA	ND
27	34	309	CLA	ND
27	34	310	CLA	ND
27	34	312	CLA	ND

All (3272) torsion outliers are listed below:

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Mol	Chain	Res	Type	Atoms
27	A	402	CLA	CBD-CGD-O2D-CED
27	A	404	CLA	C2B-C3B-CAB-CBB
27	A	404	CLA	C4B-C3B-CAB-CBB
27	B	601	CLA	C1A-C2A-CAA-CBA
27	B	601	CLA	C2B-C3B-CAB-CBB
27	B	601	CLA	C4B-C3B-CAB-CBB
27	B	601	CLA	CAD-CBD-CGD-O1D
27	B	601	CLA	CAD-CBD-CGD-O2D
27	B	603	CLA	CAD-CBD-CGD-O1D
27	B	603	CLA	CAD-CBD-CGD-O2D
27	B	604	CLA	CAD-CBD-CGD-O2D
27	B	605	CLA	C2B-C3B-CAB-CBB
27	B	605	CLA	C4B-C3B-CAB-CBB
27	B	605	CLA	C4-C3-C5-C6
27	B	610	CLA	CHA-CBD-CGD-O1D
27	B	610	CLA	CHA-CBD-CGD-O2D
27	B	611	CLA	CBD-CGD-O2D-CED
27	B	612	CLA	C1A-C2A-CAA-CBA
27	B	612	CLA	C3A-C2A-CAA-CBA
27	B	613	CLA	C2-C3-C5-C6
27	B	613	CLA	C4-C3-C5-C6
27	B	615	CLA	CHA-CBD-CGD-O1D
27	B	615	CLA	CHA-CBD-CGD-O2D
27	C	502	CLA	C1A-C2A-CAA-CBA
27	C	503	CLA	C2B-C3B-CAB-CBB
27	C	503	CLA	C4B-C3B-CAB-CBB
27	C	504	CLA	C2B-C3B-CAB-CBB
27	C	504	CLA	C4B-C3B-CAB-CBB
27	C	504	CLA	CBD-CGD-O2D-CED
27	C	505	CLA	CAD-CBD-CGD-O2D
27	C	510	CLA	CHA-CBD-CGD-O1D
27	C	510	CLA	CHA-CBD-CGD-O2D
27	C	510	CLA	CBD-CGD-O2D-CED
27	C	510	CLA	C6-C7-C8-C9
27	C	514	CLA	CBD-CGD-O2D-CED
27	D	401	CLA	C2B-C3B-CAB-CBB
27	D	401	CLA	C4B-C3B-CAB-CBB
27	D	402	CLA	C2B-C3B-CAB-CBB
27	D	402	CLA	C4B-C3B-CAB-CBB
27	D	405	CLA	C1A-C2A-CAA-CBA
27	M	102	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
27	M	102	CLA	CAD-CBD-CGD-O2D
27	M	102	CLA	C2-C3-C5-C6
27	M	102	CLA	C4-C3-C5-C6
27	Z	102	CLA	C2B-C3B-CAB-CBB
27	Z	102	CLA	C4B-C3B-CAB-CBB
27	W	102	CLA	C1A-C2A-CAA-CBA
27	a	402	CLA	CBD-CGD-O2D-CED
27	a	404	CLA	C2B-C3B-CAB-CBB
27	a	404	CLA	C4B-C3B-CAB-CBB
27	b	601	CLA	C1A-C2A-CAA-CBA
27	b	601	CLA	C2B-C3B-CAB-CBB
27	b	601	CLA	C4B-C3B-CAB-CBB
27	b	601	CLA	CAD-CBD-CGD-O1D
27	b	601	CLA	CAD-CBD-CGD-O2D
27	b	603	CLA	CAD-CBD-CGD-O1D
27	b	603	CLA	CAD-CBD-CGD-O2D
27	b	604	CLA	CAD-CBD-CGD-O2D
27	b	605	CLA	C2B-C3B-CAB-CBB
27	b	605	CLA	C4B-C3B-CAB-CBB
27	b	605	CLA	C4-C3-C5-C6
27	b	610	CLA	CHA-CBD-CGD-O1D
27	b	610	CLA	CHA-CBD-CGD-O2D
27	b	611	CLA	CBD-CGD-O2D-CED
27	b	612	CLA	C1A-C2A-CAA-CBA
27	b	612	CLA	C3A-C2A-CAA-CBA
27	b	613	CLA	C2-C3-C5-C6
27	b	613	CLA	C4-C3-C5-C6
27	b	615	CLA	CHA-CBD-CGD-O1D
27	b	615	CLA	CHA-CBD-CGD-O2D
27	c	502	CLA	C1A-C2A-CAA-CBA
27	c	503	CLA	C2B-C3B-CAB-CBB
27	c	503	CLA	C4B-C3B-CAB-CBB
27	c	504	CLA	C2B-C3B-CAB-CBB
27	c	504	CLA	C4B-C3B-CAB-CBB
27	c	504	CLA	CBD-CGD-O2D-CED
27	c	505	CLA	CAD-CBD-CGD-O2D
27	c	510	CLA	CHA-CBD-CGD-O1D
27	c	510	CLA	CHA-CBD-CGD-O2D
27	c	510	CLA	CBD-CGD-O2D-CED
27	c	510	CLA	C6-C7-C8-C9
27	c	513	CLA	C1A-C2A-CAA-CBA
27	c	514	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	d	401	CLA	C2B-C3B-CAB-CBB
27	d	401	CLA	C4B-C3B-CAB-CBB
27	d	402	CLA	C2B-C3B-CAB-CBB
27	d	402	CLA	C4B-C3B-CAB-CBB
27	d	405	CLA	C1A-C2A-CAA-CBA
27	m	101	CLA	CAD-CBD-CGD-O1D
27	m	101	CLA	CAD-CBD-CGD-O2D
27	m	101	CLA	C2-C3-C5-C6
27	m	101	CLA	C4-C3-C5-C6
27	z	102	CLA	C2B-C3B-CAB-CBB
27	z	102	CLA	C4B-C3B-CAB-CBB
27	w	102	CLA	C1A-C2A-CAA-CBA
27	11	301	CLA	C3A-C2A-CAA-CBA
27	11	303	CLA	C1A-C2A-CAA-CBA
27	11	304	CLA	CHA-CBD-CGD-O1D
27	11	304	CLA	CHA-CBD-CGD-O2D
27	11	305	CLA	C1A-C2A-CAA-CBA
27	11	305	CLA	C3A-C2A-CAA-CBA
27	11	308	CLA	C1A-C2A-CAA-CBA
27	11	308	CLA	CHA-CBD-CGD-O1D
27	11	308	CLA	CHA-CBD-CGD-O2D
27	11	309	CLA	C1A-C2A-CAA-CBA
27	11	309	CLA	C4B-C3B-CAB-CBB
27	12	305	CLA	C3A-C2A-CAA-CBA
27	12	307	CLA	C1A-C2A-CAA-CBA
27	12	308	CLA	CHA-CBD-CGD-O1D
27	12	308	CLA	CHA-CBD-CGD-O2D
27	12	309	CLA	C1A-C2A-CAA-CBA
27	12	309	CLA	C3A-C2A-CAA-CBA
27	12	312	CLA	C1A-C2A-CAA-CBA
27	12	312	CLA	CHA-CBD-CGD-O1D
27	12	312	CLA	CHA-CBD-CGD-O2D
27	12	313	CLA	C1A-C2A-CAA-CBA
27	12	313	CLA	C4B-C3B-CAB-CBB
27	13	303	CLA	C3A-C2A-CAA-CBA
27	13	305	CLA	C1A-C2A-CAA-CBA
27	13	306	CLA	CHA-CBD-CGD-O1D
27	13	306	CLA	CHA-CBD-CGD-O2D
27	13	307	CLA	C1A-C2A-CAA-CBA
27	13	307	CLA	C3A-C2A-CAA-CBA
27	13	310	CLA	C1A-C2A-CAA-CBA
27	13	310	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
27	13	310	CLA	CHA-CBD-CGD-O2D
27	13	311	CLA	C1A-C2A-CAA-CBA
27	13	311	CLA	C4B-C3B-CAB-CBB
27	14	303	CLA	C3A-C2A-CAA-CBA
27	14	305	CLA	C1A-C2A-CAA-CBA
27	14	306	CLA	CHA-CBD-CGD-O1D
27	14	306	CLA	CHA-CBD-CGD-O2D
27	14	307	CLA	C1A-C2A-CAA-CBA
27	14	307	CLA	C3A-C2A-CAA-CBA
27	14	310	CLA	C1A-C2A-CAA-CBA
27	14	310	CLA	CHA-CBD-CGD-O1D
27	14	310	CLA	CHA-CBD-CGD-O2D
27	14	311	CLA	C1A-C2A-CAA-CBA
27	14	311	CLA	C4B-C3B-CAB-CBB
27	31	301	CLA	C3A-C2A-CAA-CBA
27	31	303	CLA	C1A-C2A-CAA-CBA
27	31	304	CLA	CHA-CBD-CGD-O1D
27	31	304	CLA	CHA-CBD-CGD-O2D
27	31	305	CLA	C1A-C2A-CAA-CBA
27	31	305	CLA	C3A-C2A-CAA-CBA
27	31	308	CLA	C1A-C2A-CAA-CBA
27	31	308	CLA	CHA-CBD-CGD-O1D
27	31	308	CLA	CHA-CBD-CGD-O2D
27	31	309	CLA	C1A-C2A-CAA-CBA
27	31	309	CLA	C4B-C3B-CAB-CBB
27	32	305	CLA	C3A-C2A-CAA-CBA
27	32	307	CLA	C1A-C2A-CAA-CBA
27	32	308	CLA	CHA-CBD-CGD-O1D
27	32	308	CLA	CHA-CBD-CGD-O2D
27	32	309	CLA	C1A-C2A-CAA-CBA
27	32	309	CLA	C3A-C2A-CAA-CBA
27	32	312	CLA	C1A-C2A-CAA-CBA
27	32	312	CLA	CHA-CBD-CGD-O1D
27	32	312	CLA	CHA-CBD-CGD-O2D
27	32	313	CLA	C1A-C2A-CAA-CBA
27	32	313	CLA	C4B-C3B-CAB-CBB
27	33	303	CLA	C3A-C2A-CAA-CBA
27	33	305	CLA	C1A-C2A-CAA-CBA
27	33	306	CLA	CHA-CBD-CGD-O1D
27	33	306	CLA	CHA-CBD-CGD-O2D
27	33	307	CLA	C1A-C2A-CAA-CBA
27	33	307	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	33	310	CLA	C1A-C2A-CAA-CBA
27	33	310	CLA	CHA-CBD-CGD-O1D
27	33	310	CLA	CHA-CBD-CGD-O2D
27	33	311	CLA	C1A-C2A-CAA-CBA
27	33	311	CLA	C4B-C3B-CAB-CBB
27	34	304	CLA	C3A-C2A-CAA-CBA
27	34	306	CLA	C1A-C2A-CAA-CBA
27	34	307	CLA	CHA-CBD-CGD-O1D
27	34	307	CLA	CHA-CBD-CGD-O2D
27	34	308	CLA	C1A-C2A-CAA-CBA
27	34	308	CLA	C3A-C2A-CAA-CBA
27	34	311	CLA	C1A-C2A-CAA-CBA
27	34	311	CLA	CHA-CBD-CGD-O1D
27	34	311	CLA	CHA-CBD-CGD-O2D
27	34	312	CLA	C1A-C2A-CAA-CBA
27	34	312	CLA	C4B-C3B-CAB-CBB
29	A	405	BCR	C7-C8-C9-C10
29	A	405	BCR	C35-C13-C14-C15
29	A	405	BCR	C14-C15-C16-C17
29	A	405	BCR	C16-C17-C18-C19
29	A	405	BCR	C16-C17-C18-C36
29	A	405	BCR	C18-C19-C20-C21
29	A	409	BCR	C6-C7-C8-C9
29	A	409	BCR	C7-C8-C9-C10
29	A	409	BCR	C7-C8-C9-C34
29	B	616	BCR	C7-C8-C9-C10
29	B	616	BCR	C20-C21-C22-C37
29	B	617	BCR	C7-C8-C9-C10
29	B	623	BCR	C6-C7-C8-C9
29	B	623	BCR	C7-C8-C9-C10
29	B	623	BCR	C10-C11-C12-C13
29	B	623	BCR	C11-C12-C13-C35
29	B	623	BCR	C16-C17-C18-C36
29	B	623	BCR	C20-C21-C22-C23
29	B	623	BCR	C20-C21-C22-C37
29	C	515	BCR	C11-C12-C13-C14
29	C	515	BCR	C11-C12-C13-C35
29	C	515	BCR	C16-C17-C18-C36
29	C	515	BCR	C21-C22-C23-C24
29	C	516	BCR	C22-C23-C24-C25
29	C	520	BCR	C21-C22-C23-C24
29	F	101	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
29	F	101	BCR	C11-C10-C9-C34
29	F	101	BCR	C35-C13-C14-C15
29	F	101	BCR	C16-C17-C18-C36
29	F	101	BCR	C21-C22-C23-C24
29	F	101	BCR	C37-C22-C23-C24
29	F	101	BCR	C22-C23-C24-C25
29	H	101	BCR	C20-C21-C22-C37
29	H	101	BCR	C37-C22-C23-C24
29	Z	101	BCR	C7-C8-C9-C34
29	Z	101	BCR	C11-C12-C13-C35
29	Z	101	BCR	C17-C18-C19-C20
29	Z	101	BCR	C18-C19-C20-C21
29	Z	101	BCR	C21-C22-C23-C24
29	a	405	BCR	C7-C8-C9-C10
29	a	405	BCR	C35-C13-C14-C15
29	a	405	BCR	C14-C15-C16-C17
29	a	405	BCR	C16-C17-C18-C19
29	a	405	BCR	C16-C17-C18-C36
29	a	405	BCR	C18-C19-C20-C21
29	a	409	BCR	C6-C7-C8-C9
29	a	409	BCR	C7-C8-C9-C10
29	a	409	BCR	C7-C8-C9-C34
29	b	616	BCR	C7-C8-C9-C10
29	b	616	BCR	C20-C21-C22-C37
29	b	617	BCR	C7-C8-C9-C10
29	b	623	BCR	C6-C7-C8-C9
29	b	623	BCR	C7-C8-C9-C10
29	b	623	BCR	C10-C11-C12-C13
29	b	623	BCR	C16-C17-C18-C36
29	b	623	BCR	C20-C21-C22-C23
29	b	623	BCR	C20-C21-C22-C37
29	c	515	BCR	C11-C12-C13-C14
29	c	515	BCR	C11-C12-C13-C35
29	c	515	BCR	C16-C17-C18-C36
29	c	515	BCR	C21-C22-C23-C24
29	c	516	BCR	C22-C23-C24-C25
29	c	519	BCR	C21-C22-C23-C24
29	f	101	BCR	C7-C8-C9-C10
29	f	101	BCR	C11-C10-C9-C34
29	f	101	BCR	C35-C13-C14-C15
29	f	101	BCR	C16-C17-C18-C36
29	f	101	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
29	f	101	BCR	C37-C22-C23-C24
29	f	101	BCR	C22-C23-C24-C25
29	h	101	BCR	C20-C21-C22-C37
29	h	101	BCR	C37-C22-C23-C24
29	z	101	BCR	C7-C8-C9-C34
29	z	101	BCR	C11-C12-C13-C35
29	z	101	BCR	C17-C18-C19-C20
29	z	101	BCR	C18-C19-C20-C21
29	z	101	BCR	C21-C22-C23-C24
30	A	406	SQD	C5-C6-S-O7
30	B	620	SQD	C2-C1-O6-C44
30	L	103	SQD	O5-C1-O6-C44
30	L	103	SQD	C8-C7-O47-C45
30	L	103	SQD	O5-C5-C6-S
30	a	406	SQD	C5-C6-S-O7
30	b	620	SQD	C2-C1-O6-C44
30	l	101	SQD	O5-C1-O6-C44
30	l	101	SQD	C8-C7-O47-C45
30	l	101	SQD	O5-C5-C6-S
32	A	408	LHG	C3-O3-P-O5
32	A	408	LHG	C3-O3-P-O6
32	A	408	LHG	C4-O6-P-O3
32	A	408	LHG	C4-O6-P-O4
32	B	621	LHG	C3-O3-P-O4
32	B	621	LHG	C3-O3-P-O6
32	B	621	LHG	C4-O6-P-O3
32	B	621	LHG	C4-O6-P-O4
32	L	101	LHG	O1-C1-C2-C3
32	L	101	LHG	C3-O3-P-O4
32	L	101	LHG	C3-O3-P-O6
32	L	101	LHG	C4-O6-P-O3
32	L	102	LHG	C3-O3-P-O6
32	L	102	LHG	C4-O6-P-O5
32	a	408	LHG	C3-O3-P-O5
32	a	408	LHG	C3-O3-P-O6
32	a	408	LHG	C4-O6-P-O3
32	a	408	LHG	C4-O6-P-O4
32	b	621	LHG	C3-O3-P-O4
32	b	621	LHG	C3-O3-P-O6
32	b	621	LHG	C4-O6-P-O3
32	b	621	LHG	C4-O6-P-O4
32	l	102	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
32	l	102	LHG	C3-O3-P-O4
32	l	102	LHG	C3-O3-P-O6
32	l	102	LHG	C4-O6-P-O3
32	l	103	LHG	C3-O3-P-O6
32	l	103	LHG	C4-O6-P-O5
33	M	103	LMG	O9-C10-O7-C8
33	W	101	LMG	O6-C1-O1-C7
33	W	101	LMG	O1-C7-C8-O7
33	m	102	LMG	O9-C10-O7-C8
33	w	101	LMG	O6-C1-O1-C7
33	w	101	LMG	O1-C7-C8-O7
33	12	301	LMG	O6-C1-O1-C7
33	32	301	LMG	O6-C1-O1-C7
36	D	404	PL9	C7-C8-C9-C11
36	D	404	PL9	C37-C38-C39-C40
36	D	407	PL9	C12-C13-C14-C16
36	D	407	PL9	C42-C43-C44-C45
36	d	404	PL9	C7-C8-C9-C11
36	d	404	PL9	C37-C38-C39-C40
36	d	407	PL9	C12-C13-C14-C16
36	d	407	PL9	C42-C43-C44-C45
38	11	310	A86	O-C13-C14-C15
38	11	310	A86	C39-C38-O4-C34
38	11	310	A86	C5-C6-C8-C9
38	11	312	A86	C26-C27-C29-C30
38	11	312	A86	C28-C27-C29-C30
38	11	313	A86	C2-C1-C24-C25
38	11	313	A86	C12-C11-C13-O
38	11	314	A86	C24-C25-C26-C27
38	11	314	A86	C39-C38-O4-C34
38	11	314	A86	O5-C38-O4-C34
38	11	316	A86	C11-C13-C14-C15
38	11	316	A86	C13-C14-C15-C16
38	11	316	A86	C39-C38-O4-C34
38	11	316	A86	O5-C38-O4-C34
38	12	304	A86	C11-C13-C14-C15
38	12	304	A86	C13-C14-C15-C16
38	12	304	A86	C39-C38-O4-C34
38	12	304	A86	O5-C38-O4-C34
38	12	314	A86	O-C13-C14-C15
38	12	314	A86	C39-C38-O4-C34
38	12	314	A86	C5-C6-C8-C9

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Mol	Chain	Res	Type	Atoms
38	12	316	A86	C26-C27-C29-C30
38	12	316	A86	C28-C27-C29-C30
38	12	317	A86	C2-C1-C24-C25
38	12	317	A86	C12-C11-C13-O
38	13	302	A86	C11-C13-C14-C15
38	13	302	A86	C13-C14-C15-C16
38	13	302	A86	C39-C38-O4-C34
38	13	302	A86	O5-C38-O4-C34
38	13	312	A86	O-C13-C14-C15
38	13	312	A86	C39-C38-O4-C34
38	13	312	A86	C5-C6-C8-C9
38	13	314	A86	C26-C27-C29-C30
38	13	314	A86	C28-C27-C29-C30
38	13	315	A86	C2-C1-C24-C25
38	13	315	A86	C12-C11-C13-O
38	13	316	A86	C24-C25-C26-C27
38	13	316	A86	C39-C38-O4-C34
38	13	316	A86	O5-C38-O4-C34
38	13	317	A86	C11-C13-C14-C15
38	13	317	A86	C13-C14-C15-C16
38	13	317	A86	C39-C38-O4-C34
38	13	317	A86	O5-C38-O4-C34
38	14	301	A86	C24-C25-C26-C27
38	14	301	A86	C39-C38-O4-C34
38	14	301	A86	O5-C38-O4-C34
38	14	312	A86	O-C13-C14-C15
38	14	312	A86	C39-C38-O4-C34
38	14	312	A86	C5-C6-C8-C9
38	14	314	A86	C26-C27-C29-C30
38	14	314	A86	C28-C27-C29-C30
38	14	315	A86	C2-C1-C24-C25
38	14	315	A86	C12-C11-C13-O
38	14	316	A86	C24-C25-C26-C27
38	14	316	A86	C39-C38-O4-C34
38	14	316	A86	O5-C38-O4-C34
38	31	310	A86	O-C13-C14-C15
38	31	310	A86	C39-C38-O4-C34
38	31	310	A86	C5-C6-C8-C9
38	31	312	A86	C26-C27-C29-C30
38	31	312	A86	C28-C27-C29-C30
38	31	313	A86	C2-C1-C24-C25
38	31	313	A86	C12-C11-C13-O

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Mol	Chain	Res	Type	Atoms
38	31	314	A86	C24-C25-C26-C27
38	31	314	A86	C39-C38-O4-C34
38	31	314	A86	O5-C38-O4-C34
38	31	316	A86	C11-C13-C14-C15
38	31	316	A86	C13-C14-C15-C16
38	31	316	A86	C39-C38-O4-C34
38	31	316	A86	O5-C38-O4-C34
38	32	304	A86	C11-C13-C14-C15
38	32	304	A86	C13-C14-C15-C16
38	32	304	A86	C39-C38-O4-C34
38	32	304	A86	O5-C38-O4-C34
38	32	314	A86	O-C13-C14-C15
38	32	314	A86	C39-C38-O4-C34
38	32	314	A86	C5-C6-C8-C9
38	32	316	A86	C26-C27-C29-C30
38	32	316	A86	C28-C27-C29-C30
38	32	317	A86	C2-C1-C24-C25
38	32	317	A86	C12-C11-C13-O
38	32	318	A86	C24-C25-C26-C27
38	32	318	A86	C39-C38-O4-C34
38	32	318	A86	O5-C38-O4-C34
38	33	302	A86	C11-C13-C14-C15
38	33	302	A86	C13-C14-C15-C16
38	33	302	A86	C39-C38-O4-C34
38	33	302	A86	O5-C38-O4-C34
38	33	312	A86	O-C13-C14-C15
38	33	312	A86	C39-C38-O4-C34
38	33	312	A86	C5-C6-C8-C9
38	33	314	A86	C26-C27-C29-C30
38	33	314	A86	C28-C27-C29-C30
38	33	315	A86	C2-C1-C24-C25
38	33	315	A86	C12-C11-C13-O
38	33	316	A86	C24-C25-C26-C27
38	33	316	A86	C39-C38-O4-C34
38	33	316	A86	O5-C38-O4-C34
38	34	301	A86	C24-C25-C26-C27
38	34	301	A86	C39-C38-O4-C34
38	34	301	A86	O5-C38-O4-C34
38	34	303	A86	C11-C13-C14-C15
38	34	303	A86	C13-C14-C15-C16
38	34	303	A86	C39-C38-O4-C34
38	34	303	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
38	34	313	A86	O-C13-C14-C15
38	34	313	A86	C39-C38-O4-C34
38	34	313	A86	C5-C6-C8-C9
38	34	315	A86	C26-C27-C29-C30
38	34	315	A86	C28-C27-C29-C30
38	34	316	A86	C2-C1-C24-C25
38	34	316	A86	C12-C11-C13-O
38	11	312	A86	C39-C38-O4-C34
38	12	316	A86	C39-C38-O4-C34
38	13	314	A86	C39-C38-O4-C34
38	14	314	A86	C39-C38-O4-C34
38	31	312	A86	C39-C38-O4-C34
38	32	316	A86	C39-C38-O4-C34
38	33	314	A86	C39-C38-O4-C34
38	34	315	A86	C39-C38-O4-C34
27	A	402	CLA	O1D-CGD-O2D-CED
27	C	510	CLA	O1D-CGD-O2D-CED
27	a	402	CLA	O1D-CGD-O2D-CED
27	c	510	CLA	O1D-CGD-O2D-CED
27	11	304	CLA	O1D-CGD-O2D-CED
27	11	305	CLA	O1D-CGD-O2D-CED
27	12	308	CLA	O1D-CGD-O2D-CED
27	12	309	CLA	O1D-CGD-O2D-CED
27	13	306	CLA	O1D-CGD-O2D-CED
27	13	307	CLA	O1D-CGD-O2D-CED
27	14	306	CLA	O1D-CGD-O2D-CED
27	14	307	CLA	O1D-CGD-O2D-CED
27	31	304	CLA	O1D-CGD-O2D-CED
27	31	305	CLA	O1D-CGD-O2D-CED
27	32	308	CLA	O1D-CGD-O2D-CED
27	32	309	CLA	O1D-CGD-O2D-CED
27	33	306	CLA	O1D-CGD-O2D-CED
27	33	307	CLA	O1D-CGD-O2D-CED
27	34	307	CLA	O1D-CGD-O2D-CED
27	34	308	CLA	O1D-CGD-O2D-CED
38	11	310	A86	O5-C38-O4-C34
38	11	311	A86	C39-C38-O4-C34
38	12	314	A86	O5-C38-O4-C34
38	12	315	A86	C39-C38-O4-C34
38	13	312	A86	O5-C38-O4-C34
38	13	313	A86	C39-C38-O4-C34
38	14	312	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
38	14	313	A86	C39-C38-O4-C34
38	31	310	A86	O5-C38-O4-C34
38	31	311	A86	C39-C38-O4-C34
38	32	314	A86	O5-C38-O4-C34
38	32	315	A86	C39-C38-O4-C34
38	33	312	A86	O5-C38-O4-C34
38	33	313	A86	C39-C38-O4-C34
38	34	313	A86	O5-C38-O4-C34
38	34	314	A86	C39-C38-O4-C34
27	B	603	CLA	CBD-CGD-O2D-CED
27	B	604	CLA	CBD-CGD-O2D-CED
27	C	508	CLA	CBD-CGD-O2D-CED
27	W	103	CLA	CBD-CGD-O2D-CED
27	b	603	CLA	CBD-CGD-O2D-CED
27	b	604	CLA	CBD-CGD-O2D-CED
27	c	508	CLA	CBD-CGD-O2D-CED
27	w	103	CLA	CBD-CGD-O2D-CED
27	11	301	CLA	CBD-CGD-O2D-CED
27	11	304	CLA	CBD-CGD-O2D-CED
27	11	305	CLA	CBD-CGD-O2D-CED
27	12	305	CLA	CBD-CGD-O2D-CED
27	12	308	CLA	CBD-CGD-O2D-CED
27	12	309	CLA	CBD-CGD-O2D-CED
27	13	303	CLA	CBD-CGD-O2D-CED
27	13	306	CLA	CBD-CGD-O2D-CED
27	13	307	CLA	CBD-CGD-O2D-CED
27	14	303	CLA	CBD-CGD-O2D-CED
27	14	306	CLA	CBD-CGD-O2D-CED
27	14	307	CLA	CBD-CGD-O2D-CED
27	31	301	CLA	CBD-CGD-O2D-CED
27	31	304	CLA	CBD-CGD-O2D-CED
27	31	305	CLA	CBD-CGD-O2D-CED
27	32	305	CLA	CBD-CGD-O2D-CED
27	32	308	CLA	CBD-CGD-O2D-CED
27	32	309	CLA	CBD-CGD-O2D-CED
27	33	303	CLA	CBD-CGD-O2D-CED
27	33	306	CLA	CBD-CGD-O2D-CED
27	33	307	CLA	CBD-CGD-O2D-CED
27	34	304	CLA	CBD-CGD-O2D-CED
27	34	307	CLA	CBD-CGD-O2D-CED
27	34	308	CLA	CBD-CGD-O2D-CED
38	11	312	A86	C35-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
38	12	316	A86	C35-C34-O4-C38
38	13	314	A86	C35-C34-O4-C38
38	14	314	A86	C35-C34-O4-C38
38	31	312	A86	C35-C34-O4-C38
38	32	316	A86	C35-C34-O4-C38
38	33	314	A86	C35-C34-O4-C38
38	34	315	A86	C35-C34-O4-C38
36	D	404	PL9	C47-C48-C49-C50
36	D	404	PL9	C47-C48-C49-C51
36	d	404	PL9	C47-C48-C49-C50
36	d	404	PL9	C47-C48-C49-C51
27	B	615	CLA	O1A-CGA-O2A-C1
27	b	615	CLA	O1A-CGA-O2A-C1
27	B	611	CLA	O1D-CGD-O2D-CED
27	C	504	CLA	O1D-CGD-O2D-CED
27	W	103	CLA	O1D-CGD-O2D-CED
27	b	611	CLA	O1D-CGD-O2D-CED
27	c	504	CLA	O1D-CGD-O2D-CED
27	w	103	CLA	O1D-CGD-O2D-CED
27	C	514	CLA	O1D-CGD-O2D-CED
27	c	514	CLA	O1D-CGD-O2D-CED
38	11	312	A86	O5-C38-O4-C34
38	12	316	A86	O5-C38-O4-C34
38	13	314	A86	O5-C38-O4-C34
38	14	314	A86	O5-C38-O4-C34
38	31	312	A86	O5-C38-O4-C34
38	32	316	A86	O5-C38-O4-C34
38	33	314	A86	O5-C38-O4-C34
38	34	315	A86	O5-C38-O4-C34
30	L	103	SQD	O49-C7-O47-C45
30	l	101	SQD	O49-C7-O47-C45
27	B	607	CLA	C3-C5-C6-C7
27	C	513	CLA	C3-C5-C6-C7
27	M	102	CLA	C3-C5-C6-C7
27	b	607	CLA	C3-C5-C6-C7
27	c	513	CLA	C3-C5-C6-C7
27	m	101	CLA	C3-C5-C6-C7
27	B	615	CLA	CBA-CGA-O2A-C1
27	Z	102	CLA	CBA-CGA-O2A-C1
27	b	615	CLA	CBA-CGA-O2A-C1
27	z	102	CLA	CBA-CGA-O2A-C1
27	B	602	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	B	609	CLA	CBD-CGD-O2D-CED
27	B	614	CLA	CBD-CGD-O2D-CED
27	C	507	CLA	CBD-CGD-O2D-CED
27	b	602	CLA	CBD-CGD-O2D-CED
27	b	609	CLA	CBD-CGD-O2D-CED
27	b	614	CLA	CBD-CGD-O2D-CED
27	c	507	CLA	CBD-CGD-O2D-CED
27	11	303	CLA	CBD-CGD-O2D-CED
27	11	309	CLA	CBD-CGD-O2D-CED
27	12	307	CLA	CBD-CGD-O2D-CED
27	12	313	CLA	CBD-CGD-O2D-CED
27	13	305	CLA	CBD-CGD-O2D-CED
27	13	311	CLA	CBD-CGD-O2D-CED
27	14	305	CLA	CBD-CGD-O2D-CED
27	14	311	CLA	CBD-CGD-O2D-CED
27	31	303	CLA	CBD-CGD-O2D-CED
27	31	309	CLA	CBD-CGD-O2D-CED
27	32	307	CLA	CBD-CGD-O2D-CED
27	32	313	CLA	CBD-CGD-O2D-CED
27	33	305	CLA	CBD-CGD-O2D-CED
27	33	311	CLA	CBD-CGD-O2D-CED
27	34	306	CLA	CBD-CGD-O2D-CED
27	34	312	CLA	CBD-CGD-O2D-CED
33	M	103	LMG	C11-C10-O7-C8
33	m	102	LMG	C11-C10-O7-C8
38	11	313	A86	C39-C38-O4-C34
38	12	317	A86	C39-C38-O4-C34
38	13	315	A86	C39-C38-O4-C34
38	14	315	A86	C39-C38-O4-C34
38	31	313	A86	C39-C38-O4-C34
38	32	317	A86	C39-C38-O4-C34
38	33	315	A86	C39-C38-O4-C34
38	34	316	A86	C39-C38-O4-C34
27	B	602	CLA	C4-C3-C5-C6
27	B	603	CLA	C4-C3-C5-C6
27	b	602	CLA	C4-C3-C5-C6
27	b	603	CLA	C4-C3-C5-C6
27	B	602	CLA	C2-C3-C5-C6
27	B	605	CLA	C2-C3-C5-C6
27	b	602	CLA	C2-C3-C5-C6
27	b	605	CLA	C2-C3-C5-C6
27	C	508	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	c	508	CLA	O1D-CGD-O2D-CED
27	C	505	CLA	C3-C5-C6-C7
27	c	505	CLA	C3-C5-C6-C7
28	A	403	PHO	C3-C5-C6-C7
28	a	403	PHO	C3-C5-C6-C7
27	C	508	CLA	CBA-CGA-O2A-C1
27	c	508	CLA	CBA-CGA-O2A-C1
35	H	102	DGD	C4D-C5D-C6D-O5D
35	h	102	DGD	C4D-C5D-C6D-O5D
36	D	404	PL9	C37-C38-C39-C41
36	D	407	PL9	C7-C8-C9-C11
36	D	407	PL9	C42-C43-C44-C46
36	d	404	PL9	C37-C38-C39-C41
36	d	407	PL9	C7-C8-C9-C11
36	d	407	PL9	C42-C43-C44-C46
38	11	311	A86	O5-C38-O4-C34
38	12	315	A86	O5-C38-O4-C34
38	13	313	A86	O5-C38-O4-C34
38	14	313	A86	O5-C38-O4-C34
38	31	311	A86	O5-C38-O4-C34
38	32	315	A86	O5-C38-O4-C34
38	33	313	A86	O5-C38-O4-C34
38	34	314	A86	O5-C38-O4-C34
33	W	101	LMG	O6-C5-C6-O5
33	w	101	LMG	O6-C5-C6-O5
38	11	311	A86	C24-C25-C26-C27
38	12	315	A86	C24-C25-C26-C27
38	13	313	A86	C24-C25-C26-C27
38	14	313	A86	C24-C25-C26-C27
38	31	311	A86	C24-C25-C26-C27
38	32	315	A86	C24-C25-C26-C27
38	33	313	A86	C24-C25-C26-C27
38	34	314	A86	C24-C25-C26-C27
27	Z	102	CLA	O1A-CGA-O2A-C1
27	z	102	CLA	O1A-CGA-O2A-C1
27	11	301	CLA	O1A-CGA-O2A-C1
27	12	305	CLA	O1A-CGA-O2A-C1
27	13	303	CLA	O1A-CGA-O2A-C1
27	14	303	CLA	O1A-CGA-O2A-C1
27	31	301	CLA	O1A-CGA-O2A-C1
27	32	305	CLA	O1A-CGA-O2A-C1
27	33	303	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	34	304	CLA	O1A-CGA-O2A-C1
27	B	607	CLA	CBD-CGD-O2D-CED
27	C	502	CLA	CBD-CGD-O2D-CED
27	b	607	CLA	CBD-CGD-O2D-CED
27	c	502	CLA	CBD-CGD-O2D-CED
27	11	301	CLA	O1D-CGD-O2D-CED
27	12	305	CLA	O1D-CGD-O2D-CED
27	13	303	CLA	O1D-CGD-O2D-CED
27	14	303	CLA	O1D-CGD-O2D-CED
27	31	301	CLA	O1D-CGD-O2D-CED
27	32	305	CLA	O1D-CGD-O2D-CED
27	33	303	CLA	O1D-CGD-O2D-CED
27	34	304	CLA	O1D-CGD-O2D-CED
27	C	512	CLA	CBA-CGA-O2A-C1
27	C	513	CLA	CBA-CGA-O2A-C1
27	c	512	CLA	CBA-CGA-O2A-C1
27	c	513	CLA	CBA-CGA-O2A-C1
27	11	301	CLA	CBA-CGA-O2A-C1
27	12	305	CLA	CBA-CGA-O2A-C1
27	13	303	CLA	CBA-CGA-O2A-C1
27	14	303	CLA	CBA-CGA-O2A-C1
27	31	301	CLA	CBA-CGA-O2A-C1
27	32	305	CLA	CBA-CGA-O2A-C1
27	33	303	CLA	CBA-CGA-O2A-C1
27	34	304	CLA	CBA-CGA-O2A-C1
27	B	603	CLA	O1D-CGD-O2D-CED
27	b	603	CLA	O1D-CGD-O2D-CED
27	B	622	CLA	C3-C5-C6-C7
27	D	401	CLA	C3-C5-C6-C7
27	b	622	CLA	C3-C5-C6-C7
27	d	401	CLA	C3-C5-C6-C7
27	C	512	CLA	CBD-CGD-O2D-CED
27	c	512	CLA	CBD-CGD-O2D-CED
33	B	618	LMG	O6-C5-C6-O5
33	b	618	LMG	O6-C5-C6-O5
33	W	101	LMG	C4-C5-C6-O5
33	w	101	LMG	C4-C5-C6-O5
27	C	502	CLA	C4-C3-C5-C6
27	c	502	CLA	C4-C3-C5-C6
27	C	508	CLA	O1A-CGA-O2A-C1
27	C	513	CLA	O1A-CGA-O2A-C1
27	c	508	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	c	513	CLA	O1A-CGA-O2A-C1
27	b	604	CLA	O1D-CGD-O2D-CED
36	D	404	PL9	C19-C21-C22-C23
36	D	404	PL9	C24-C26-C27-C28
36	D	404	PL9	C44-C46-C47-C48
36	d	404	PL9	C19-C21-C22-C23
36	d	404	PL9	C24-C26-C27-C28
36	d	404	PL9	C44-C46-C47-C48
27	B	604	CLA	O1D-CGD-O2D-CED
28	A	403	PHO	C10-C11-C12-C13
28	a	403	PHO	C10-C11-C12-C13
39	12	302	LMU	O5B-C5B-C6B-O6B
27	11	307	CLA	C2A-CAA-CBA-CGA
27	12	311	CLA	C2A-CAA-CBA-CGA
27	13	309	CLA	C2A-CAA-CBA-CGA
27	14	309	CLA	C2A-CAA-CBA-CGA
27	31	307	CLA	C2A-CAA-CBA-CGA
27	32	311	CLA	C2A-CAA-CBA-CGA
27	33	309	CLA	C2A-CAA-CBA-CGA
27	34	310	CLA	C2A-CAA-CBA-CGA
35	C	518	DGD	O6E-C1E-O5D-C6D
35	c	518	DGD	O6E-C1E-O5D-C6D
33	12	301	LMG	O6-C5-C6-O5
39	32	302	LMU	O5B-C5B-C6B-O6B
27	A	402	CLA	CBA-CGA-O2A-C1
27	C	511	CLA	CBA-CGA-O2A-C1
27	c	511	CLA	CBA-CGA-O2A-C1
27	B	610	CLA	CBD-CGD-O2D-CED
27	B	622	CLA	CBD-CGD-O2D-CED
27	M	102	CLA	CBD-CGD-O2D-CED
27	b	610	CLA	CBD-CGD-O2D-CED
27	b	622	CLA	CBD-CGD-O2D-CED
27	m	101	CLA	CBD-CGD-O2D-CED
35	H	102	DGD	O6E-C5E-C6E-O5E
35	h	102	DGD	O6E-C5E-C6E-O5E
27	C	512	CLA	O1A-CGA-O2A-C1
27	c	512	CLA	O1A-CGA-O2A-C1
29	B	623	BCR	C15-C16-C17-C18
29	b	623	BCR	C15-C16-C17-C18
38	11	310	A86	C24-C25-C26-C27
38	11	312	A86	C24-C25-C26-C27
38	12	314	A86	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
38	12	316	A86	C24-C25-C26-C27
38	13	312	A86	C24-C25-C26-C27
38	13	314	A86	C24-C25-C26-C27
38	14	312	A86	C24-C25-C26-C27
38	14	314	A86	C24-C25-C26-C27
38	31	310	A86	C24-C25-C26-C27
38	31	312	A86	C24-C25-C26-C27
38	32	314	A86	C24-C25-C26-C27
38	32	316	A86	C24-C25-C26-C27
38	33	312	A86	C24-C25-C26-C27
38	33	314	A86	C24-C25-C26-C27
38	34	313	A86	C24-C25-C26-C27
38	34	315	A86	C24-C25-C26-C27
27	C	505	CLA	CBA-CGA-O2A-C1
27	C	506	CLA	CBA-CGA-O2A-C1
27	a	402	CLA	CBA-CGA-O2A-C1
27	c	505	CLA	CBA-CGA-O2A-C1
27	c	506	CLA	CBA-CGA-O2A-C1
30	B	620	SQD	C24-C23-O48-C46
30	b	620	SQD	C24-C23-O48-C46
27	C	503	CLA	CBD-CGD-O2D-CED
27	c	503	CLA	CBD-CGD-O2D-CED
27	B	602	CLA	O1D-CGD-O2D-CED
27	C	507	CLA	O1D-CGD-O2D-CED
27	c	507	CLA	O1D-CGD-O2D-CED
27	b	602	CLA	O1D-CGD-O2D-CED
27	B	603	CLA	C2-C3-C5-C6
27	C	502	CLA	C2-C3-C5-C6
27	b	603	CLA	C2-C3-C5-C6
27	c	502	CLA	C2-C3-C5-C6
27	B	602	CLA	C3-C5-C6-C7
27	b	602	CLA	C3-C5-C6-C7
27	B	601	CLA	C11-C10-C8-C9
27	B	604	CLA	C11-C10-C8-C9
27	B	610	CLA	C11-C12-C13-C14
27	C	506	CLA	C11-C12-C13-C14
27	M	102	CLA	C6-C7-C8-C9
27	Z	102	CLA	C11-C12-C13-C14
27	b	601	CLA	C11-C10-C8-C9
27	b	604	CLA	C11-C10-C8-C9
27	b	610	CLA	C11-C12-C13-C14
27	c	506	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
27	m	101	CLA	C6-C7-C8-C9
27	z	102	CLA	C11-C12-C13-C14
28	A	403	PHO	C11-C10-C8-C9
28	D	403	PHO	C6-C7-C8-C9
28	a	403	PHO	C11-C10-C8-C9
28	d	403	PHO	C6-C7-C8-C9
27	B	614	CLA	O1D-CGD-O2D-CED
27	b	614	CLA	O1D-CGD-O2D-CED
27	C	511	CLA	O1A-CGA-O2A-C1
27	c	511	CLA	O1A-CGA-O2A-C1
29	B	623	BCR	C7-C8-C9-C34
29	B	623	BCR	C37-C22-C23-C24
29	F	101	BCR	C7-C8-C9-C34
29	Z	101	BCR	C37-C22-C23-C24
29	b	623	BCR	C7-C8-C9-C34
29	b	623	BCR	C11-C12-C13-C35
29	b	623	BCR	C37-C22-C23-C24
29	f	101	BCR	C7-C8-C9-C34
29	z	101	BCR	C37-C22-C23-C24
38	11	310	A86	C7-C6-C8-C9
38	11	313	A86	C-C1-C24-C25
38	12	314	A86	C7-C6-C8-C9
38	12	317	A86	C-C1-C24-C25
38	13	312	A86	C7-C6-C8-C9
38	13	315	A86	C-C1-C24-C25
38	14	312	A86	C7-C6-C8-C9
38	14	315	A86	C-C1-C24-C25
38	31	310	A86	C7-C6-C8-C9
38	31	313	A86	C-C1-C24-C25
38	32	314	A86	C7-C6-C8-C9
38	32	317	A86	C-C1-C24-C25
38	33	312	A86	C7-C6-C8-C9
38	33	315	A86	C-C1-C24-C25
38	34	313	A86	C7-C6-C8-C9
38	34	316	A86	C-C1-C24-C25
35	H	102	DGD	C4E-C5E-C6E-O5E
35	h	102	DGD	C4E-C5E-C6E-O5E
27	C	506	CLA	O1A-CGA-O2A-C1
27	c	506	CLA	O1A-CGA-O2A-C1
33	32	301	LMG	O6-C5-C6-O5
32	L	101	LHG	C8-C7-O7-C5
32	l	102	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
27	11	307	CLA	CBA-CGA-O2A-C1
27	12	311	CLA	CBA-CGA-O2A-C1
27	13	309	CLA	CBA-CGA-O2A-C1
27	14	309	CLA	CBA-CGA-O2A-C1
27	31	307	CLA	CBA-CGA-O2A-C1
27	32	311	CLA	CBA-CGA-O2A-C1
27	33	309	CLA	CBA-CGA-O2A-C1
27	34	310	CLA	CBA-CGA-O2A-C1
27	B	610	CLA	C15-C16-C17-C18
27	b	610	CLA	C15-C16-C17-C18
27	b	622	CLA	C5-C6-C7-C8
27	11	307	CLA	C8-C10-C11-C12
27	12	311	CLA	C8-C10-C11-C12
27	13	309	CLA	C8-C10-C11-C12
27	14	309	CLA	C8-C10-C11-C12
27	31	307	CLA	C8-C10-C11-C12
27	32	311	CLA	C8-C10-C11-C12
27	33	309	CLA	C8-C10-C11-C12
27	34	310	CLA	C8-C10-C11-C12
27	B	609	CLA	O1D-CGD-O2D-CED
27	b	609	CLA	O1D-CGD-O2D-CED
36	D	407	PL9	C7-C8-C9-C10
27	B	601	CLA	C8-C10-C11-C12
27	B	611	CLA	C10-C11-C12-C13
27	B	622	CLA	C5-C6-C7-C8
27	M	102	CLA	C13-C15-C16-C17
27	W	103	CLA	C13-C15-C16-C17
27	b	601	CLA	C8-C10-C11-C12
27	b	611	CLA	C10-C11-C12-C13
27	m	101	CLA	C13-C15-C16-C17
27	w	103	CLA	C13-C15-C16-C17
33	C	519	LMG	O6-C5-C6-O5
33	q	301	LMG	O6-C5-C6-O5
33	B	618	LMG	C4-C5-C6-O5
33	b	618	LMG	C4-C5-C6-O5
27	11	306	CLA	CBD-CGD-O2D-CED
27	12	310	CLA	CBD-CGD-O2D-CED
27	13	308	CLA	CBD-CGD-O2D-CED
27	14	308	CLA	CBD-CGD-O2D-CED
27	31	306	CLA	CBD-CGD-O2D-CED
27	32	310	CLA	CBD-CGD-O2D-CED
27	33	308	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	34	309	CLA	CBD-CGD-O2D-CED
33	12	301	LMG	C4-C5-C6-O5
27	C	504	CLA	C6-C7-C8-C10
27	W	103	CLA	C12-C13-C15-C16
27	c	504	CLA	C6-C7-C8-C10
27	w	103	CLA	C12-C13-C15-C16
28	A	403	PHO	C15-C16-C17-C18
28	a	403	PHO	C15-C16-C17-C18
27	11	303	CLA	O1D-CGD-O2D-CED
27	34	306	CLA	O1D-CGD-O2D-CED
33	32	301	LMG	C10-C11-C12-C13
38	11	313	A86	C24-C25-C26-C27
38	11	316	A86	C11-C10-C9-C8
38	12	304	A86	C11-C10-C9-C8
38	12	317	A86	C24-C25-C26-C27
38	13	302	A86	C11-C10-C9-C8
38	13	315	A86	C24-C25-C26-C27
38	13	317	A86	C11-C10-C9-C8
38	14	315	A86	C24-C25-C26-C27
38	31	313	A86	C24-C25-C26-C27
38	31	316	A86	C11-C10-C9-C8
38	32	304	A86	C11-C10-C9-C8
38	32	317	A86	C24-C25-C26-C27
38	33	302	A86	C11-C10-C9-C8
38	33	315	A86	C24-C25-C26-C27
38	34	303	A86	C11-C10-C9-C8
38	34	316	A86	C24-C25-C26-C27
27	12	307	CLA	O1D-CGD-O2D-CED
27	13	305	CLA	O1D-CGD-O2D-CED
27	14	305	CLA	O1D-CGD-O2D-CED
27	31	303	CLA	O1D-CGD-O2D-CED
27	32	307	CLA	O1D-CGD-O2D-CED
27	33	305	CLA	O1D-CGD-O2D-CED
36	D	404	PL9	C29-C31-C32-C33
36	D	404	PL9	C34-C36-C37-C38
36	D	404	PL9	C39-C41-C42-C43
36	d	404	PL9	C29-C31-C32-C33
36	d	404	PL9	C34-C36-C37-C38
36	d	404	PL9	C39-C41-C42-C43
32	L	101	LHG	C7-C8-C9-C10
32	l	102	LHG	C7-C8-C9-C10
27	c	505	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	B	608	CLA	C15-C16-C17-C18
27	B	615	CLA	C8-C10-C11-C12
27	B	615	CLA	C13-C15-C16-C17
27	C	514	CLA	C8-C10-C11-C12
27	Z	102	CLA	C8-C10-C11-C12
27	b	608	CLA	C15-C16-C17-C18
27	b	615	CLA	C8-C10-C11-C12
27	b	615	CLA	C13-C15-C16-C17
27	c	514	CLA	C8-C10-C11-C12
27	z	102	CLA	C8-C10-C11-C12
27	A	402	CLA	C2A-CAA-CBA-CGA
27	B	601	CLA	C2A-CAA-CBA-CGA
27	B	606	CLA	C2A-CAA-CBA-CGA
27	B	610	CLA	C2A-CAA-CBA-CGA
27	C	503	CLA	C2A-CAA-CBA-CGA
27	C	513	CLA	C2A-CAA-CBA-CGA
27	W	103	CLA	C2A-CAA-CBA-CGA
27	a	402	CLA	C2A-CAA-CBA-CGA
27	b	601	CLA	C2A-CAA-CBA-CGA
27	b	606	CLA	C2A-CAA-CBA-CGA
27	b	610	CLA	C2A-CAA-CBA-CGA
27	c	503	CLA	C2A-CAA-CBA-CGA
27	c	513	CLA	C2A-CAA-CBA-CGA
27	w	103	CLA	C2A-CAA-CBA-CGA
27	11	301	CLA	C2A-CAA-CBA-CGA
27	11	306	CLA	C2A-CAA-CBA-CGA
27	12	305	CLA	C2A-CAA-CBA-CGA
27	12	310	CLA	C2A-CAA-CBA-CGA
27	13	303	CLA	C2A-CAA-CBA-CGA
27	13	308	CLA	C2A-CAA-CBA-CGA
27	14	303	CLA	C2A-CAA-CBA-CGA
27	14	308	CLA	C2A-CAA-CBA-CGA
27	31	301	CLA	C2A-CAA-CBA-CGA
27	31	306	CLA	C2A-CAA-CBA-CGA
27	32	305	CLA	C2A-CAA-CBA-CGA
27	32	310	CLA	C2A-CAA-CBA-CGA
27	33	303	CLA	C2A-CAA-CBA-CGA
27	33	308	CLA	C2A-CAA-CBA-CGA
27	34	304	CLA	C2A-CAA-CBA-CGA
27	34	309	CLA	C2A-CAA-CBA-CGA
27	A	404	CLA	C8-C10-C11-C12
27	B	601	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	D	402	CLA	C15-C16-C17-C18
27	W	103	CLA	C10-C11-C12-C13
27	a	404	CLA	C8-C10-C11-C12
27	b	601	CLA	C5-C6-C7-C8
27	b	622	CLA	C13-C15-C16-C17
27	d	402	CLA	C15-C16-C17-C18
27	w	103	CLA	C10-C11-C12-C13
39	32	302	LMU	C4B-C5B-C6B-O6B
33	12	301	LMG	C10-C11-C12-C13
27	C	505	CLA	O1A-CGA-O2A-C1
30	B	620	SQD	O5-C1-O6-C44
30	b	620	SQD	O5-C1-O6-C44
39	12	302	LMU	C4B-C5B-C6B-O6B
27	B	604	CLA	C8-C10-C11-C12
27	B	606	CLA	C10-C11-C12-C13
27	B	613	CLA	C10-C11-C12-C13
27	B	622	CLA	C13-C15-C16-C17
27	C	508	CLA	C8-C10-C11-C12
27	C	509	CLA	C8-C10-C11-C12
27	C	511	CLA	C8-C10-C11-C12
27	W	102	CLA	C10-C11-C12-C13
27	b	604	CLA	C8-C10-C11-C12
27	b	606	CLA	C10-C11-C12-C13
27	b	613	CLA	C10-C11-C12-C13
27	c	508	CLA	C8-C10-C11-C12
27	c	509	CLA	C8-C10-C11-C12
27	c	511	CLA	C8-C10-C11-C12
27	w	102	CLA	C10-C11-C12-C13
27	C	513	CLA	CBD-CGD-O2D-CED
33	B	618	LMG	C28-C29-C30-C31
33	b	618	LMG	C28-C29-C30-C31
27	C	513	CLA	C8-C10-C11-C12
27	c	502	CLA	O1D-CGD-O2D-CED
36	d	407	PL9	C7-C8-C9-C10
27	C	502	CLA	O1D-CGD-O2D-CED
27	34	312	CLA	O1D-CGD-O2D-CED
27	B	602	CLA	C5-C6-C7-C8
27	c	513	CLA	C8-C10-C11-C12
27	c	513	CLA	CBD-CGD-O2D-CED
27	A	402	CLA	O1A-CGA-O2A-C1
27	a	402	CLA	O1A-CGA-O2A-C1
27	11	307	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	12	311	CLA	O1A-CGA-O2A-C1
27	13	309	CLA	O1A-CGA-O2A-C1
27	14	309	CLA	O1A-CGA-O2A-C1
27	31	307	CLA	O1A-CGA-O2A-C1
27	32	311	CLA	O1A-CGA-O2A-C1
32	B	621	LHG	C23-C24-C25-C26
32	b	621	LHG	C23-C24-C25-C26
27	11	309	CLA	O1D-CGD-O2D-CED
27	12	313	CLA	O1D-CGD-O2D-CED
27	13	311	CLA	O1D-CGD-O2D-CED
27	14	311	CLA	O1D-CGD-O2D-CED
27	31	309	CLA	O1D-CGD-O2D-CED
27	32	313	CLA	O1D-CGD-O2D-CED
27	33	311	CLA	O1D-CGD-O2D-CED
27	C	504	CLA	C5-C6-C7-C8
27	C	505	CLA	C15-C16-C17-C18
27	b	602	CLA	C5-C6-C7-C8
27	c	504	CLA	C5-C6-C7-C8
27	c	505	CLA	C15-C16-C17-C18
27	B	607	CLA	CBA-CGA-O2A-C1
27	D	406	CLA	CBA-CGA-O2A-C1
27	b	607	CLA	CBA-CGA-O2A-C1
27	d	406	CLA	CBA-CGA-O2A-C1
33	W	101	LMG	C29-C28-O8-C9
33	w	101	LMG	C29-C28-O8-C9
35	J	101	DGD	C2A-C1A-O1G-C1G
35	j	101	DGD	C2A-C1A-O1G-C1G
33	W	101	LMG	C11-C10-O7-C8
33	w	101	LMG	C11-C10-O7-C8
38	12	304	A86	C35-C34-O4-C38
27	33	309	CLA	O1A-CGA-O2A-C1
27	34	310	CLA	O1A-CGA-O2A-C1
27	M	102	CLA	C8-C10-C11-C12
32	A	408	LHG	O9-C7-O7-C5
32	a	408	LHG	O9-C7-O7-C5
27	W	103	CLA	CBA-CGA-O2A-C1
27	w	103	CLA	CBA-CGA-O2A-C1
33	B	619	LMG	C29-C28-O8-C9
33	b	619	LMG	C29-C28-O8-C9
38	11	316	A86	C35-C34-O4-C38
38	13	302	A86	C35-C34-O4-C38
38	13	317	A86	C35-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
38	31	316	A86	C35-C34-O4-C38
38	32	304	A86	C35-C34-O4-C38
38	33	302	A86	C35-C34-O4-C38
38	34	303	A86	C35-C34-O4-C38
27	B	612	CLA	C10-C11-C12-C13
27	C	505	CLA	C8-C10-C11-C12
27	C	507	CLA	C10-C11-C12-C13
27	C	508	CLA	C10-C11-C12-C13
27	C	508	CLA	C15-C16-C17-C18
27	D	402	CLA	C10-C11-C12-C13
27	b	612	CLA	C10-C11-C12-C13
27	c	505	CLA	C8-C10-C11-C12
27	c	507	CLA	C10-C11-C12-C13
27	c	508	CLA	C10-C11-C12-C13
27	d	402	CLA	C10-C11-C12-C13
27	m	101	CLA	C8-C10-C11-C12
27	W	102	CLA	CBD-CGD-O2D-CED
27	w	102	CLA	CBD-CGD-O2D-CED
27	B	607	CLA	O1D-CGD-O2D-CED
27	b	607	CLA	O1D-CGD-O2D-CED
27	C	504	CLA	C10-C11-C12-C13
27	C	505	CLA	C13-C15-C16-C17
27	C	507	CLA	C15-C16-C17-C18
27	W	102	CLA	C8-C10-C11-C12
27	c	507	CLA	C15-C16-C17-C18
27	c	508	CLA	C15-C16-C17-C18
27	w	102	CLA	C8-C10-C11-C12
38	31	313	A86	O5-C38-O4-C34
27	B	602	CLA	C15-C16-C17-C18
27	C	510	CLA	C13-C15-C16-C17
27	Z	102	CLA	C13-C15-C16-C17
27	b	602	CLA	C15-C16-C17-C18
27	c	504	CLA	C10-C11-C12-C13
27	c	505	CLA	C13-C15-C16-C17
27	c	510	CLA	C13-C15-C16-C17
27	z	102	CLA	C13-C15-C16-C17
38	11	313	A86	O5-C38-O4-C34
38	12	317	A86	O5-C38-O4-C34
38	13	315	A86	O5-C38-O4-C34
38	14	315	A86	O5-C38-O4-C34
38	32	317	A86	O5-C38-O4-C34
38	33	315	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
38	34	316	A86	O5-C38-O4-C34
27	D	406	CLA	C4-C3-C5-C6
27	d	406	CLA	C4-C3-C5-C6
27	B	613	CLA	C5-C6-C7-C8
27	b	613	CLA	C5-C6-C7-C8
27	B	615	CLA	C3-C5-C6-C7
27	b	615	CLA	C3-C5-C6-C7
27	C	511	CLA	C11-C12-C13-C14
27	c	511	CLA	C11-C12-C13-C14
35	C	518	DGD	C2E-C1E-O5D-C6D
35	J	101	DGD	C2E-C1E-O5D-C6D
35	c	518	DGD	C2E-C1E-O5D-C6D
35	j	101	DGD	C2E-C1E-O5D-C6D
27	B	608	CLA	C8-C10-C11-C12
27	D	405	CLA	C15-C16-C17-C18
27	b	608	CLA	C8-C10-C11-C12
27	d	405	CLA	C15-C16-C17-C18
33	B	619	LMG	C10-C11-C12-C13
33	b	619	LMG	C10-C11-C12-C13
27	B	612	CLA	CBA-CGA-O2A-C1
27	b	612	CLA	CBA-CGA-O2A-C1
27	b	611	CLA	C16-C17-C18-C19
29	B	617	BCR	C16-C17-C18-C36
29	C	515	BCR	C11-C10-C9-C34
29	C	515	BCR	C20-C21-C22-C37
29	C	516	BCR	C20-C21-C22-C37
29	M	101	BCR	C16-C17-C18-C36
29	M	101	BCR	C20-C21-C22-C37
29	Z	101	BCR	C11-C10-C9-C34
29	b	617	BCR	C16-C17-C18-C36
29	c	515	BCR	C11-C10-C9-C34
29	c	515	BCR	C20-C21-C22-C37
29	c	516	BCR	C20-C21-C22-C37
29	m	103	BCR	C16-C17-C18-C36
29	m	103	BCR	C20-C21-C22-C37
29	z	101	BCR	C11-C10-C9-C34
33	32	301	LMG	C4-C5-C6-O5
37	E	101	HEM	C1A-C2A-CAA-CBA
37	f	102	HEM	C1A-C2A-CAA-CBA
27	D	401	CLA	C13-C15-C16-C17
27	d	401	CLA	C13-C15-C16-C17
29	C	515	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
29	C	516	BCR	C11-C12-C13-C35
29	C	516	BCR	C37-C22-C23-C24
29	C	520	BCR	C37-C22-C23-C24
29	c	515	BCR	C37-C22-C23-C24
29	c	516	BCR	C11-C12-C13-C35
29	c	516	BCR	C37-C22-C23-C24
29	c	519	BCR	C37-C22-C23-C24
29	B	623	BCR	C21-C22-C23-C24
29	M	101	BCR	C21-C22-C23-C24
29	Z	101	BCR	C11-C12-C13-C14
29	b	623	BCR	C21-C22-C23-C24
29	m	103	BCR	C21-C22-C23-C24
29	z	101	BCR	C11-C12-C13-C14
27	B	607	CLA	O1A-CGA-O2A-C1
27	W	103	CLA	O1A-CGA-O2A-C1
27	b	607	CLA	O1A-CGA-O2A-C1
27	w	103	CLA	O1A-CGA-O2A-C1
33	M	103	LMG	O10-C28-O8-C9
33	m	102	LMG	O10-C28-O8-C9
30	L	103	SQD	C46-C45-O47-C7
30	l	101	SQD	C46-C45-O47-C7
27	B	611	CLA	C16-C17-C18-C19
27	D	406	CLA	O1A-CGA-O2A-C1
27	d	406	CLA	O1A-CGA-O2A-C1
29	A	405	BCR	C20-C21-C22-C23
29	B	623	BCR	C12-C13-C14-C15
29	B	623	BCR	C16-C17-C18-C19
29	C	515	BCR	C12-C13-C14-C15
29	C	515	BCR	C16-C17-C18-C19
29	F	101	BCR	C20-C21-C22-C23
29	Z	101	BCR	C12-C13-C14-C15
29	Z	101	BCR	C20-C21-C22-C23
29	a	405	BCR	C20-C21-C22-C23
29	b	623	BCR	C12-C13-C14-C15
29	b	623	BCR	C16-C17-C18-C19
29	c	515	BCR	C12-C13-C14-C15
29	c	515	BCR	C16-C17-C18-C19
29	f	101	BCR	C20-C21-C22-C23
29	z	101	BCR	C12-C13-C14-C15
29	z	101	BCR	C20-C21-C22-C23
35	C	517	DGD	O6D-C1D-O3G-C3G
35	J	101	DGD	O6E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
35	c	517	DGD	O6D-C1D-O3G-C3G
35	j	101	DGD	O6E-C1E-O5D-C6D
27	C	512	CLA	O1D-CGD-O2D-CED
27	c	512	CLA	O1D-CGD-O2D-CED
27	B	612	CLA	C2-C1-O2A-CGA
27	b	612	CLA	C2-C1-O2A-CGA
27	B	605	CLA	C16-C17-C18-C20
27	b	605	CLA	C16-C17-C18-C20
33	B	618	LMG	C31-C32-C33-C34
33	b	618	LMG	C31-C32-C33-C34
39	12	302	LMU	C5-C6-C7-C8
30	A	406	SQD	C10-C11-C12-C13
32	B	621	LHG	C11-C10-C9-C8
32	b	621	LHG	C11-C10-C9-C8
33	C	519	LMG	C32-C33-C34-C35
33	q	301	LMG	C32-C33-C34-C35
33	12	301	LMG	C12-C13-C14-C15
39	32	302	LMU	C5-C6-C7-C8
30	A	406	SQD	C11-C12-C13-C14
30	a	406	SQD	C10-C11-C12-C13
30	a	406	SQD	C11-C12-C13-C14
33	D	408	LMG	C35-C36-C37-C38
33	d	408	LMG	C35-C36-C37-C38
35	H	102	DGD	C7A-C8A-C9A-CAA
35	h	102	DGD	C7A-C8A-C9A-CAA
32	L	102	LHG	C16-C17-C18-C19
32	l	103	LHG	C16-C17-C18-C19
39	12	302	LMU	C2-C1-O1'-C1'
30	L	103	SQD	C15-C16-C17-C18
30	L	103	SQD	C32-C33-C34-C35
30	l	101	SQD	C15-C16-C17-C18
30	l	101	SQD	C32-C33-C34-C35
32	A	408	LHG	C15-C16-C17-C18
32	a	408	LHG	C15-C16-C17-C18
27	A	404	CLA	C5-C6-C7-C8
27	a	404	CLA	C5-C6-C7-C8
27	B	622	CLA	C4B-C3B-CAB-CBB
27	C	505	CLA	C4B-C3B-CAB-CBB
27	C	513	CLA	C4B-C3B-CAB-CBB
27	D	406	CLA	C4B-C3B-CAB-CBB
27	W	103	CLA	C4B-C3B-CAB-CBB
27	b	622	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
27	c	505	CLA	C4B-C3B-CAB-CBB
27	c	513	CLA	C4B-C3B-CAB-CBB
27	d	406	CLA	C4B-C3B-CAB-CBB
27	w	103	CLA	C4B-C3B-CAB-CBB
27	11	308	CLA	C4B-C3B-CAB-CBB
27	12	312	CLA	C4B-C3B-CAB-CBB
27	13	310	CLA	C4B-C3B-CAB-CBB
27	14	310	CLA	C4B-C3B-CAB-CBB
27	31	308	CLA	C4B-C3B-CAB-CBB
27	32	312	CLA	C4B-C3B-CAB-CBB
27	33	310	CLA	C4B-C3B-CAB-CBB
27	34	311	CLA	C4B-C3B-CAB-CBB
35	H	102	DGD	C1B-C2B-C3B-C4B
35	h	102	DGD	C1B-C2B-C3B-C4B
33	M	103	LMG	C15-C16-C17-C18
33	m	102	LMG	C15-C16-C17-C18
27	B	605	CLA	C16-C17-C18-C19
27	b	605	CLA	C16-C17-C18-C19
33	32	301	LMG	C12-C13-C14-C15
27	C	508	CLA	C13-C15-C16-C17
27	c	508	CLA	C13-C15-C16-C17
32	a	408	LHG	C29-C30-C31-C32
32	L	102	LHG	C23-C24-C25-C26
32	l	103	LHG	C23-C24-C25-C26
33	b	619	LMG	C28-C29-C30-C31
32	A	408	LHG	C29-C30-C31-C32
27	B	601	CLA	C3-C5-C6-C7
27	b	601	CLA	C3-C5-C6-C7
27	B	622	CLA	C3A-C2A-CAA-CBA
27	D	405	CLA	C3A-C2A-CAA-CBA
27	W	102	CLA	C3A-C2A-CAA-CBA
27	W	103	CLA	C3A-C2A-CAA-CBA
27	d	405	CLA	C3A-C2A-CAA-CBA
27	w	102	CLA	C3A-C2A-CAA-CBA
27	w	103	CLA	C3A-C2A-CAA-CBA
27	11	303	CLA	C3A-C2A-CAA-CBA
27	11	304	CLA	C3A-C2A-CAA-CBA
27	11	306	CLA	C3A-C2A-CAA-CBA
27	11	308	CLA	C3A-C2A-CAA-CBA
27	12	307	CLA	C3A-C2A-CAA-CBA
27	12	308	CLA	C3A-C2A-CAA-CBA
27	12	310	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	12	312	CLA	C3A-C2A-CAA-CBA
27	13	305	CLA	C3A-C2A-CAA-CBA
27	13	306	CLA	C3A-C2A-CAA-CBA
27	13	308	CLA	C3A-C2A-CAA-CBA
27	13	310	CLA	C3A-C2A-CAA-CBA
27	14	305	CLA	C3A-C2A-CAA-CBA
27	14	306	CLA	C3A-C2A-CAA-CBA
27	14	308	CLA	C3A-C2A-CAA-CBA
27	14	310	CLA	C3A-C2A-CAA-CBA
27	31	303	CLA	C3A-C2A-CAA-CBA
27	31	304	CLA	C3A-C2A-CAA-CBA
27	31	306	CLA	C3A-C2A-CAA-CBA
27	31	308	CLA	C3A-C2A-CAA-CBA
27	32	307	CLA	C3A-C2A-CAA-CBA
27	32	308	CLA	C3A-C2A-CAA-CBA
27	32	310	CLA	C3A-C2A-CAA-CBA
27	32	312	CLA	C3A-C2A-CAA-CBA
27	33	305	CLA	C3A-C2A-CAA-CBA
27	33	306	CLA	C3A-C2A-CAA-CBA
27	33	308	CLA	C3A-C2A-CAA-CBA
27	33	310	CLA	C3A-C2A-CAA-CBA
27	34	306	CLA	C3A-C2A-CAA-CBA
27	34	307	CLA	C3A-C2A-CAA-CBA
27	34	309	CLA	C3A-C2A-CAA-CBA
27	34	311	CLA	C3A-C2A-CAA-CBA
33	W	101	LMG	C20-C21-C22-C23
33	w	101	LMG	C20-C21-C22-C23
27	C	504	CLA	C8-C10-C11-C12
27	c	504	CLA	C8-C10-C11-C12
32	A	408	LHG	C23-C24-C25-C26
32	a	408	LHG	C23-C24-C25-C26
33	B	619	LMG	C28-C29-C30-C31
30	L	103	SQD	C33-C34-C35-C36
30	l	101	SQD	C33-C34-C35-C36
38	11	316	A86	C3-C4-C5-C6
38	12	304	A86	C3-C4-C5-C6
38	13	302	A86	C3-C4-C5-C6
38	13	317	A86	C3-C4-C5-C6
38	31	316	A86	C3-C4-C5-C6
38	32	304	A86	C3-C4-C5-C6
38	33	302	A86	C3-C4-C5-C6
38	34	303	A86	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
33	D	408	LMG	C30-C31-C32-C33
33	d	408	LMG	C30-C31-C32-C33
33	M	103	LMG	C33-C34-C35-C36
33	W	101	LMG	C19-C20-C21-C22
33	m	102	LMG	C33-C34-C35-C36
27	b	622	CLA	O1D-CGD-O2D-CED
27	C	504	CLA	CBA-CGA-O2A-C1
27	M	102	CLA	CBA-CGA-O2A-C1
27	c	504	CLA	CBA-CGA-O2A-C1
27	m	101	CLA	CBA-CGA-O2A-C1
36	D	404	PL9	C9-C11-C12-C13
36	d	404	PL9	C9-C11-C12-C13
33	w	101	LMG	C19-C20-C21-C22
35	C	518	DGD	C2A-C3A-C4A-C5A
35	c	518	DGD	C2A-C3A-C4A-C5A
32	A	408	LHG	C7-C8-C9-C10
32	a	408	LHG	C7-C8-C9-C10
27	11	307	CLA	C5-C6-C7-C8
27	12	311	CLA	C5-C6-C7-C8
27	13	309	CLA	C5-C6-C7-C8
27	14	309	CLA	C5-C6-C7-C8
27	31	307	CLA	C5-C6-C7-C8
27	32	311	CLA	C5-C6-C7-C8
27	33	309	CLA	C5-C6-C7-C8
27	34	310	CLA	C5-C6-C7-C8
35	C	518	DGD	O6E-C5E-C6E-O5E
35	c	518	DGD	O6E-C5E-C6E-O5E
27	B	612	CLA	O1A-CGA-O2A-C1
27	b	612	CLA	O1A-CGA-O2A-C1
27	B	610	CLA	O1D-CGD-O2D-CED
27	M	102	CLA	O1D-CGD-O2D-CED
27	b	610	CLA	O1D-CGD-O2D-CED
27	m	101	CLA	O1D-CGD-O2D-CED
32	L	102	LHG	C32-C33-C34-C35
32	l	103	LHG	C32-C33-C34-C35
30	A	406	SQD	C32-C33-C34-C35
30	a	406	SQD	C32-C33-C34-C35
35	H	102	DGD	C3A-C4A-C5A-C6A
35	h	102	DGD	C3A-C4A-C5A-C6A
27	B	611	CLA	C16-C17-C18-C20
27	b	611	CLA	C16-C17-C18-C20
27	B	622	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
27	W	103	CLA	C2B-C3B-CAB-CBB
27	w	103	CLA	C2B-C3B-CAB-CBB
27	11	309	CLA	C2B-C3B-CAB-CBB
27	12	313	CLA	C2B-C3B-CAB-CBB
27	13	311	CLA	C2B-C3B-CAB-CBB
27	14	311	CLA	C2B-C3B-CAB-CBB
27	31	309	CLA	C2B-C3B-CAB-CBB
27	32	313	CLA	C2B-C3B-CAB-CBB
27	33	311	CLA	C2B-C3B-CAB-CBB
27	34	312	CLA	C2B-C3B-CAB-CBB
29	B	616	BCR	C1-C6-C7-C8
29	B	623	BCR	C1-C6-C7-C8
29	B	623	BCR	C5-C6-C7-C8
29	C	515	BCR	C5-C6-C7-C8
29	C	520	BCR	C23-C24-C25-C30
29	M	101	BCR	C1-C6-C7-C8
29	M	101	BCR	C5-C6-C7-C8
29	b	616	BCR	C1-C6-C7-C8
29	b	623	BCR	C1-C6-C7-C8
29	b	623	BCR	C5-C6-C7-C8
29	c	515	BCR	C5-C6-C7-C8
29	c	519	BCR	C23-C24-C25-C30
29	m	103	BCR	C1-C6-C7-C8
29	m	103	BCR	C5-C6-C7-C8
27	c	505	CLA	CBD-CGD-O2D-CED
33	D	408	LMG	C36-C37-C38-C39
33	d	408	LMG	C36-C37-C38-C39
27	B	622	CLA	O1D-CGD-O2D-CED
27	C	502	CLA	C2A-CAA-CBA-CGA
27	c	502	CLA	C2A-CAA-CBA-CGA
32	l	102	LHG	C24-C25-C26-C27
27	M	102	CLA	O1A-CGA-O2A-C1
27	m	101	CLA	O1A-CGA-O2A-C1
27	C	505	CLA	CBD-CGD-O2D-CED
32	L	101	LHG	C24-C25-C26-C27
32	L	101	LHG	O9-C7-O7-C5
32	l	102	LHG	O9-C7-O7-C5
27	C	503	CLA	O1D-CGD-O2D-CED
32	L	101	LHG	C25-C26-C27-C28
32	l	102	LHG	C25-C26-C27-C28
33	M	103	LMG	C14-C15-C16-C17
33	W	101	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
33	m	102	LMG	C14-C15-C16-C17
33	w	101	LMG	C14-C15-C16-C17
29	B	616	BCR	C10-C11-C12-C13
29	C	515	BCR	C10-C11-C12-C13
29	F	101	BCR	C10-C11-C12-C13
29	b	616	BCR	C10-C11-C12-C13
29	c	515	BCR	C10-C11-C12-C13
29	f	101	BCR	C10-C11-C12-C13
27	D	406	CLA	C2-C3-C5-C6
27	d	406	CLA	C2-C3-C5-C6
38	11	316	A86	C33-C34-O4-C38
38	31	316	A86	C33-C34-O4-C38
38	33	302	A86	C33-C34-O4-C38
30	L	103	SQD	C14-C15-C16-C17
30	l	101	SQD	C14-C15-C16-C17
32	A	408	LHG	C28-C29-C30-C31
32	a	408	LHG	C28-C29-C30-C31
27	B	602	CLA	CBA-CGA-O2A-C1
27	b	602	CLA	CBA-CGA-O2A-C1
33	B	618	LMG	C29-C28-O8-C9
33	b	618	LMG	C29-C28-O8-C9
35	H	102	DGD	O6D-C5D-C6D-O5D
30	b	620	SQD	C11-C10-C9-C8
33	B	619	LMG	C18-C19-C20-C21
33	M	103	LMG	C31-C32-C33-C34
33	m	102	LMG	C31-C32-C33-C34
27	C	512	CLA	C5-C6-C7-C8
27	c	512	CLA	C5-C6-C7-C8
30	B	620	SQD	C11-C10-C9-C8
30	L	103	SQD	C31-C32-C33-C34
30	l	101	SQD	C31-C32-C33-C34
32	B	621	LHG	C30-C31-C32-C33
32	b	621	LHG	C30-C31-C32-C33
33	b	619	LMG	C18-C19-C20-C21
35	C	518	DGD	CAA-CBA-CCA-CDA
35	c	518	DGD	CAA-CBA-CCA-CDA
27	c	503	CLA	O1D-CGD-O2D-CED
32	L	102	LHG	C28-C29-C30-C31
32	l	103	LHG	C28-C29-C30-C31
35	C	517	DGD	C3A-C4A-C5A-C6A
35	c	517	DGD	C3A-C4A-C5A-C6A
38	12	304	A86	C33-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
38	13	302	A86	C33-C34-O4-C38
38	13	317	A86	C33-C34-O4-C38
38	32	304	A86	C33-C34-O4-C38
38	34	303	A86	C33-C34-O4-C38
35	h	102	DGD	O6D-C5D-C6D-O5D
32	L	101	LHG	C13-C14-C15-C16
32	l	102	LHG	C13-C14-C15-C16
27	c	510	CLA	C3-C5-C6-C7
29	B	623	BCR	C13-C14-C15-C16
29	b	623	BCR	C13-C14-C15-C16
27	B	602	CLA	C16-C17-C18-C19
27	b	602	CLA	C16-C17-C18-C19
33	B	619	LMG	C11-C10-O7-C8
33	b	619	LMG	C11-C10-O7-C8
30	L	103	SQD	C7-C8-C9-C10
30	l	101	SQD	C7-C8-C9-C10
33	C	519	LMG	C19-C20-C21-C22
33	q	301	LMG	C19-C20-C21-C22
30	A	406	SQD	C12-C13-C14-C15
30	a	406	SQD	C12-C13-C14-C15
33	C	519	LMG	C4-C5-C6-O5
33	q	301	LMG	C4-C5-C6-O5
35	J	101	DGD	C8A-C9A-CAA-CBA
27	C	510	CLA	C3-C5-C6-C7
29	a	405	BCR	C11-C12-C13-C14
35	C	517	DGD	CCA-CDA-CEA-CFA
35	c	517	DGD	CCA-CDA-CEA-CFA
35	j	101	DGD	C8A-C9A-CAA-CBA
27	C	507	CLA	C2A-CAA-CBA-CGA
27	c	507	CLA	C2A-CAA-CBA-CGA
27	B	602	CLA	C16-C17-C18-C20
27	B	610	CLA	C16-C17-C18-C20
27	b	602	CLA	C16-C17-C18-C20
27	b	610	CLA	C16-C17-C18-C20
33	B	618	LMG	C29-C30-C31-C32
27	C	507	CLA	C4-C3-C5-C6
27	c	507	CLA	C4-C3-C5-C6
33	b	618	LMG	C29-C30-C31-C32
33	q	301	LMG	C18-C19-C20-C21
33	C	519	LMG	C18-C19-C20-C21
39	12	302	LMU	C1-C2-C3-C4
33	C	519	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
33	q	301	LMG	C10-C11-C12-C13
30	A	406	SQD	C14-C15-C16-C17
30	a	406	SQD	C14-C15-C16-C17
27	W	102	CLA	C5-C6-C7-C8
27	c	514	CLA	C15-C16-C17-C18
35	C	517	DGD	C7B-C8B-C9B-CAB
35	c	517	DGD	C7B-C8B-C9B-CAB
33	W	101	LMG	C12-C13-C14-C15
33	w	101	LMG	C12-C13-C14-C15
27	C	502	CLA	C10-C11-C12-C13
27	C	514	CLA	C15-C16-C17-C18
27	c	502	CLA	C10-C11-C12-C13
27	w	102	CLA	C5-C6-C7-C8
30	B	620	SQD	O47-C45-C46-O48
30	b	620	SQD	O47-C45-C46-O48
27	D	405	CLA	C5-C6-C7-C8
27	M	102	CLA	C5-C6-C7-C8
32	L	101	LHG	C31-C32-C33-C34
32	l	102	LHG	C31-C32-C33-C34
32	b	621	LHG	C9-C10-C11-C12
33	W	101	LMG	C37-C38-C39-C40
33	w	101	LMG	C37-C38-C39-C40
27	C	507	CLA	C13-C15-C16-C17
27	c	507	CLA	C13-C15-C16-C17
27	d	405	CLA	C5-C6-C7-C8
27	m	101	CLA	C5-C6-C7-C8
32	A	408	LHG	C14-C15-C16-C17
32	B	621	LHG	C9-C10-C11-C12
32	L	101	LHG	C29-C30-C31-C32
32	a	408	LHG	C14-C15-C16-C17
32	l	102	LHG	C29-C30-C31-C32
39	12	302	LMU	C2-C3-C4-C5
33	C	519	LMG	O9-C10-O7-C8
33	W	101	LMG	O9-C10-O7-C8
33	w	101	LMG	O9-C10-O7-C8
27	B	615	CLA	C2A-CAA-CBA-CGA
27	b	615	CLA	C2A-CAA-CBA-CGA
30	L	103	SQD	C12-C13-C14-C15
30	l	101	SQD	C12-C13-C14-C15
33	C	519	LMG	C17-C18-C19-C20
33	D	408	LMG	C17-C18-C19-C20
33	q	301	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
35	C	517	DGD	C3B-C4B-C5B-C6B
33	d	408	LMG	C17-C18-C19-C20
27	b	614	CLA	C15-C16-C17-C18
33	D	408	LMG	O6-C5-C6-O5
33	d	408	LMG	O6-C5-C6-O5
35	c	517	DGD	C3B-C4B-C5B-C6B
27	B	614	CLA	C15-C16-C17-C18
32	L	101	LHG	O1-C1-C2-O2
32	l	102	LHG	O1-C1-C2-O2
27	B	602	CLA	O1A-CGA-O2A-C1
27	C	504	CLA	O1A-CGA-O2A-C1
27	b	602	CLA	O1A-CGA-O2A-C1
27	c	504	CLA	O1A-CGA-O2A-C1
30	A	406	SQD	C17-C18-C19-C20
30	a	406	SQD	C17-C18-C19-C20
27	A	404	CLA	C1A-C2A-CAA-CBA
27	B	604	CLA	C1A-C2A-CAA-CBA
27	B	606	CLA	C1A-C2A-CAA-CBA
27	B	607	CLA	C1A-C2A-CAA-CBA
27	B	611	CLA	C1A-C2A-CAA-CBA
27	B	622	CLA	C1A-C2A-CAA-CBA
27	C	504	CLA	C1A-C2A-CAA-CBA
27	C	512	CLA	C1A-C2A-CAA-CBA
27	C	513	CLA	C1A-C2A-CAA-CBA
27	D	401	CLA	C1A-C2A-CAA-CBA
27	D	402	CLA	C1A-C2A-CAA-CBA
27	M	102	CLA	C1A-C2A-CAA-CBA
27	W	103	CLA	C1A-C2A-CAA-CBA
27	a	404	CLA	C1A-C2A-CAA-CBA
27	b	604	CLA	C1A-C2A-CAA-CBA
27	b	606	CLA	C1A-C2A-CAA-CBA
27	b	607	CLA	C1A-C2A-CAA-CBA
27	b	611	CLA	C1A-C2A-CAA-CBA
27	b	622	CLA	C1A-C2A-CAA-CBA
27	c	504	CLA	C1A-C2A-CAA-CBA
27	c	512	CLA	C1A-C2A-CAA-CBA
27	d	401	CLA	C1A-C2A-CAA-CBA
27	d	402	CLA	C1A-C2A-CAA-CBA
27	m	101	CLA	C1A-C2A-CAA-CBA
27	w	103	CLA	C1A-C2A-CAA-CBA
27	11	301	CLA	C1A-C2A-CAA-CBA
27	11	304	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	11	306	CLA	C1A-C2A-CAA-CBA
27	12	305	CLA	C1A-C2A-CAA-CBA
27	12	308	CLA	C1A-C2A-CAA-CBA
27	12	310	CLA	C1A-C2A-CAA-CBA
27	13	303	CLA	C1A-C2A-CAA-CBA
27	13	306	CLA	C1A-C2A-CAA-CBA
27	13	308	CLA	C1A-C2A-CAA-CBA
27	14	303	CLA	C1A-C2A-CAA-CBA
27	14	306	CLA	C1A-C2A-CAA-CBA
27	14	308	CLA	C1A-C2A-CAA-CBA
27	31	301	CLA	C1A-C2A-CAA-CBA
27	31	304	CLA	C1A-C2A-CAA-CBA
27	31	306	CLA	C1A-C2A-CAA-CBA
27	32	305	CLA	C1A-C2A-CAA-CBA
27	32	308	CLA	C1A-C2A-CAA-CBA
27	32	310	CLA	C1A-C2A-CAA-CBA
27	33	303	CLA	C1A-C2A-CAA-CBA
27	33	306	CLA	C1A-C2A-CAA-CBA
27	33	308	CLA	C1A-C2A-CAA-CBA
27	34	304	CLA	C1A-C2A-CAA-CBA
27	34	307	CLA	C1A-C2A-CAA-CBA
27	34	309	CLA	C1A-C2A-CAA-CBA
27	C	503	CLA	C13-C15-C16-C17
27	c	503	CLA	C13-C15-C16-C17
39	32	302	LMU	C2-C3-C4-C5
27	C	507	CLA	C8-C10-C11-C12
27	c	507	CLA	C8-C10-C11-C12
32	B	621	LHG	O6-C4-C5-C6
32	b	621	LHG	O6-C4-C5-C6
33	q	301	LMG	O9-C10-O7-C8
27	B	601	CLA	C11-C10-C8-C7
27	B	612	CLA	C6-C7-C8-C10
27	B	622	CLA	C11-C10-C8-C7
27	C	503	CLA	C11-C12-C13-C15
27	C	505	CLA	C11-C12-C13-C15
27	C	513	CLA	C11-C10-C8-C7
27	D	402	CLA	C12-C13-C15-C16
27	M	102	CLA	C6-C7-C8-C10
27	b	601	CLA	C11-C10-C8-C7
27	b	612	CLA	C6-C7-C8-C10
27	b	622	CLA	C11-C10-C8-C7
27	c	503	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
27	c	505	CLA	C11-C12-C13-C15
27	c	513	CLA	C11-C10-C8-C7
27	d	402	CLA	C12-C13-C15-C16
27	m	101	CLA	C6-C7-C8-C10
27	11	301	CLA	C11-C10-C8-C7
27	12	305	CLA	C11-C10-C8-C7
27	13	303	CLA	C11-C10-C8-C7
27	14	303	CLA	C11-C10-C8-C7
27	31	301	CLA	C11-C10-C8-C7
27	32	305	CLA	C11-C10-C8-C7
27	33	303	CLA	C11-C10-C8-C7
27	34	304	CLA	C11-C10-C8-C7
33	W	101	LMG	C18-C19-C20-C21
33	w	101	LMG	C18-C19-C20-C21
27	B	610	CLA	C16-C17-C18-C19
27	b	610	CLA	C16-C17-C18-C19
30	A	406	SQD	C7-C8-C9-C10
30	a	406	SQD	C7-C8-C9-C10
27	C	507	CLA	C2-C3-C5-C6
27	c	507	CLA	C2-C3-C5-C6
27	C	505	CLA	C10-C11-C12-C13
27	c	505	CLA	C10-C11-C12-C13
27	M	102	CLA	C2A-CAA-CBA-CGA
27	m	101	CLA	C2A-CAA-CBA-CGA
27	B	606	CLA	C11-C10-C8-C9
27	C	505	CLA	C11-C12-C13-C14
27	C	506	CLA	C14-C13-C15-C16
27	C	507	CLA	C11-C12-C13-C14
27	Z	102	CLA	C6-C7-C8-C9
27	b	606	CLA	C11-C10-C8-C9
27	c	505	CLA	C11-C12-C13-C14
27	c	506	CLA	C14-C13-C15-C16
27	c	507	CLA	C11-C12-C13-C14
27	z	102	CLA	C6-C7-C8-C9
27	11	301	CLA	C11-C10-C8-C9
27	12	305	CLA	C11-C10-C8-C9
27	13	303	CLA	C11-C10-C8-C9
27	14	303	CLA	C11-C10-C8-C9
27	31	301	CLA	C11-C10-C8-C9
27	32	305	CLA	C11-C10-C8-C9
27	33	303	CLA	C11-C10-C8-C9
27	34	304	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
32	L	101	LHG	C33-C34-C35-C36
32	l	102	LHG	C33-C34-C35-C36
33	12	301	LMG	C32-C33-C34-C35
39	32	302	LMU	C1-C2-C3-C4
27	C	502	CLA	CBA-CGA-O2A-C1
27	c	502	CLA	CBA-CGA-O2A-C1
27	B	601	CLA	C10-C11-C12-C13
27	b	601	CLA	C10-C11-C12-C13
33	b	619	LMG	C31-C32-C33-C34
33	32	301	LMG	C32-C33-C34-C35
32	A	408	LHG	C4-C5-C6-O8
32	a	408	LHG	C4-C5-C6-O8
33	D	408	LMG	O1-C7-C8-C9
33	W	101	LMG	O1-C7-C8-C9
33	d	408	LMG	O1-C7-C8-C9
33	w	101	LMG	O1-C7-C8-C9
33	B	619	LMG	C31-C32-C33-C34
33	12	301	LMG	C14-C15-C16-C17
35	j	101	DGD	C6A-C7A-C8A-C9A
30	L	103	SQD	C17-C18-C19-C20
30	l	101	SQD	C17-C18-C19-C20
33	B	619	LMG	C11-C12-C13-C14
33	b	619	LMG	C11-C12-C13-C14
35	J	101	DGD	C6A-C7A-C8A-C9A
30	L	103	SQD	C24-C23-O48-C46
30	l	101	SQD	C24-C23-O48-C46
35	C	517	DGD	O6E-C5E-C6E-O5E
35	c	517	DGD	O6E-C5E-C6E-O5E
27	Z	102	CLA	C16-C17-C18-C19
27	z	102	CLA	C16-C17-C18-C19
32	l	103	LHG	O10-C23-O8-C6
27	C	511	CLA	C5-C6-C7-C8
27	M	102	CLA	C10-C11-C12-C13
27	m	101	CLA	C10-C11-C12-C13
32	L	102	LHG	O10-C23-O8-C6
32	A	408	LHG	C13-C14-C15-C16
32	a	408	LHG	C13-C14-C15-C16
28	A	403	PHO	C2-C3-C5-C6
28	a	403	PHO	C2-C3-C5-C6
27	B	604	CLA	C13-C15-C16-C17
27	C	509	CLA	C5-C6-C7-C8
27	b	604	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
27	c	509	CLA	C5-C6-C7-C8
27	c	511	CLA	C5-C6-C7-C8
29	B	617	BCR	C7-C8-C9-C34
29	b	617	BCR	C7-C8-C9-C34
38	11	316	A86	C7-C6-C8-C9
38	12	304	A86	C7-C6-C8-C9
38	13	302	A86	C7-C6-C8-C9
38	13	317	A86	C7-C6-C8-C9
38	31	316	A86	C7-C6-C8-C9
38	32	304	A86	C7-C6-C8-C9
38	33	302	A86	C7-C6-C8-C9
38	34	303	A86	C7-C6-C8-C9
35	J	101	DGD	O1B-C1B-O2G-C2G
35	j	101	DGD	O1B-C1B-O2G-C2G
39	12	302	LMU	C4-C5-C6-C7
29	A	405	BCR	C11-C12-C13-C14
29	H	101	BCR	C21-C22-C23-C24
29	h	101	BCR	C21-C22-C23-C24
38	11	314	A86	C2-C1-C24-C25
38	13	316	A86	C2-C1-C24-C25
38	14	301	A86	C2-C1-C24-C25
38	14	316	A86	C2-C1-C24-C25
38	31	314	A86	C2-C1-C24-C25
38	32	318	A86	C2-C1-C24-C25
38	33	316	A86	C2-C1-C24-C25
38	34	301	A86	C2-C1-C24-C25
27	11	307	CLA	C15-C16-C17-C18
27	12	311	CLA	C15-C16-C17-C18
27	13	309	CLA	C15-C16-C17-C18
27	14	309	CLA	C15-C16-C17-C18
27	31	307	CLA	C15-C16-C17-C18
27	32	311	CLA	C15-C16-C17-C18
27	33	309	CLA	C15-C16-C17-C18
27	34	310	CLA	C15-C16-C17-C18
28	A	403	PHO	C8-C10-C11-C12
28	a	403	PHO	C8-C10-C11-C12
32	L	101	LHG	C28-C29-C30-C31
32	l	102	LHG	C28-C29-C30-C31
27	11	303	CLA	CBA-CGA-O2A-C1
27	11	315	CLA	CBA-CGA-O2A-C1
27	12	303	CLA	CBA-CGA-O2A-C1
27	12	307	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	13	301	CLA	CBA-CGA-O2A-C1
27	13	305	CLA	CBA-CGA-O2A-C1
27	14	302	CLA	CBA-CGA-O2A-C1
27	14	305	CLA	CBA-CGA-O2A-C1
27	31	303	CLA	CBA-CGA-O2A-C1
27	31	315	CLA	CBA-CGA-O2A-C1
27	32	303	CLA	CBA-CGA-O2A-C1
27	32	307	CLA	CBA-CGA-O2A-C1
27	33	301	CLA	CBA-CGA-O2A-C1
27	33	305	CLA	CBA-CGA-O2A-C1
27	34	302	CLA	CBA-CGA-O2A-C1
27	34	306	CLA	CBA-CGA-O2A-C1
27	B	611	CLA	C15-C16-C17-C18
27	b	611	CLA	C15-C16-C17-C18
32	L	101	LHG	C32-C33-C34-C35
32	l	102	LHG	C32-C33-C34-C35
33	32	301	LMG	C15-C16-C17-C18
35	H	102	DGD	CBA-CCA-CDA-CEA
35	c	517	DGD	CBA-CCA-CDA-CEA
35	h	102	DGD	CBA-CCA-CDA-CEA
35	C	517	DGD	CBA-CCA-CDA-CEA
32	B	621	LHG	C33-C34-C35-C36
32	b	621	LHG	C33-C34-C35-C36
33	W	101	LMG	C17-C18-C19-C20
33	w	101	LMG	C17-C18-C19-C20
33	M	103	LMG	C29-C28-O8-C9
33	m	102	LMG	C29-C28-O8-C9
35	H	102	DGD	CBB-CCB-CDB-CEB
35	h	102	DGD	CBB-CCB-CDB-CEB
27	B	609	CLA	C2-C3-C5-C6
27	b	609	CLA	C2-C3-C5-C6
39	32	302	LMU	C4-C5-C6-C7
33	W	101	LMG	C30-C31-C32-C33
33	w	101	LMG	C30-C31-C32-C33
33	12	301	LMG	O1-C7-C8-O7
35	C	517	DGD	O2G-C2G-C3G-O3G
35	c	517	DGD	O2G-C2G-C3G-O3G
32	A	408	LHG	C30-C31-C32-C33
33	B	618	LMG	C30-C31-C32-C33
33	b	618	LMG	C30-C31-C32-C33
32	a	408	LHG	C30-C31-C32-C33
33	B	619	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
33	b	619	LMG	C34-C35-C36-C37
27	11	307	CLA	CAA-CBA-CGA-O2A
27	12	311	CLA	CAA-CBA-CGA-O2A
27	13	309	CLA	CAA-CBA-CGA-O2A
27	14	309	CLA	CAA-CBA-CGA-O2A
27	31	307	CLA	CAA-CBA-CGA-O2A
27	32	311	CLA	CAA-CBA-CGA-O2A
27	33	309	CLA	CAA-CBA-CGA-O2A
27	34	310	CLA	CAA-CBA-CGA-O2A
33	B	619	LMG	C13-C14-C15-C16
33	C	519	LMG	C37-C38-C39-C40
33	q	301	LMG	C37-C38-C39-C40
33	b	619	LMG	C13-C14-C15-C16
27	B	608	CLA	C13-C15-C16-C17
27	b	608	CLA	C13-C15-C16-C17
27	Z	102	CLA	C16-C17-C18-C20
27	z	102	CLA	C16-C17-C18-C20
32	L	102	LHG	C13-C14-C15-C16
32	l	103	LHG	C13-C14-C15-C16
27	B	611	CLA	CBA-CGA-O2A-C1
32	B	621	LHG	C27-C28-C29-C30
28	D	403	PHO	C5-C6-C7-C8
28	d	403	PHO	C5-C6-C7-C8
32	b	621	LHG	C27-C28-C29-C30
27	34	309	CLA	O1D-CGD-O2D-CED
27	11	306	CLA	O1D-CGD-O2D-CED
27	12	310	CLA	O1D-CGD-O2D-CED
27	13	308	CLA	O1D-CGD-O2D-CED
27	14	308	CLA	O1D-CGD-O2D-CED
27	31	306	CLA	O1D-CGD-O2D-CED
27	32	310	CLA	O1D-CGD-O2D-CED
27	33	308	CLA	O1D-CGD-O2D-CED
27	b	611	CLA	CBA-CGA-O2A-C1
35	H	102	DGD	C1A-C2A-C3A-C4A
35	h	102	DGD	C1A-C2A-C3A-C4A
39	32	302	LMU	C2-C1-O1'-C1'
27	B	605	CLA	C11-C12-C13-C14
27	B	607	CLA	C14-C13-C15-C16
27	B	622	CLA	C6-C7-C8-C9
27	B	622	CLA	C11-C10-C8-C9
27	C	504	CLA	C11-C12-C13-C14
27	C	513	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
27	C	514	CLA	C14-C13-C15-C16
27	D	402	CLA	C11-C10-C8-C9
27	D	402	CLA	C14-C13-C15-C16
27	W	103	CLA	C14-C13-C15-C16
27	b	605	CLA	C11-C12-C13-C14
27	b	607	CLA	C14-C13-C15-C16
27	b	622	CLA	C6-C7-C8-C9
27	b	622	CLA	C11-C10-C8-C9
27	c	513	CLA	C11-C10-C8-C9
27	c	514	CLA	C14-C13-C15-C16
27	d	402	CLA	C11-C10-C8-C9
27	d	402	CLA	C14-C13-C15-C16
27	w	103	CLA	C14-C13-C15-C16
27	11	303	CLA	C11-C12-C13-C14
27	11	315	CLA	C14-C13-C15-C16
27	12	303	CLA	C14-C13-C15-C16
27	12	307	CLA	C11-C12-C13-C14
27	13	301	CLA	C14-C13-C15-C16
27	13	305	CLA	C11-C12-C13-C14
27	14	302	CLA	C14-C13-C15-C16
27	14	305	CLA	C11-C12-C13-C14
27	31	303	CLA	C11-C12-C13-C14
27	31	315	CLA	C14-C13-C15-C16
27	32	303	CLA	C14-C13-C15-C16
27	32	307	CLA	C11-C12-C13-C14
27	33	301	CLA	C14-C13-C15-C16
27	33	305	CLA	C11-C12-C13-C14
27	34	302	CLA	C14-C13-C15-C16
27	34	306	CLA	C11-C12-C13-C14
27	C	513	CLA	O1D-CGD-O2D-CED
27	c	513	CLA	O1D-CGD-O2D-CED
27	B	605	CLA	C5-C6-C7-C8
27	W	102	CLA	C15-C16-C17-C18
27	b	605	CLA	C5-C6-C7-C8
27	w	102	CLA	C15-C16-C17-C18
27	B	602	CLA	C4B-C3B-CAB-CBB
27	B	609	CLA	C4B-C3B-CAB-CBB
27	B	610	CLA	C4B-C3B-CAB-CBB
27	B	611	CLA	C4B-C3B-CAB-CBB
27	C	506	CLA	C4B-C3B-CAB-CBB
27	C	512	CLA	C4B-C3B-CAB-CBB
27	b	602	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
27	b	609	CLA	C4B-C3B-CAB-CBB
27	b	610	CLA	C4B-C3B-CAB-CBB
27	b	611	CLA	C4B-C3B-CAB-CBB
27	c	506	CLA	C4B-C3B-CAB-CBB
27	c	512	CLA	C4B-C3B-CAB-CBB
27	11	301	CLA	C4B-C3B-CAB-CBB
27	11	306	CLA	C4B-C3B-CAB-CBB
27	12	305	CLA	C4B-C3B-CAB-CBB
27	12	310	CLA	C4B-C3B-CAB-CBB
27	13	303	CLA	C4B-C3B-CAB-CBB
27	13	308	CLA	C4B-C3B-CAB-CBB
27	14	303	CLA	C4B-C3B-CAB-CBB
27	14	308	CLA	C4B-C3B-CAB-CBB
27	31	301	CLA	C4B-C3B-CAB-CBB
27	31	306	CLA	C4B-C3B-CAB-CBB
27	32	305	CLA	C4B-C3B-CAB-CBB
27	32	310	CLA	C4B-C3B-CAB-CBB
27	33	303	CLA	C4B-C3B-CAB-CBB
27	33	308	CLA	C4B-C3B-CAB-CBB
27	34	304	CLA	C4B-C3B-CAB-CBB
27	34	309	CLA	C4B-C3B-CAB-CBB
33	W	101	LMG	C15-C16-C17-C18
33	w	101	LMG	C15-C16-C17-C18
27	B	606	CLA	C13-C15-C16-C17
27	b	606	CLA	C13-C15-C16-C17
35	j	101	DGD	CDA-CEA-CFA-CGA
36	D	407	PL9	C32-C33-C34-C36
36	d	407	PL9	C32-C33-C34-C36
35	J	101	DGD	CDA-CEA-CFA-CGA
32	L	101	LHG	O6-C4-C5-C6
32	l	102	LHG	O6-C4-C5-C6
32	L	101	LHG	C27-C28-C29-C30
32	l	102	LHG	C27-C28-C29-C30
32	A	408	LHG	C32-C33-C34-C35
32	a	408	LHG	C32-C33-C34-C35
27	B	605	CLA	C11-C12-C13-C15
27	B	606	CLA	C11-C10-C8-C7
27	B	607	CLA	C12-C13-C15-C16
27	B	614	CLA	C11-C10-C8-C7
27	B	622	CLA	C6-C7-C8-C10
27	C	506	CLA	C12-C13-C15-C16
27	C	507	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
27	C	514	CLA	C12-C13-C15-C16
27	D	402	CLA	C11-C10-C8-C7
27	Z	102	CLA	C6-C7-C8-C10
27	b	605	CLA	C11-C12-C13-C15
27	b	606	CLA	C11-C10-C8-C7
27	b	607	CLA	C12-C13-C15-C16
27	b	614	CLA	C11-C10-C8-C7
27	b	622	CLA	C6-C7-C8-C10
27	c	506	CLA	C12-C13-C15-C16
27	c	507	CLA	C11-C12-C13-C15
27	c	514	CLA	C12-C13-C15-C16
27	d	402	CLA	C11-C10-C8-C7
27	z	102	CLA	C6-C7-C8-C10
27	11	303	CLA	C11-C12-C13-C15
27	11	315	CLA	C12-C13-C15-C16
27	12	303	CLA	C12-C13-C15-C16
27	12	307	CLA	C11-C12-C13-C15
27	13	301	CLA	C12-C13-C15-C16
27	13	305	CLA	C11-C12-C13-C15
27	14	302	CLA	C12-C13-C15-C16
27	14	305	CLA	C11-C12-C13-C15
27	31	303	CLA	C11-C12-C13-C15
27	31	315	CLA	C12-C13-C15-C16
27	32	303	CLA	C12-C13-C15-C16
27	32	307	CLA	C11-C12-C13-C15
27	33	301	CLA	C12-C13-C15-C16
27	33	305	CLA	C11-C12-C13-C15
27	34	302	CLA	C12-C13-C15-C16
27	34	306	CLA	C11-C12-C13-C15
33	M	103	LMG	C16-C17-C18-C19
33	m	102	LMG	C16-C17-C18-C19
27	11	303	CLA	O1A-CGA-O2A-C1
27	12	307	CLA	O1A-CGA-O2A-C1
27	13	305	CLA	O1A-CGA-O2A-C1
27	14	305	CLA	O1A-CGA-O2A-C1
27	31	303	CLA	O1A-CGA-O2A-C1
27	32	307	CLA	O1A-CGA-O2A-C1
27	33	305	CLA	O1A-CGA-O2A-C1
27	34	306	CLA	O1A-CGA-O2A-C1
33	B	619	LMG	C21-C22-C23-C24
33	b	619	LMG	C21-C22-C23-C24
27	B	601	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	B	609	CLA	C4-C3-C5-C6
27	C	506	CLA	C4-C3-C5-C6
27	C	513	CLA	C3A-C2A-CAA-CBA
27	b	601	CLA	C3A-C2A-CAA-CBA
27	b	609	CLA	C4-C3-C5-C6
27	b	622	CLA	C3A-C2A-CAA-CBA
27	c	506	CLA	C4-C3-C5-C6
27	c	513	CLA	C3A-C2A-CAA-CBA
28	A	403	PHO	C4-C3-C5-C6
28	a	403	PHO	C4-C3-C5-C6
27	C	502	CLA	O1A-CGA-O2A-C1
27	c	502	CLA	O1A-CGA-O2A-C1
38	11	312	A86	C3-C4-C5-C6
38	11	314	A86	C1-C2-C3-C4
38	12	316	A86	C3-C4-C5-C6
38	13	314	A86	C3-C4-C5-C6
38	13	316	A86	C1-C2-C3-C4
38	14	301	A86	C1-C2-C3-C4
38	14	314	A86	C3-C4-C5-C6
38	14	316	A86	C1-C2-C3-C4
38	31	312	A86	C3-C4-C5-C6
38	31	314	A86	C1-C2-C3-C4
38	32	316	A86	C3-C4-C5-C6
38	32	318	A86	C1-C2-C3-C4
38	33	314	A86	C3-C4-C5-C6
38	33	316	A86	C1-C2-C3-C4
38	34	301	A86	C1-C2-C3-C4
38	34	315	A86	C3-C4-C5-C6
35	h	102	DGD	C5A-C6A-C7A-C8A
27	11	315	CLA	O1A-CGA-O2A-C1
27	12	303	CLA	O1A-CGA-O2A-C1
27	13	301	CLA	O1A-CGA-O2A-C1
27	14	302	CLA	O1A-CGA-O2A-C1
27	31	315	CLA	O1A-CGA-O2A-C1
27	32	303	CLA	O1A-CGA-O2A-C1
27	33	301	CLA	O1A-CGA-O2A-C1
27	34	302	CLA	O1A-CGA-O2A-C1
35	H	102	DGD	C5A-C6A-C7A-C8A
27	C	513	CLA	C13-C15-C16-C17
27	c	513	CLA	C13-C15-C16-C17
35	C	518	DGD	C5A-C6A-C7A-C8A
35	H	102	DGD	CCB-CDB-CEB-CFB

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Mol	Chain	Res	Type	Atoms
35	c	518	DGD	C5A-C6A-C7A-C8A
27	C	514	CLA	CBA-CGA-O2A-C1
27	c	514	CLA	CBA-CGA-O2A-C1
35	h	102	DGD	CCB-CDB-CEB-CFB
30	B	620	SQD	C44-C45-C46-O48
30	L	103	SQD	C44-C45-C46-O48
30	b	620	SQD	C44-C45-C46-O48
30	l	101	SQD	C44-C45-C46-O48
33	C	519	LMG	O1-C7-C8-C9
33	W	101	LMG	C7-C8-C9-O8
33	q	301	LMG	O1-C7-C8-C9
33	w	101	LMG	C7-C8-C9-O8
35	C	517	DGD	C1G-C2G-C3G-O3G
35	c	517	DGD	C1G-C2G-C3G-O3G
32	B	621	LHG	C32-C33-C34-C35
32	b	621	LHG	C32-C33-C34-C35
32	l	103	LHG	C30-C31-C32-C33
33	B	618	LMG	C13-C14-C15-C16
33	D	408	LMG	C20-C21-C22-C23
33	b	618	LMG	C13-C14-C15-C16
35	C	517	DGD	C5A-C6A-C7A-C8A
35	c	517	DGD	C5A-C6A-C7A-C8A
35	c	518	DGD	C4A-C5A-C6A-C7A
32	L	102	LHG	C30-C31-C32-C33
33	d	408	LMG	C20-C21-C22-C23
35	C	518	DGD	C4A-C5A-C6A-C7A
27	C	511	CLA	C4-C3-C5-C6
27	c	511	CLA	C4-C3-C5-C6
27	C	506	CLA	C2-C3-C5-C6
27	c	506	CLA	C2-C3-C5-C6
38	11	313	A86	C10-C11-C13-O
38	12	317	A86	C10-C11-C13-O
38	13	315	A86	C10-C11-C13-O
38	14	315	A86	C10-C11-C13-O
38	31	313	A86	C10-C11-C13-O
38	32	317	A86	C10-C11-C13-O
38	33	315	A86	C10-C11-C13-O
38	34	316	A86	C10-C11-C13-O
27	D	402	CLA	C16-C17-C18-C19
27	d	402	CLA	C16-C17-C18-C19
32	B	621	LHG	O6-C4-C5-O7
32	L	101	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
32	b	621	LHG	O6-C4-C5-O7
32	l	102	LHG	O6-C4-C5-O7
33	B	618	LMG	C36-C37-C38-C39
33	C	519	LMG	C29-C30-C31-C32
33	b	618	LMG	C36-C37-C38-C39
33	q	301	LMG	C29-C30-C31-C32
27	b	622	CLA	C2B-C3B-CAB-CBB
29	A	405	BCR	C1-C6-C7-C8
29	A	409	BCR	C1-C6-C7-C8
29	B	617	BCR	C1-C6-C7-C8
29	C	515	BCR	C1-C6-C7-C8
29	C	515	BCR	C23-C24-C25-C30
29	C	516	BCR	C1-C6-C7-C8
29	C	520	BCR	C1-C6-C7-C8
29	C	520	BCR	C23-C24-C25-C26
29	F	101	BCR	C1-C6-C7-C8
29	F	101	BCR	C5-C6-C7-C8
29	H	101	BCR	C1-C6-C7-C8
29	M	101	BCR	C23-C24-C25-C30
29	a	405	BCR	C1-C6-C7-C8
29	a	409	BCR	C1-C6-C7-C8
29	b	617	BCR	C1-C6-C7-C8
29	c	515	BCR	C1-C6-C7-C8
29	c	515	BCR	C23-C24-C25-C30
29	c	516	BCR	C1-C6-C7-C8
29	c	519	BCR	C1-C6-C7-C8
29	c	519	BCR	C23-C24-C25-C26
29	f	101	BCR	C1-C6-C7-C8
29	f	101	BCR	C5-C6-C7-C8
29	h	101	BCR	C1-C6-C7-C8
29	m	103	BCR	C23-C24-C25-C30
32	A	408	LHG	C8-C7-O7-C5
32	a	408	LHG	C12-C13-C14-C15
30	L	103	SQD	C25-C26-C27-C28
32	A	408	LHG	C12-C13-C14-C15
30	L	103	SQD	O47-C45-C46-O48
30	l	101	SQD	O47-C45-C46-O48
32	A	408	LHG	O7-C5-C6-O8
32	a	408	LHG	O7-C5-C6-O8
33	D	408	LMG	O1-C7-C8-O7
33	d	408	LMG	O1-C7-C8-O7
35	C	518	DGD	C4E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
35	c	518	DGD	C4E-C5E-C6E-O5E
30	l	101	SQD	C25-C26-C27-C28
27	B	609	CLA	C5-C6-C7-C8
30	a	406	SQD	C28-C29-C30-C31
33	W	101	LMG	C32-C33-C34-C35
33	W	101	LMG	C22-C23-C24-C25
33	w	101	LMG	C22-C23-C24-C25
30	A	406	SQD	C28-C29-C30-C31
32	L	102	LHG	C9-C10-C11-C12
32	l	103	LHG	C9-C10-C11-C12
33	D	408	LMG	C34-C35-C36-C37
33	w	101	LMG	C32-C33-C34-C35
27	b	609	CLA	C5-C6-C7-C8
27	C	511	CLA	C2-C3-C5-C6
27	c	511	CLA	C2-C3-C5-C6
33	d	408	LMG	C34-C35-C36-C37
32	a	408	LHG	C8-C7-O7-C5
33	C	519	LMG	C11-C10-O7-C8
27	B	614	CLA	C11-C10-C8-C9
27	C	510	CLA	C14-C13-C15-C16
27	b	614	CLA	C11-C10-C8-C9
27	c	504	CLA	C11-C12-C13-C14
27	c	510	CLA	C14-C13-C15-C16
33	B	619	LMG	C19-C20-C21-C22
29	B	616	BCR	C6-C7-C8-C9
29	B	617	BCR	C22-C23-C24-C25
29	b	616	BCR	C6-C7-C8-C9
29	b	617	BCR	C22-C23-C24-C25
33	b	619	LMG	C19-C20-C21-C22
27	c	505	CLA	O1D-CGD-O2D-CED
27	C	505	CLA	O1D-CGD-O2D-CED
27	W	102	CLA	O1D-CGD-O2D-CED
27	w	102	CLA	O1D-CGD-O2D-CED
35	H	102	DGD	C6A-C7A-C8A-C9A
35	h	102	DGD	C6A-C7A-C8A-C9A
32	L	102	LHG	C29-C30-C31-C32
32	l	103	LHG	C29-C30-C31-C32
27	B	613	CLA	C8-C10-C11-C12
27	b	613	CLA	C8-C10-C11-C12
27	B	604	CLA	CBA-CGA-O2A-C1
27	C	503	CLA	CBA-CGA-O2A-C1
27	c	503	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
36	D	404	PL9	C28-C29-C31-C32
36	d	404	PL9	C28-C29-C31-C32
27	C	507	CLA	C16-C17-C18-C19
27	D	402	CLA	C16-C17-C18-C20
27	c	507	CLA	C16-C17-C18-C19
27	d	402	CLA	C16-C17-C18-C20
33	q	301	LMG	C11-C10-O7-C8
29	C	516	BCR	C35-C13-C14-C15
29	c	516	BCR	C35-C13-C14-C15
27	b	604	CLA	CBA-CGA-O2A-C1
32	L	102	LHG	C10-C11-C12-C13
32	l	103	LHG	C10-C11-C12-C13
33	C	519	LMG	C30-C31-C32-C33
33	q	301	LMG	C30-C31-C32-C33
32	L	102	LHG	O6-C4-C5-C6
32	l	103	LHG	O6-C4-C5-C6
35	C	518	DGD	O1A-C1A-O1G-C1G
38	11	314	A86	C-C1-C24-C25
38	13	316	A86	C-C1-C24-C25
38	14	301	A86	C-C1-C24-C25
38	14	316	A86	C-C1-C24-C25
38	31	314	A86	C-C1-C24-C25
38	32	318	A86	C-C1-C24-C25
38	33	316	A86	C-C1-C24-C25
38	34	301	A86	C-C1-C24-C25
35	H	102	DGD	C3B-C4B-C5B-C6B
27	B	612	CLA	C11-C10-C8-C7
27	C	504	CLA	C11-C12-C13-C15
27	C	508	CLA	C12-C13-C15-C16
27	C	510	CLA	C12-C13-C15-C16
27	D	405	CLA	C11-C12-C13-C15
27	Z	102	CLA	C12-C13-C15-C16
27	b	612	CLA	C11-C10-C8-C7
27	c	504	CLA	C11-C12-C13-C15
27	c	508	CLA	C12-C13-C15-C16
27	c	510	CLA	C12-C13-C15-C16
27	d	405	CLA	C11-C12-C13-C15
27	z	102	CLA	C12-C13-C15-C16
27	11	307	CLA	C12-C13-C15-C16
27	12	311	CLA	C12-C13-C15-C16
27	13	309	CLA	C12-C13-C15-C16
27	14	309	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
27	31	307	CLA	C12-C13-C15-C16
27	32	311	CLA	C12-C13-C15-C16
27	33	309	CLA	C12-C13-C15-C16
27	34	310	CLA	C12-C13-C15-C16
28	A	403	PHO	C11-C10-C8-C7
28	a	403	PHO	C11-C10-C8-C7
33	C	519	LMG	C28-C29-C30-C31
33	q	301	LMG	C28-C29-C30-C31
32	L	101	LHG	C17-C18-C19-C20
33	B	618	LMG	C38-C39-C40-C41
35	h	102	DGD	C3B-C4B-C5B-C6B
32	l	102	LHG	C17-C18-C19-C20
33	D	408	LMG	C39-C40-C41-C42
33	b	618	LMG	C38-C39-C40-C41
33	d	408	LMG	C39-C40-C41-C42
27	C	509	CLA	C13-C15-C16-C17
27	D	402	CLA	C13-C15-C16-C17
27	c	509	CLA	C13-C15-C16-C17
27	d	402	CLA	C13-C15-C16-C17
38	11	316	A86	C5-C6-C8-C9
38	12	304	A86	C5-C6-C8-C9
38	13	302	A86	C5-C6-C8-C9
38	13	317	A86	C5-C6-C8-C9
38	31	316	A86	C5-C6-C8-C9
38	32	304	A86	C5-C6-C8-C9
38	33	302	A86	C5-C6-C8-C9
38	34	303	A86	C5-C6-C8-C9
27	B	611	CLA	O1A-CGA-O2A-C1
27	b	611	CLA	O1A-CGA-O2A-C1
35	c	518	DGD	O1A-C1A-O1G-C1G
27	D	405	CLA	C2A-CAA-CBA-CGA
27	d	405	CLA	C2A-CAA-CBA-CGA
27	11	302	CLA	C2A-CAA-CBA-CGA
27	12	306	CLA	C2A-CAA-CBA-CGA
27	13	304	CLA	C2A-CAA-CBA-CGA
27	14	304	CLA	C2A-CAA-CBA-CGA
27	31	302	CLA	C2A-CAA-CBA-CGA
27	32	306	CLA	C2A-CAA-CBA-CGA
27	33	304	CLA	C2A-CAA-CBA-CGA
27	34	305	CLA	C2A-CAA-CBA-CGA
33	B	619	LMG	C17-C18-C19-C20
35	C	517	DGD	C9A-CAA-CBA-CCA

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Mol	Chain	Res	Type	Atoms
35	c	517	DGD	C9A-CAA-CBA-CCA
35	c	517	DGD	C6B-C7B-C8B-C9B
27	B	605	CLA	CBD-CGD-O2D-CED
35	C	517	DGD	C6B-C7B-C8B-C9B
27	C	504	CLA	C4-C3-C5-C6
27	c	504	CLA	C4-C3-C5-C6
27	C	514	CLA	O1A-CGA-O2A-C1
27	c	514	CLA	O1A-CGA-O2A-C1
33	b	619	LMG	C17-C18-C19-C20
27	b	605	CLA	CBD-CGD-O2D-CED
33	12	301	LMG	C13-C14-C15-C16
29	C	520	BCR	C19-C20-C21-C22
29	c	519	BCR	C19-C20-C21-C22
38	11	316	A86	C24-C25-C26-C27
38	12	304	A86	C24-C25-C26-C27
38	13	302	A86	C24-C25-C26-C27
38	13	317	A86	C24-C25-C26-C27
38	31	316	A86	C24-C25-C26-C27
38	32	304	A86	C24-C25-C26-C27
38	33	302	A86	C24-C25-C26-C27
38	34	303	A86	C24-C25-C26-C27
33	C	519	LMG	C33-C34-C35-C36
33	q	301	LMG	C33-C34-C35-C36
33	32	301	LMG	C11-C12-C13-C14
29	A	409	BCR	C11-C10-C9-C8
29	a	409	BCR	C11-C10-C9-C8
35	J	101	DGD	O6D-C1D-O3G-C3G
35	j	101	DGD	O6D-C1D-O3G-C3G
33	B	619	LMG	O1-C7-C8-C9
33	b	619	LMG	O1-C7-C8-C9
33	32	301	LMG	O1-C7-C8-C9
27	b	613	CLA	CBD-CGD-O2D-CED
37	V	201	HEM	C4C-C3C-CAC-CBC
37	v	201	HEM	C4C-C3C-CAC-CBC
33	12	301	LMG	C11-C12-C13-C14
27	D	401	CLA	C4-C3-C5-C6
27	d	401	CLA	C4-C3-C5-C6
30	A	406	SQD	O6-C44-C45-O47
30	a	406	SQD	O6-C44-C45-O47
33	B	619	LMG	O1-C7-C8-O7
33	C	519	LMG	O1-C7-C8-O7
33	W	101	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
33	b	619	LMG	O1-C7-C8-O7
33	q	301	LMG	O1-C7-C8-O7
33	w	101	LMG	O7-C8-C9-O8
33	32	301	LMG	O1-C7-C8-O7
27	A	404	CLA	C11-C10-C8-C9
27	B	605	CLA	C6-C7-C8-C9
27	B	610	CLA	C14-C13-C15-C16
27	B	612	CLA	C11-C10-C8-C9
27	C	508	CLA	C14-C13-C15-C16
27	W	103	CLA	C11-C12-C13-C14
27	a	404	CLA	C11-C10-C8-C9
27	b	605	CLA	C6-C7-C8-C9
27	b	610	CLA	C14-C13-C15-C16
27	b	612	CLA	C11-C10-C8-C9
27	c	508	CLA	C14-C13-C15-C16
27	w	103	CLA	C11-C12-C13-C14
35	J	101	DGD	C4A-C5A-C6A-C7A
32	B	621	LHG	C34-C35-C36-C37
32	b	621	LHG	C34-C35-C36-C37
35	j	101	DGD	C4A-C5A-C6A-C7A
27	A	402	CLA	C13-C15-C16-C17
27	D	401	CLA	C10-C11-C12-C13
27	a	402	CLA	C13-C15-C16-C17
27	B	613	CLA	CBD-CGD-O2D-CED
38	11	316	A86	C13-C14-C15-O1
38	12	304	A86	C13-C14-C15-O1
38	13	302	A86	C13-C14-C15-O1
38	13	317	A86	C13-C14-C15-O1
38	31	316	A86	C13-C14-C15-O1
38	32	304	A86	C13-C14-C15-O1
38	33	302	A86	C13-C14-C15-O1
38	34	303	A86	C13-C14-C15-O1
27	d	401	CLA	C10-C11-C12-C13
27	C	503	CLA	O1A-CGA-O2A-C1
27	c	503	CLA	O1A-CGA-O2A-C1
32	l	103	LHG	C33-C34-C35-C36
32	L	102	LHG	C33-C34-C35-C36
37	E	101	HEM	C2A-CAA-CBA-CGA
37	f	102	HEM	C2A-CAA-CBA-CGA
27	D	401	CLA	C16-C17-C18-C19
27	d	401	CLA	C16-C17-C18-C19
32	L	102	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
32	l	103	LHG	C27-C28-C29-C30
35	C	518	DGD	C1B-C2B-C3B-C4B
35	c	518	DGD	C1B-C2B-C3B-C4B
33	W	101	LMG	C16-C17-C18-C19
33	w	101	LMG	C16-C17-C18-C19
33	B	618	LMG	C12-C13-C14-C15
33	b	618	LMG	C12-C13-C14-C15
27	c	510	CLA	C5-C6-C7-C8
27	33	303	CLA	C5-C6-C7-C8
27	b	604	CLA	O1A-CGA-O2A-C1
28	D	403	PHO	C16-C17-C18-C20
27	B	604	CLA	O1A-CGA-O2A-C1
35	C	517	DGD	C4D-C5D-C6D-O5D
27	B	608	CLA	C4B-C3B-CAB-CBB
27	C	509	CLA	C1A-C2A-CAA-CBA
27	W	102	CLA	C4B-C3B-CAB-CBB
27	b	608	CLA	C4B-C3B-CAB-CBB
27	c	509	CLA	C1A-C2A-CAA-CBA
27	w	102	CLA	C4B-C3B-CAB-CBB
27	11	315	CLA	C4B-C3B-CAB-CBB
27	12	303	CLA	C4B-C3B-CAB-CBB
27	13	301	CLA	C4B-C3B-CAB-CBB
27	14	302	CLA	C4B-C3B-CAB-CBB
27	31	315	CLA	C4B-C3B-CAB-CBB
27	32	303	CLA	C4B-C3B-CAB-CBB
27	33	301	CLA	C4B-C3B-CAB-CBB
27	34	302	CLA	C4B-C3B-CAB-CBB
38	11	312	A86	O-C13-C14-C15
38	11	316	A86	O-C13-C14-C15
38	12	304	A86	O-C13-C14-C15
38	12	316	A86	O-C13-C14-C15
38	13	302	A86	O-C13-C14-C15
38	13	314	A86	O-C13-C14-C15
38	13	317	A86	O-C13-C14-C15
38	14	314	A86	O-C13-C14-C15
38	31	312	A86	O-C13-C14-C15
38	31	316	A86	O-C13-C14-C15
38	32	304	A86	O-C13-C14-C15
38	32	316	A86	O-C13-C14-C15
38	33	302	A86	O-C13-C14-C15
38	33	314	A86	O-C13-C14-C15
38	34	303	A86	O-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
38	34	315	A86	O-C13-C14-C15
27	C	510	CLA	C5-C6-C7-C8
27	11	301	CLA	C5-C6-C7-C8
27	13	303	CLA	C5-C6-C7-C8
27	14	303	CLA	C5-C6-C7-C8
27	32	305	CLA	C5-C6-C7-C8
28	d	403	PHO	C16-C17-C18-C20
27	12	305	CLA	C5-C6-C7-C8
27	34	304	CLA	C5-C6-C7-C8
35	c	517	DGD	C4D-C5D-C6D-O5D
27	31	301	CLA	C5-C6-C7-C8
35	c	518	DGD	C6B-C7B-C8B-C9B
33	B	618	LMG	C19-C20-C21-C22
35	C	518	DGD	C6B-C7B-C8B-C9B
27	B	601	CLA	C12-C13-C15-C16
27	B	610	CLA	C12-C13-C15-C16
27	C	506	CLA	C11-C12-C13-C15
27	C	509	CLA	C6-C7-C8-C10
27	Z	102	CLA	C11-C12-C13-C15
27	b	601	CLA	C12-C13-C15-C16
27	b	610	CLA	C12-C13-C15-C16
27	c	506	CLA	C11-C12-C13-C15
27	c	509	CLA	C6-C7-C8-C10
27	z	102	CLA	C11-C12-C13-C15
33	b	618	LMG	C19-C20-C21-C22
27	C	507	CLA	C16-C17-C18-C20
27	c	507	CLA	C16-C17-C18-C20
35	C	518	DGD	CBB-CCB-CDB-CEB
35	c	518	DGD	CBB-CCB-CDB-CEB
32	B	621	LHG	C28-C29-C30-C31
32	b	621	LHG	C28-C29-C30-C31
27	31	303	CLA	C10-C11-C12-C13
27	32	307	CLA	C10-C11-C12-C13
27	33	305	CLA	C10-C11-C12-C13
27	34	306	CLA	C10-C11-C12-C13
33	b	618	LMG	C18-C19-C20-C21
27	11	309	CLA	C3A-C2A-CAA-CBA
27	12	313	CLA	C3A-C2A-CAA-CBA
27	13	311	CLA	C3A-C2A-CAA-CBA
27	14	311	CLA	C3A-C2A-CAA-CBA
27	31	309	CLA	C3A-C2A-CAA-CBA
27	32	313	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	33	311	CLA	C3A-C2A-CAA-CBA
27	34	312	CLA	C3A-C2A-CAA-CBA
27	C	514	CLA	C16-C17-C18-C19
27	c	514	CLA	C16-C17-C18-C19
27	B	613	CLA	O1D-CGD-O2D-CED
33	B	618	LMG	C18-C19-C20-C21
27	D	401	CLA	C2-C3-C5-C6
27	d	401	CLA	C2-C3-C5-C6
27	11	303	CLA	C10-C11-C12-C13
27	12	307	CLA	C10-C11-C12-C13
27	14	305	CLA	C10-C11-C12-C13
32	L	102	LHG	O6-C4-C5-O7
32	l	103	LHG	O6-C4-C5-O7
33	12	301	LMG	C30-C31-C32-C33
27	13	305	CLA	C10-C11-C12-C13
27	11	304	CLA	C2A-CAA-CBA-CGA
27	12	308	CLA	C2A-CAA-CBA-CGA
27	13	306	CLA	C2A-CAA-CBA-CGA
27	14	306	CLA	C2A-CAA-CBA-CGA
27	31	304	CLA	C2A-CAA-CBA-CGA
27	32	308	CLA	C2A-CAA-CBA-CGA
27	33	306	CLA	C2A-CAA-CBA-CGA
27	34	307	CLA	C2A-CAA-CBA-CGA
27	D	405	CLA	C11-C12-C13-C14
27	Z	102	CLA	C14-C13-C15-C16
27	d	405	CLA	C11-C12-C13-C14
27	z	102	CLA	C14-C13-C15-C16
27	11	307	CLA	C14-C13-C15-C16
27	12	311	CLA	C14-C13-C15-C16
27	13	309	CLA	C14-C13-C15-C16
27	14	309	CLA	C14-C13-C15-C16
27	31	307	CLA	C14-C13-C15-C16
27	32	311	CLA	C14-C13-C15-C16
27	33	309	CLA	C14-C13-C15-C16
27	34	310	CLA	C14-C13-C15-C16
29	C	520	BCR	C9-C10-C11-C12
29	c	519	BCR	C9-C10-C11-C12
35	C	517	DGD	O6D-C5D-C6D-O5D
35	c	517	DGD	O6D-C5D-C6D-O5D
33	b	619	LMG	C22-C23-C24-C25
27	b	613	CLA	O1D-CGD-O2D-CED
27	C	508	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	D	405	CLA	C13-C15-C16-C17
27	c	508	CLA	C5-C6-C7-C8
27	d	405	CLA	C13-C15-C16-C17
33	B	619	LMG	C22-C23-C24-C25
35	H	102	DGD	CCA-CDA-CEA-CFA
35	C	517	DGD	C2D-C1D-O3G-C3G
35	c	517	DGD	C2D-C1D-O3G-C3G
35	h	102	DGD	CCA-CDA-CEA-CFA
27	B	609	CLA	CAD-CBD-CGD-O2D
27	B	612	CLA	CAD-CBD-CGD-O2D
27	C	503	CLA	CAD-CBD-CGD-O2D
27	C	506	CLA	CAD-CBD-CGD-O2D
27	C	507	CLA	CAD-CBD-CGD-O2D
27	b	609	CLA	CAD-CBD-CGD-O2D
27	b	612	CLA	CAD-CBD-CGD-O2D
27	c	503	CLA	CAD-CBD-CGD-O2D
27	c	506	CLA	CAD-CBD-CGD-O2D
27	c	507	CLA	CAD-CBD-CGD-O2D
27	11	303	CLA	CAD-CBD-CGD-O2D
27	11	305	CLA	CAD-CBD-CGD-O2D
27	12	307	CLA	CAD-CBD-CGD-O2D
27	12	309	CLA	CAD-CBD-CGD-O2D
27	13	305	CLA	CAD-CBD-CGD-O2D
27	13	307	CLA	CAD-CBD-CGD-O2D
27	14	305	CLA	CAD-CBD-CGD-O2D
27	14	307	CLA	CAD-CBD-CGD-O2D
27	31	303	CLA	CAD-CBD-CGD-O2D
27	31	305	CLA	CAD-CBD-CGD-O2D
27	32	307	CLA	CAD-CBD-CGD-O2D
27	32	309	CLA	CAD-CBD-CGD-O2D
27	33	305	CLA	CAD-CBD-CGD-O2D
27	33	307	CLA	CAD-CBD-CGD-O2D
27	34	306	CLA	CAD-CBD-CGD-O2D
27	34	308	CLA	CAD-CBD-CGD-O2D
27	B	615	CLA	C5-C6-C7-C8
27	b	615	CLA	C5-C6-C7-C8
35	C	518	DGD	C7B-C8B-C9B-CAB
35	c	518	DGD	C7B-C8B-C9B-CAB
27	B	604	CLA	CAD-CBD-CGD-O1D
27	B	609	CLA	CAD-CBD-CGD-O1D
27	B	612	CLA	CAD-CBD-CGD-O1D
27	C	503	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
27	C	505	CLA	CAD-CBD-CGD-O1D
27	C	506	CLA	CAD-CBD-CGD-O1D
27	C	507	CLA	CAD-CBD-CGD-O1D
27	C	508	CLA	CAD-CBD-CGD-O1D
27	C	511	CLA	CHA-CBD-CGD-O1D
27	C	511	CLA	CHA-CBD-CGD-O2D
27	b	604	CLA	CAD-CBD-CGD-O1D
27	b	609	CLA	CAD-CBD-CGD-O1D
27	b	612	CLA	CAD-CBD-CGD-O1D
27	c	503	CLA	CAD-CBD-CGD-O1D
27	c	505	CLA	CAD-CBD-CGD-O1D
27	c	506	CLA	CAD-CBD-CGD-O1D
27	c	507	CLA	CAD-CBD-CGD-O1D
27	c	508	CLA	CAD-CBD-CGD-O1D
27	c	511	CLA	CHA-CBD-CGD-O1D
27	c	511	CLA	CHA-CBD-CGD-O2D
27	11	303	CLA	CAD-CBD-CGD-O1D
27	11	305	CLA	CAD-CBD-CGD-O1D
27	11	309	CLA	CHA-CBD-CGD-O1D
27	11	309	CLA	CHA-CBD-CGD-O2D
27	12	307	CLA	CAD-CBD-CGD-O1D
27	12	309	CLA	CAD-CBD-CGD-O1D
27	12	313	CLA	CHA-CBD-CGD-O1D
27	12	313	CLA	CHA-CBD-CGD-O2D
27	13	305	CLA	CAD-CBD-CGD-O1D
27	13	307	CLA	CAD-CBD-CGD-O1D
27	13	311	CLA	CHA-CBD-CGD-O1D
27	13	311	CLA	CHA-CBD-CGD-O2D
27	14	305	CLA	CAD-CBD-CGD-O1D
27	14	307	CLA	CAD-CBD-CGD-O1D
27	14	311	CLA	CHA-CBD-CGD-O1D
27	14	311	CLA	CHA-CBD-CGD-O2D
27	31	303	CLA	CAD-CBD-CGD-O1D
27	31	305	CLA	CAD-CBD-CGD-O1D
27	31	309	CLA	CHA-CBD-CGD-O1D
27	31	309	CLA	CHA-CBD-CGD-O2D
27	32	307	CLA	CAD-CBD-CGD-O1D
27	32	309	CLA	CAD-CBD-CGD-O1D
27	32	313	CLA	CHA-CBD-CGD-O1D
27	32	313	CLA	CHA-CBD-CGD-O2D
27	33	305	CLA	CAD-CBD-CGD-O1D
27	33	307	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
27	33	311	CLA	CHA-CBD-CGD-O1D
27	33	311	CLA	CHA-CBD-CGD-O2D
27	34	306	CLA	CAD-CBD-CGD-O1D
27	34	308	CLA	CAD-CBD-CGD-O1D
27	34	312	CLA	CHA-CBD-CGD-O1D
27	34	312	CLA	CHA-CBD-CGD-O2D
32	A	408	LHG	C3-O3-P-O4
32	B	621	LHG	C3-O3-P-O5
32	L	101	LHG	C4-O6-P-O5
32	L	102	LHG	C3-O3-P-O5
32	L	102	LHG	C4-O6-P-O3
32	a	408	LHG	C3-O3-P-O4
32	b	621	LHG	C3-O3-P-O5
32	l	102	LHG	C4-O6-P-O5
32	l	103	LHG	C3-O3-P-O5
32	l	103	LHG	C4-O6-P-O3
38	11	313	A86	C10-C11-C13-C14
38	12	317	A86	C10-C11-C13-C14
38	13	315	A86	C10-C11-C13-C14
38	14	315	A86	C10-C11-C13-C14
38	31	313	A86	C10-C11-C13-C14
38	32	317	A86	C10-C11-C13-C14
38	33	315	A86	C10-C11-C13-C14
38	34	316	A86	C10-C11-C13-C14
33	w	101	LMG	C38-C39-C40-C41
27	B	602	CLA	C2B-C3B-CAB-CBB
27	B	610	CLA	C2B-C3B-CAB-CBB
27	C	505	CLA	C2B-C3B-CAB-CBB
27	C	506	CLA	C2B-C3B-CAB-CBB
27	C	513	CLA	C2B-C3B-CAB-CBB
27	b	602	CLA	C2B-C3B-CAB-CBB
27	b	610	CLA	C2B-C3B-CAB-CBB
27	c	505	CLA	C2B-C3B-CAB-CBB
27	c	506	CLA	C2B-C3B-CAB-CBB
27	c	513	CLA	C2B-C3B-CAB-CBB
27	11	308	CLA	C2B-C3B-CAB-CBB
27	12	312	CLA	C2B-C3B-CAB-CBB
27	13	310	CLA	C2B-C3B-CAB-CBB
27	14	310	CLA	C2B-C3B-CAB-CBB
27	31	308	CLA	C2B-C3B-CAB-CBB
27	32	312	CLA	C2B-C3B-CAB-CBB
27	33	310	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
27	34	311	CLA	C2B-C3B-CAB-CBB
29	A	409	BCR	C5-C6-C7-C8
29	a	409	BCR	C5-C6-C7-C8
33	W	101	LMG	C38-C39-C40-C41
33	b	618	LMG	C16-C17-C18-C19
35	h	102	DGD	C5B-C6B-C7B-C8B
29	B	616	BCR	C11-C12-C13-C35
29	b	616	BCR	C11-C12-C13-C35
35	H	102	DGD	C5B-C6B-C7B-C8B
33	32	301	LMG	C16-C17-C18-C19
33	B	618	LMG	C16-C17-C18-C19
32	L	102	LHG	C35-C36-C37-C38
32	l	103	LHG	C35-C36-C37-C38
27	z	102	CLA	CBD-CGD-O2D-CED
38	11	313	A86	C12-C11-C13-C14
38	12	317	A86	C12-C11-C13-C14
38	13	315	A86	C12-C11-C13-C14
38	14	315	A86	C12-C11-C13-C14
38	31	313	A86	C12-C11-C13-C14
38	32	317	A86	C12-C11-C13-C14
38	33	315	A86	C12-C11-C13-C14
38	34	316	A86	C12-C11-C13-C14
36	D	404	PL9	C4-C3-C7-C8
36	d	404	PL9	C4-C3-C7-C8
35	C	518	DGD	C1A-C2A-C3A-C4A
35	c	518	DGD	C1A-C2A-C3A-C4A
33	b	619	LMG	O10-C28-O8-C9
27	Z	102	CLA	C5-C6-C7-C8
27	11	315	CLA	C13-C15-C16-C17
27	12	303	CLA	C13-C15-C16-C17
27	14	302	CLA	C13-C15-C16-C17
27	31	315	CLA	C13-C15-C16-C17
27	32	303	CLA	C13-C15-C16-C17
27	34	302	CLA	C13-C15-C16-C17
32	L	102	LHG	C12-C13-C14-C15
33	w	101	LMG	C36-C37-C38-C39
27	z	102	CLA	C5-C6-C7-C8
27	13	301	CLA	C13-C15-C16-C17
27	33	301	CLA	C13-C15-C16-C17
28	A	403	PHO	C5-C6-C7-C8
32	l	103	LHG	C12-C13-C14-C15
33	w	101	LMG	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
35	J	101	DGD	CDB-CEB-CFB-CGB
33	W	101	LMG	C21-C22-C23-C24
33	W	101	LMG	C36-C37-C38-C39
33	B	619	LMG	O10-C28-O8-C9
27	Z	102	CLA	CBD-CGD-O2D-CED
35	j	101	DGD	CDB-CEB-CFB-CGB
27	B	622	CLA	C11-C12-C13-C14
27	C	502	CLA	C14-C13-C15-C16
27	C	503	CLA	C11-C12-C13-C14
27	W	102	CLA	C14-C13-C15-C16
27	b	622	CLA	C11-C12-C13-C14
27	c	502	CLA	C14-C13-C15-C16
27	c	503	CLA	C11-C12-C13-C14
27	w	102	CLA	C14-C13-C15-C16
27	W	103	CLA	C11-C12-C13-C15
27	w	103	CLA	C11-C12-C13-C15
28	a	403	PHO	C5-C6-C7-C8
37	E	101	HEM	C3A-C2A-CAA-CBA
32	b	621	LHG	C29-C30-C31-C32
32	B	621	LHG	C29-C30-C31-C32
27	B	603	CLA	C16-C17-C18-C20
27	D	401	CLA	C16-C17-C18-C20
27	b	603	CLA	C16-C17-C18-C20
27	d	401	CLA	C16-C17-C18-C20
27	C	513	CLA	C10-C11-C12-C13
27	c	513	CLA	C10-C11-C12-C13
32	L	101	LHG	C23-C24-C25-C26
29	c	515	BCR	C19-C20-C21-C22
30	l	101	SQD	C24-C25-C26-C27
27	B	614	CLA	C13-C15-C16-C17
37	f	102	HEM	C3A-C2A-CAA-CBA
32	l	102	LHG	C23-C24-C25-C26
27	b	614	CLA	C13-C15-C16-C17
30	L	103	SQD	C24-C25-C26-C27
35	H	102	DGD	C4A-C5A-C6A-C7A
35	h	102	DGD	C4A-C5A-C6A-C7A
27	11	315	CLA	O1D-CGD-O2D-CED
27	W	103	CLA	C2-C1-O2A-CGA
27	w	103	CLA	C2-C1-O2A-CGA
35	H	102	DGD	O2G-C1B-C2B-C3B
35	h	102	DGD	O2G-C1B-C2B-C3B
35	C	517	DGD	C8A-C9A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	32	303	CLA	O1D-CGD-O2D-CED
33	32	301	LMG	C13-C14-C15-C16
33	B	619	LMG	C32-C33-C34-C35
33	b	619	LMG	C32-C33-C34-C35
27	12	303	CLA	O1D-CGD-O2D-CED
27	13	301	CLA	O1D-CGD-O2D-CED
35	c	517	DGD	C8A-C9A-CAA-CBA
27	14	302	CLA	O1D-CGD-O2D-CED
27	33	301	CLA	O1D-CGD-O2D-CED
35	C	518	DGD	C5D-C6D-O5D-C1E
35	c	518	DGD	C5D-C6D-O5D-C1E
27	B	603	CLA	C2A-CAA-CBA-CGA
27	C	506	CLA	C2A-CAA-CBA-CGA
27	b	603	CLA	C2A-CAA-CBA-CGA
27	c	506	CLA	C2A-CAA-CBA-CGA
27	34	302	CLA	O1D-CGD-O2D-CED
29	C	515	BCR	C19-C20-C21-C22
27	B	605	CLA	O1D-CGD-O2D-CED
27	31	315	CLA	O1D-CGD-O2D-CED
27	C	509	CLA	CBA-CGA-O2A-C1
27	c	509	CLA	CBA-CGA-O2A-C1
38	11	310	A86	C13-C14-C15-C16
38	12	314	A86	C13-C14-C15-C16
38	13	312	A86	C13-C14-C15-C16
38	14	312	A86	C13-C14-C15-C16
38	31	310	A86	C13-C14-C15-C16
38	32	314	A86	C13-C14-C15-C16
38	33	312	A86	C13-C14-C15-C16
38	34	313	A86	C13-C14-C15-C16
27	34	302	CLA	C3-C5-C6-C7
27	B	608	CLA	CBD-CGD-O2D-CED
27	C	509	CLA	C6-C7-C8-C9
27	W	103	CLA	C6-C7-C8-C9
27	c	509	CLA	C6-C7-C8-C9
27	w	103	CLA	C6-C7-C8-C9
27	b	605	CLA	O1D-CGD-O2D-CED
32	A	408	LHG	C24-C23-O8-C6
32	a	408	LHG	C24-C23-O8-C6
27	Z	102	CLA	O1D-CGD-O2D-CED
27	z	102	CLA	O1D-CGD-O2D-CED
27	11	303	CLA	C4B-C3B-CAB-CBB
27	12	307	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
27	13	305	CLA	C4B-C3B-CAB-CBB
27	14	305	CLA	C4B-C3B-CAB-CBB
27	31	303	CLA	C4B-C3B-CAB-CBB
27	32	307	CLA	C4B-C3B-CAB-CBB
27	33	305	CLA	C4B-C3B-CAB-CBB
27	34	306	CLA	C4B-C3B-CAB-CBB
27	11	315	CLA	C3-C5-C6-C7
27	13	301	CLA	C3-C5-C6-C7
27	B	606	CLA	C8-C10-C11-C12
33	C	519	LMG	C29-C28-O8-C9
33	q	301	LMG	C29-C28-O8-C9
27	b	606	CLA	C8-C10-C11-C12
27	W	102	CLA	C4-C3-C5-C6
27	w	102	CLA	C4-C3-C5-C6
30	B	620	SQD	O10-C23-O48-C46
30	b	620	SQD	O10-C23-O48-C46
27	b	605	CLA	C8-C10-C11-C12
32	L	101	LHG	C10-C11-C12-C13
32	l	102	LHG	C10-C11-C12-C13
33	b	618	LMG	C20-C21-C22-C23
35	C	518	DGD	C5B-C6B-C7B-C8B
27	B	615	CLA	C6-C7-C8-C10
27	C	505	CLA	C6-C7-C8-C10
27	W	102	CLA	C11-C12-C13-C15
27	b	615	CLA	C6-C7-C8-C10
27	c	505	CLA	C6-C7-C8-C10
27	w	102	CLA	C11-C12-C13-C15
27	b	608	CLA	CBD-CGD-O2D-CED
33	B	618	LMG	C20-C21-C22-C23
27	12	303	CLA	C3-C5-C6-C7
27	14	302	CLA	C3-C5-C6-C7
27	31	315	CLA	C3-C5-C6-C7
27	32	303	CLA	C3-C5-C6-C7
27	33	301	CLA	C3-C5-C6-C7
35	c	518	DGD	C5B-C6B-C7B-C8B
27	B	622	CLA	O1A-CGA-O2A-C1
27	B	601	CLA	CAA-CBA-CGA-O2A
27	b	601	CLA	CAA-CBA-CGA-O2A
32	L	101	LHG	C30-C31-C32-C33
27	B	603	CLA	C16-C17-C18-C19
27	b	603	CLA	C16-C17-C18-C19
35	H	102	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
27	12	311	CLA	CAA-CBA-CGA-O1A
27	14	309	CLA	CAA-CBA-CGA-O1A
27	31	307	CLA	CAA-CBA-CGA-O1A
27	33	309	CLA	CAA-CBA-CGA-O1A
35	h	102	DGD	C2B-C3B-C4B-C5B
27	B	605	CLA	C8-C10-C11-C12
27	b	622	CLA	O1A-CGA-O2A-C1
32	l	102	LHG	C30-C31-C32-C33
33	12	301	LMG	O7-C8-C9-O8
27	C	507	CLA	C3A-C2A-CAA-CBA
27	c	507	CLA	C3A-C2A-CAA-CBA
27	32	311	CLA	CAA-CBA-CGA-O1A
30	L	103	SQD	C11-C12-C13-C14
33	12	301	LMG	C15-C16-C17-C18
32	A	408	LHG	C31-C32-C33-C34
32	a	408	LHG	C31-C32-C33-C34
27	11	307	CLA	CAA-CBA-CGA-O1A
27	13	309	CLA	CAA-CBA-CGA-O1A
27	34	310	CLA	CAA-CBA-CGA-O1A
27	C	509	CLA	C10-C11-C12-C13
27	c	509	CLA	C10-C11-C12-C13
30	l	101	SQD	C11-C12-C13-C14
27	D	401	CLA	C2-C1-O2A-CGA
27	d	401	CLA	C2-C1-O2A-CGA
35	c	517	DGD	C8B-C9B-CAB-CBB
27	b	612	CLA	C5-C6-C7-C8
35	C	517	DGD	C8B-C9B-CAB-CBB
27	B	612	CLA	C5-C6-C7-C8
35	J	101	DGD	C3A-C4A-C5A-C6A
35	j	101	DGD	C3A-C4A-C5A-C6A
27	C	514	CLA	C10-C11-C12-C13
27	c	514	CLA	C10-C11-C12-C13
27	33	301	CLA	C8-C10-C11-C12
33	12	301	LMG	O1-C7-C8-C9
33	12	301	LMG	C7-C8-C9-O8
38	11	316	A86	C12-C11-C13-O
38	12	304	A86	C12-C11-C13-O
38	13	302	A86	C12-C11-C13-O
38	13	317	A86	C12-C11-C13-O
38	31	316	A86	C12-C11-C13-O
38	32	304	A86	C12-C11-C13-O
38	33	302	A86	C12-C11-C13-O

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Mol	Chain	Res	Type	Atoms
38	34	303	A86	C12-C11-C13-O
33	W	101	LMG	C34-C35-C36-C37
30	B	620	SQD	C12-C13-C14-C15
30	b	620	SQD	C12-C13-C14-C15
27	31	315	CLA	C8-C10-C11-C12
27	34	302	CLA	C8-C10-C11-C12
33	w	101	LMG	C34-C35-C36-C37
27	11	304	CLA	CAA-CBA-CGA-O1A
27	13	306	CLA	CAA-CBA-CGA-O1A
27	14	306	CLA	CAA-CBA-CGA-O1A
27	33	306	CLA	CAA-CBA-CGA-O1A
27	33	306	CLA	CAA-CBA-CGA-O2A
27	34	307	CLA	CAA-CBA-CGA-O1A
27	34	307	CLA	CAA-CBA-CGA-O2A
27	B	605	CLA	C11-C10-C8-C9
27	C	505	CLA	C6-C7-C8-C9
27	b	605	CLA	C11-C10-C8-C9
27	c	505	CLA	C6-C7-C8-C9
35	j	101	DGD	O1A-C1A-O1G-C1G
27	11	304	CLA	CAA-CBA-CGA-O2A
27	12	308	CLA	CAA-CBA-CGA-O1A
27	31	304	CLA	CAA-CBA-CGA-O1A
27	32	308	CLA	CAA-CBA-CGA-O1A
27	11	315	CLA	C8-C10-C11-C12
27	13	301	CLA	C8-C10-C11-C12
27	14	302	CLA	C8-C10-C11-C12
27	32	303	CLA	C8-C10-C11-C12
28	a	403	PHO	C13-C15-C16-C17
27	12	308	CLA	CAA-CBA-CGA-O2A
27	13	306	CLA	CAA-CBA-CGA-O2A
27	14	306	CLA	CAA-CBA-CGA-O2A
27	31	304	CLA	CAA-CBA-CGA-O2A
27	32	308	CLA	CAA-CBA-CGA-O2A
37	E	101	HEM	CAA-CBA-CGA-O1A
37	f	102	HEM	CAA-CBA-CGA-O1A
27	C	514	CLA	C16-C17-C18-C20
35	c	518	DGD	C8B-C9B-CAB-CBB
27	c	509	CLA	O1A-CGA-O2A-C1
35	J	101	DGD	O1A-C1A-O1G-C1G
27	11	308	CLA	CAA-CBA-CGA-O1A
27	12	312	CLA	CAA-CBA-CGA-O1A
27	14	310	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
27	31	308	CLA	CAA-CBA-CGA-O1A
27	32	312	CLA	CAA-CBA-CGA-O1A
27	34	311	CLA	CAA-CBA-CGA-O1A
37	E	101	HEM	CAD-CBD-CGD-O1D
37	f	102	HEM	CAD-CBD-CGD-O1D
35	C	518	DGD	C8B-C9B-CAB-CBB
27	12	303	CLA	C8-C10-C11-C12
28	A	403	PHO	C13-C15-C16-C17
27	B	603	CLA	C1A-C2A-CAA-CBA
27	Z	102	CLA	C1A-C2A-CAA-CBA
27	b	603	CLA	C1A-C2A-CAA-CBA
27	z	102	CLA	C1A-C2A-CAA-CBA
27	11	302	CLA	C1A-C2A-CAA-CBA
27	12	306	CLA	C1A-C2A-CAA-CBA
27	13	304	CLA	C1A-C2A-CAA-CBA
27	14	304	CLA	C1A-C2A-CAA-CBA
27	31	302	CLA	C1A-C2A-CAA-CBA
27	32	306	CLA	C1A-C2A-CAA-CBA
27	33	304	CLA	C1A-C2A-CAA-CBA
27	34	305	CLA	C1A-C2A-CAA-CBA
38	11	316	A86	C10-C11-C13-O
38	12	304	A86	C10-C11-C13-O
38	13	302	A86	C10-C11-C13-O
38	13	317	A86	C10-C11-C13-O
38	31	316	A86	C10-C11-C13-O
38	32	304	A86	C10-C11-C13-O
38	33	302	A86	C10-C11-C13-O
38	34	303	A86	C10-C11-C13-O
27	c	514	CLA	C16-C17-C18-C20
27	33	310	CLA	CAA-CBA-CGA-O1A
35	C	517	DGD	C2A-C3A-C4A-C5A
35	c	517	DGD	C2A-C3A-C4A-C5A
27	C	509	CLA	O1A-CGA-O2A-C1
27	B	609	CLA	C2B-C3B-CAB-CBB
27	B	611	CLA	C2B-C3B-CAB-CBB
27	C	507	CLA	C2B-C3B-CAB-CBB
27	C	512	CLA	C2B-C3B-CAB-CBB
27	D	406	CLA	C2B-C3B-CAB-CBB
27	M	102	CLA	C2B-C3B-CAB-CBB
27	W	102	CLA	C2B-C3B-CAB-CBB
27	b	609	CLA	C2B-C3B-CAB-CBB
27	b	611	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
27	c	507	CLA	C2B-C3B-CAB-CBB
27	c	512	CLA	C2B-C3B-CAB-CBB
27	d	406	CLA	C2B-C3B-CAB-CBB
27	m	101	CLA	C2B-C3B-CAB-CBB
27	w	102	CLA	C2B-C3B-CAB-CBB
27	11	305	CLA	C2B-C3B-CAB-CBB
27	11	306	CLA	C2B-C3B-CAB-CBB
27	11	307	CLA	C2B-C3B-CAB-CBB
27	11	315	CLA	C2B-C3B-CAB-CBB
27	12	303	CLA	C2B-C3B-CAB-CBB
27	12	309	CLA	C2B-C3B-CAB-CBB
27	12	311	CLA	C2B-C3B-CAB-CBB
27	13	301	CLA	C2B-C3B-CAB-CBB
27	13	307	CLA	C2B-C3B-CAB-CBB
27	13	309	CLA	C2B-C3B-CAB-CBB
27	14	302	CLA	C2B-C3B-CAB-CBB
27	14	307	CLA	C2B-C3B-CAB-CBB
27	14	309	CLA	C2B-C3B-CAB-CBB
27	31	305	CLA	C2B-C3B-CAB-CBB
27	31	307	CLA	C2B-C3B-CAB-CBB
27	31	315	CLA	C2B-C3B-CAB-CBB
27	32	303	CLA	C2B-C3B-CAB-CBB
27	32	309	CLA	C2B-C3B-CAB-CBB
27	32	311	CLA	C2B-C3B-CAB-CBB
27	33	301	CLA	C2B-C3B-CAB-CBB
27	33	307	CLA	C2B-C3B-CAB-CBB
27	33	309	CLA	C2B-C3B-CAB-CBB
27	34	302	CLA	C2B-C3B-CAB-CBB
27	34	308	CLA	C2B-C3B-CAB-CBB
27	34	310	CLA	C2B-C3B-CAB-CBB
29	A	405	BCR	C5-C6-C7-C8
29	A	405	BCR	C23-C24-C25-C30
29	A	409	BCR	C23-C24-C25-C30
29	B	616	BCR	C5-C6-C7-C8
29	B	617	BCR	C5-C6-C7-C8
29	C	515	BCR	C23-C24-C25-C26
29	C	516	BCR	C5-C6-C7-C8
29	C	520	BCR	C5-C6-C7-C8
29	F	101	BCR	C23-C24-C25-C30
29	H	101	BCR	C5-C6-C7-C8
29	M	101	BCR	C23-C24-C25-C26
29	Z	101	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	Z	101	BCR	C5-C6-C7-C8
29	Z	101	BCR	C23-C24-C25-C30
29	a	405	BCR	C5-C6-C7-C8
29	a	405	BCR	C23-C24-C25-C30
29	a	409	BCR	C23-C24-C25-C30
29	b	616	BCR	C5-C6-C7-C8
29	b	617	BCR	C5-C6-C7-C8
29	c	515	BCR	C23-C24-C25-C26
29	c	516	BCR	C5-C6-C7-C8
29	c	519	BCR	C5-C6-C7-C8
29	f	101	BCR	C23-C24-C25-C30
29	h	101	BCR	C5-C6-C7-C8
29	m	103	BCR	C23-C24-C25-C26
29	z	101	BCR	C1-C6-C7-C8
29	z	101	BCR	C5-C6-C7-C8
29	z	101	BCR	C23-C24-C25-C30
27	13	310	CLA	CAA-CBA-CGA-O1A
37	f	102	HEM	CAA-CBA-CGA-O2A
32	L	101	LHG	C35-C36-C37-C38
32	l	102	LHG	C35-C36-C37-C38
37	E	101	HEM	CAA-CBA-CGA-O2A
36	D	407	PL9	C15-C14-C16-C17
36	d	407	PL9	C15-C14-C16-C17
27	W	102	CLA	C2-C3-C5-C6
27	w	102	CLA	C2-C3-C5-C6
27	C	510	CLA	C6-C7-C8-C10
27	W	102	CLA	C12-C13-C15-C16
27	W	103	CLA	C6-C7-C8-C10
27	c	510	CLA	C6-C7-C8-C10
27	w	102	CLA	C12-C13-C15-C16
27	w	103	CLA	C6-C7-C8-C10
27	C	511	CLA	C2A-CAA-CBA-CGA
27	c	511	CLA	C2A-CAA-CBA-CGA
35	j	101	DGD	C3B-C4B-C5B-C6B
32	b	621	LHG	C14-C15-C16-C17
35	J	101	DGD	C3B-C4B-C5B-C6B
32	B	621	LHG	C14-C15-C16-C17
33	D	408	LMG	C15-C16-C17-C18
27	B	615	CLA	C6-C7-C8-C9
27	b	615	CLA	C6-C7-C8-C9
27	11	307	CLA	C6-C7-C8-C9
27	12	311	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
27	13	309	CLA	C6-C7-C8-C9
27	14	309	CLA	C6-C7-C8-C9
27	31	307	CLA	C6-C7-C8-C9
27	32	311	CLA	C6-C7-C8-C9
27	33	309	CLA	C6-C7-C8-C9
27	34	310	CLA	C6-C7-C8-C9
33	d	408	LMG	C15-C16-C17-C18
32	L	101	LHG	C9-C10-C11-C12
33	B	618	LMG	C11-C12-C13-C14
33	b	618	LMG	C11-C12-C13-C14
32	l	102	LHG	C9-C10-C11-C12
33	C	519	LMG	C35-C36-C37-C38
37	E	101	HEM	CAD-CBD-CGD-O2D
37	f	102	HEM	CAD-CBD-CGD-O2D
33	q	301	LMG	C35-C36-C37-C38
27	C	504	CLA	C2-C3-C5-C6
27	c	504	CLA	C2-C3-C5-C6
27	12	303	CLA	CBD-CGD-O2D-CED
27	b	601	CLA	CBA-CGA-O2A-C1
27	B	601	CLA	O1A-CGA-O2A-C1
27	b	601	CLA	O1A-CGA-O2A-C1
33	B	619	LMG	C36-C37-C38-C39
33	b	619	LMG	C36-C37-C38-C39
35	H	102	DGD	C9B-CAB-CBB-CCB
35	h	102	DGD	C9B-CAB-CBB-CCB
35	H	102	DGD	C1G-C2G-C3G-O3G
35	h	102	DGD	C1G-C2G-C3G-O3G
36	D	407	PL9	C39-C41-C42-C43
36	d	407	PL9	C39-C41-C42-C43
30	l	101	SQD	C9-C10-C11-C12
27	Z	102	CLA	C2A-CAA-CBA-CGA
27	z	102	CLA	C2A-CAA-CBA-CGA
30	L	103	SQD	C9-C10-C11-C12
27	31	315	CLA	CBD-CGD-O2D-CED
33	12	301	LMG	C31-C32-C33-C34
27	B	601	CLA	CBA-CGA-O2A-C1
27	B	604	CLA	C4-C3-C5-C6
27	b	604	CLA	C4-C3-C5-C6
33	B	618	LMG	C34-C35-C36-C37
27	34	302	CLA	CBD-CGD-O2D-CED
35	C	518	DGD	CCB-CDB-CEB-CFB
35	c	518	DGD	CCB-CDB-CEB-CFB

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Mol	Chain	Res	Type	Atoms
27	B	603	CLA	C4B-C3B-CAB-CBB
27	b	603	CLA	C4B-C3B-CAB-CBB
27	A	404	CLA	O1A-CGA-O2A-C1
27	a	404	CLA	O1A-CGA-O2A-C1
30	L	103	SQD	C19-C20-C21-C22
33	b	618	LMG	C34-C35-C36-C37
27	32	303	CLA	CBD-CGD-O2D-CED
27	33	301	CLA	CBD-CGD-O2D-CED
28	D	403	PHO	CAA-CBA-CGA-O2A
28	d	403	PHO	CAA-CBA-CGA-O2A
30	l	101	SQD	C19-C20-C21-C22
27	11	315	CLA	CBD-CGD-O2D-CED
27	13	301	CLA	CBD-CGD-O2D-CED
28	D	403	PHO	CHA-CBD-CGD-O1D
28	d	403	PHO	CHA-CBD-CGD-O1D
29	Z	101	BCR	C16-C17-C18-C36
29	z	101	BCR	C16-C17-C18-C36
27	14	302	CLA	CBD-CGD-O2D-CED
36	D	404	PL9	C30-C29-C31-C32
36	d	404	PL9	C30-C29-C31-C32
27	11	307	CLA	C6-C7-C8-C10
27	12	311	CLA	C6-C7-C8-C10
27	13	309	CLA	C6-C7-C8-C10
27	14	309	CLA	C6-C7-C8-C10
27	31	307	CLA	C6-C7-C8-C10
27	32	311	CLA	C6-C7-C8-C10
27	33	309	CLA	C6-C7-C8-C10
27	34	310	CLA	C6-C7-C8-C10
29	M	101	BCR	C19-C20-C21-C22
29	m	103	BCR	C19-C20-C21-C22
33	D	408	LMG	C28-C29-C30-C31
33	d	408	LMG	C28-C29-C30-C31
33	C	519	LMG	C16-C17-C18-C19
33	q	301	LMG	C16-C17-C18-C19
27	b	608	CLA	O1D-CGD-O2D-CED
27	C	504	CLA	C6-C7-C8-C9
27	c	504	CLA	C6-C7-C8-C9
30	A	406	SQD	C5-C6-S-O8
30	a	406	SQD	C5-C6-S-O8
33	M	103	LMG	C8-C7-O1-C1
33	m	102	LMG	C8-C7-O1-C1
27	A	404	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	a	404	CLA	CBA-CGA-O2A-C1
27	11	308	CLA	CAA-CBA-CGA-O2A
27	12	312	CLA	CAA-CBA-CGA-O2A
27	13	310	CLA	CAA-CBA-CGA-O2A
27	14	308	CLA	CAA-CBA-CGA-O2A
27	14	310	CLA	CAA-CBA-CGA-O2A
27	31	308	CLA	CAA-CBA-CGA-O2A
27	32	312	CLA	CAA-CBA-CGA-O2A
27	33	308	CLA	CAA-CBA-CGA-O2A
27	33	310	CLA	CAA-CBA-CGA-O2A
27	34	311	CLA	CAA-CBA-CGA-O2A
27	B	605	CLA	C13-C15-C16-C17
27	b	605	CLA	C13-C15-C16-C17
27	11	306	CLA	CAA-CBA-CGA-O2A
27	12	310	CLA	CAA-CBA-CGA-O2A
27	13	308	CLA	CAA-CBA-CGA-O2A
27	31	306	CLA	CAA-CBA-CGA-O2A
27	32	310	CLA	CAA-CBA-CGA-O2A
27	34	309	CLA	CAA-CBA-CGA-O2A
28	D	403	PHO	O1D-CGD-O2D-CED
28	d	403	PHO	O1D-CGD-O2D-CED
27	B	622	CLA	CBA-CGA-O2A-C1
27	B	608	CLA	O1D-CGD-O2D-CED
36	D	404	PL9	C32-C33-C34-C36
36	d	404	PL9	C32-C33-C34-C36
29	F	101	BCR	C11-C10-C9-C8
29	f	101	BCR	C11-C10-C9-C8
35	H	102	DGD	C4B-C5B-C6B-C7B
27	12	310	CLA	CAA-CBA-CGA-O1A
27	13	308	CLA	CAA-CBA-CGA-O1A
35	h	102	DGD	C4B-C5B-C6B-C7B
27	C	505	CLA	C5-C6-C7-C8
27	11	306	CLA	CAA-CBA-CGA-O1A
27	14	308	CLA	CAA-CBA-CGA-O1A
27	31	306	CLA	CAA-CBA-CGA-O1A
27	32	310	CLA	CAA-CBA-CGA-O1A
27	33	308	CLA	CAA-CBA-CGA-O1A
27	34	309	CLA	CAA-CBA-CGA-O1A
27	c	505	CLA	C5-C6-C7-C8
33	w	101	LMG	C39-C40-C41-C42
33	w	101	LMG	O10-C28-O8-C9
32	b	621	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
33	W	101	LMG	C39-C40-C41-C42
27	b	622	CLA	CBA-CGA-O2A-C1
32	B	621	LHG	C10-C11-C12-C13
27	B	608	CLA	C4-C3-C5-C6
27	b	608	CLA	C4-C3-C5-C6
32	A	408	LHG	C16-C17-C18-C19
32	a	408	LHG	C16-C17-C18-C19
30	B	620	SQD	C24-C25-C26-C27
27	11	301	CLA	C8-C10-C11-C12
27	B	601	CLA	C14-C13-C15-C16
27	B	602	CLA	C6-C7-C8-C9
27	B	615	CLA	C14-C13-C15-C16
27	Z	102	CLA	C11-C10-C8-C9
27	b	601	CLA	C14-C13-C15-C16
27	b	602	CLA	C6-C7-C8-C9
27	b	615	CLA	C14-C13-C15-C16
27	z	102	CLA	C11-C10-C8-C9
27	14	303	CLA	C8-C10-C11-C12
27	31	301	CLA	C8-C10-C11-C12
27	32	305	CLA	C8-C10-C11-C12
33	W	101	LMG	O10-C28-O8-C9
30	b	620	SQD	C24-C25-C26-C27
29	A	409	BCR	C17-C18-C19-C20
29	a	409	BCR	C17-C18-C19-C20
27	13	303	CLA	C8-C10-C11-C12
27	33	303	CLA	C8-C10-C11-C12
27	c	513	CLA	C15-C16-C17-C18
27	12	305	CLA	C8-C10-C11-C12
27	34	304	CLA	C8-C10-C11-C12
35	J	101	DGD	O1G-C1A-C2A-C3A
35	j	101	DGD	O1G-C1A-C2A-C3A
27	B	605	CLA	C2A-CAA-CBA-CGA
27	b	605	CLA	C2A-CAA-CBA-CGA
27	B	604	CLA	C11-C10-C8-C7
27	B	604	CLA	C11-C12-C13-C15
27	B	610	CLA	C11-C10-C8-C7
27	C	508	CLA	C11-C10-C8-C7
27	b	604	CLA	C11-C10-C8-C7
27	b	604	CLA	C11-C12-C13-C15
27	b	610	CLA	C11-C10-C8-C7
27	c	508	CLA	C11-C10-C8-C7
27	C	513	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
27	B	603	CLA	C2B-C3B-CAB-CBB
27	b	603	CLA	C2B-C3B-CAB-CBB
27	11	301	CLA	C2B-C3B-CAB-CBB
27	11	303	CLA	C2B-C3B-CAB-CBB
27	12	305	CLA	C2B-C3B-CAB-CBB
27	12	307	CLA	C2B-C3B-CAB-CBB
27	12	310	CLA	C2B-C3B-CAB-CBB
27	13	303	CLA	C2B-C3B-CAB-CBB
27	13	305	CLA	C2B-C3B-CAB-CBB
27	13	308	CLA	C2B-C3B-CAB-CBB
27	14	303	CLA	C2B-C3B-CAB-CBB
27	14	305	CLA	C2B-C3B-CAB-CBB
27	14	308	CLA	C2B-C3B-CAB-CBB
27	31	301	CLA	C2B-C3B-CAB-CBB
27	31	303	CLA	C2B-C3B-CAB-CBB
27	31	306	CLA	C2B-C3B-CAB-CBB
27	32	305	CLA	C2B-C3B-CAB-CBB
27	32	307	CLA	C2B-C3B-CAB-CBB
27	32	310	CLA	C2B-C3B-CAB-CBB
27	33	303	CLA	C2B-C3B-CAB-CBB
27	33	305	CLA	C2B-C3B-CAB-CBB
27	33	308	CLA	C2B-C3B-CAB-CBB
27	34	304	CLA	C2B-C3B-CAB-CBB
27	34	306	CLA	C2B-C3B-CAB-CBB
27	34	309	CLA	C2B-C3B-CAB-CBB
29	A	405	BCR	C23-C24-C25-C26
29	A	409	BCR	C23-C24-C25-C26
29	B	616	BCR	C23-C24-C25-C26
29	B	617	BCR	C23-C24-C25-C26
29	F	101	BCR	C23-C24-C25-C26
29	H	101	BCR	C23-C24-C25-C26
29	H	101	BCR	C23-C24-C25-C30
29	Z	101	BCR	C23-C24-C25-C26
29	a	405	BCR	C23-C24-C25-C26
29	a	409	BCR	C23-C24-C25-C26
29	b	616	BCR	C23-C24-C25-C26
29	b	617	BCR	C23-C24-C25-C26
29	f	101	BCR	C23-C24-C25-C26
29	h	101	BCR	C23-C24-C25-C26
29	h	101	BCR	C23-C24-C25-C30
29	z	101	BCR	C23-C24-C25-C26
35	C	518	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
35	c	518	DGD	O1B-C1B-O2G-C2G
27	A	402	CLA	C2-C1-O2A-CGA
27	A	404	CLA	C2-C1-O2A-CGA
27	B	615	CLA	C2-C1-O2A-CGA
27	C	511	CLA	C2-C1-O2A-CGA
27	a	402	CLA	C2-C1-O2A-CGA
27	a	404	CLA	C2-C1-O2A-CGA
27	b	615	CLA	C2-C1-O2A-CGA
27	c	511	CLA	C2-C1-O2A-CGA
27	C	509	CLA	C3-C5-C6-C7
36	D	407	PL9	C29-C31-C32-C33
36	d	407	PL9	C29-C31-C32-C33
27	c	509	CLA	C3-C5-C6-C7
27	C	502	CLA	CAA-CBA-CGA-O2A
27	c	502	CLA	CAA-CBA-CGA-O2A
27	w	103	CLA	CAA-CBA-CGA-O2A
33	d	408	LMG	C16-C17-C18-C19
27	11	305	CLA	C2A-CAA-CBA-CGA
27	12	309	CLA	C2A-CAA-CBA-CGA
27	13	307	CLA	C2A-CAA-CBA-CGA
27	14	307	CLA	C2A-CAA-CBA-CGA
27	31	305	CLA	C2A-CAA-CBA-CGA
27	32	309	CLA	C2A-CAA-CBA-CGA
27	33	307	CLA	C2A-CAA-CBA-CGA
27	34	308	CLA	C2A-CAA-CBA-CGA
28	D	403	PHO	CBD-CGD-O2D-CED
28	d	403	PHO	CBD-CGD-O2D-CED
27	D	402	CLA	C4C-C3C-CAC-CBC
27	d	402	CLA	C4C-C3C-CAC-CBC
33	D	408	LMG	C16-C17-C18-C19
27	W	103	CLA	CAA-CBA-CGA-O2A
36	D	407	PL9	C4-C3-C7-C8
36	d	407	PL9	C4-C3-C7-C8
32	l	102	LHG	C11-C12-C13-C14
32	L	101	LHG	C11-C12-C13-C14
27	A	404	CLA	CAA-CBA-CGA-O2A
27	a	404	CLA	CAA-CBA-CGA-O2A
35	h	102	DGD	CDB-CEB-CFB-CGB
27	B	611	CLA	C2A-CAA-CBA-CGA
27	b	611	CLA	C2A-CAA-CBA-CGA
35	H	102	DGD	CDB-CEB-CFB-CGB
27	b	605	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	A	406	SQD	C30-C31-C32-C33
30	a	406	SQD	C30-C31-C32-C33
32	l	103	LHG	C11-C10-C9-C8
28	D	403	PHO	C8-C10-C11-C12
28	d	403	PHO	C8-C10-C11-C12
38	12	316	A86	C-C1-C24-C25
38	34	315	A86	C-C1-C24-C25
32	L	102	LHG	C11-C10-C9-C8
27	C	506	CLA	C10-C11-C12-C13
27	C	507	CLA	C4B-C3B-CAB-CBB
27	M	102	CLA	C4B-C3B-CAB-CBB
27	c	507	CLA	C4B-C3B-CAB-CBB
27	m	101	CLA	C4B-C3B-CAB-CBB
27	11	305	CLA	C4B-C3B-CAB-CBB
27	11	307	CLA	C4B-C3B-CAB-CBB
27	12	309	CLA	C4B-C3B-CAB-CBB
27	12	311	CLA	C4B-C3B-CAB-CBB
27	13	307	CLA	C4B-C3B-CAB-CBB
27	13	309	CLA	C4B-C3B-CAB-CBB
27	14	307	CLA	C4B-C3B-CAB-CBB
27	14	309	CLA	C4B-C3B-CAB-CBB
27	31	305	CLA	C4B-C3B-CAB-CBB
27	31	307	CLA	C4B-C3B-CAB-CBB
27	32	309	CLA	C4B-C3B-CAB-CBB
27	32	311	CLA	C4B-C3B-CAB-CBB
27	33	307	CLA	C4B-C3B-CAB-CBB
27	33	309	CLA	C4B-C3B-CAB-CBB
27	34	308	CLA	C4B-C3B-CAB-CBB
27	34	310	CLA	C4B-C3B-CAB-CBB
27	B	605	CLA	CBA-CGA-O2A-C1
36	D	407	PL9	C12-C11-C9-C10
36	d	407	PL9	C12-C11-C9-C10
27	B	605	CLA	C10-C11-C12-C13
27	b	605	CLA	C10-C11-C12-C13
27	c	506	CLA	C10-C11-C12-C13
33	B	619	LMG	O6-C1-O1-C7
33	C	519	LMG	O6-C1-O1-C7
33	b	619	LMG	O6-C1-O1-C7
33	q	301	LMG	O6-C1-O1-C7
35	C	518	DGD	O1G-C1G-C2G-O2G
35	c	518	DGD	O1G-C1G-C2G-O2G
38	11	314	A86	C5-C6-C8-C9

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Mol	Chain	Res	Type	Atoms
38	13	316	A86	C5-C6-C8-C9
38	14	301	A86	C5-C6-C8-C9
38	14	316	A86	C5-C6-C8-C9
38	31	314	A86	C5-C6-C8-C9
38	32	318	A86	C5-C6-C8-C9
38	33	316	A86	C5-C6-C8-C9
38	34	301	A86	C5-C6-C8-C9
29	Z	101	BCR	C19-C20-C21-C22
29	z	101	BCR	C19-C20-C21-C22
30	A	406	SQD	C35-C36-C37-C38
30	a	406	SQD	C35-C36-C37-C38
27	d	401	CLA	CBD-CGD-O2D-CED
32	B	621	LHG	C11-C12-C13-C14
32	a	408	LHG	C18-C19-C20-C21
32	A	408	LHG	C18-C19-C20-C21
32	L	102	LHG	C17-C18-C19-C20
32	b	621	LHG	C11-C12-C13-C14
33	B	618	LMG	C37-C38-C39-C40
27	B	610	CLA	C2-C1-O2A-CGA
27	b	610	CLA	C2-C1-O2A-CGA
33	b	618	LMG	C37-C38-C39-C40
27	A	402	CLA	C11-C10-C8-C7
27	B	610	CLA	C11-C12-C13-C15
27	a	402	CLA	C11-C10-C8-C7
27	b	610	CLA	C11-C12-C13-C15
33	C	519	LMG	C39-C40-C41-C42
32	l	103	LHG	C17-C18-C19-C20
33	q	301	LMG	C39-C40-C41-C42
27	B	607	CLA	C10-C11-C12-C13
27	b	607	CLA	C10-C11-C12-C13
33	32	301	LMG	C31-C32-C33-C34
32	L	101	LHG	C16-C17-C18-C19
32	l	102	LHG	C16-C17-C18-C19
32	l	102	LHG	C34-C35-C36-C37
32	L	101	LHG	C34-C35-C36-C37
27	12	313	CLA	CAA-CBA-CGA-O1A
27	32	313	CLA	CAA-CBA-CGA-O1A
27	D	401	CLA	CBD-CGD-O2D-CED
27	C	502	CLA	C3A-C2A-CAA-CBA
27	Z	102	CLA	C3A-C2A-CAA-CBA
27	c	502	CLA	C3A-C2A-CAA-CBA
27	z	102	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	11	302	CLA	C3A-C2A-CAA-CBA
27	12	306	CLA	C3A-C2A-CAA-CBA
27	13	304	CLA	C3A-C2A-CAA-CBA
27	14	304	CLA	C3A-C2A-CAA-CBA
27	31	302	CLA	C3A-C2A-CAA-CBA
27	32	306	CLA	C3A-C2A-CAA-CBA
27	33	304	CLA	C3A-C2A-CAA-CBA
27	34	305	CLA	C3A-C2A-CAA-CBA
27	13	311	CLA	CAA-CBA-CGA-O1A
27	31	309	CLA	CAA-CBA-CGA-O1A
27	33	311	CLA	CAA-CBA-CGA-O1A
27	34	312	CLA	CAA-CBA-CGA-O1A
33	M	103	LMG	C8-C9-O8-C28
27	W	103	CLA	CAA-CBA-CGA-O1A
27	w	103	CLA	CAA-CBA-CGA-O1A
35	j	101	DGD	CCA-CDA-CEA-CFA
27	b	607	CLA	C8-C10-C11-C12
35	C	518	DGD	CCA-CDA-CEA-CFA
35	J	101	DGD	CCA-CDA-CEA-CFA
27	11	309	CLA	CAA-CBA-CGA-O1A
27	14	311	CLA	CAA-CBA-CGA-O1A
35	c	518	DGD	CCA-CDA-CEA-CFA
27	B	607	CLA	C8-C10-C11-C12
33	12	301	LMG	C16-C17-C18-C19
27	C	508	CLA	C11-C10-C8-C9
27	c	508	CLA	C11-C10-C8-C9
33	C	519	LMG	C34-C35-C36-C37
33	q	301	LMG	C34-C35-C36-C37
33	m	102	LMG	C8-C9-O8-C28
38	13	314	A86	C-C1-C24-C25
36	D	404	PL9	C12-C11-C9-C8
36	d	404	PL9	C12-C11-C9-C8
27	B	602	CLA	C13-C15-C16-C17
27	b	602	CLA	C13-C15-C16-C17
27	B	605	CLA	O1A-CGA-O2A-C1
27	C	502	CLA	CAA-CBA-CGA-O1A
27	c	502	CLA	CAA-CBA-CGA-O1A
35	C	518	DGD	C2G-C3G-O3G-C1D
35	c	518	DGD	C2G-C3G-O3G-C1D
27	b	605	CLA	O1A-CGA-O2A-C1
33	b	619	LMG	C20-C21-C22-C23
27	c	508	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
33	B	619	LMG	C20-C21-C22-C23
38	11	312	A86	C12-C11-C13-O
38	12	316	A86	C12-C11-C13-O
38	13	314	A86	C12-C11-C13-O
38	14	314	A86	C12-C11-C13-O
38	31	312	A86	C12-C11-C13-O
38	32	316	A86	C12-C11-C13-O
38	33	314	A86	C12-C11-C13-O
38	34	315	A86	C12-C11-C13-O
27	C	508	CLA	CAA-CBA-CGA-O2A
27	W	102	CLA	CAD-CBD-CGD-O2D
27	W	103	CLA	CAD-CBD-CGD-O2D
27	w	102	CLA	CAD-CBD-CGD-O2D
27	w	103	CLA	CAD-CBD-CGD-O2D
27	11	306	CLA	CAD-CBD-CGD-O2D
27	12	310	CLA	CAD-CBD-CGD-O2D
27	13	308	CLA	CAD-CBD-CGD-O2D
27	14	308	CLA	CAD-CBD-CGD-O2D
27	31	306	CLA	CAD-CBD-CGD-O2D
27	32	310	CLA	CAD-CBD-CGD-O2D
27	33	308	CLA	CAD-CBD-CGD-O2D
27	34	309	CLA	CAD-CBD-CGD-O2D
27	C	504	CLA	C3-C5-C6-C7
27	a	404	CLA	CAA-CBA-CGA-O1A
29	H	101	BCR	C22-C23-C24-C25
29	h	101	BCR	C22-C23-C24-C25
27	C	506	CLA	C2-C1-O2A-CGA
27	A	404	CLA	CAA-CBA-CGA-O1A
27	c	504	CLA	C3-C5-C6-C7
27	C	508	CLA	CAA-CBA-CGA-O1A
27	c	508	CLA	CAA-CBA-CGA-O1A
27	B	622	CLA	C10-C11-C12-C13
27	c	511	CLA	CAA-CBA-CGA-O2A
33	d	408	LMG	O9-C10-C11-C12
27	Z	102	CLA	CAA-CBA-CGA-O2A
27	z	102	CLA	CAA-CBA-CGA-O2A
33	D	408	LMG	O9-C10-C11-C12
35	C	517	DGD	O1B-C1B-C2B-C3B
35	c	517	DGD	O1B-C1B-C2B-C3B

There are no ring outliers.

251 monomers are involved in 639 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	b	601	CLA	3	0
27	b	613	CLA	4	0
27	32	308	CLA	3	0
27	34	310	CLA	2	0
27	B	605	CLA	2	0
27	d	402	CLA	3	0
33	C	519	LMG	2	0
29	Z	101	BCR	2	0
38	32	315	A86	9	0
27	11	302	CLA	2	0
27	c	509	CLA	6	0
27	B	603	CLA	1	0
27	C	506	CLA	1	0
27	c	513	CLA	3	0
27	B	609	CLA	2	0
27	11	315	CLA	4	0
29	B	617	BCR	2	0
38	31	312	A86	4	0
38	33	302	A86	10	0
29	C	515	BCR	2	0
33	m	102	LMG	3	0
27	33	309	CLA	2	0
27	B	610	CLA	2	0
27	34	305	CLA	1	0
27	d	405	CLA	7	0
28	d	403	PHO	2	0
27	b	622	CLA	2	0
27	32	311	CLA	2	0
29	b	616	BCR	2	0
27	C	509	CLA	6	0
27	11	301	CLA	8	0
27	b	607	CLA	2	0
38	34	314	A86	9	0
27	14	302	CLA	3	0
33	b	618	LMG	3	0
33	q	301	LMG	1	0
27	B	613	CLA	2	0
38	13	314	A86	2	0
38	31	314	A86	2	0
27	c	512	CLA	2	0
33	d	408	LMG	1	0
27	32	303	CLA	4	0
27	13	308	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	b	614	CLA	5	0
38	33	314	A86	3	0
27	32	312	CLA	1	0
38	11	313	A86	5	0
27	13	305	CLA	3	0
27	11	307	CLA	2	0
27	c	502	CLA	4	0
27	d	401	CLA	4	0
29	C	516	BCR	3	0
27	M	102	CLA	1	0
27	14	303	CLA	7	0
27	D	402	CLA	2	0
33	b	619	LMG	1	0
38	13	317	A86	6	0
34	c	501	OEX	1	0
38	14	314	A86	4	0
27	32	310	CLA	2	0
27	33	304	CLA	2	0
35	h	102	DGD	3	0
29	c	519	BCR	2	0
29	B	623	BCR	2	0
27	B	601	CLA	6	0
27	11	303	CLA	3	0
27	14	308	CLA	1	0
27	31	315	CLA	3	0
27	w	103	CLA	2	0
38	32	318	A86	2	0
27	31	308	CLA	1	0
27	11	306	CLA	1	0
27	33	303	CLA	11	0
38	34	301	A86	3	0
27	32	309	CLA	1	0
27	D	405	CLA	5	0
30	b	620	SQD	1	0
38	32	304	A86	7	0
27	32	306	CLA	2	0
27	c	508	CLA	2	0
27	12	309	CLA	2	0
31	a	407	BCT	1	0
27	31	307	CLA	2	0
27	34	304	CLA	9	0
27	13	304	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	13	303	CLA	9	0
38	32	316	A86	4	0
27	31	305	CLA	2	0
27	B	608	CLA	2	0
33	B	618	LMG	4	0
27	13	310	CLA	1	0
27	C	508	CLA	2	0
27	c	510	CLA	3	0
27	B	612	CLA	4	0
27	C	514	CLA	3	0
38	12	315	A86	9	0
36	d	407	PL9	4	0
27	12	305	CLA	9	0
27	11	308	CLA	1	0
27	b	604	CLA	7	0
38	14	316	A86	2	0
27	33	310	CLA	1	0
27	A	404	CLA	7	0
27	13	307	CLA	2	0
27	11	305	CLA	2	0
27	B	611	CLA	3	0
27	12	307	CLA	3	0
32	l	103	LHG	1	0
34	C	501	OEX	1	0
37	f	102	HEM	2	0
38	31	316	A86	9	0
27	C	507	CLA	6	0
27	m	101	CLA	2	0
27	B	606	CLA	3	0
27	13	309	CLA	2	0
33	B	619	LMG	2	0
27	W	103	CLA	3	0
38	31	311	A86	9	0
27	b	608	CLA	2	0
27	Z	102	CLA	2	0
27	12	311	CLA	2	0
27	z	102	CLA	2	0
27	34	306	CLA	3	0
27	b	610	CLA	2	0
37	v	201	HEM	2	0
27	12	306	CLA	1	0
27	C	511	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	32	317	A86	3	0
27	C	504	CLA	3	0
27	B	607	CLA	3	0
27	a	402	CLA	1	0
27	b	612	CLA	4	0
38	13	315	A86	5	0
27	11	304	CLA	2	0
27	33	308	CLA	1	0
27	34	309	CLA	1	0
38	13	316	A86	3	0
27	31	304	CLA	2	0
35	H	102	DGD	5	0
27	12	303	CLA	5	0
38	33	315	A86	5	0
38	33	313	A86	9	0
38	33	316	A86	2	0
27	12	310	CLA	2	0
27	B	614	CLA	4	0
29	M	101	BCR	2	0
27	d	406	CLA	1	0
38	13	302	A86	9	0
27	D	401	CLA	4	0
29	m	103	BCR	3	0
38	14	315	A86	5	0
38	14	313	A86	9	0
27	C	502	CLA	2	0
27	14	307	CLA	2	0
33	M	103	LMG	2	0
27	C	505	CLA	1	0
27	31	306	CLA	1	0
32	A	408	LHG	6	0
29	a	405	BCR	1	0
27	w	102	CLA	3	0
29	f	101	BCR	2	0
38	31	313	A86	5	0
27	12	312	CLA	1	0
30	l	101	SQD	3	0
29	H	101	BCR	3	0
29	A	409	BCR	2	0
38	12	304	A86	7	0
33	12	301	LMG	3	0
32	a	408	LHG	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	32	301	LMG	3	0
27	b	602	CLA	6	0
27	D	406	CLA	1	0
27	33	306	CLA	2	0
37	E	101	HEM	2	0
38	11	316	A86	10	0
27	32	305	CLA	8	0
27	c	511	CLA	4	0
27	34	311	CLA	1	0
27	c	504	CLA	2	0
27	32	307	CLA	3	0
27	b	611	CLA	2	0
27	C	503	CLA	3	0
27	34	308	CLA	2	0
29	C	520	BCR	1	0
29	a	409	BCR	1	0
31	A	407	BCT	1	0
27	31	302	CLA	2	0
27	b	609	CLA	2	0
29	b	617	BCR	3	0
29	c	515	BCR	4	0
36	D	404	PL9	3	0
27	31	303	CLA	3	0
27	c	507	CLA	5	0
29	h	101	BCR	3	0
27	a	404	CLA	6	0
29	c	516	BCR	2	0
38	11	312	A86	3	0
38	34	315	A86	3	0
29	b	623	BCR	1	0
27	C	513	CLA	4	0
27	c	503	CLA	3	0
28	D	403	PHO	2	0
38	34	316	A86	4	0
33	W	101	LMG	4	0
27	b	615	CLA	3	0
29	F	101	BCR	2	0
32	L	102	LHG	1	0
38	12	316	A86	4	0
27	13	301	CLA	3	0
27	31	301	CLA	9	0
38	11	311	A86	9	0

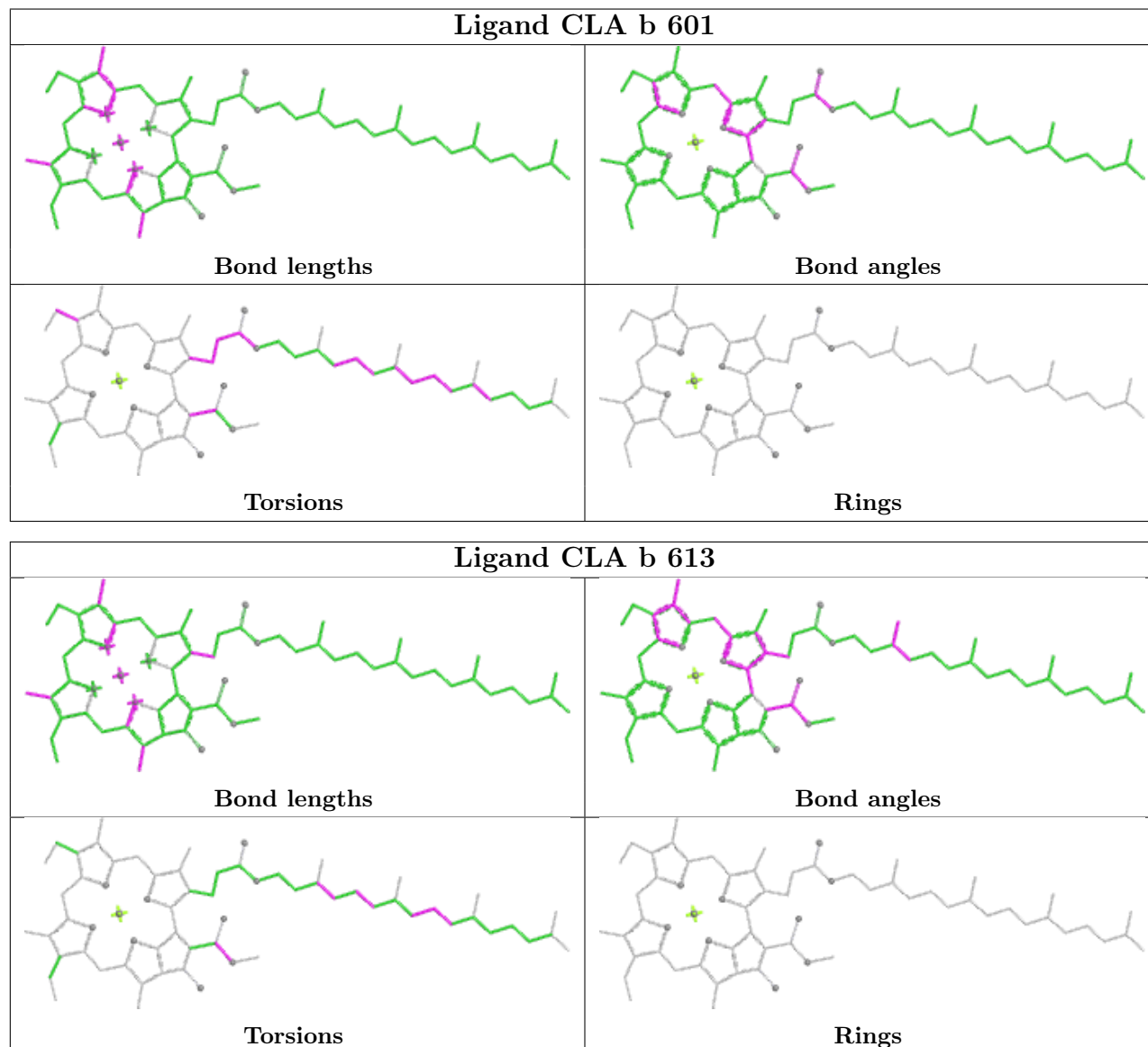
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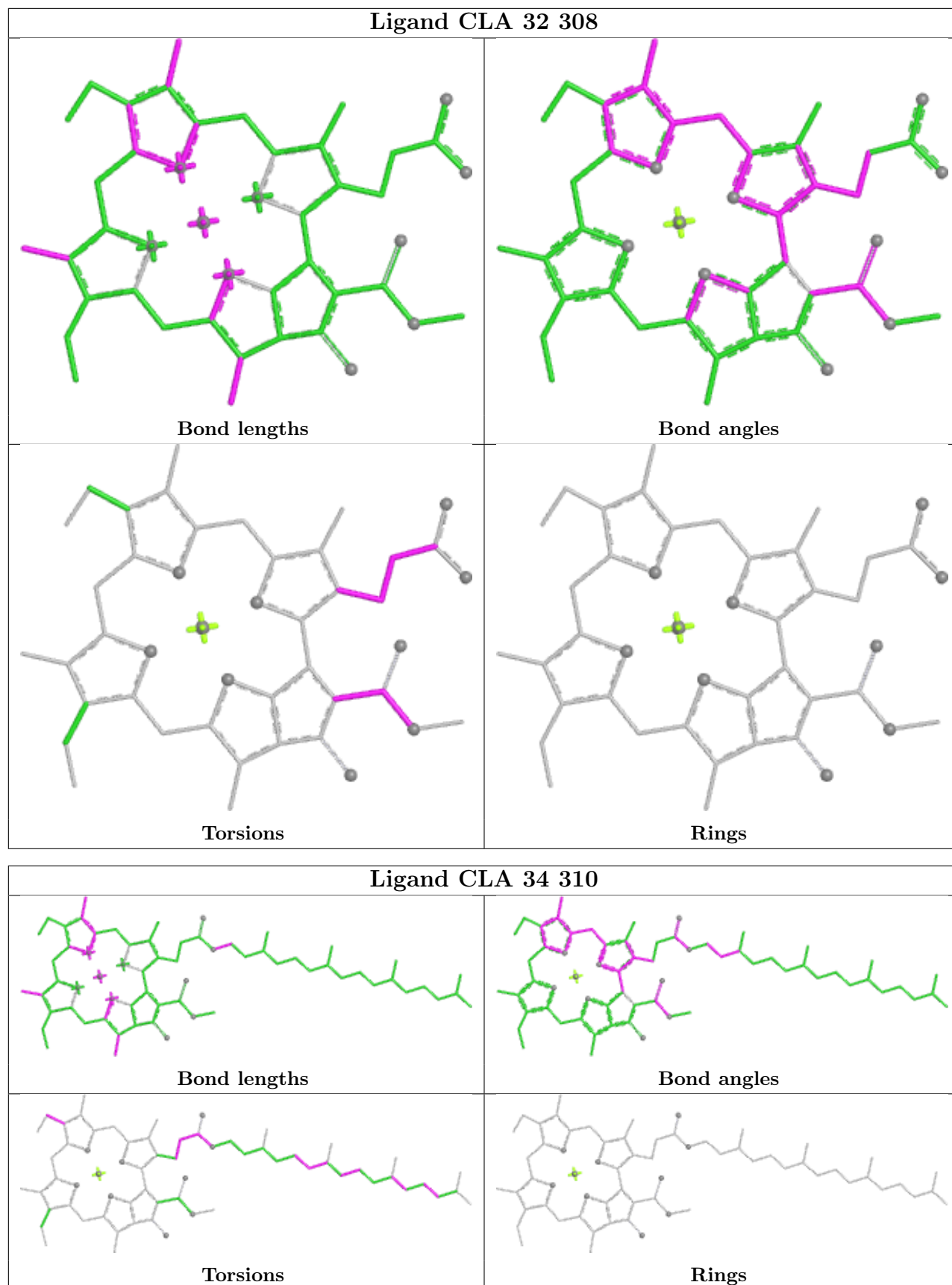
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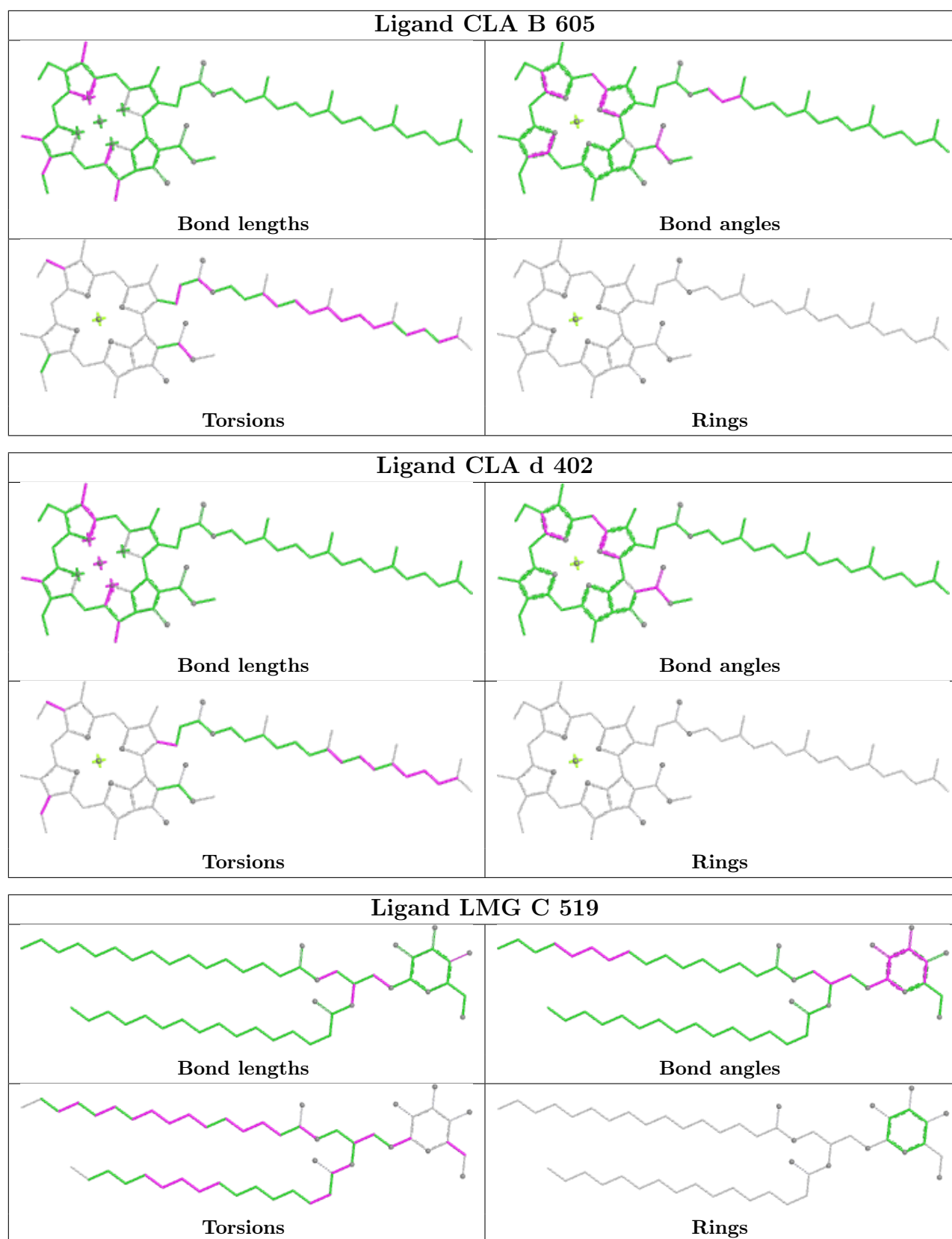
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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33	w	101	LMG	4	0
27	12	308	CLA	3	0
27	14	310	CLA	1	0
27	b	605	CLA	3	0
32	l	102	LHG	3	0
37	V	201	HEM	2	0
27	33	301	CLA	5	0
33	D	408	LMG	1	0
35	j	101	DGD	2	0
27	33	305	CLA	3	0
38	11	314	A86	3	0
36	d	404	PL9	2	0
38	34	303	A86	7	0
27	b	603	CLA	1	0
38	14	301	A86	3	0
27	B	602	CLA	7	0
27	W	102	CLA	4	0
27	b	606	CLA	4	0
27	C	512	CLA	1	0
27	c	505	CLA	2	0
30	L	103	SQD	3	0
32	L	101	LHG	6	0
38	12	317	A86	5	0
27	14	305	CLA	3	0
27	14	304	CLA	2	0
27	C	510	CLA	2	0
27	B	604	CLA	4	0
27	c	514	CLA	3	0
27	A	402	CLA	1	0
27	13	306	CLA	1	0
27	B	615	CLA	4	0
27	14	309	CLA	2	0
27	33	307	CLA	2	0
27	34	302	CLA	4	0
29	z	101	BCR	2	0
36	D	407	PL9	4	0
27	B	622	CLA	2	0
29	B	616	BCR	3	0
38	13	313	A86	9	0

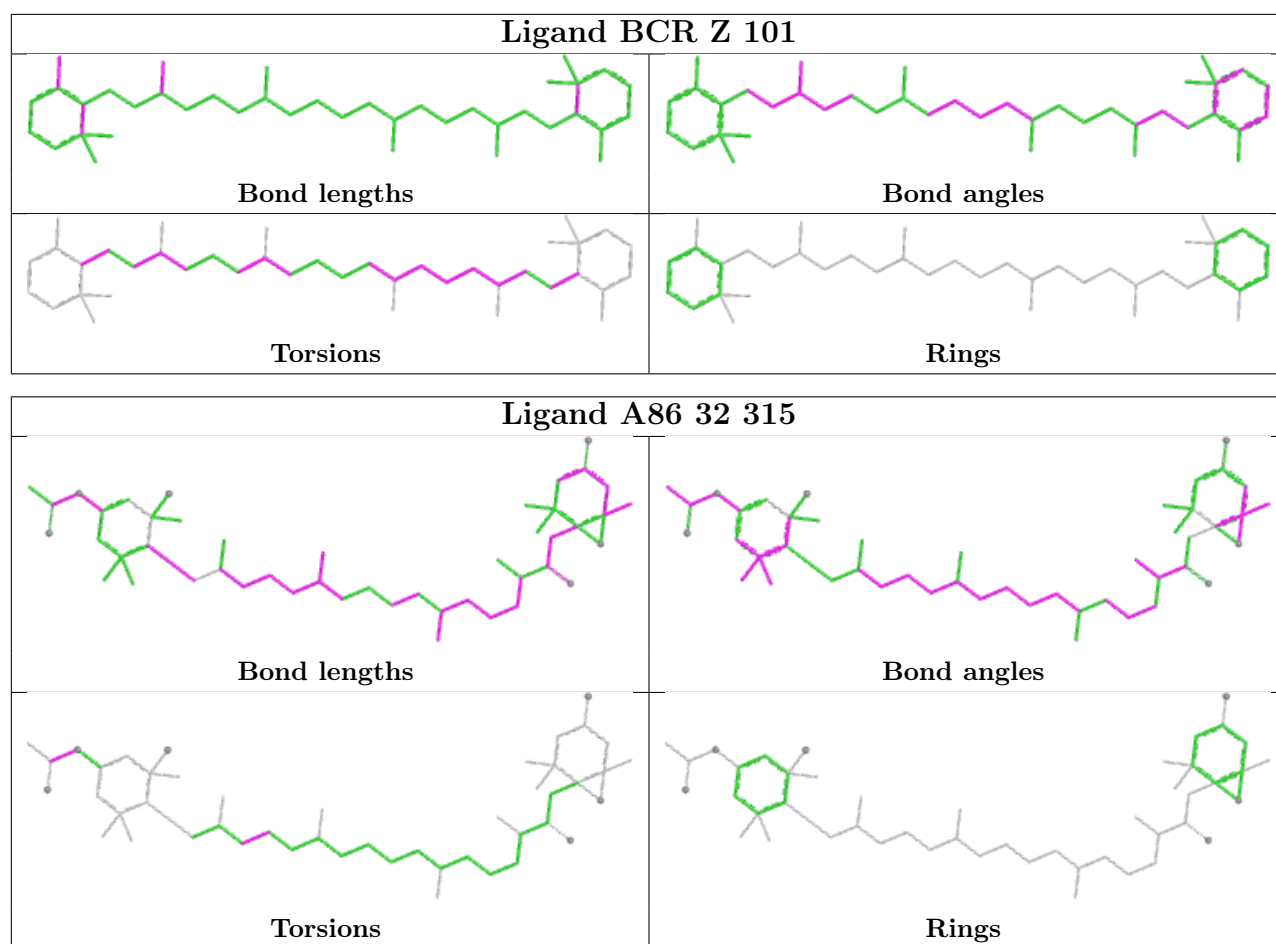
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

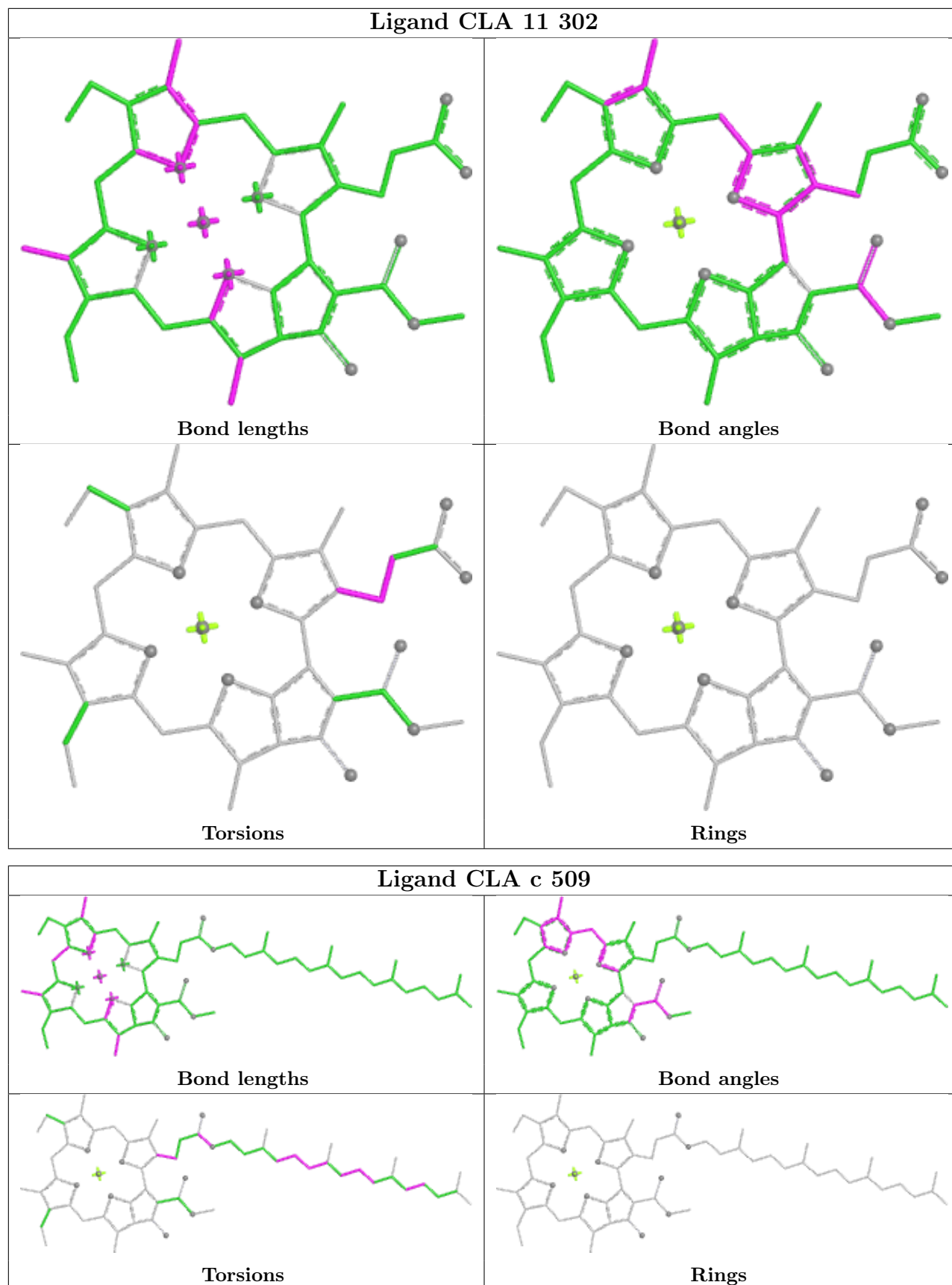
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

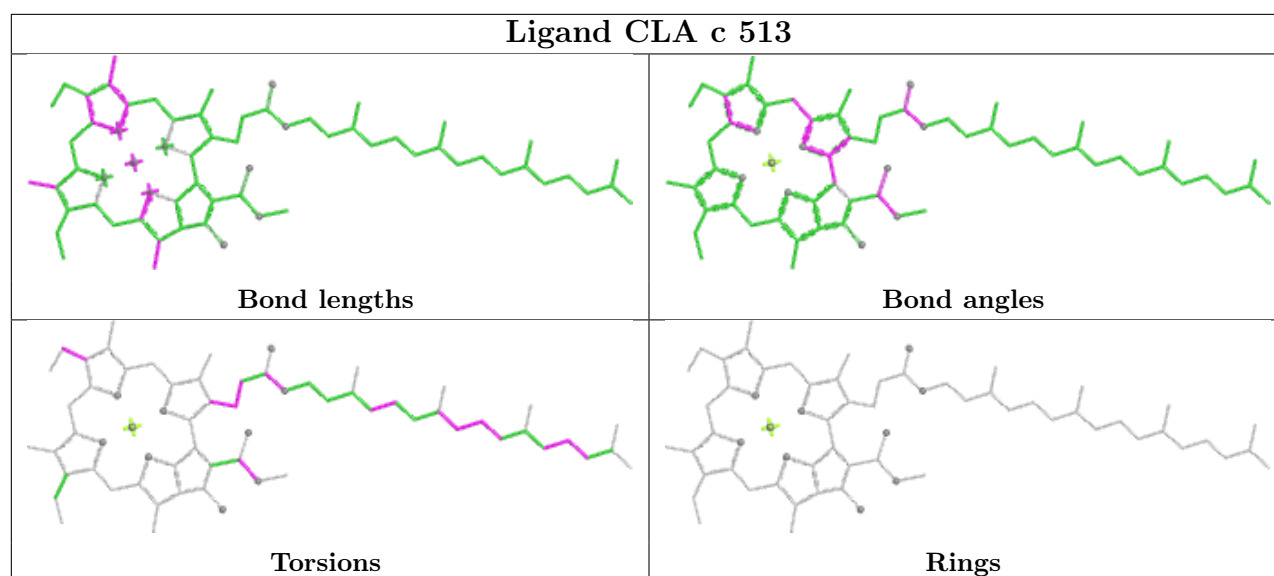
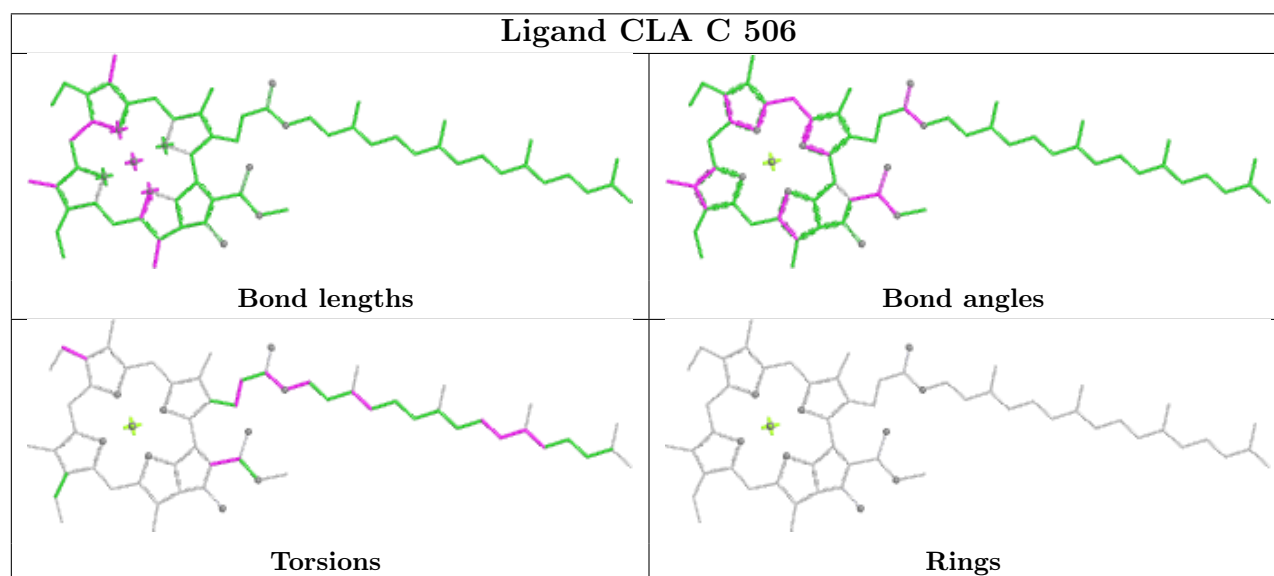
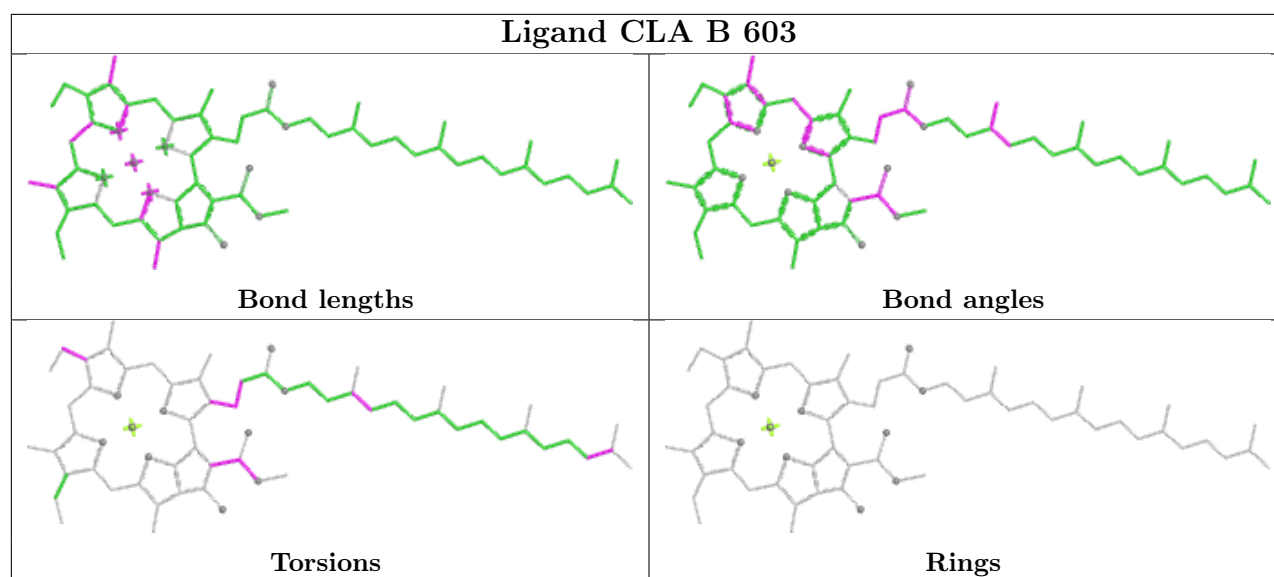


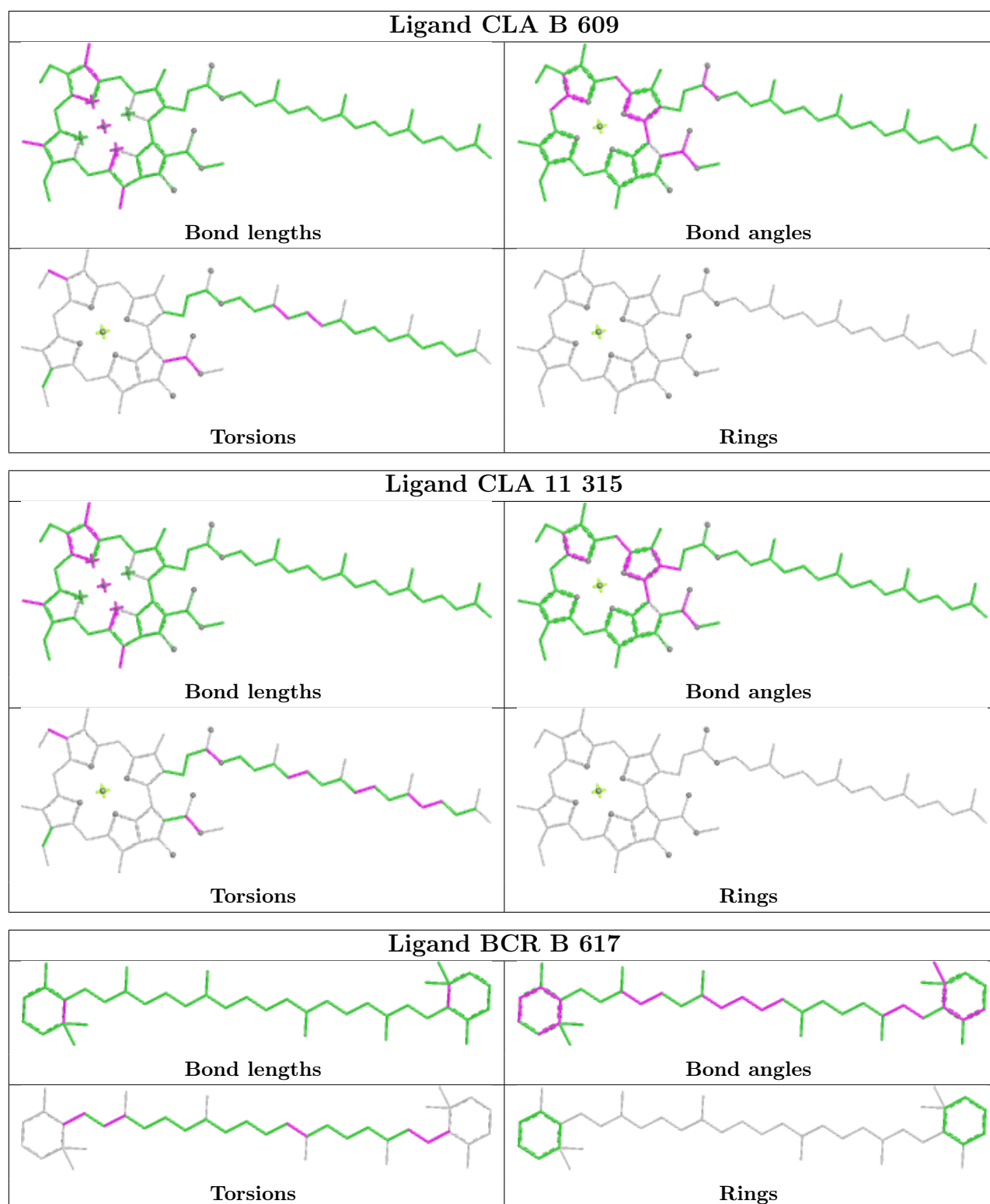


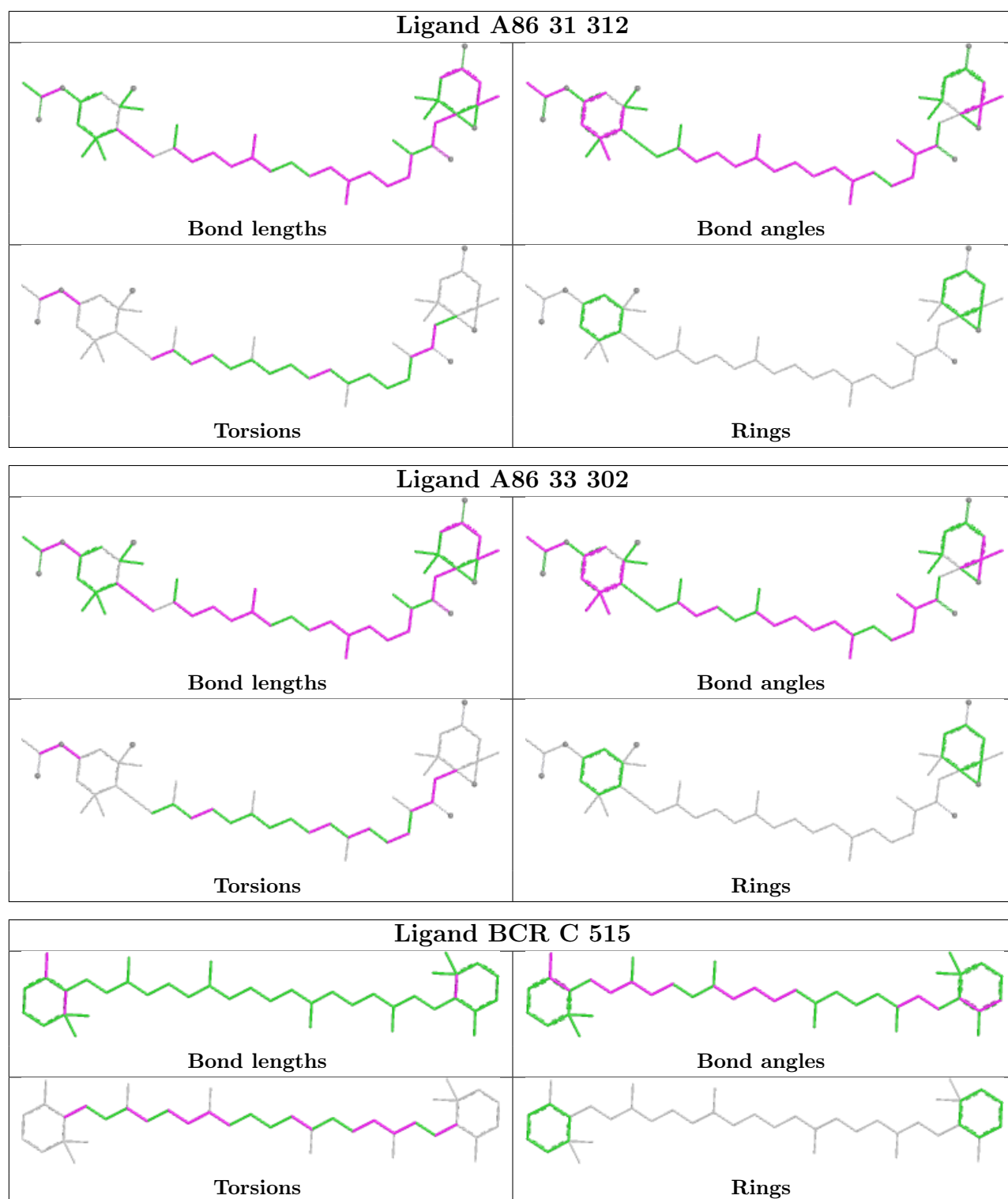


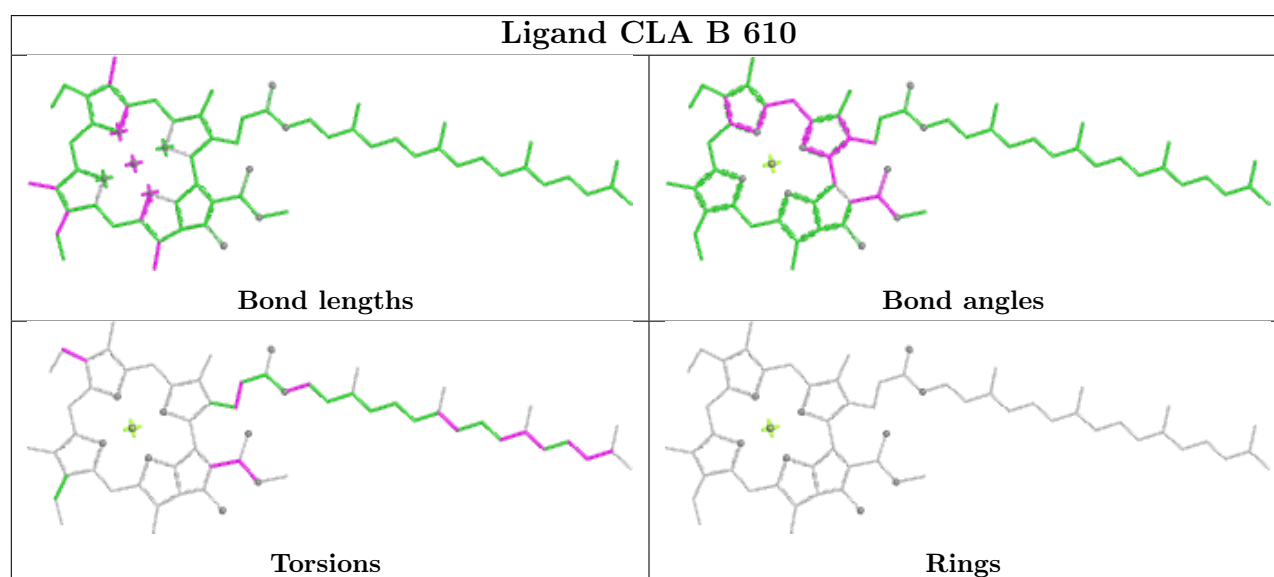
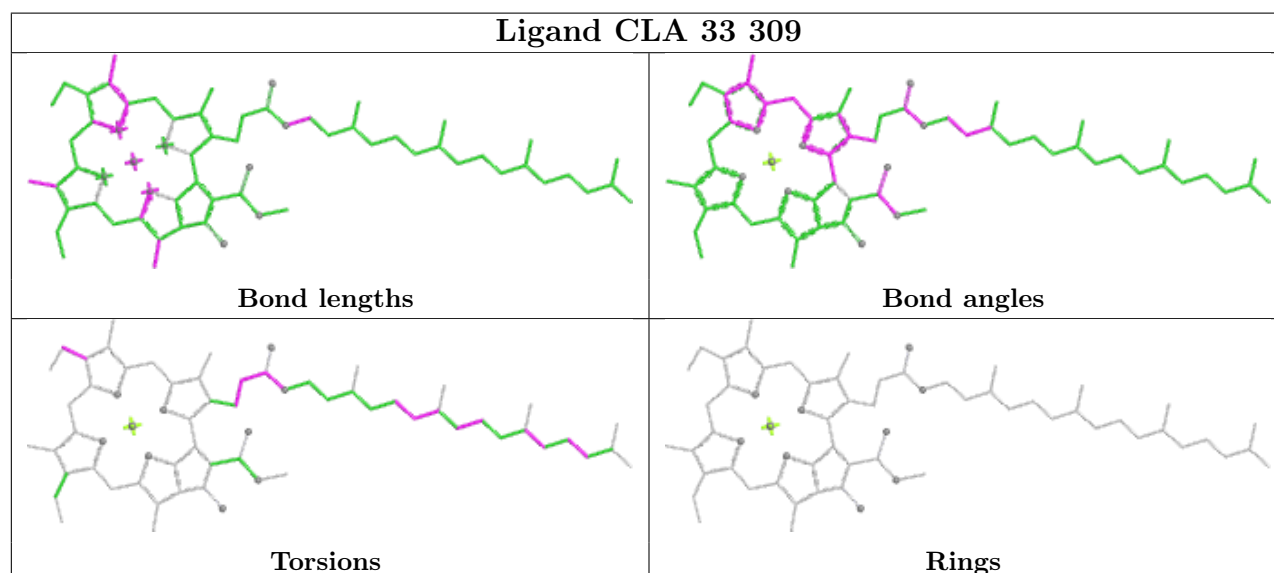
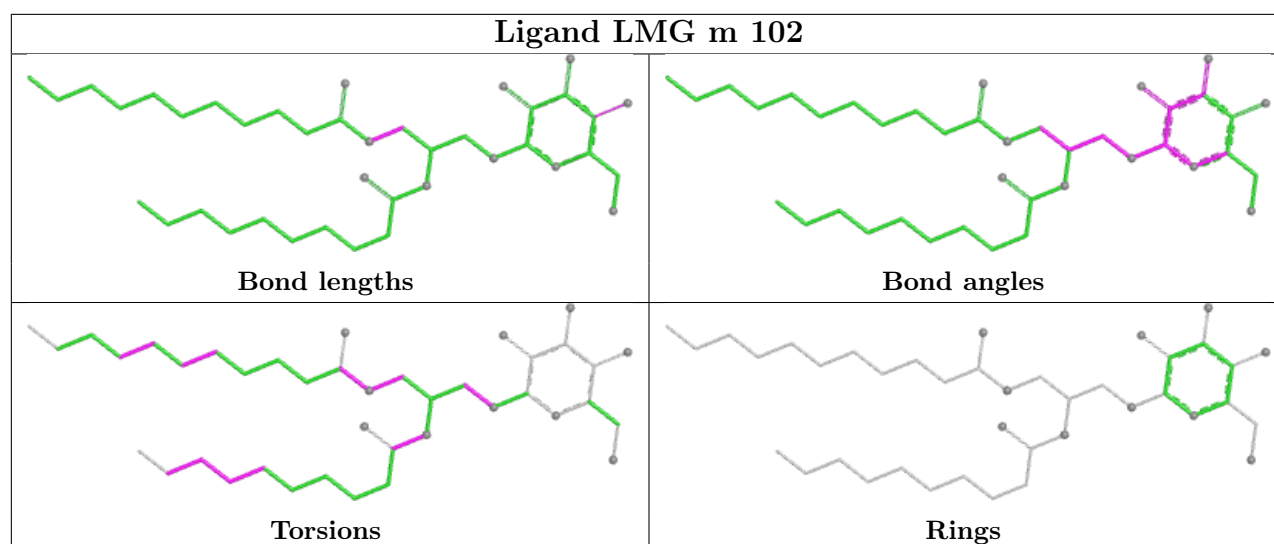


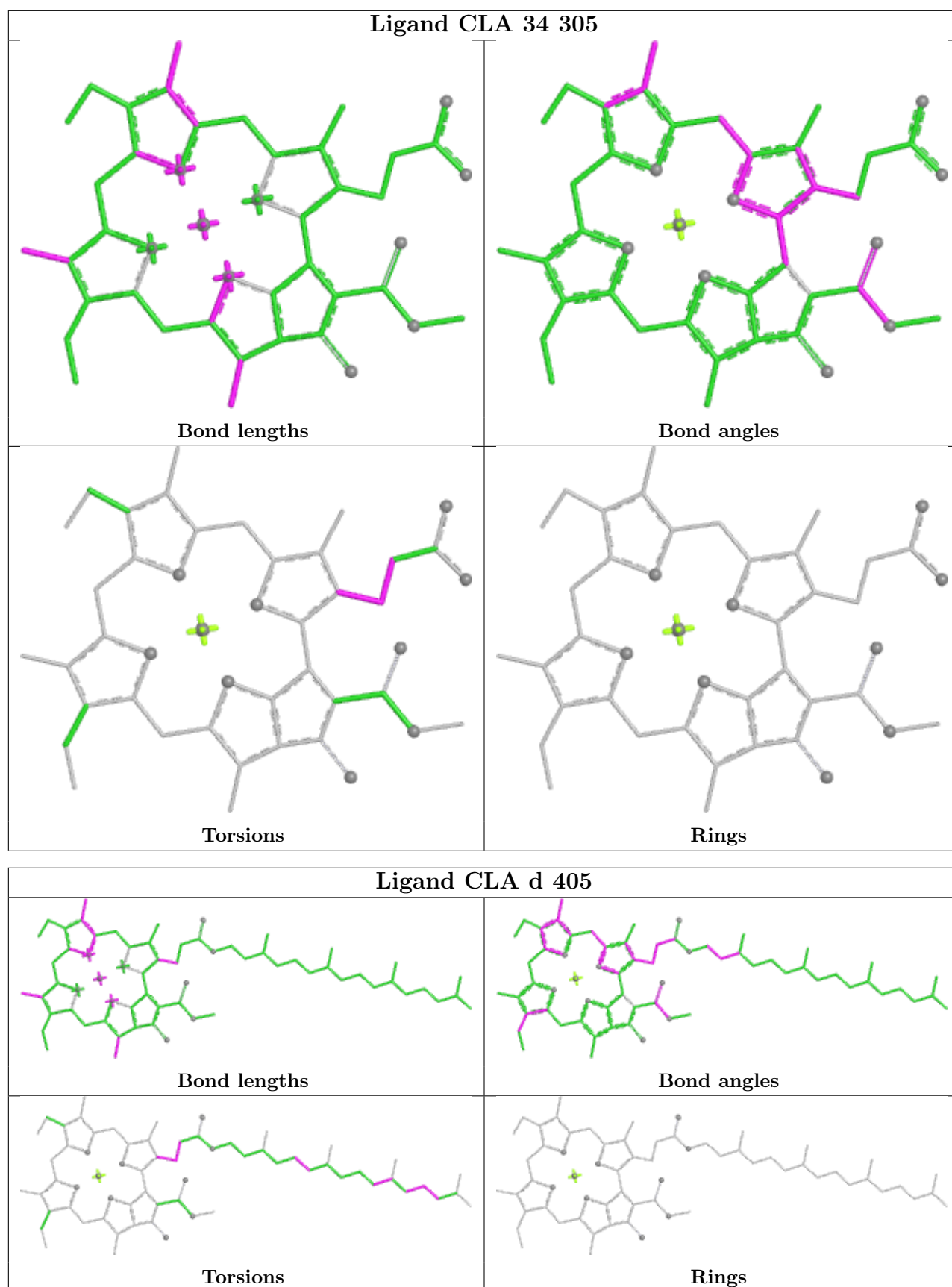


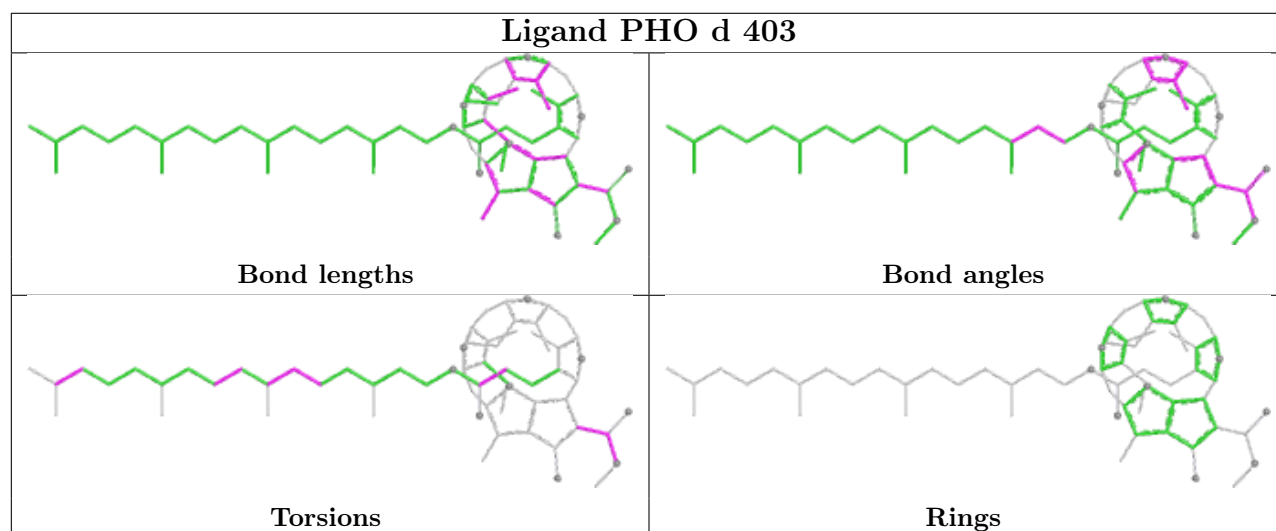
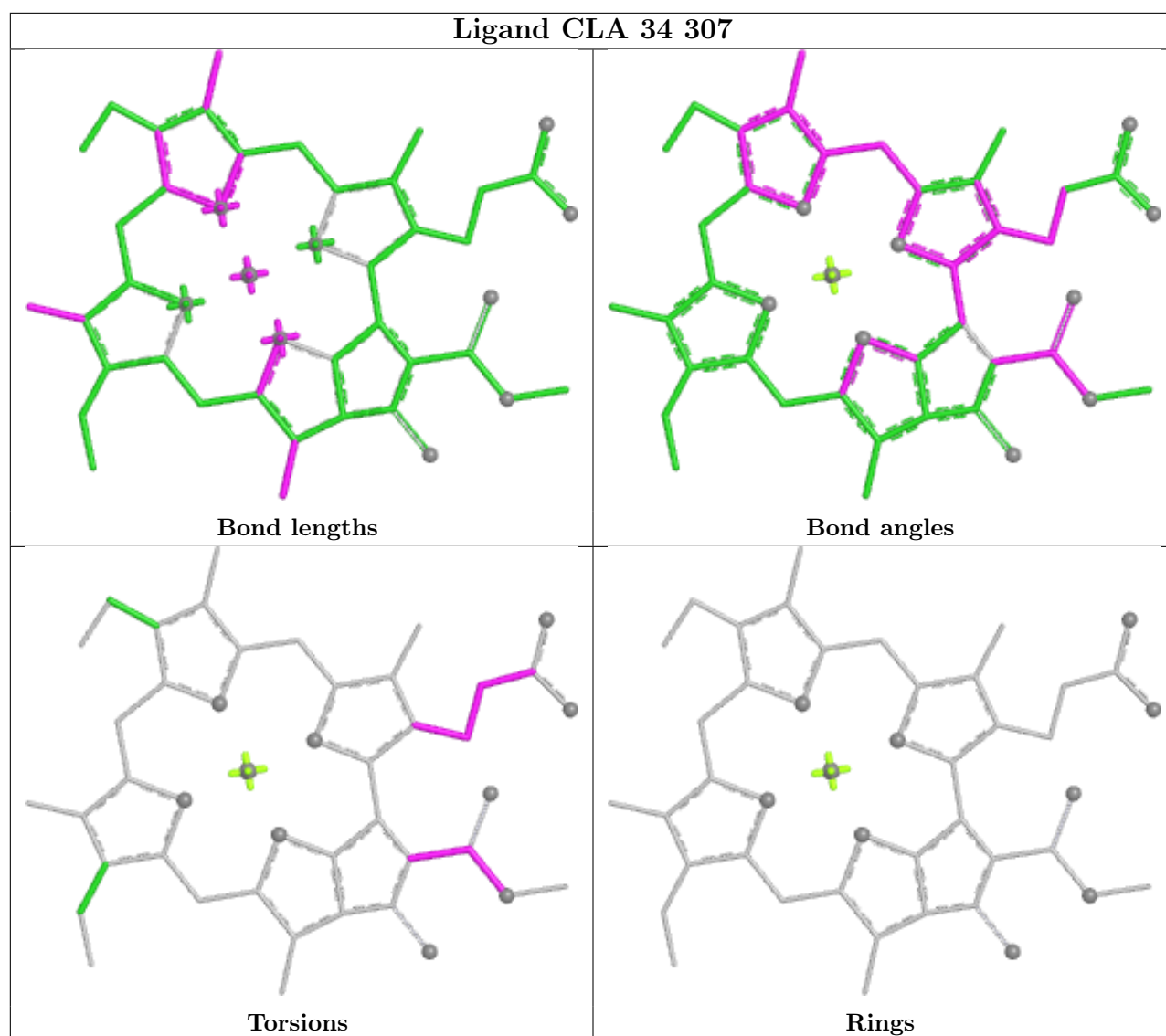


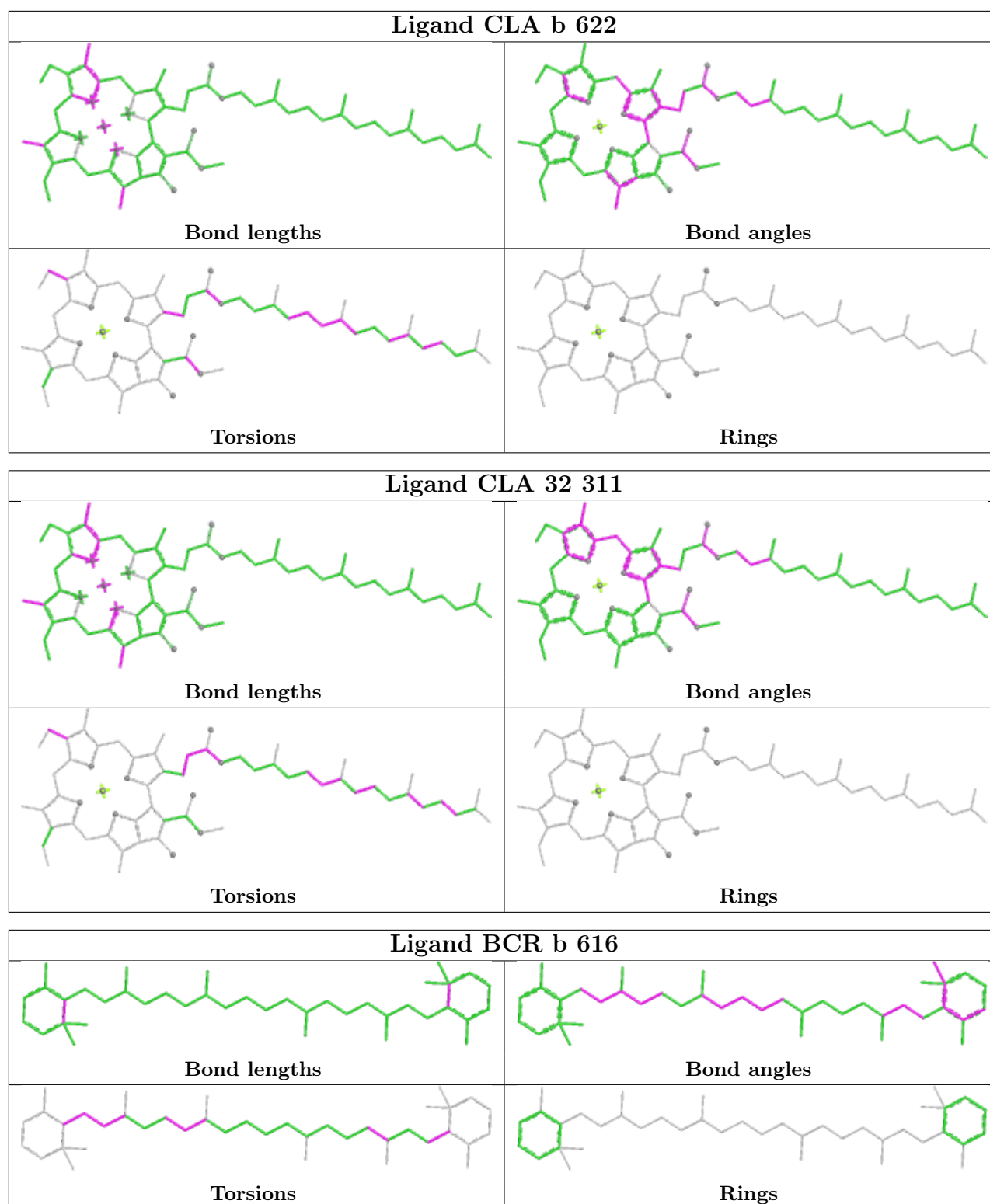


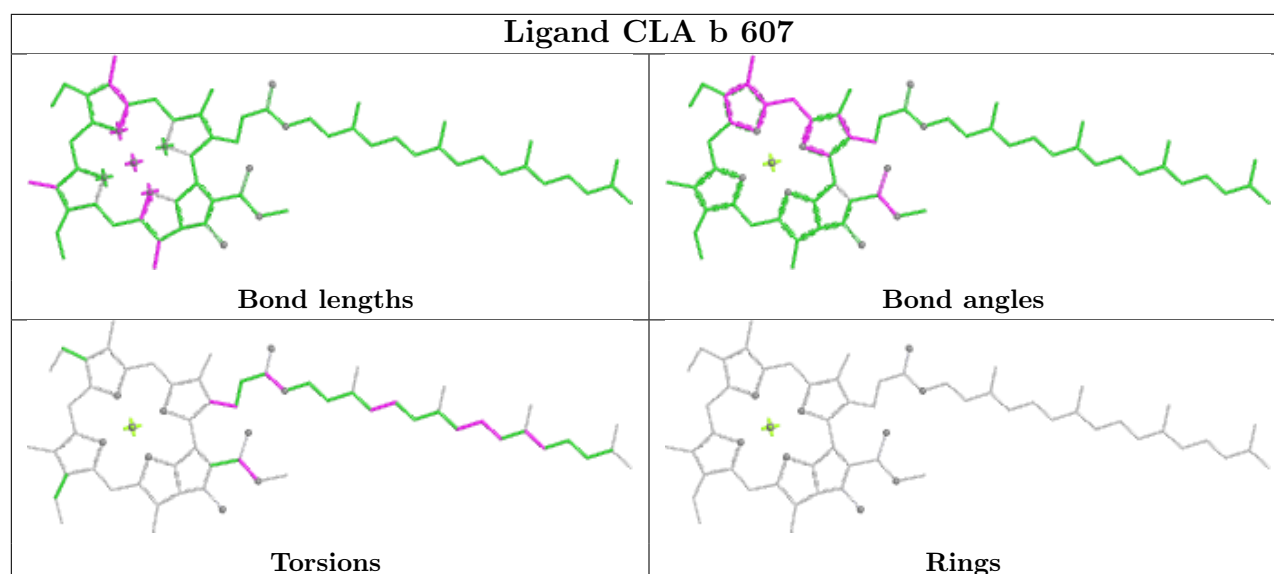
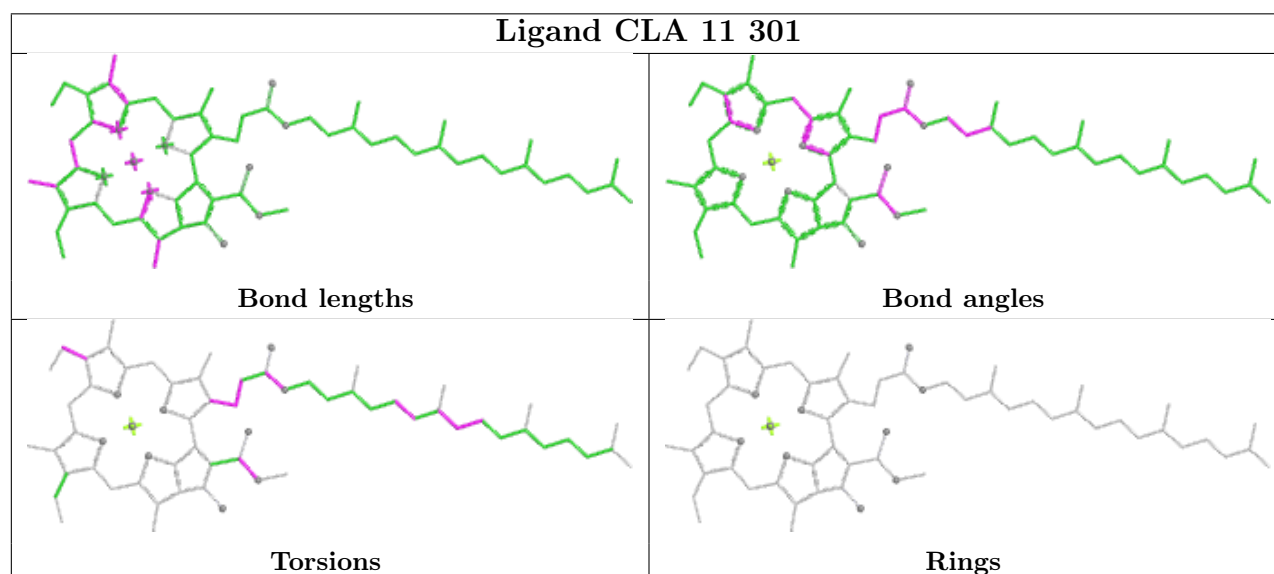
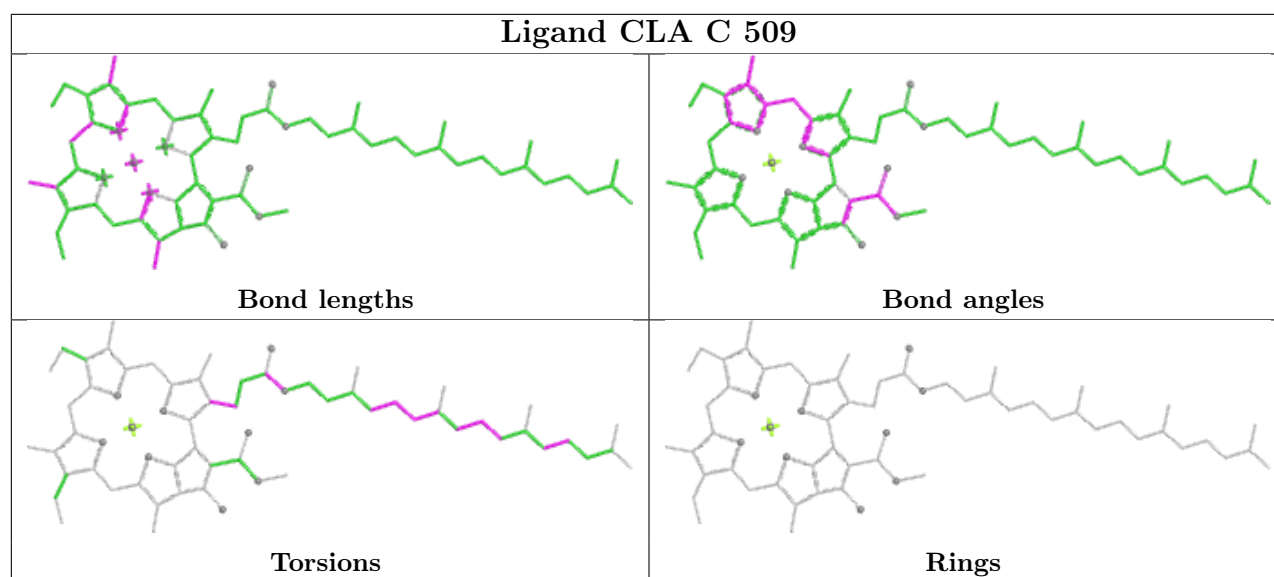


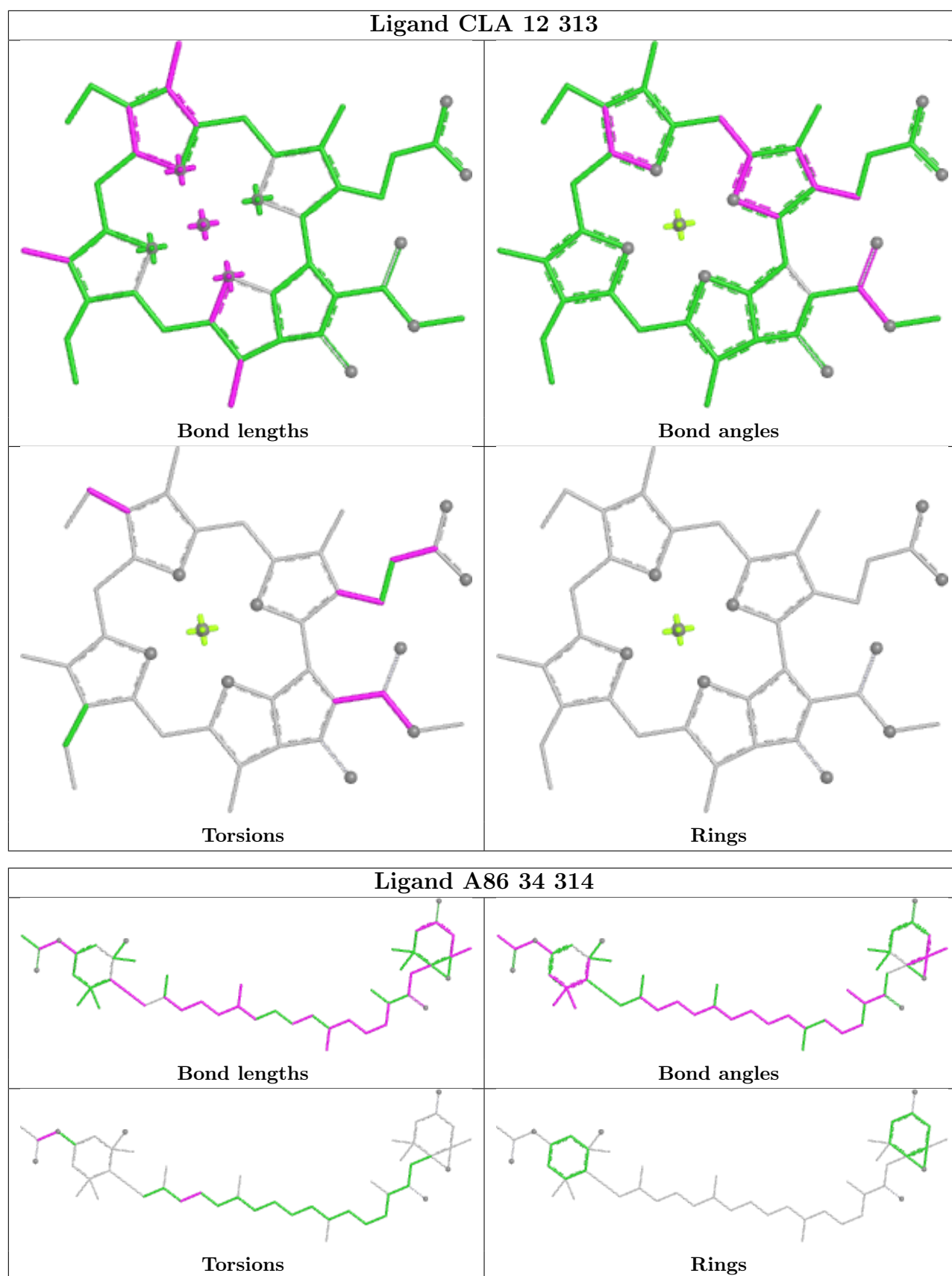


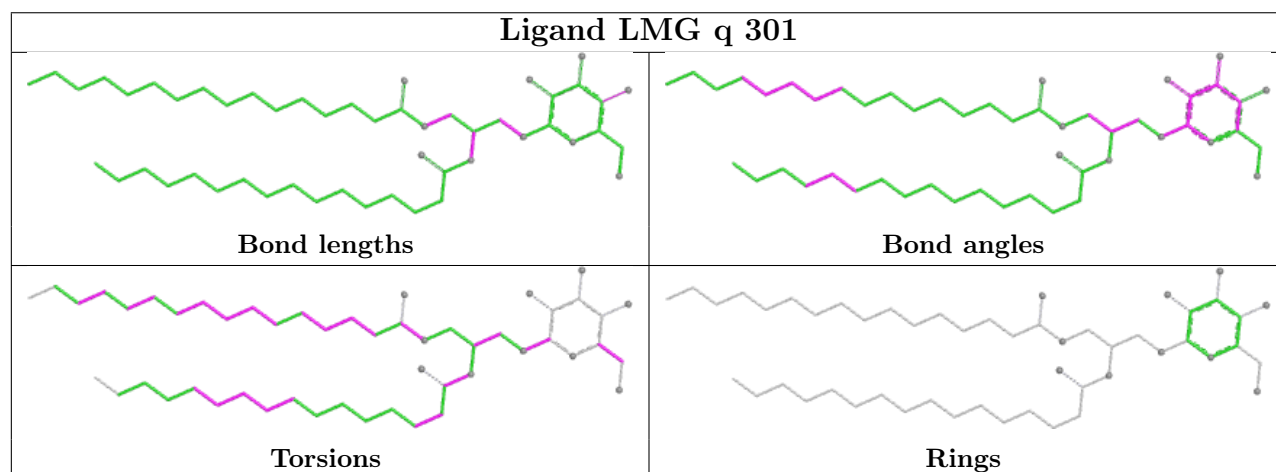
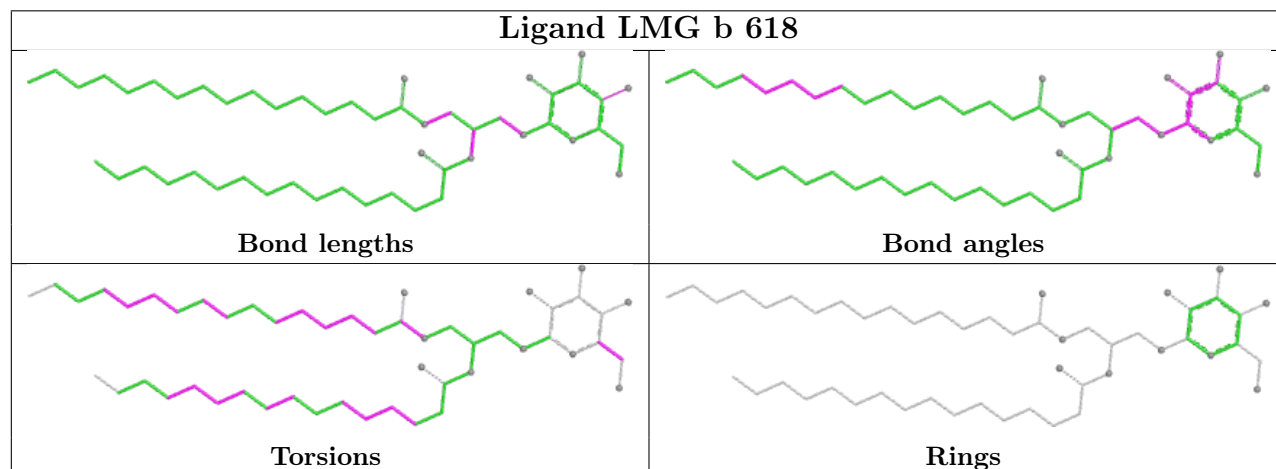
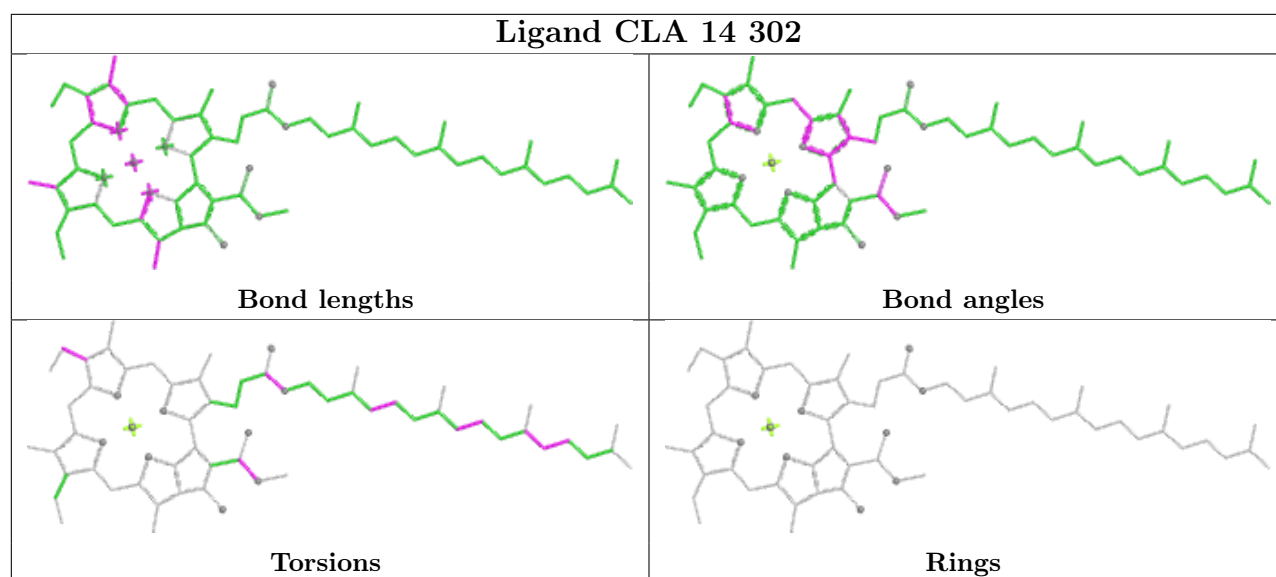


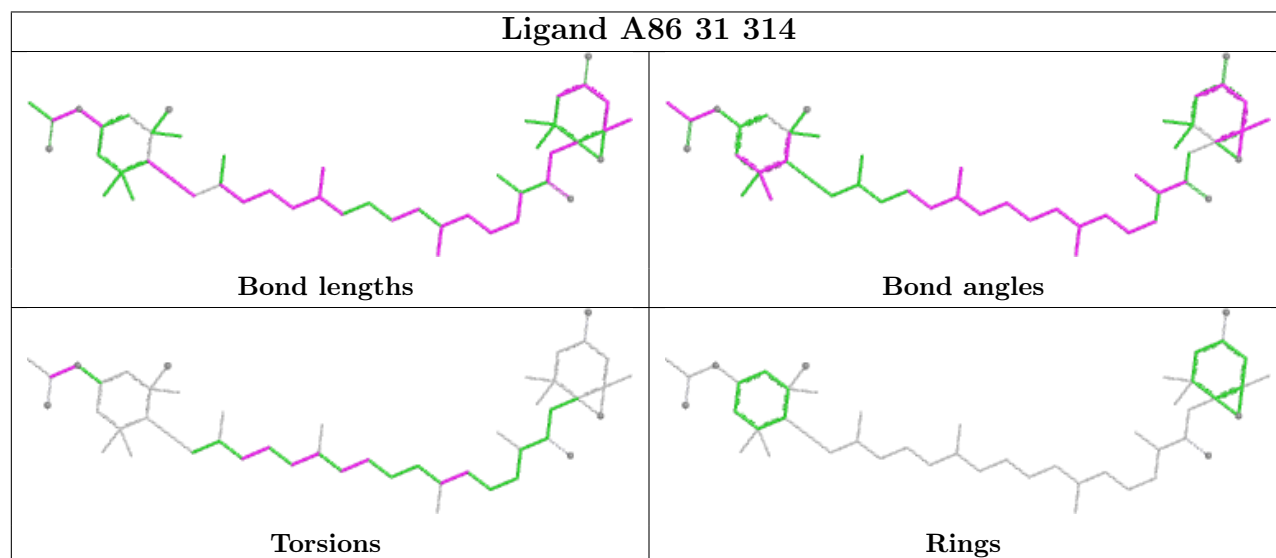
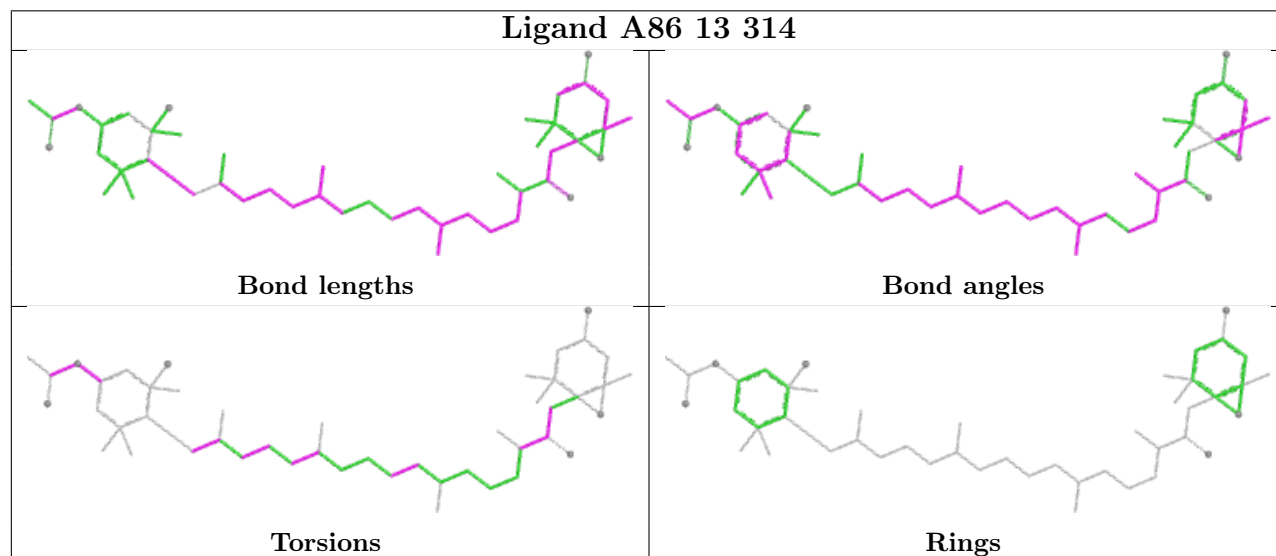
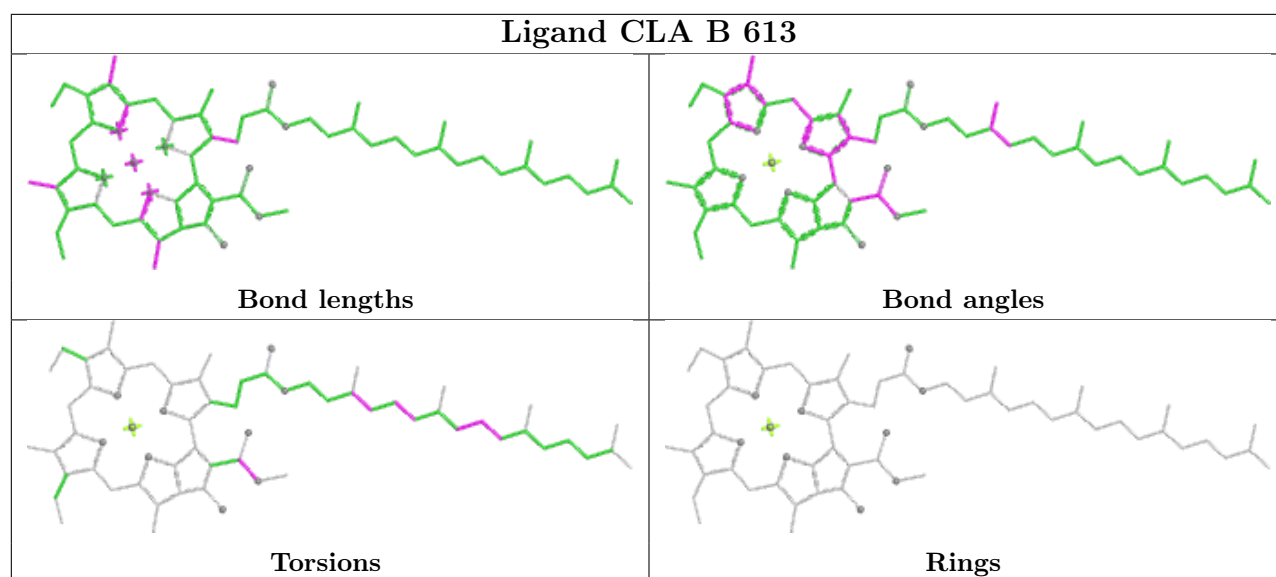


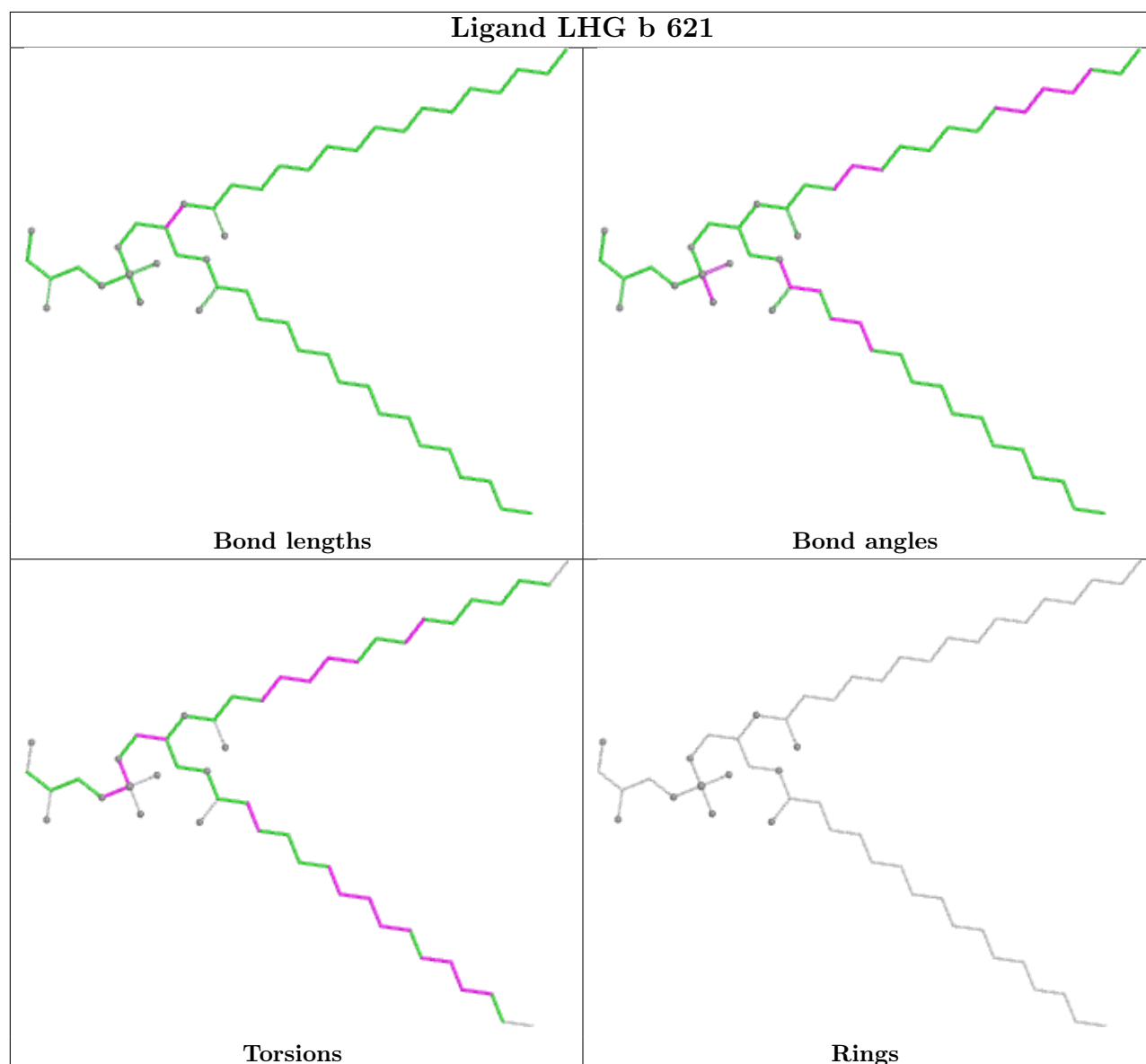
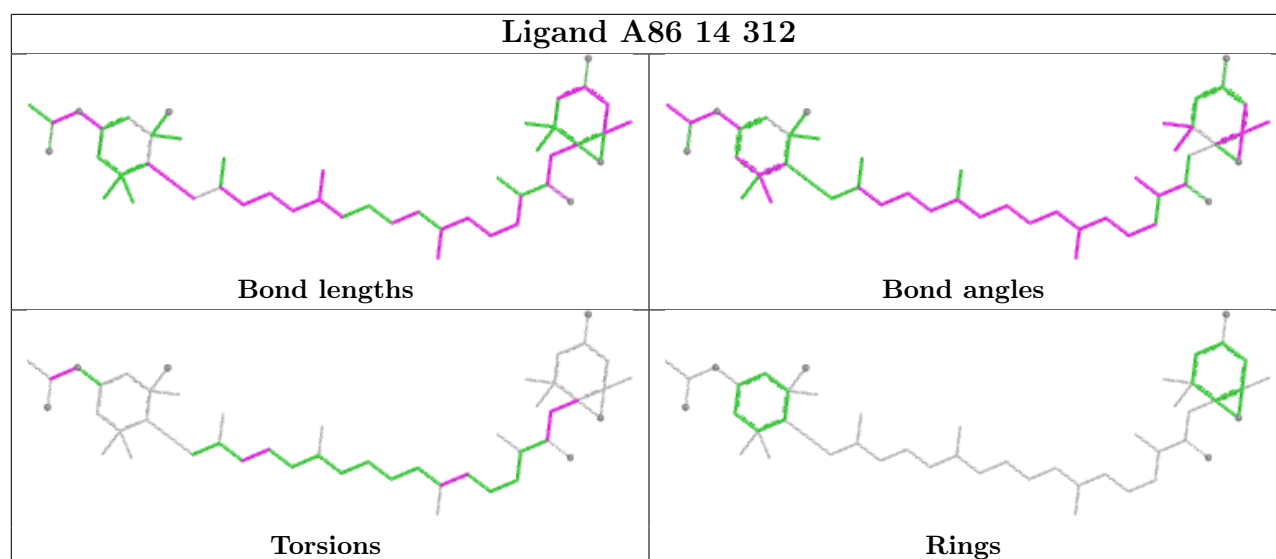


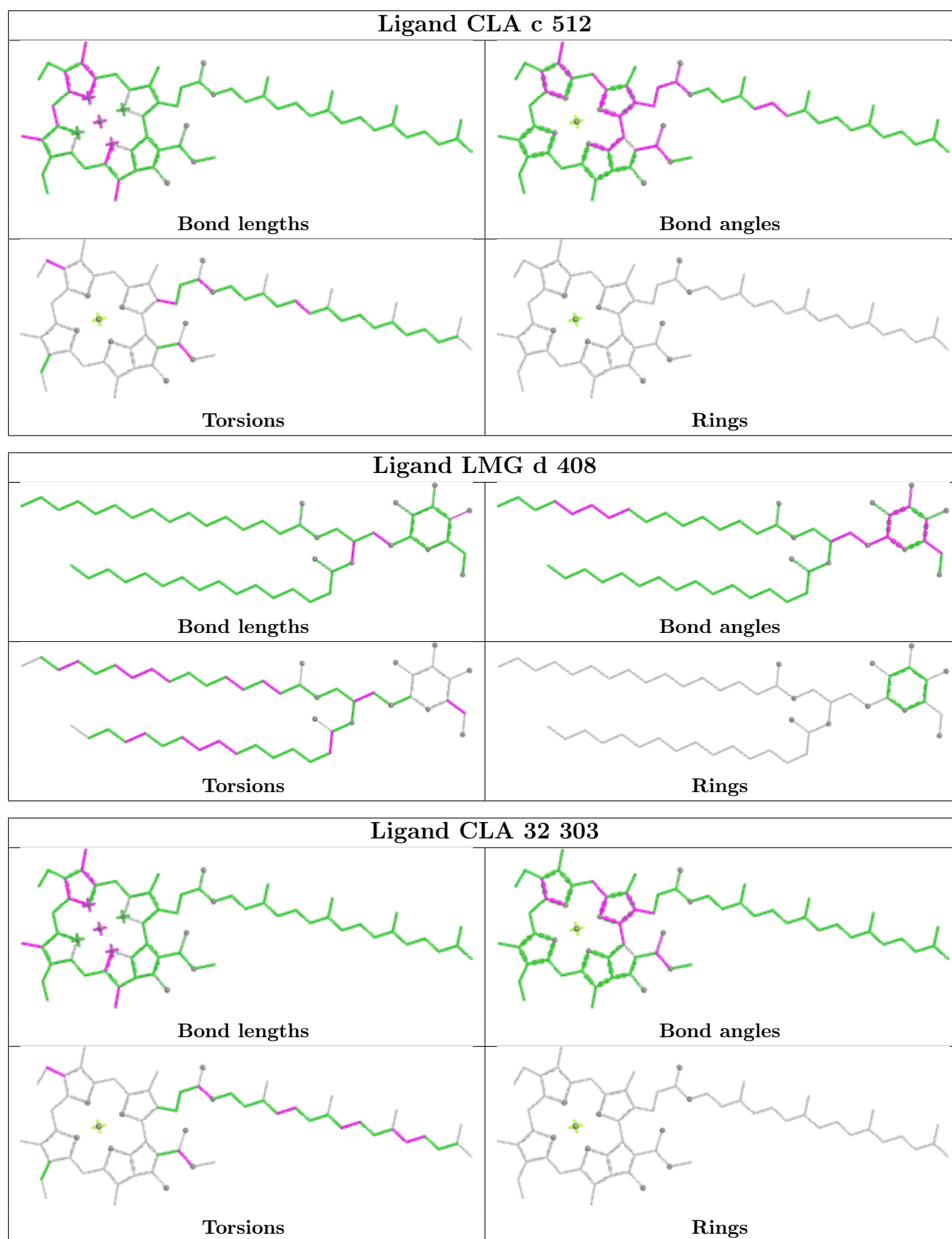


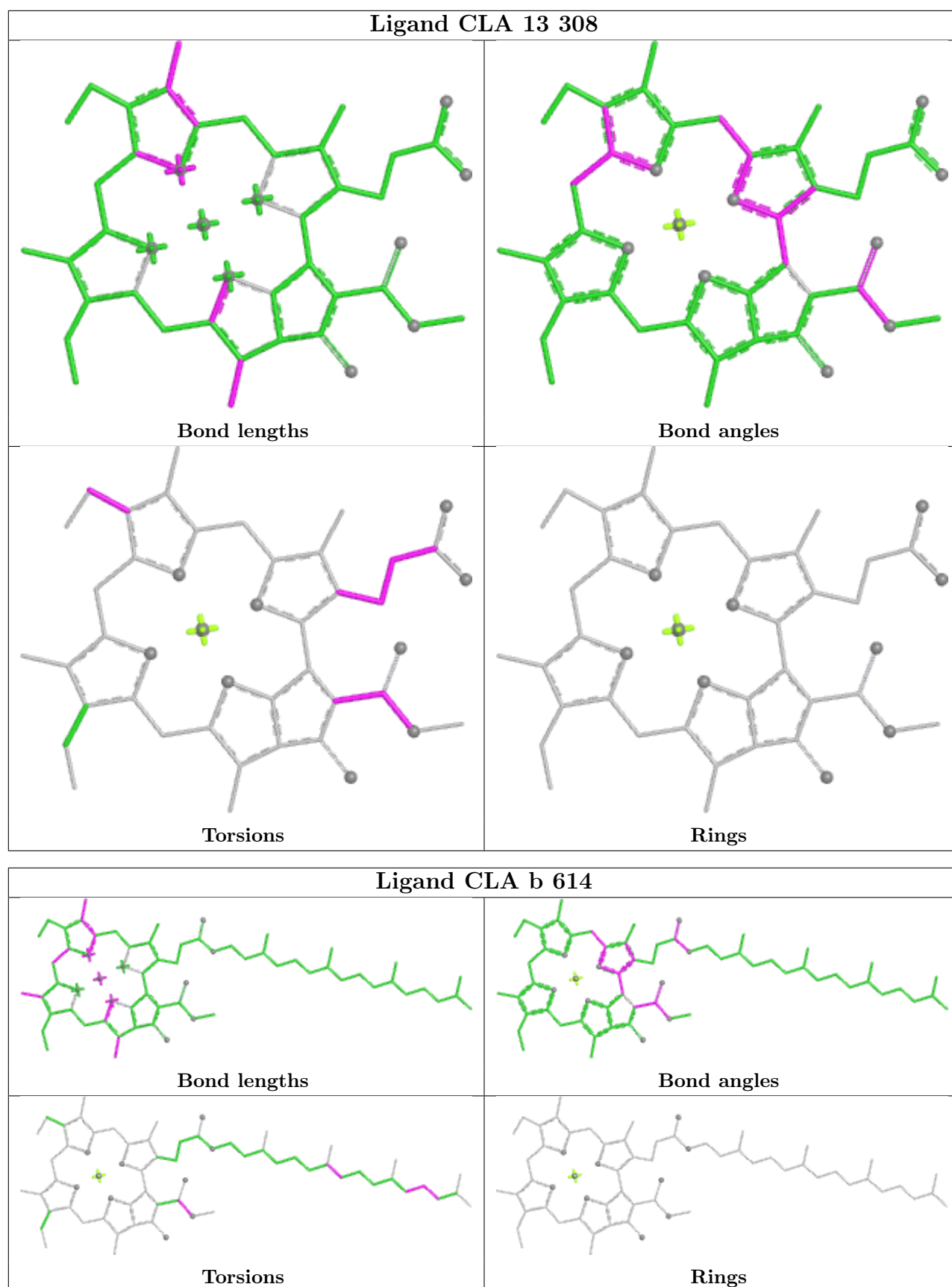


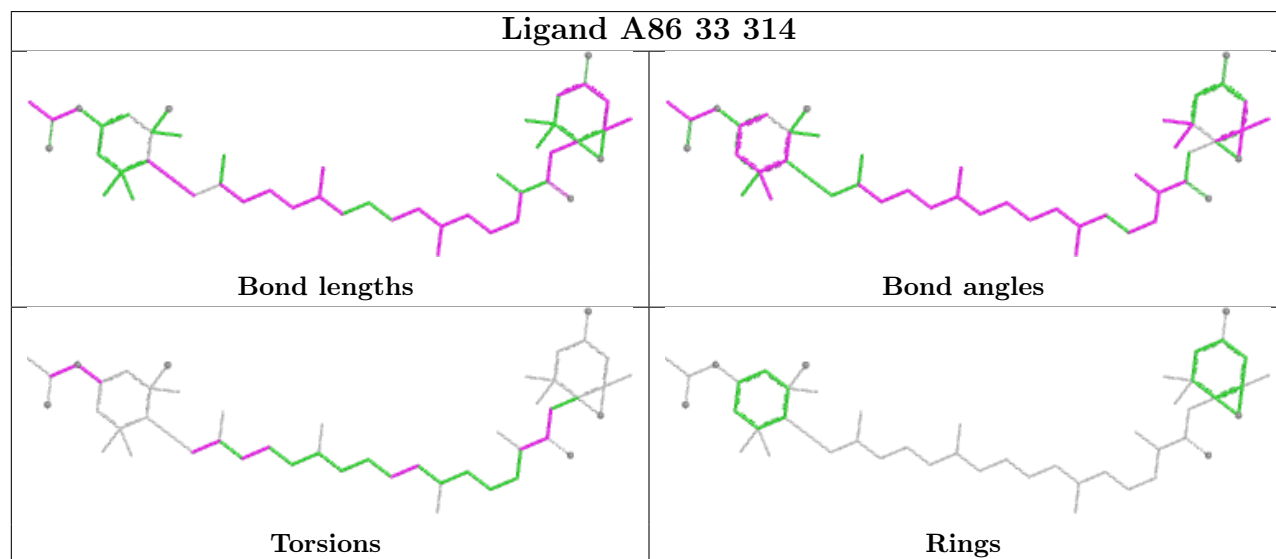
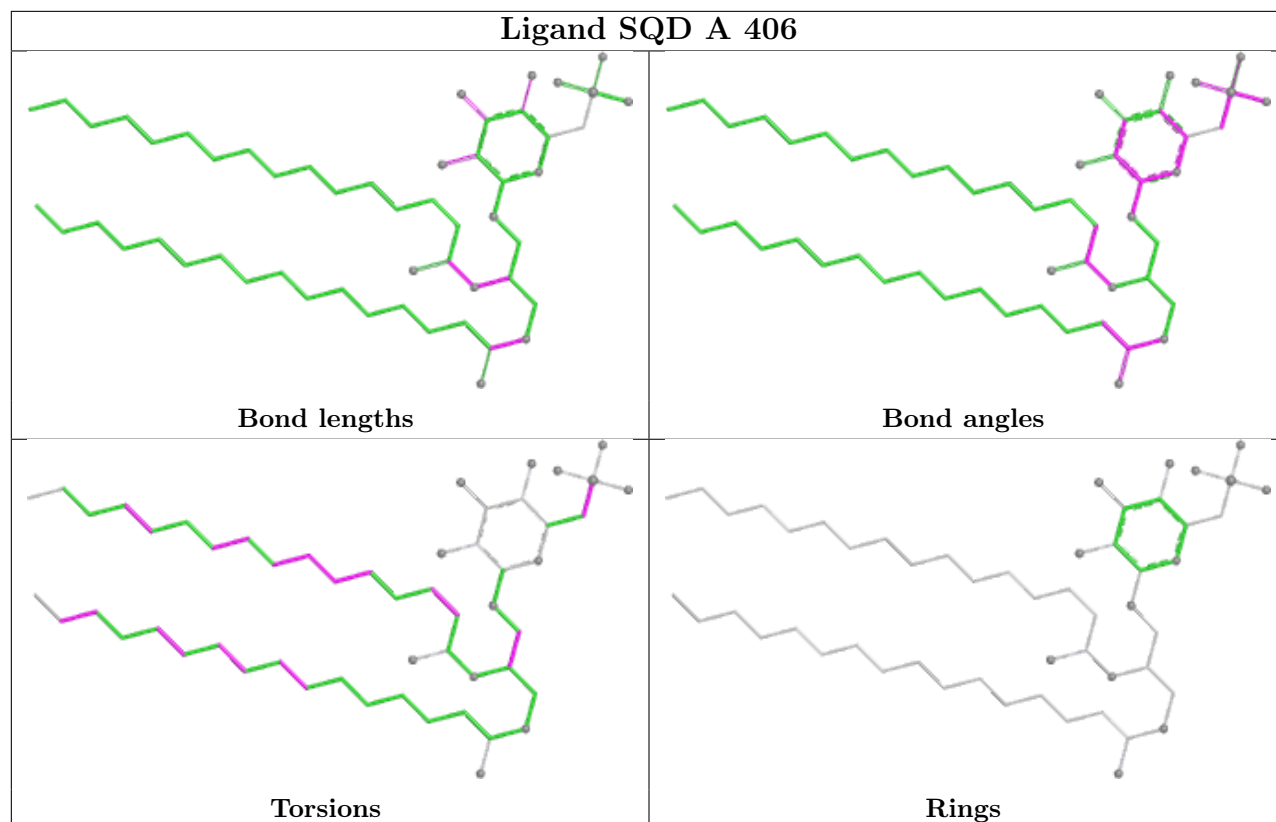


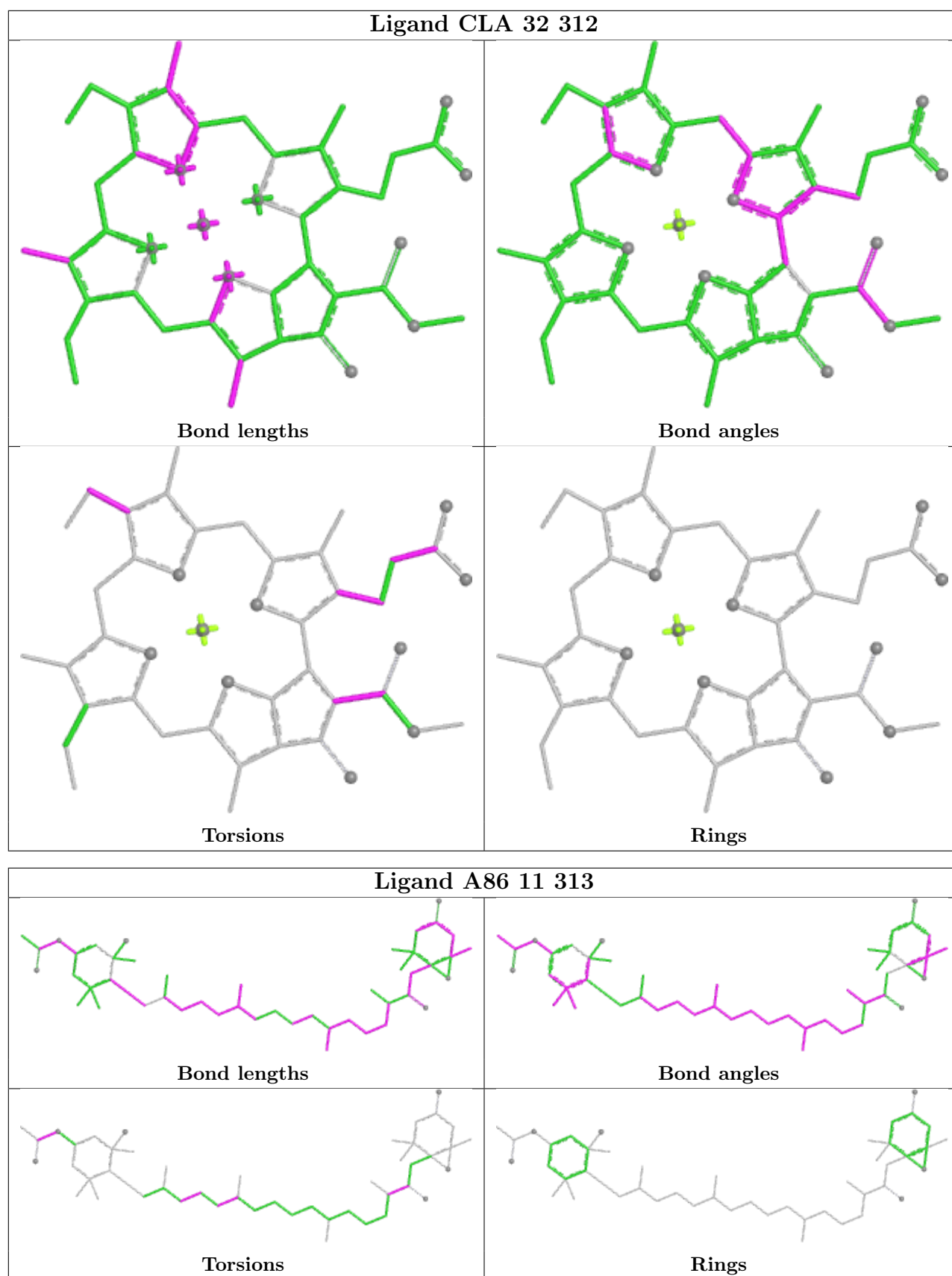


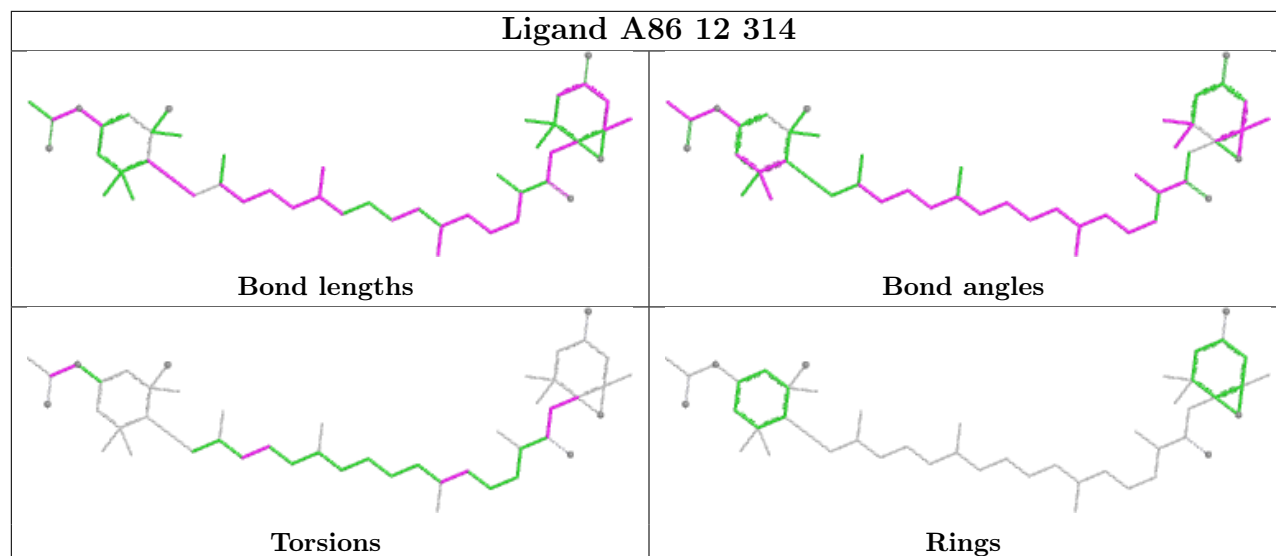
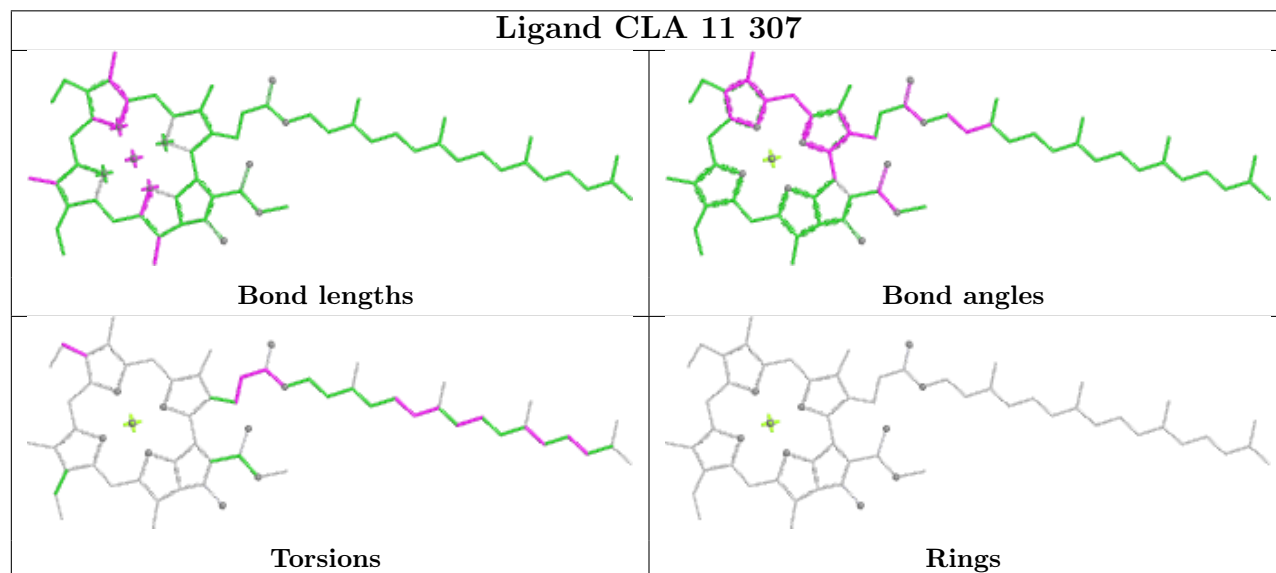
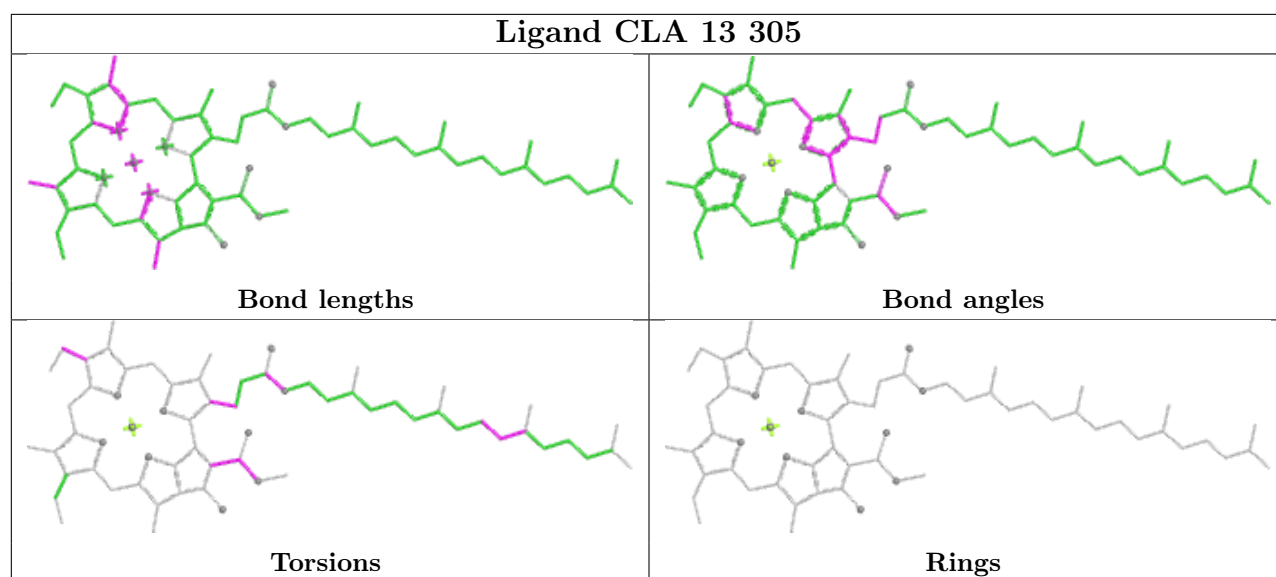


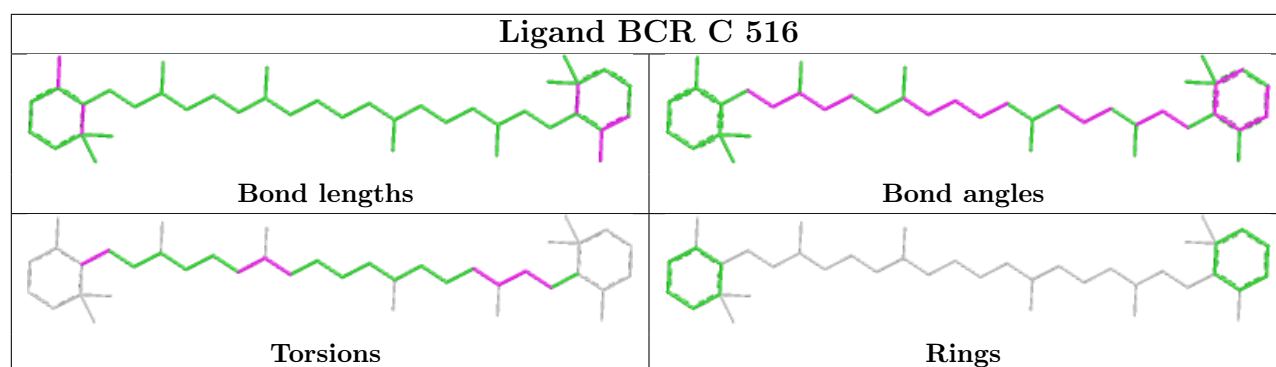
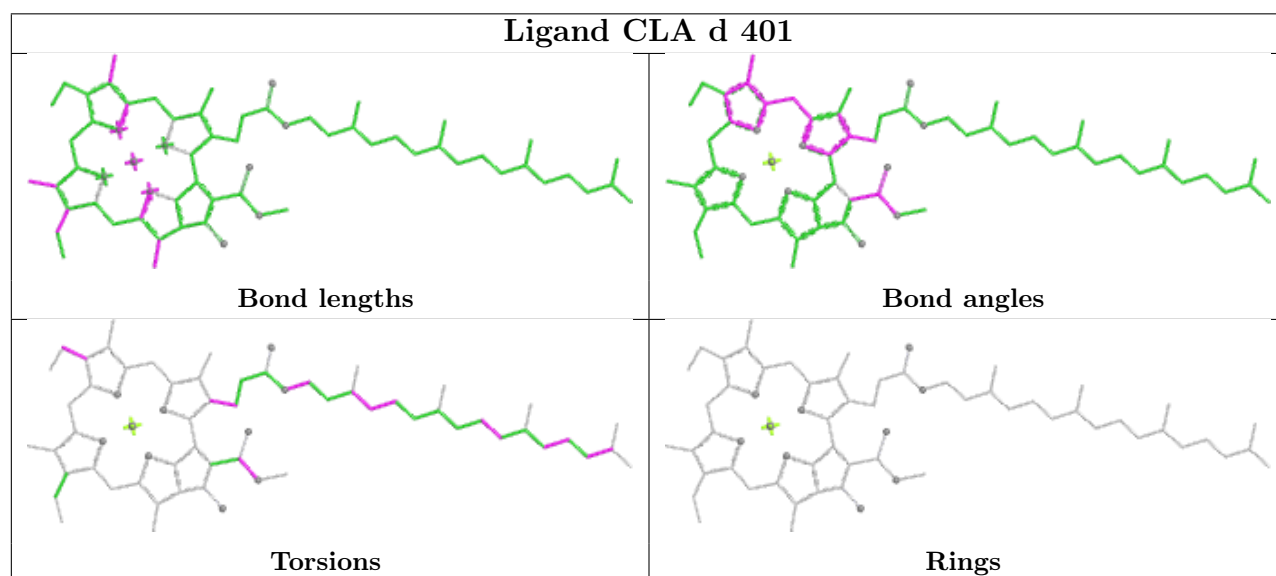
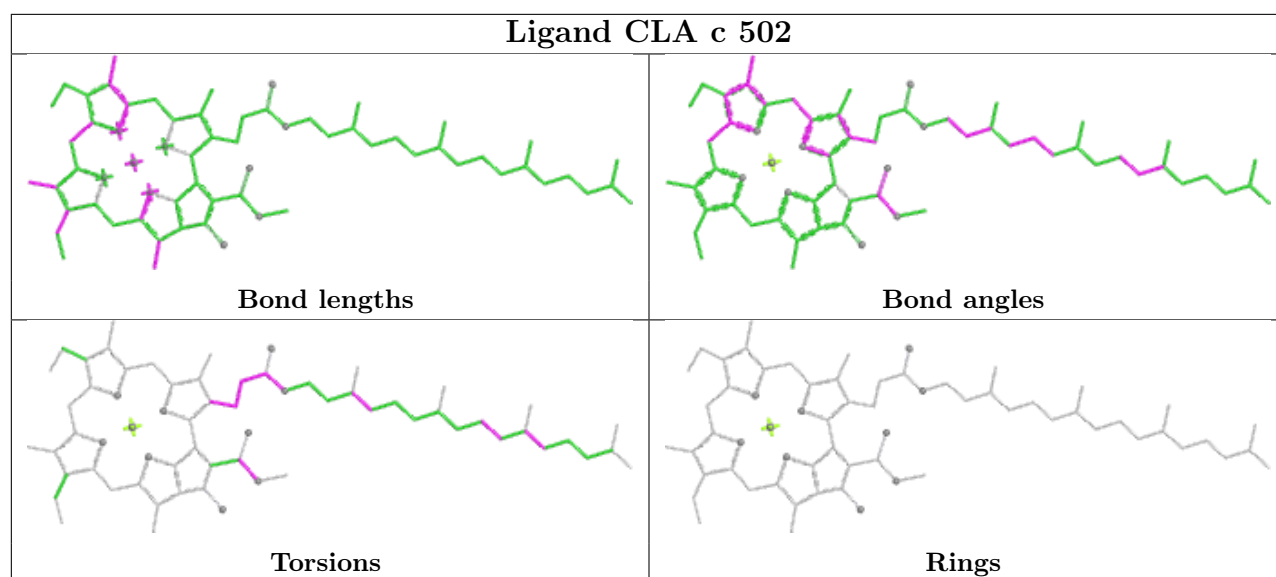


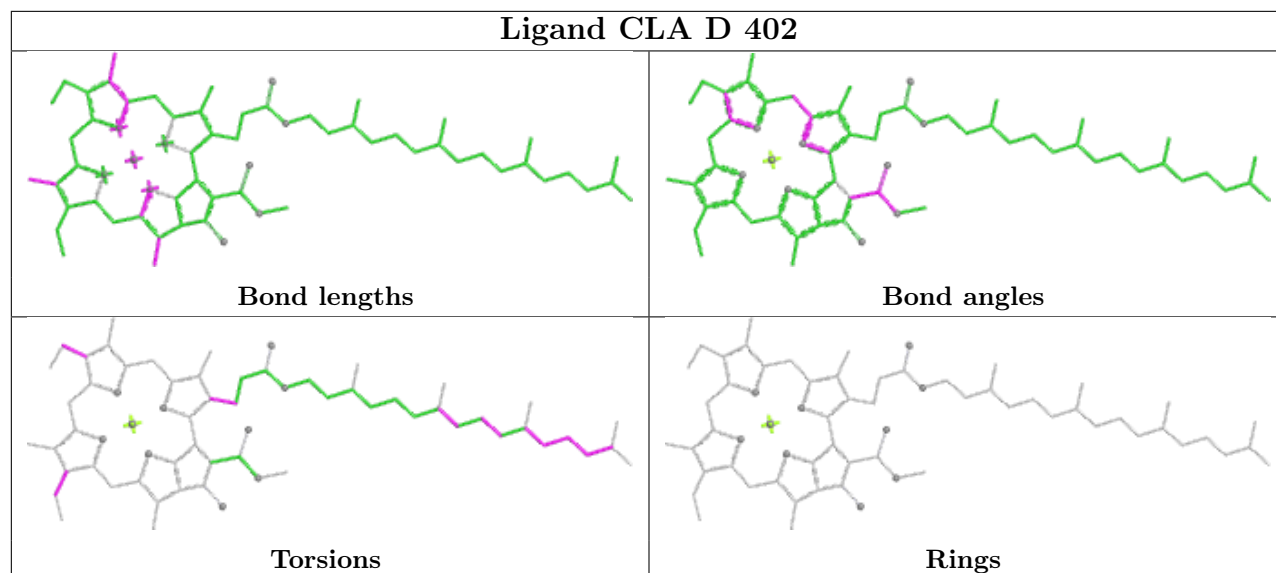
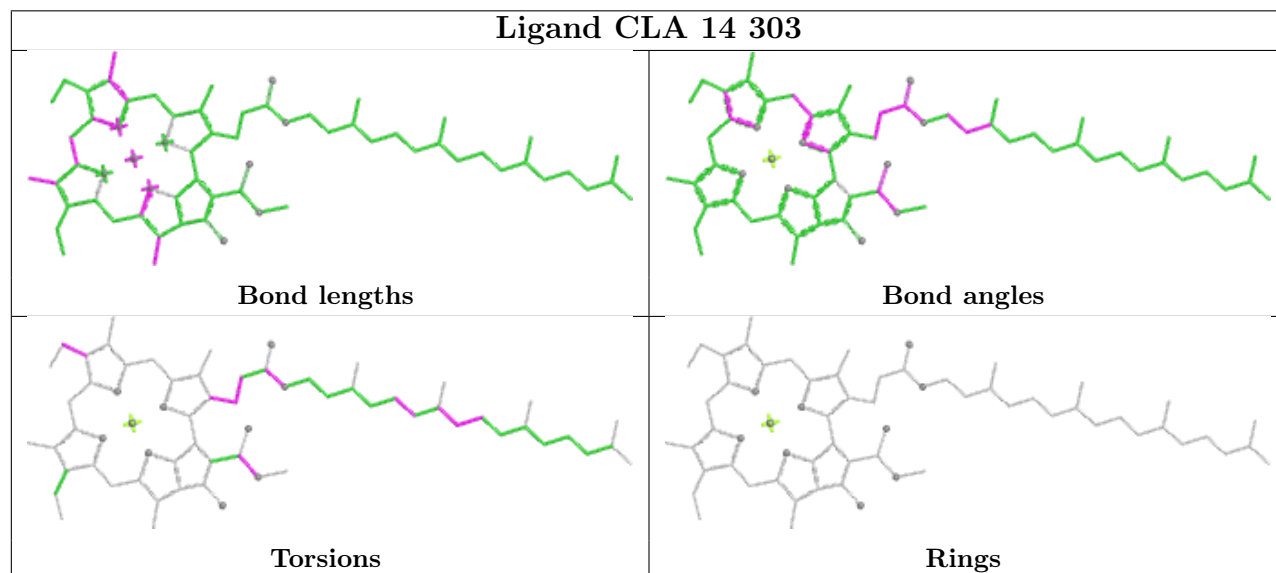
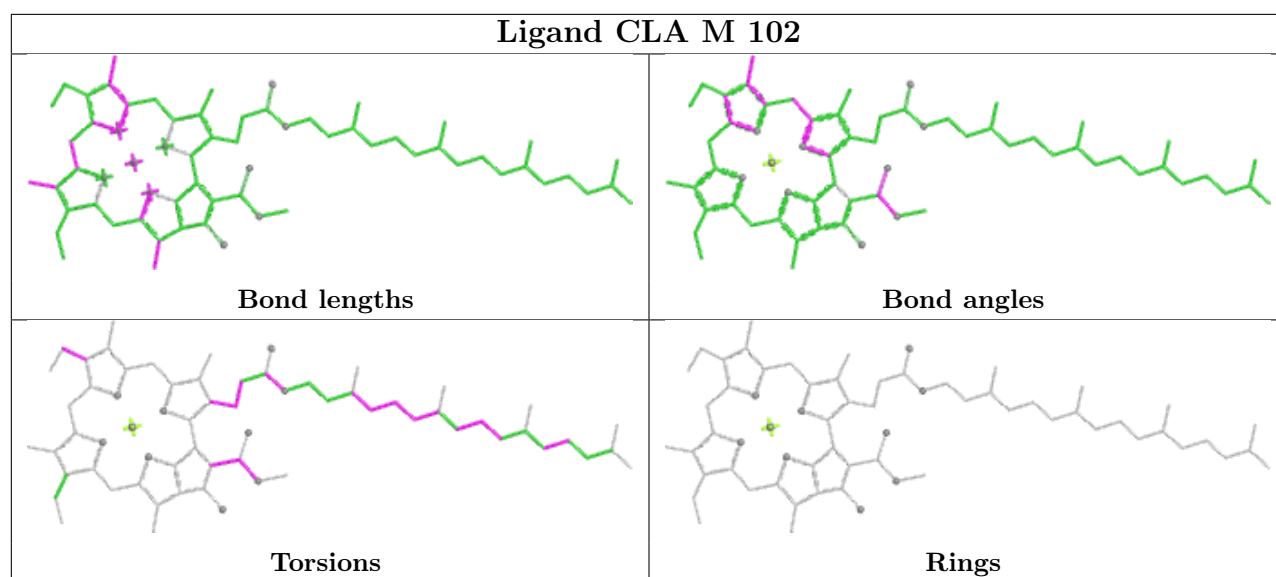


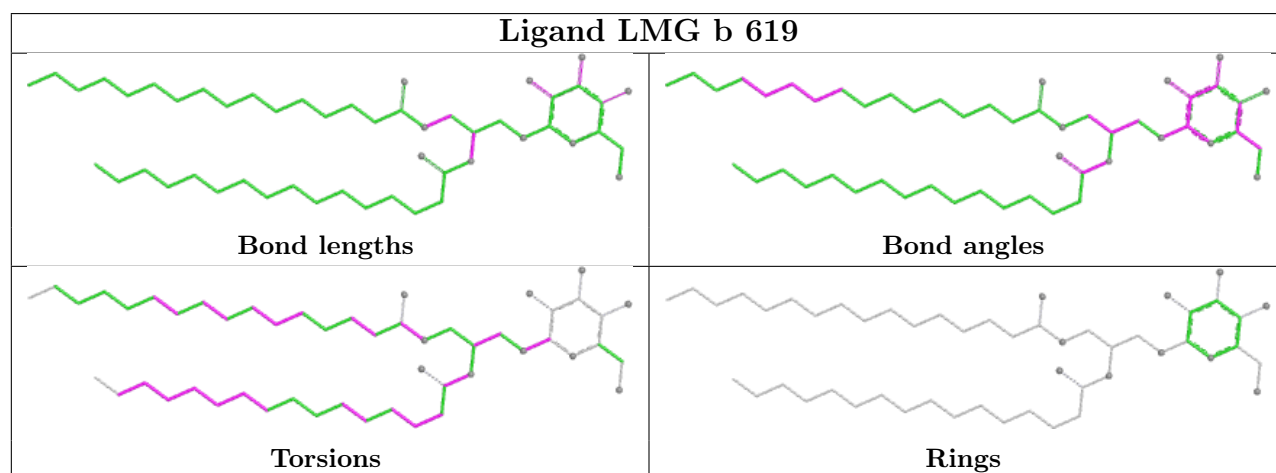
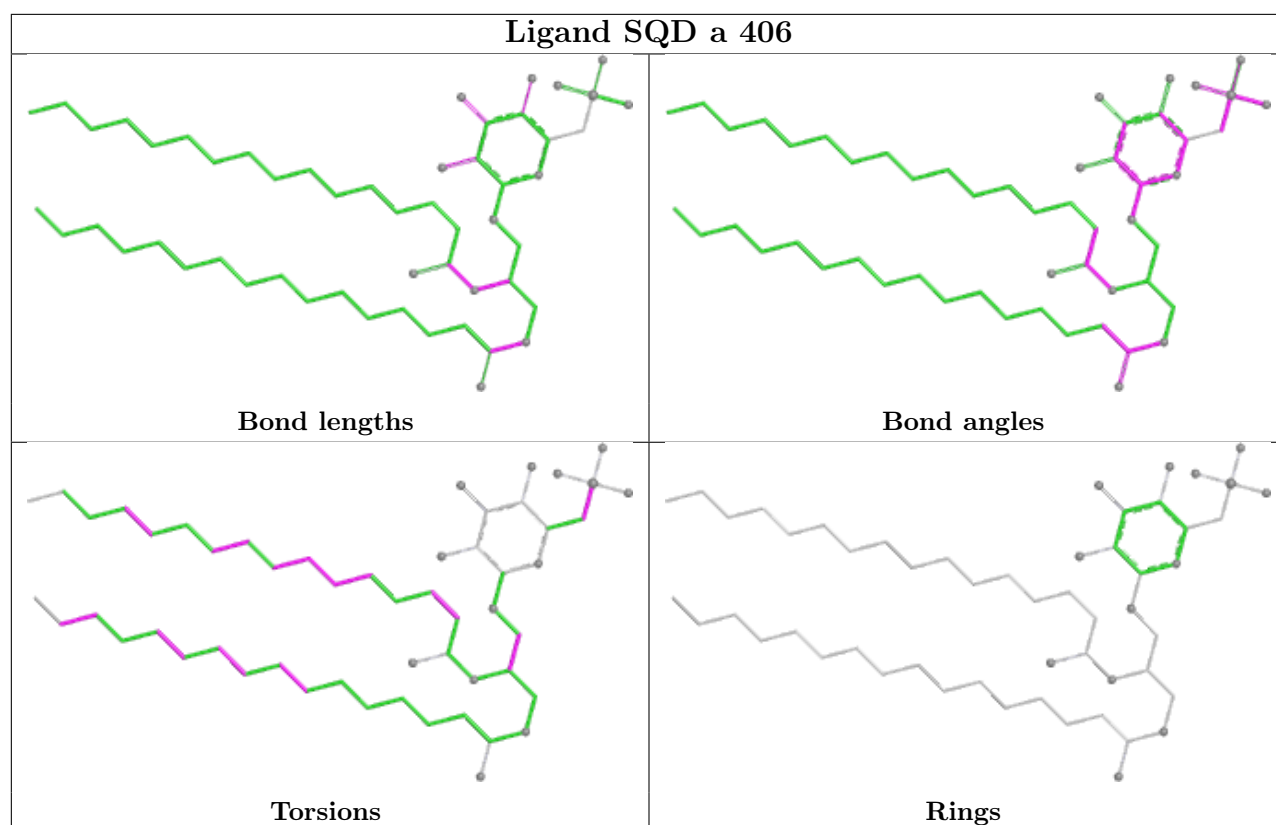


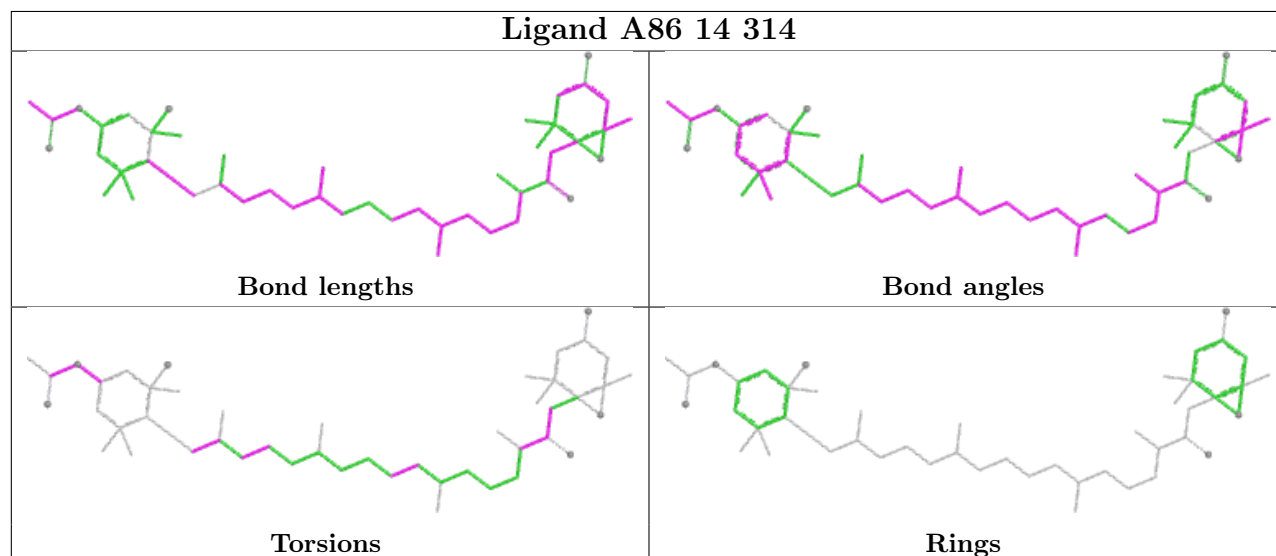
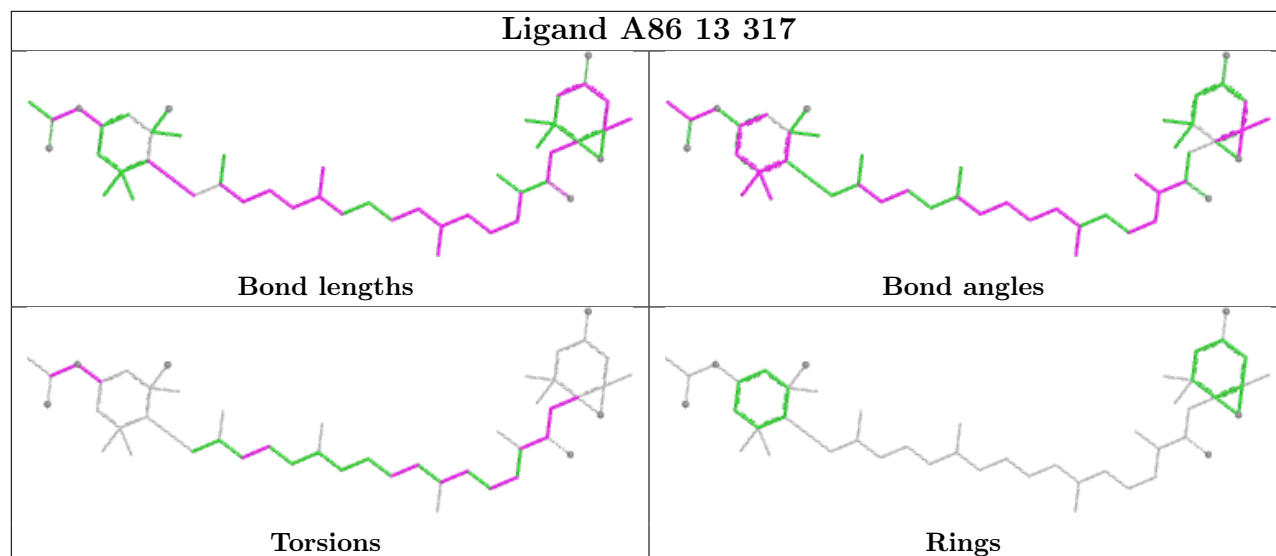


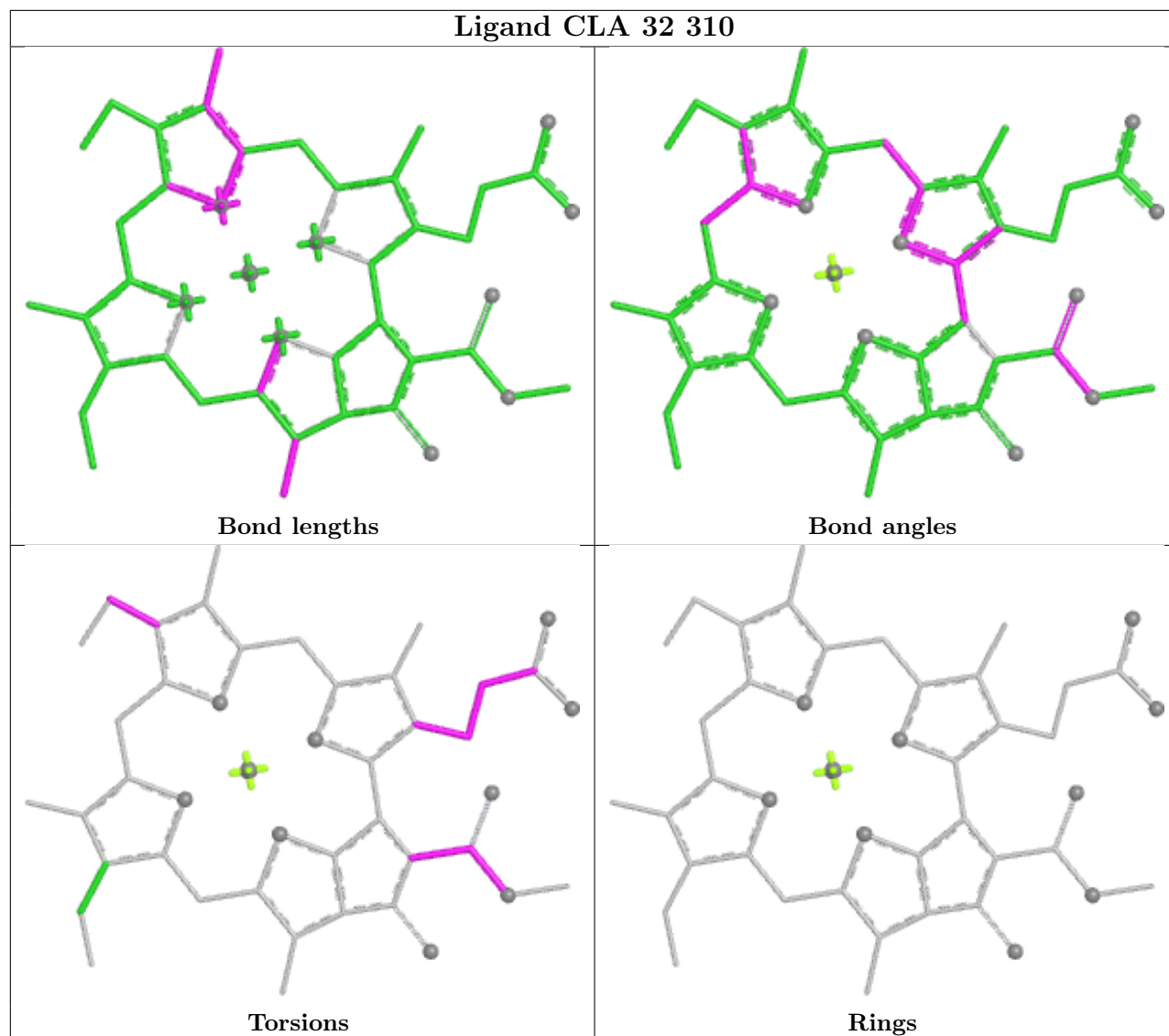


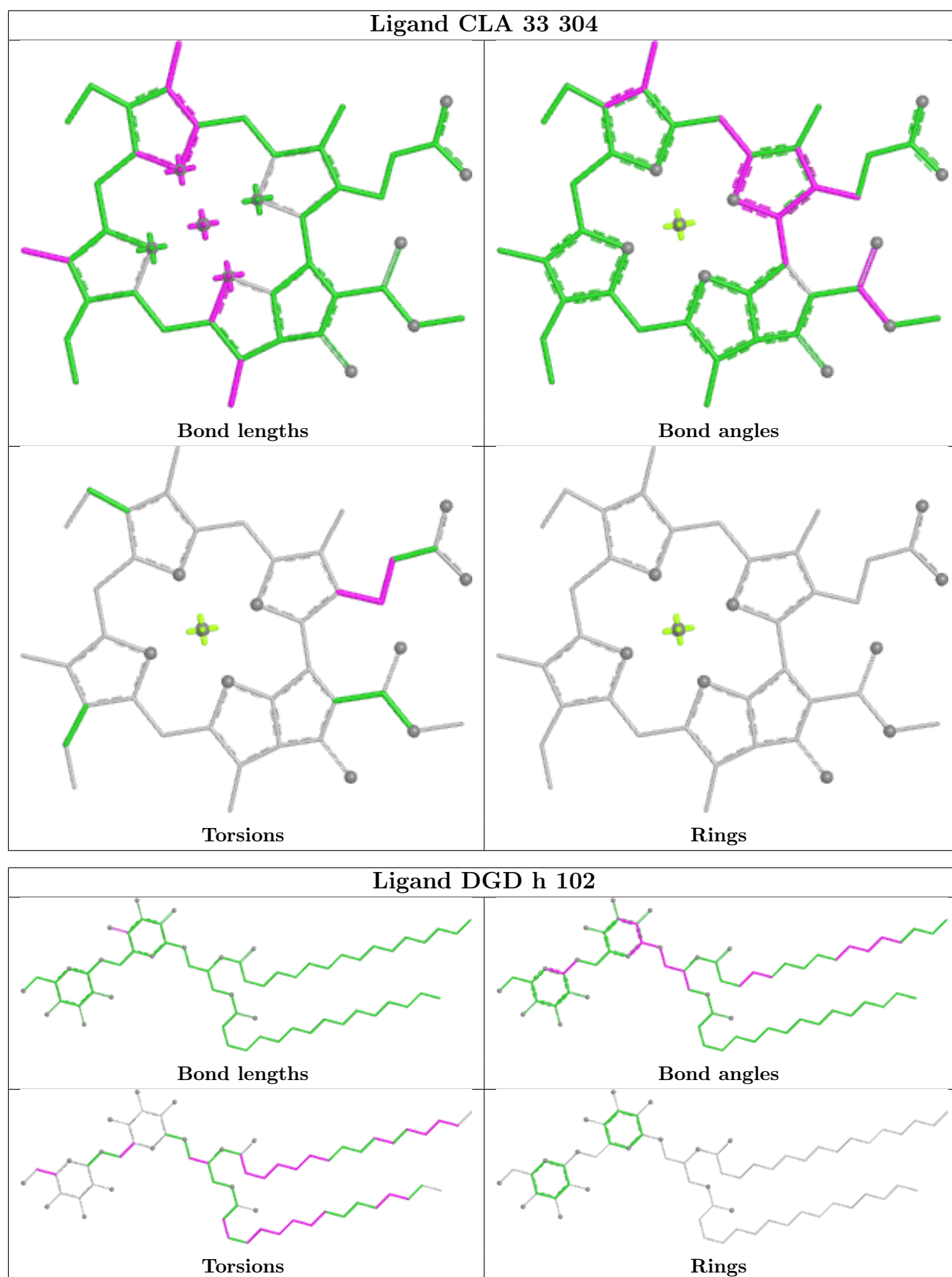


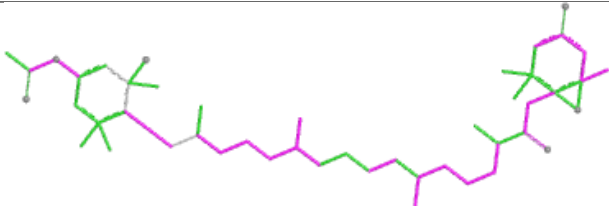
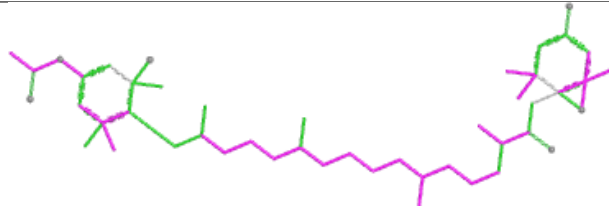
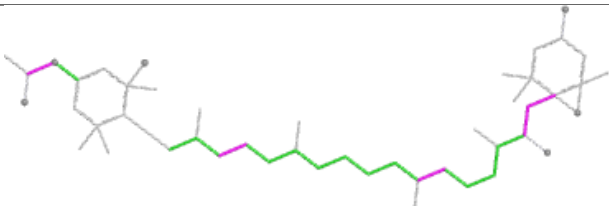
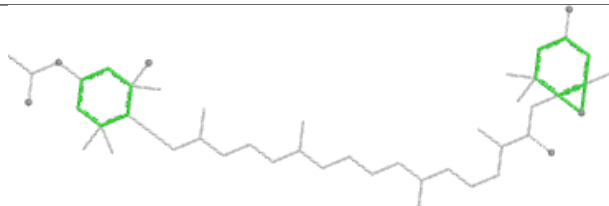


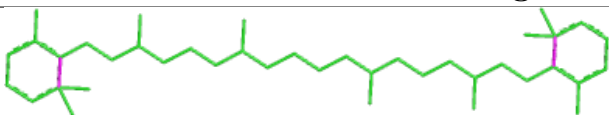
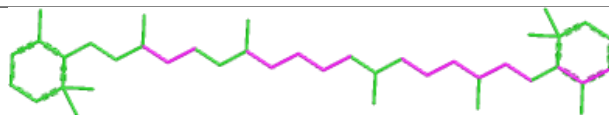
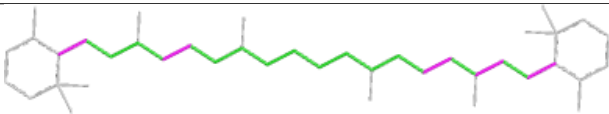
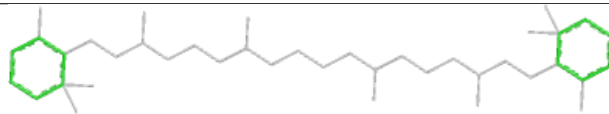


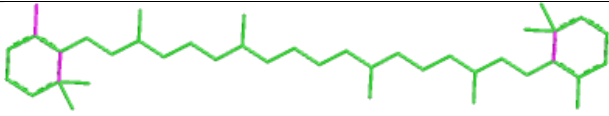
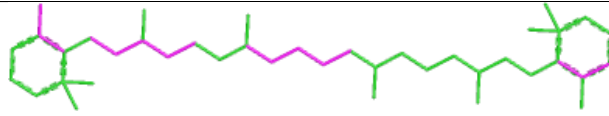
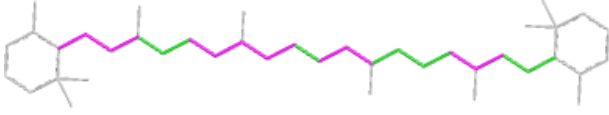
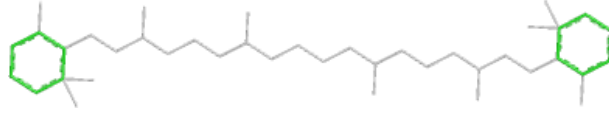


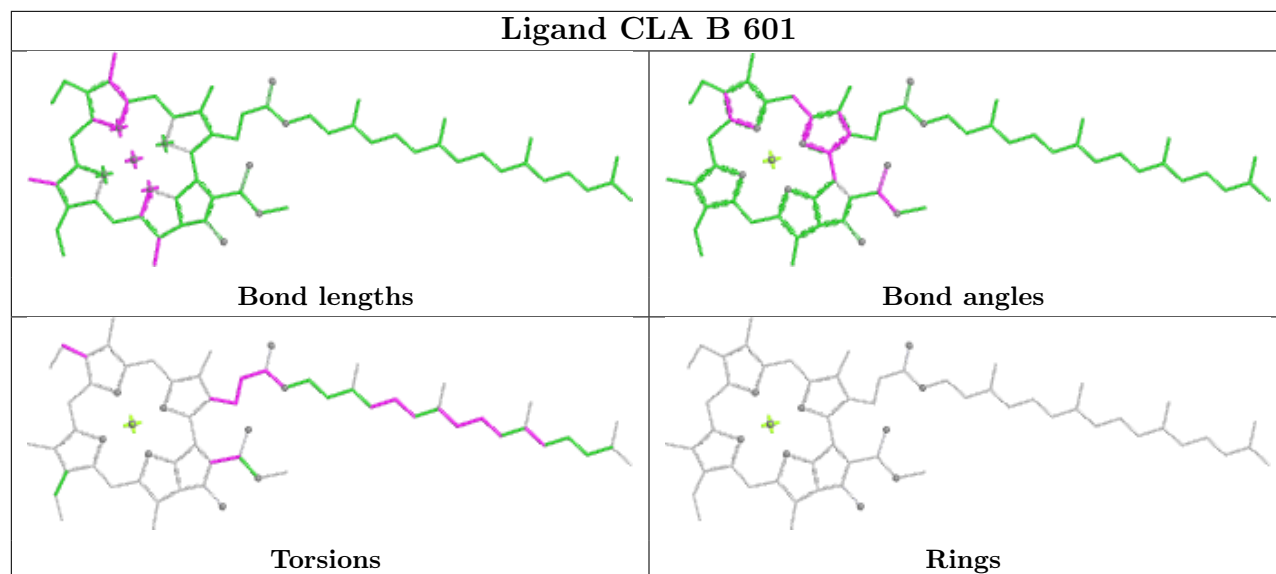
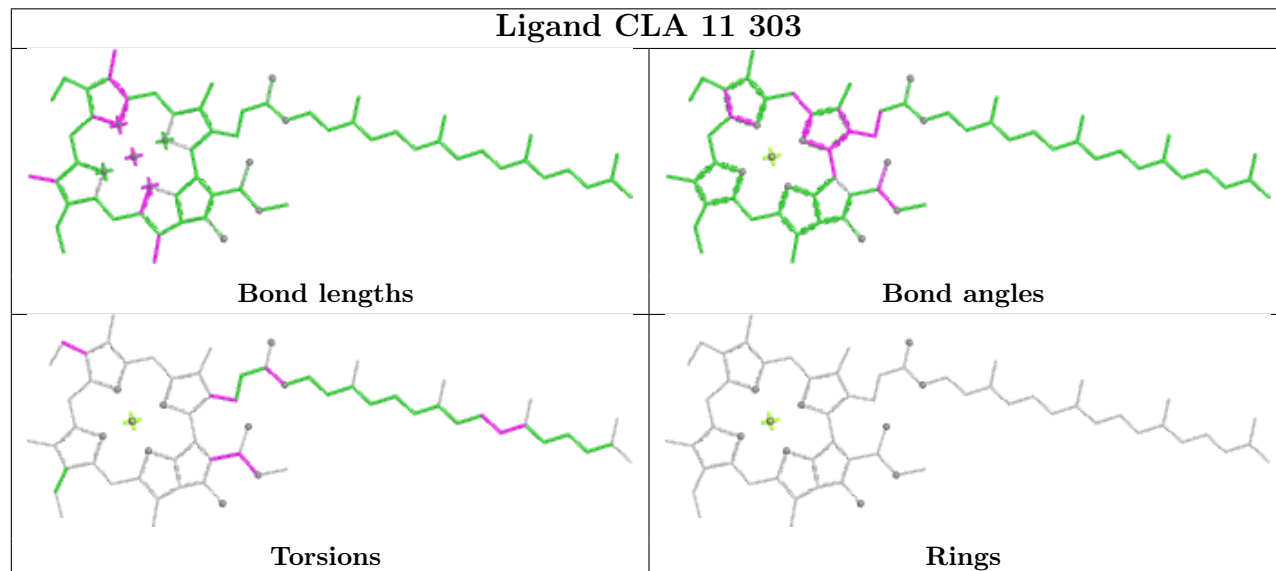


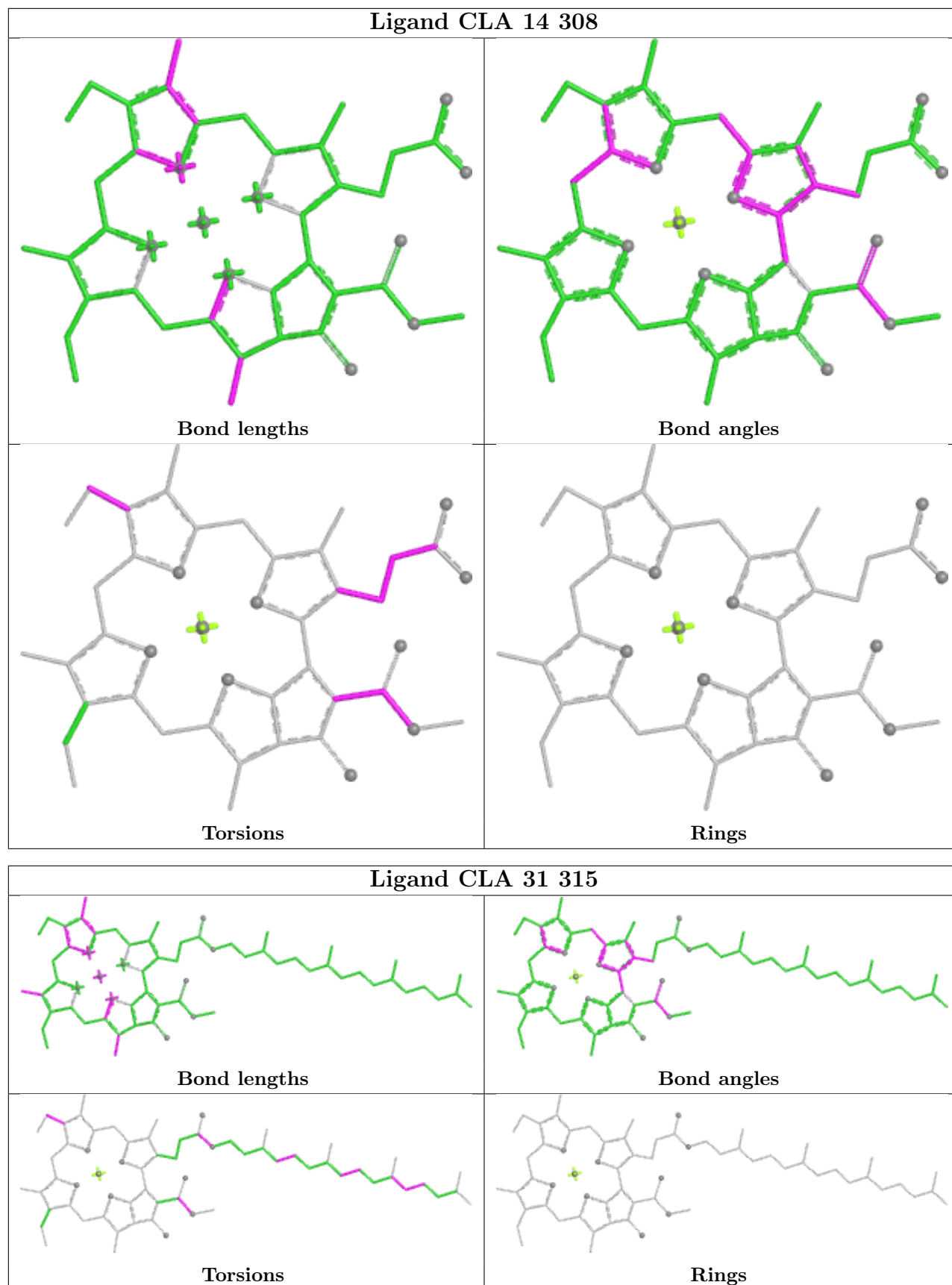


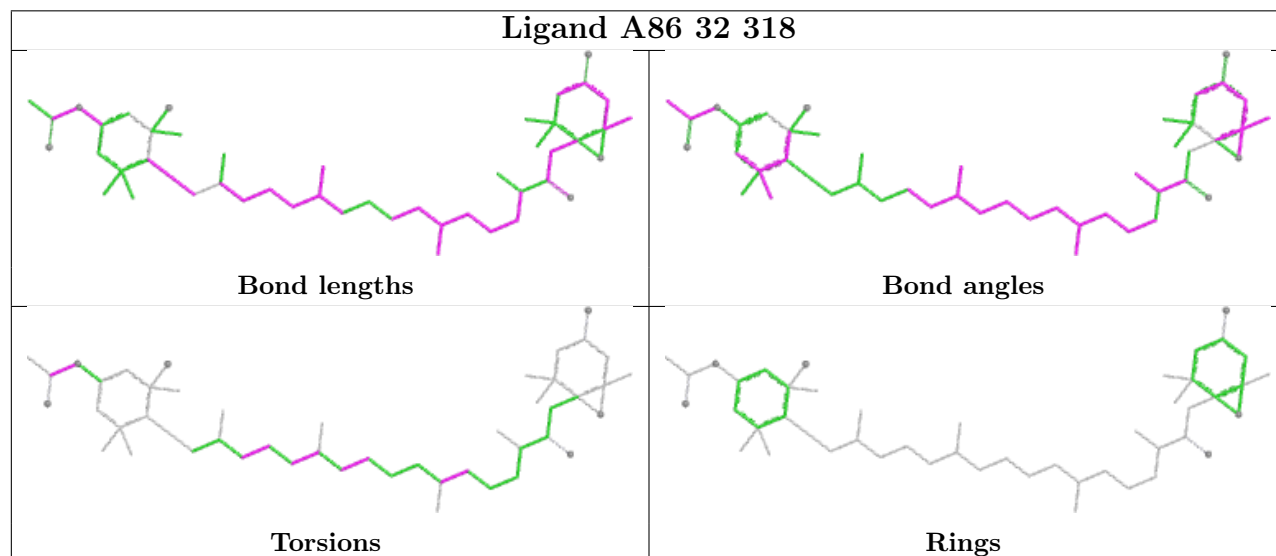
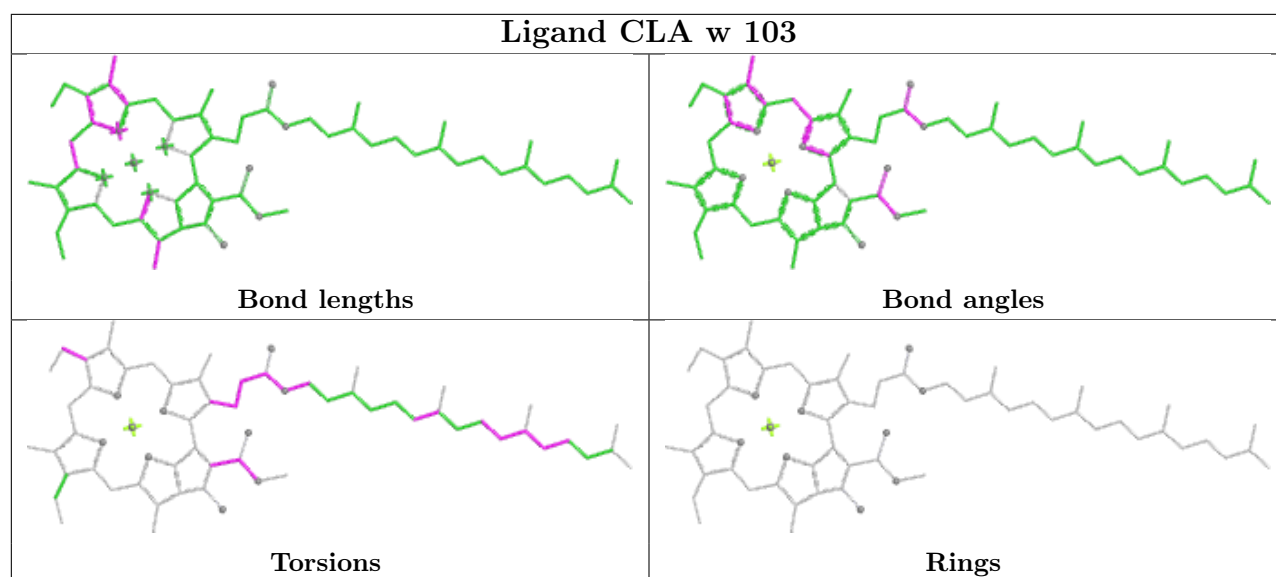
Ligand A86 33 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

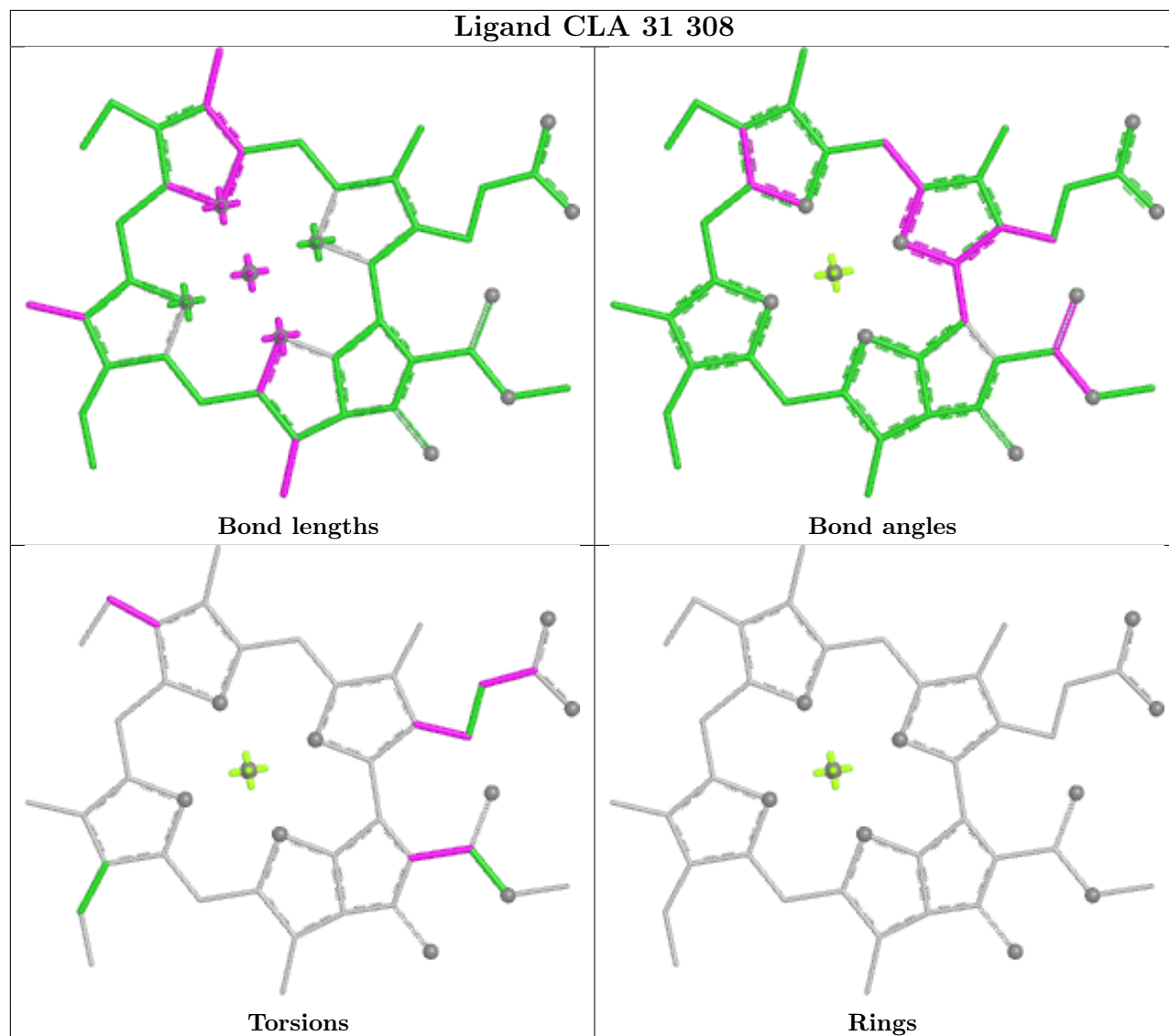
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Bond lengths	Bond angles
	
Torsions	Rings

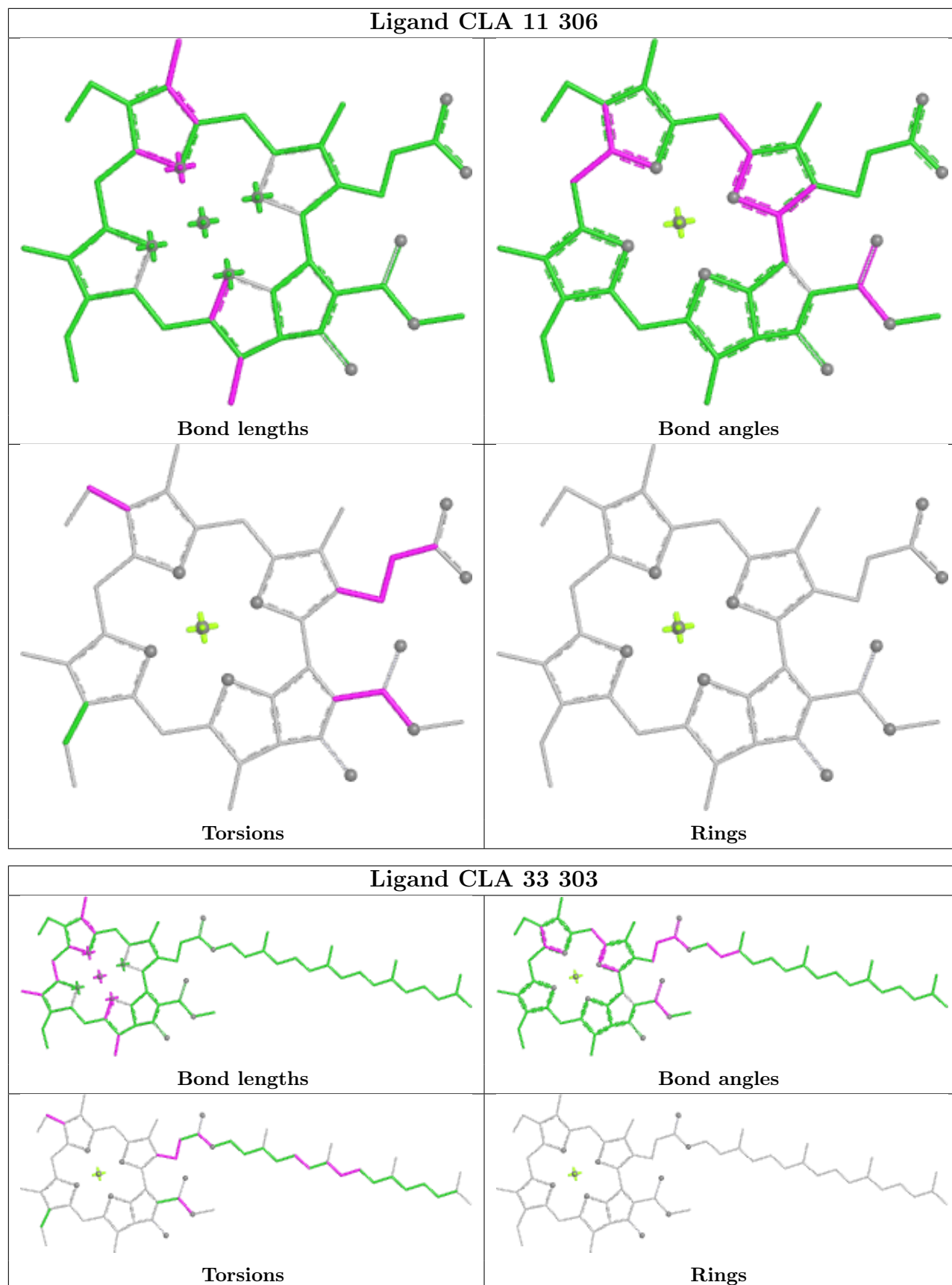
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Bond lengths	Bond angles
	
Torsions	Rings

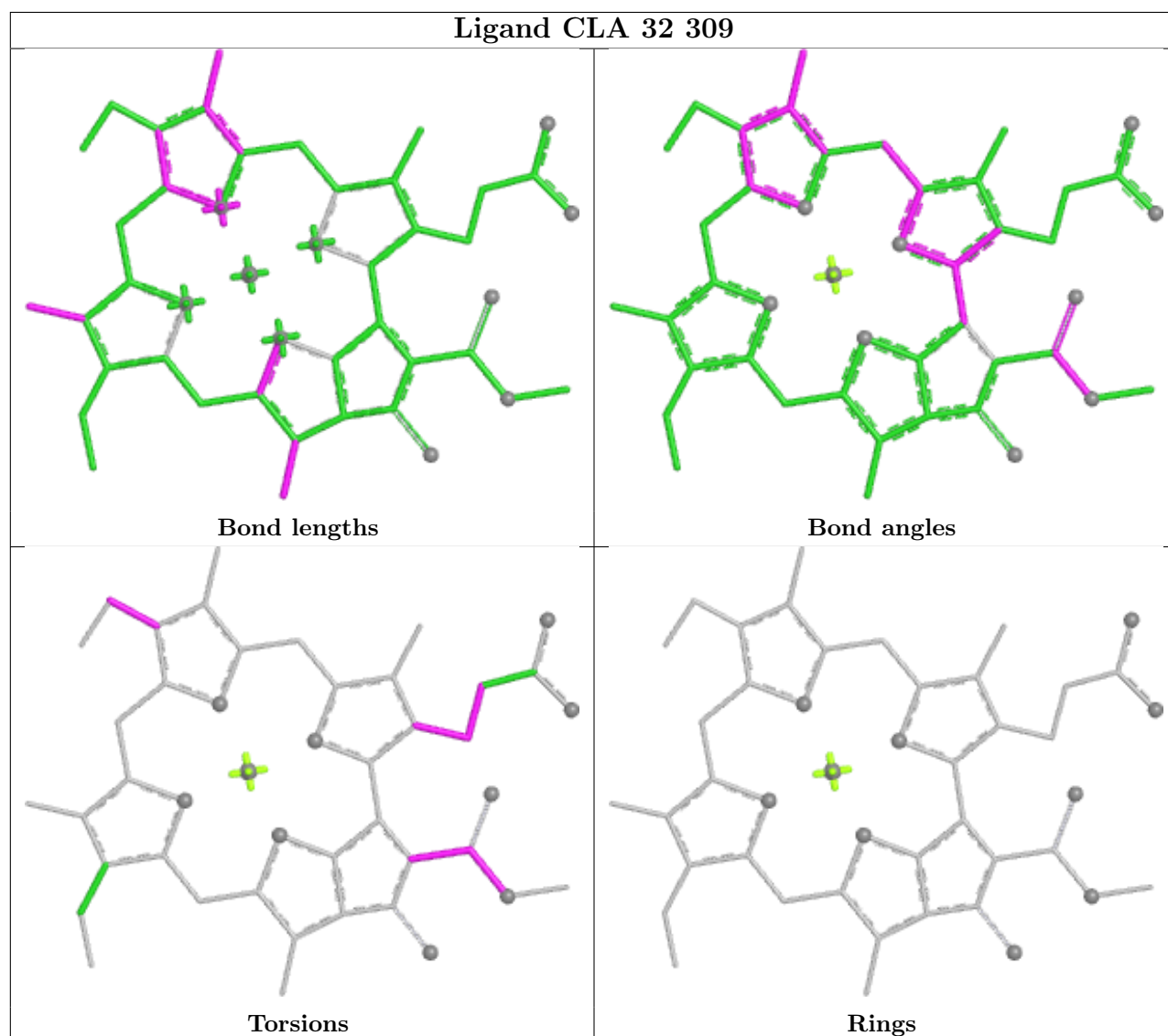
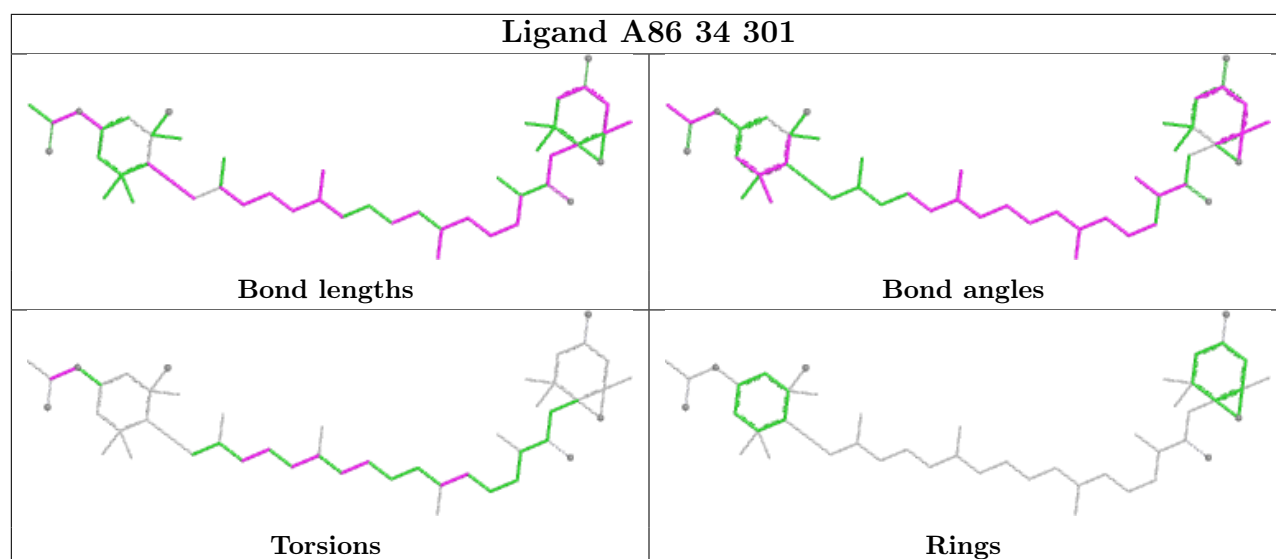
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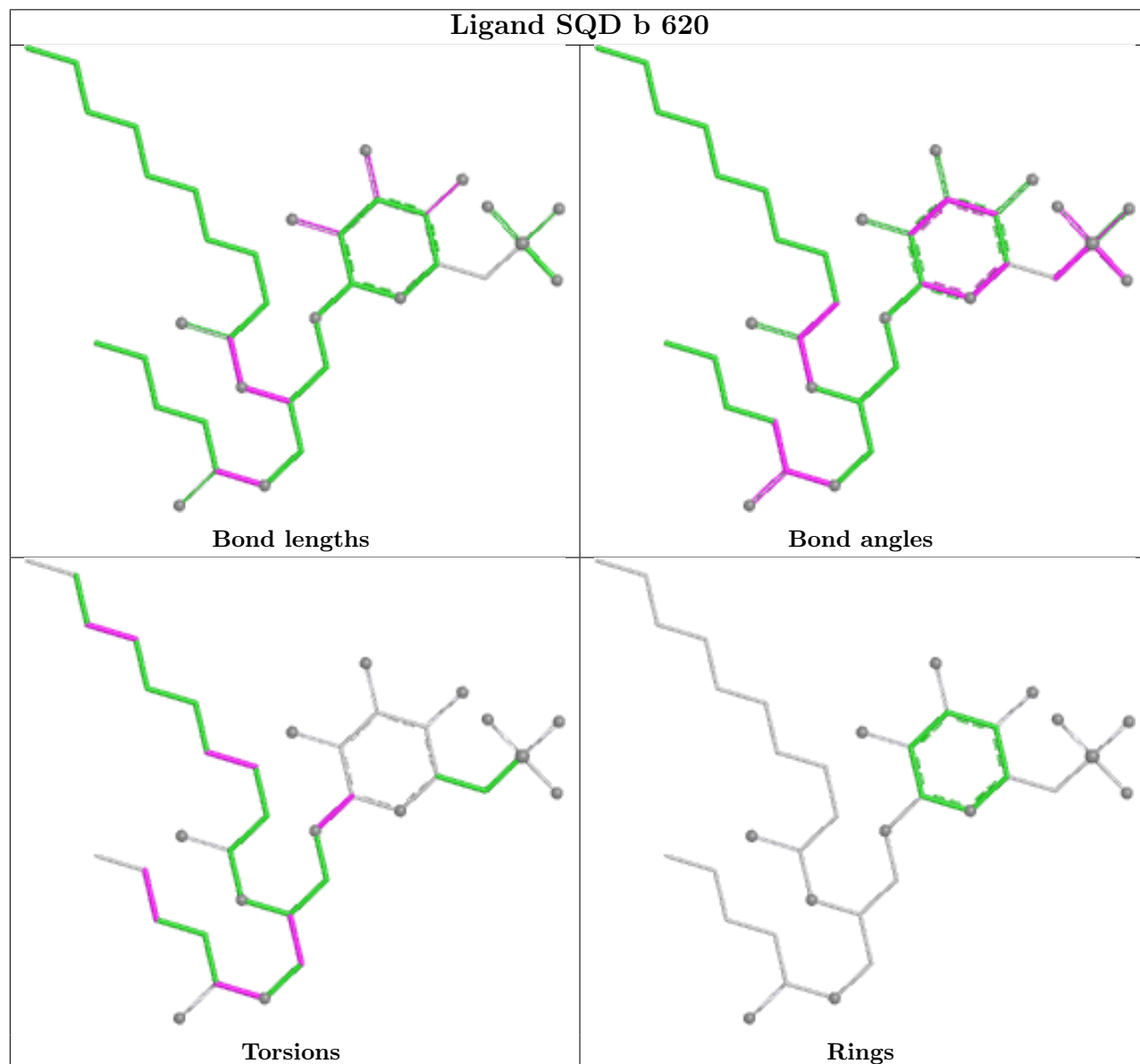
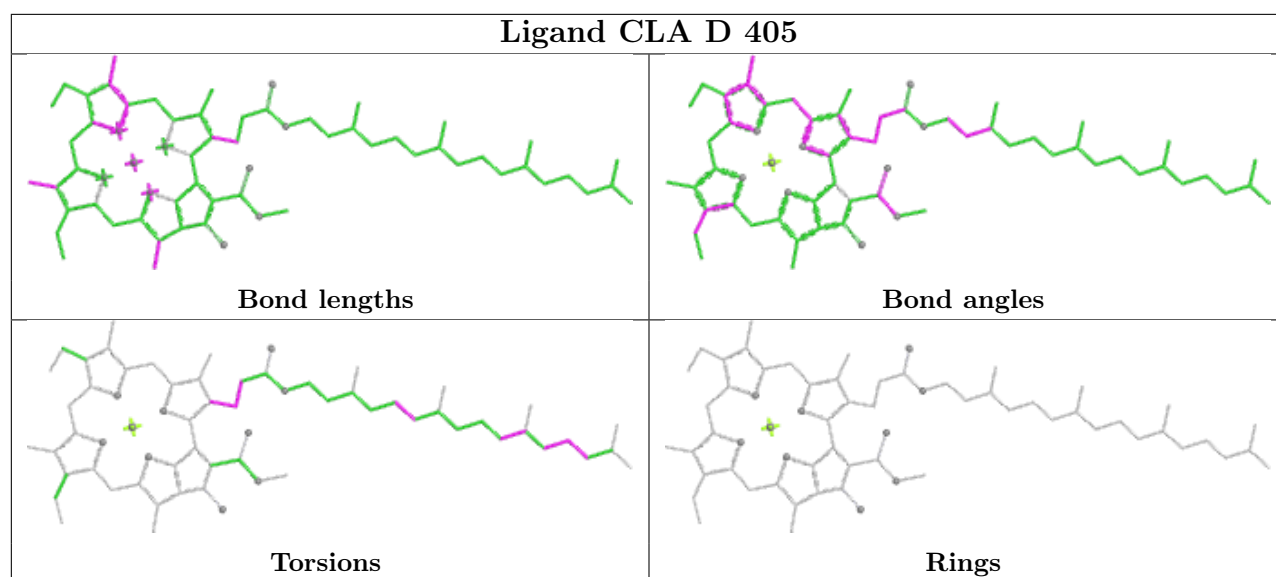


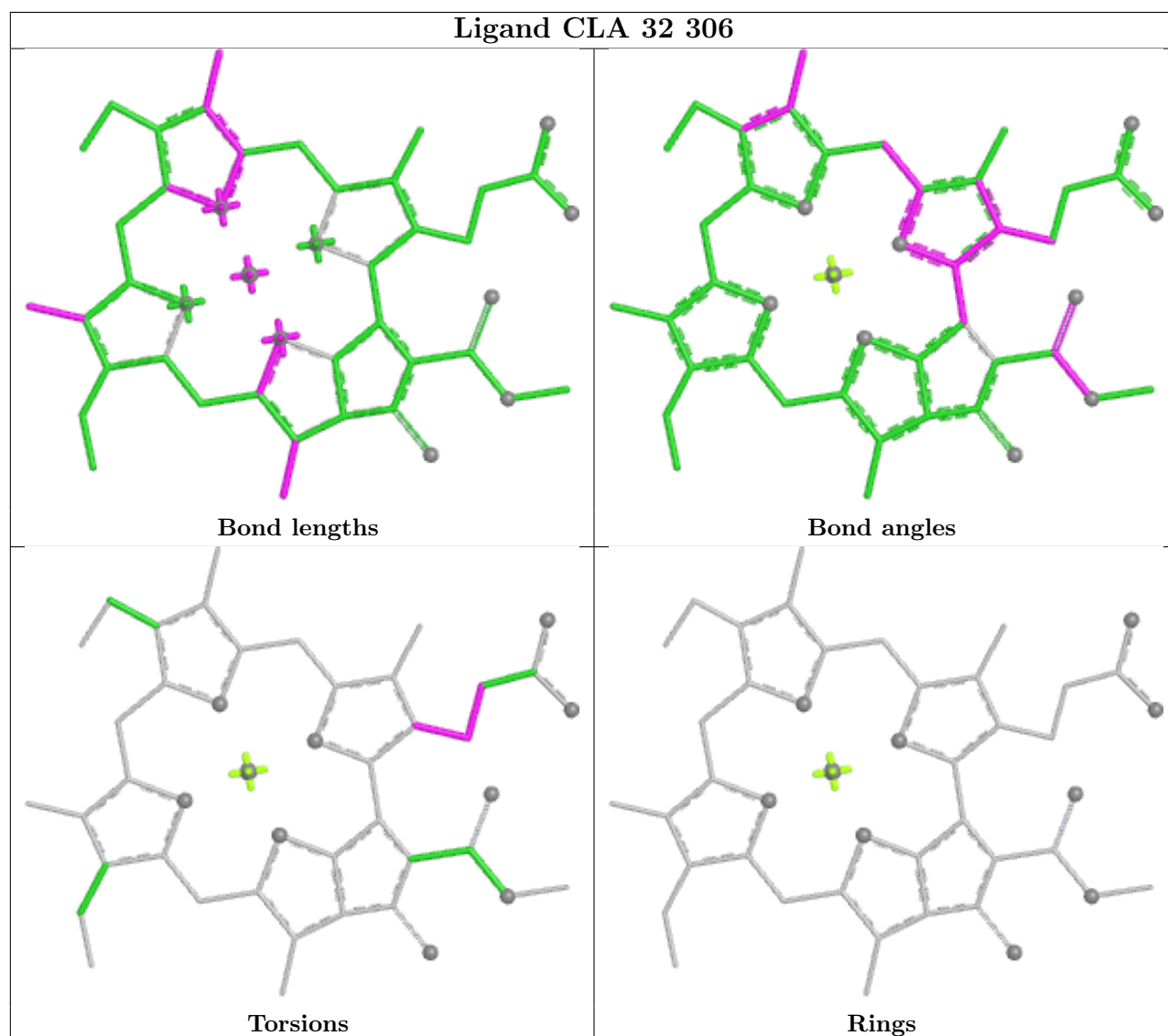
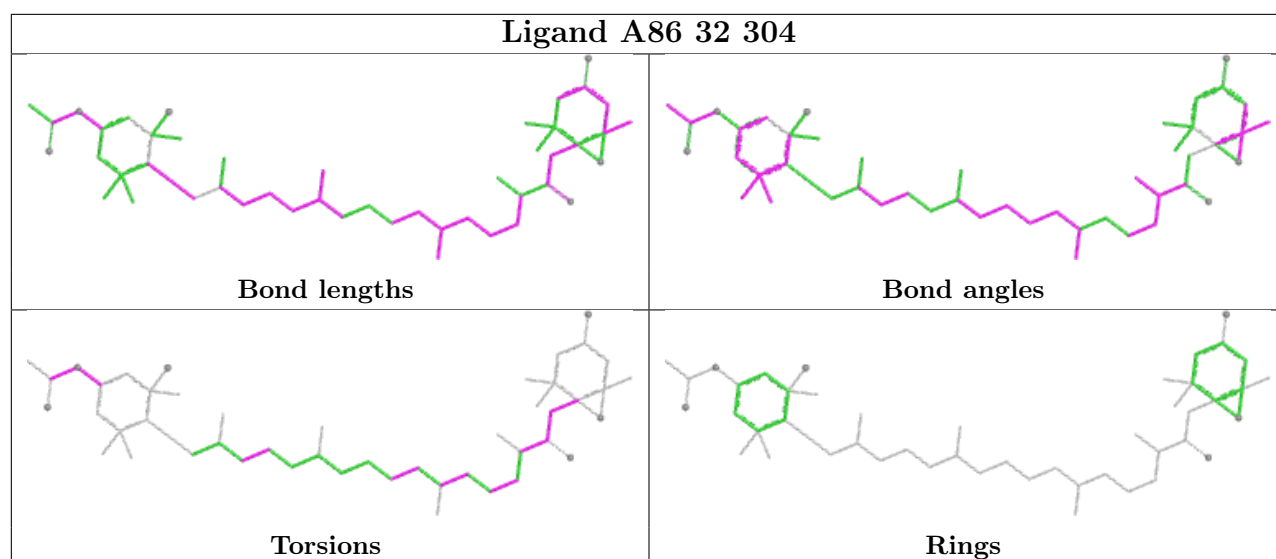


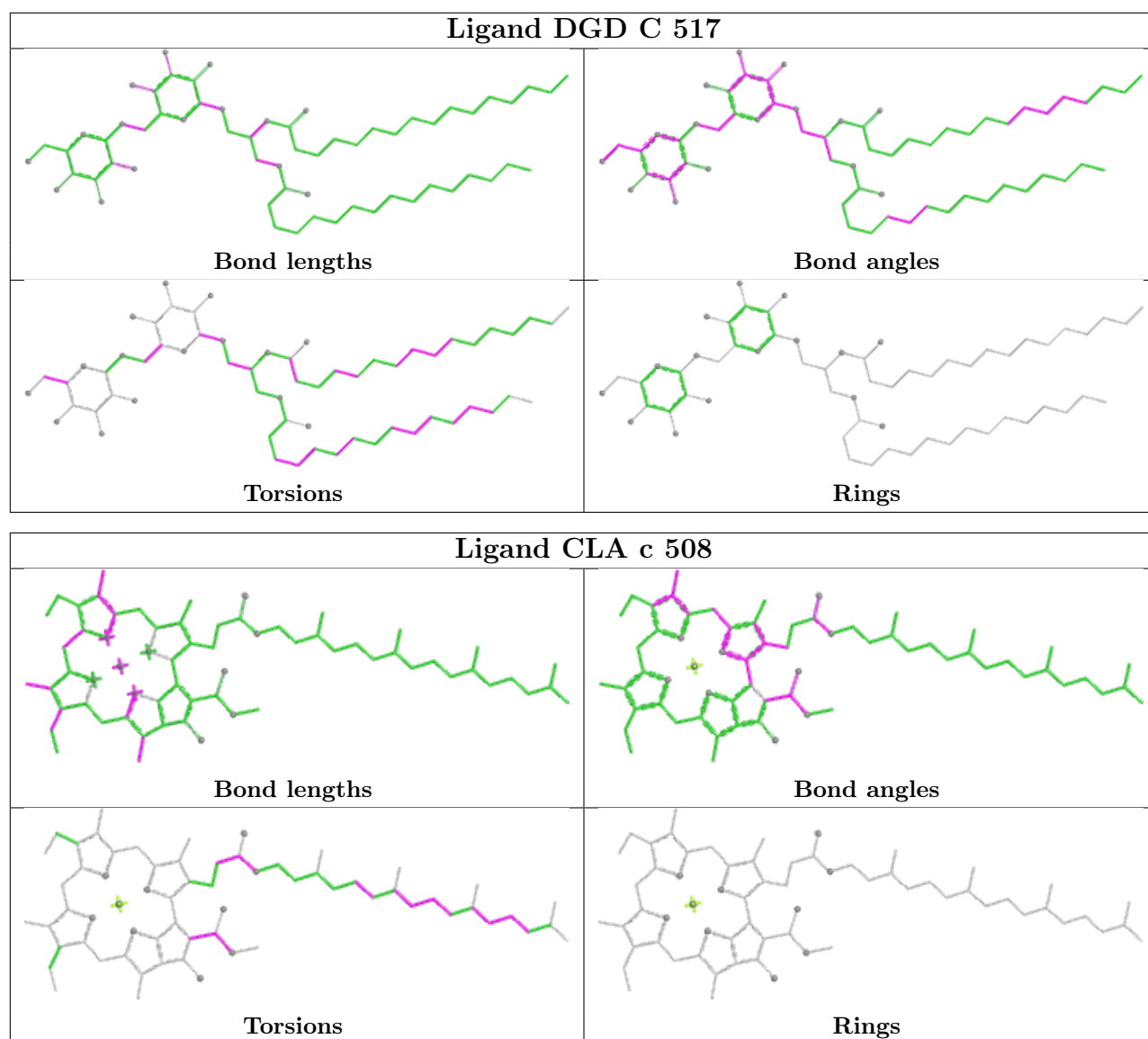


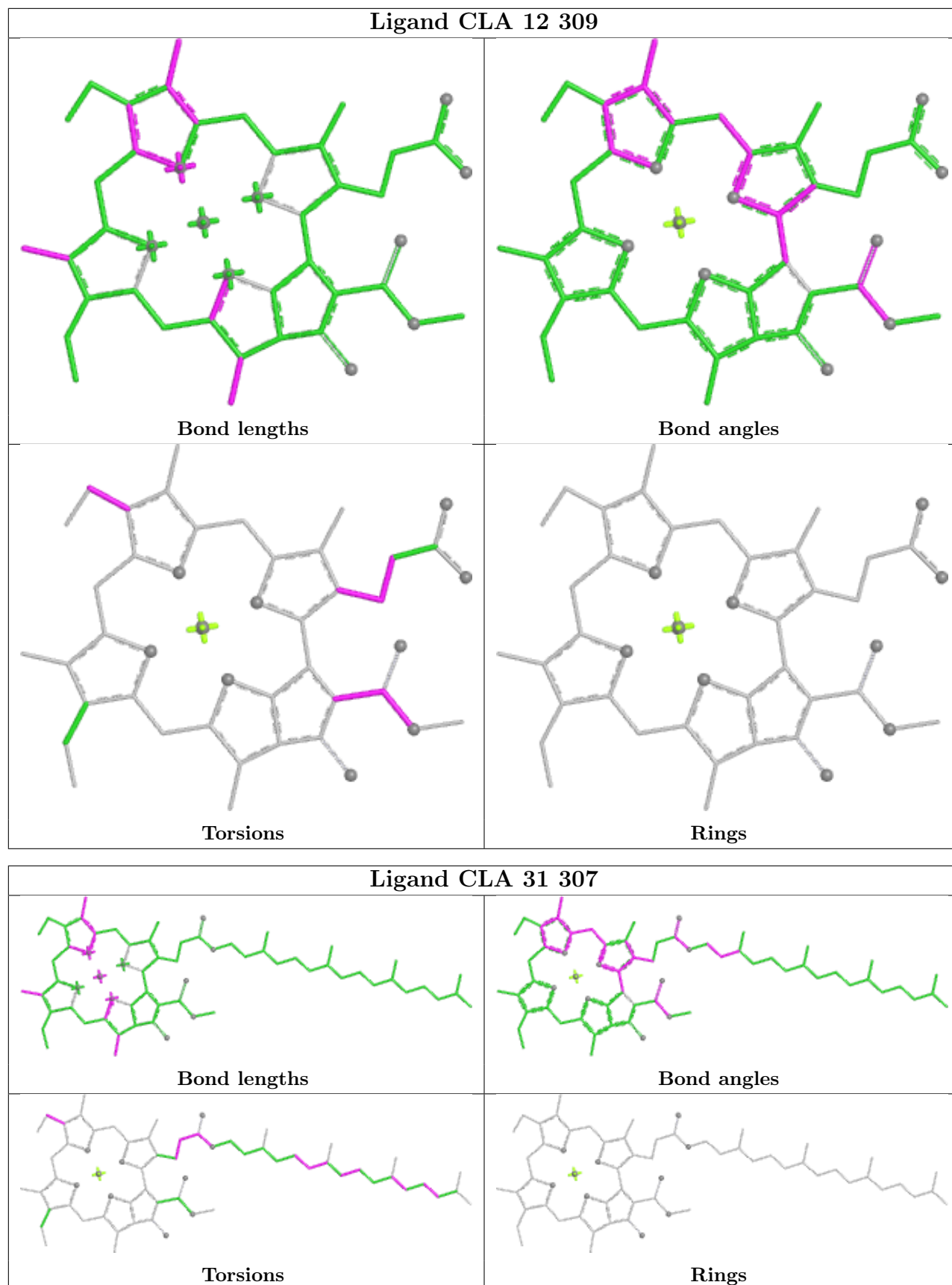


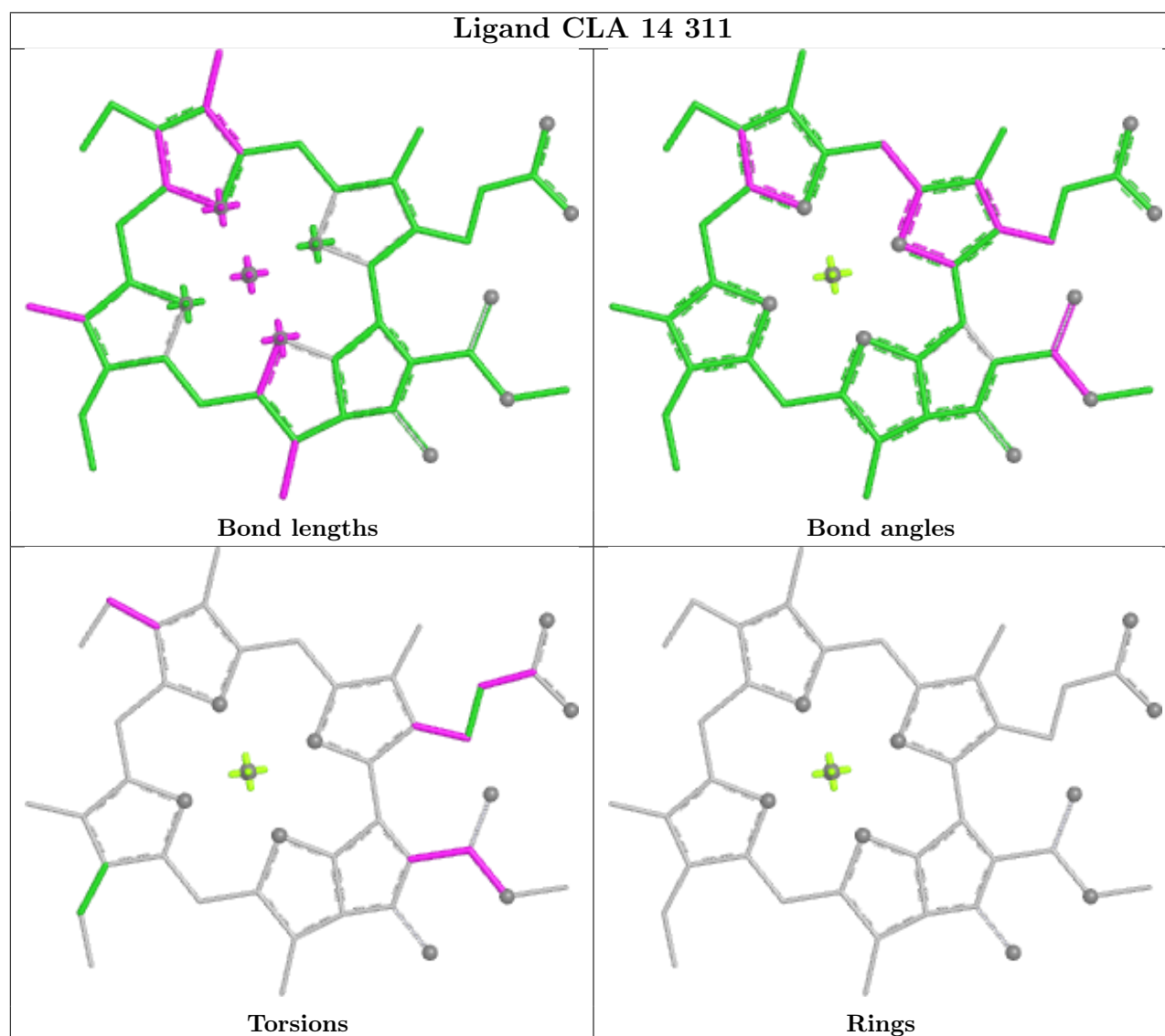
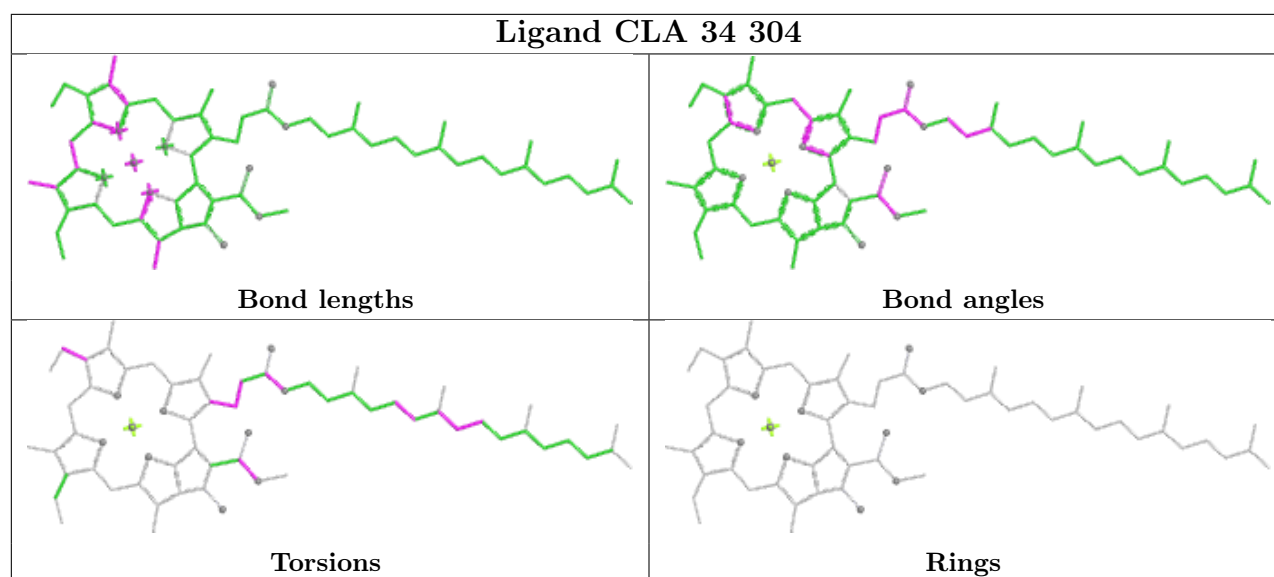


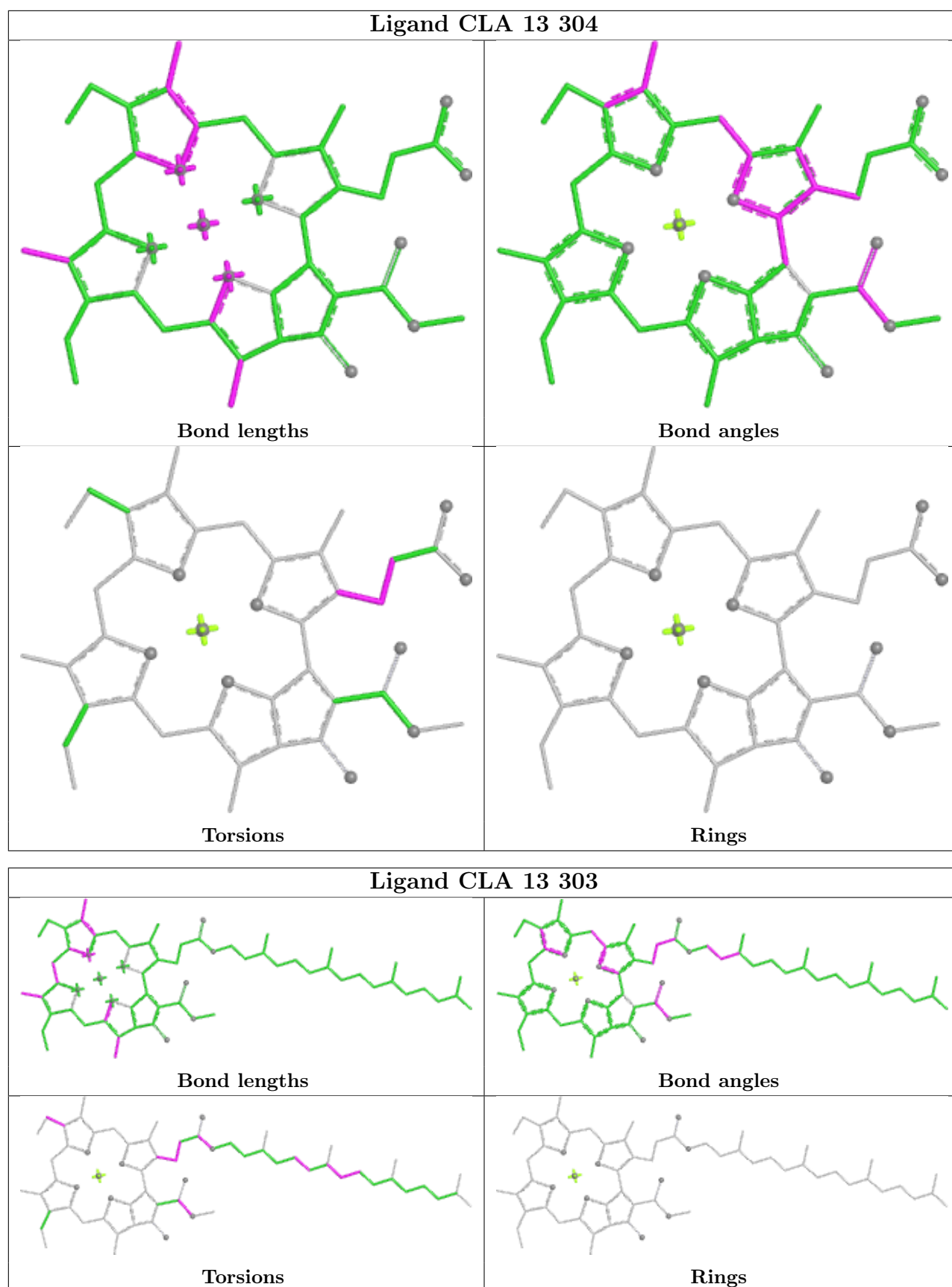




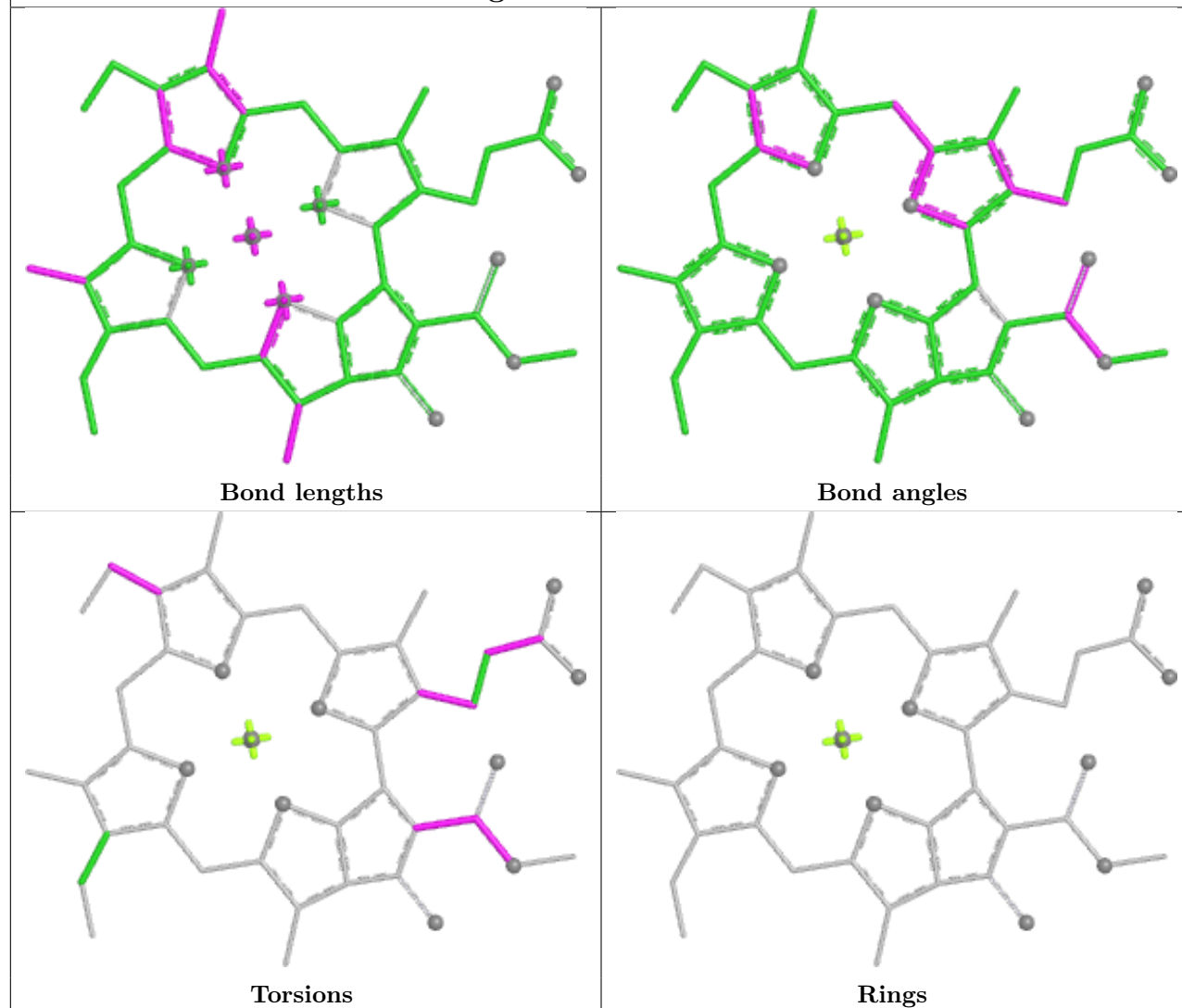




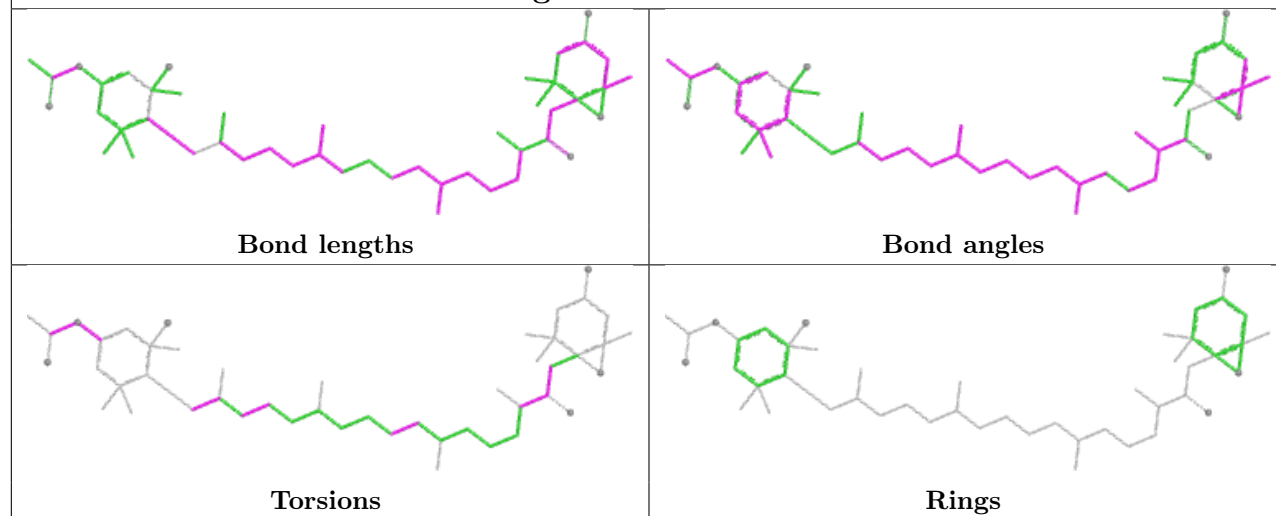


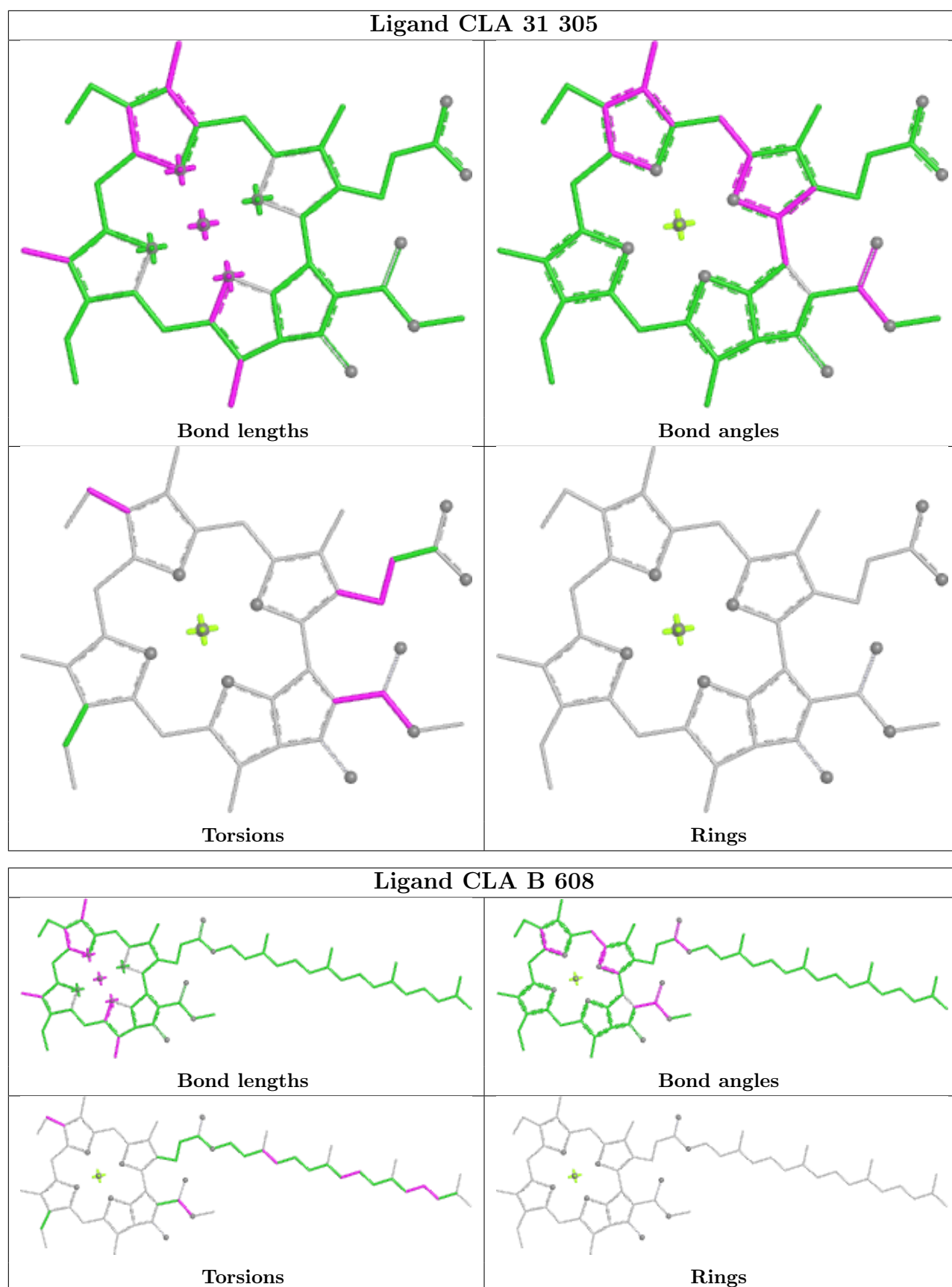


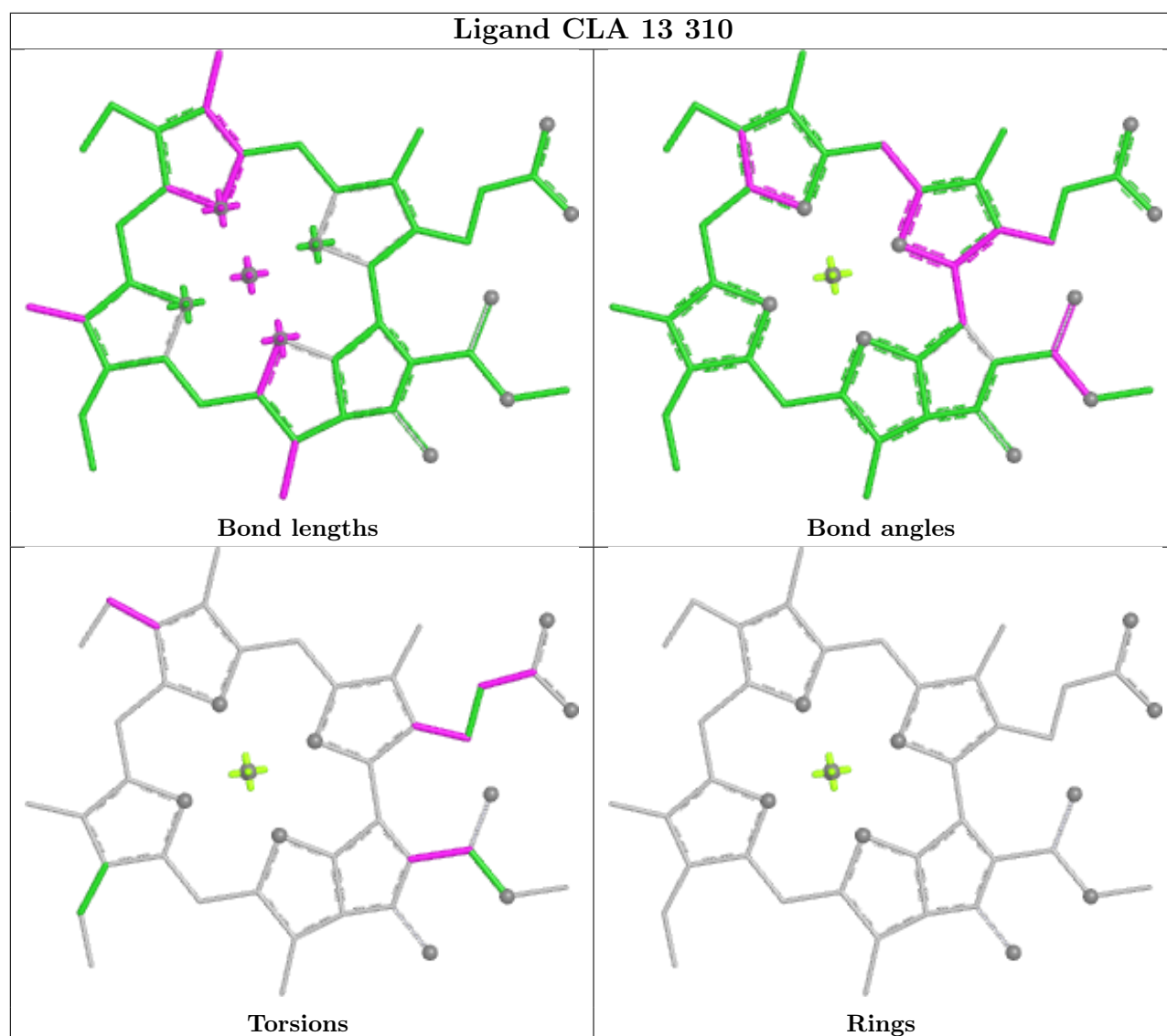
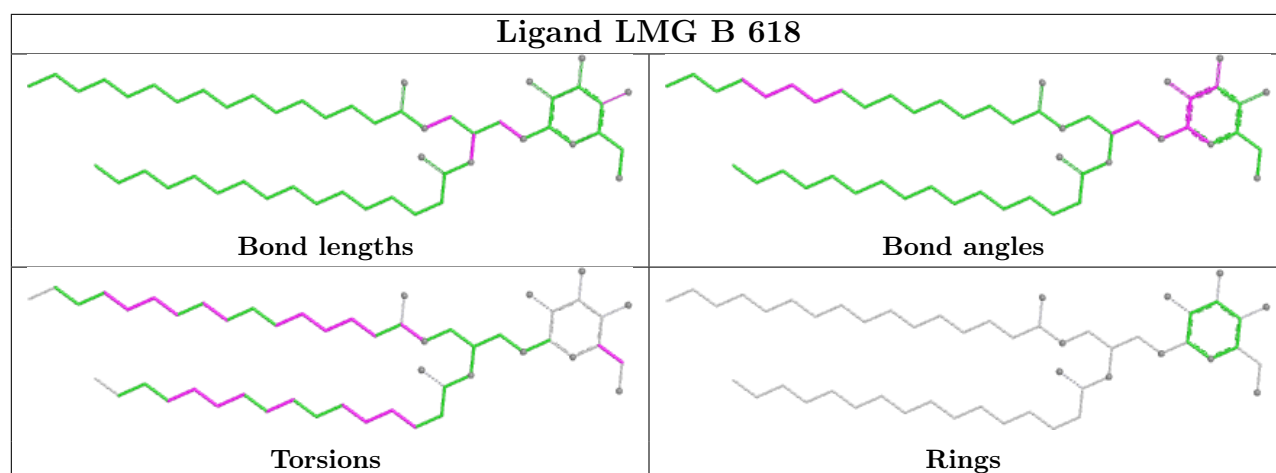
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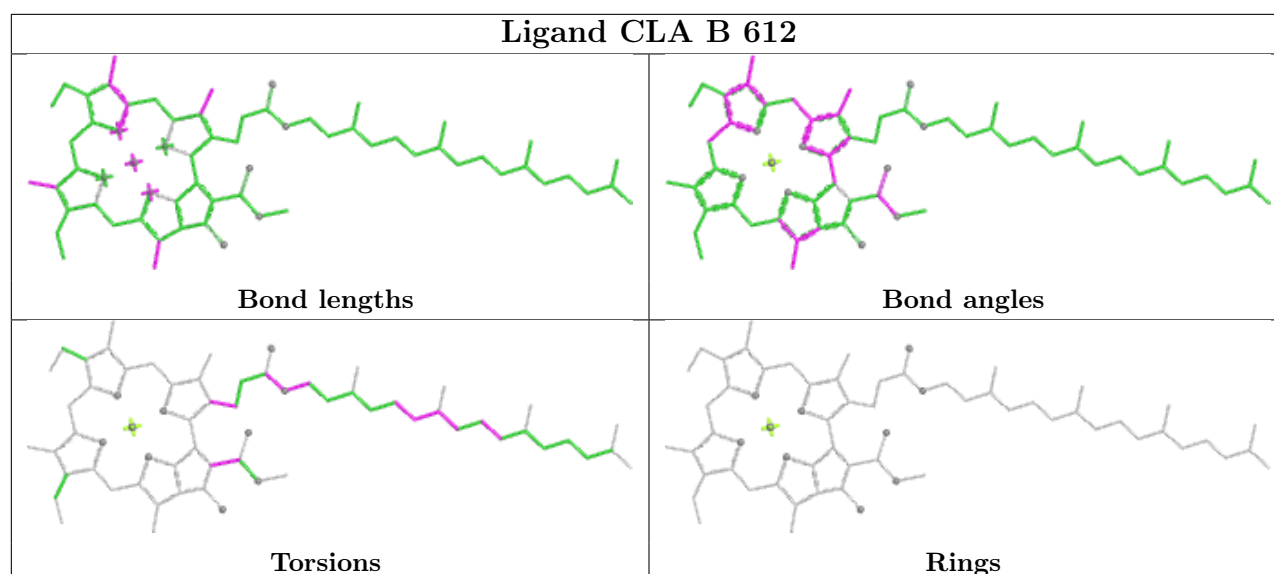
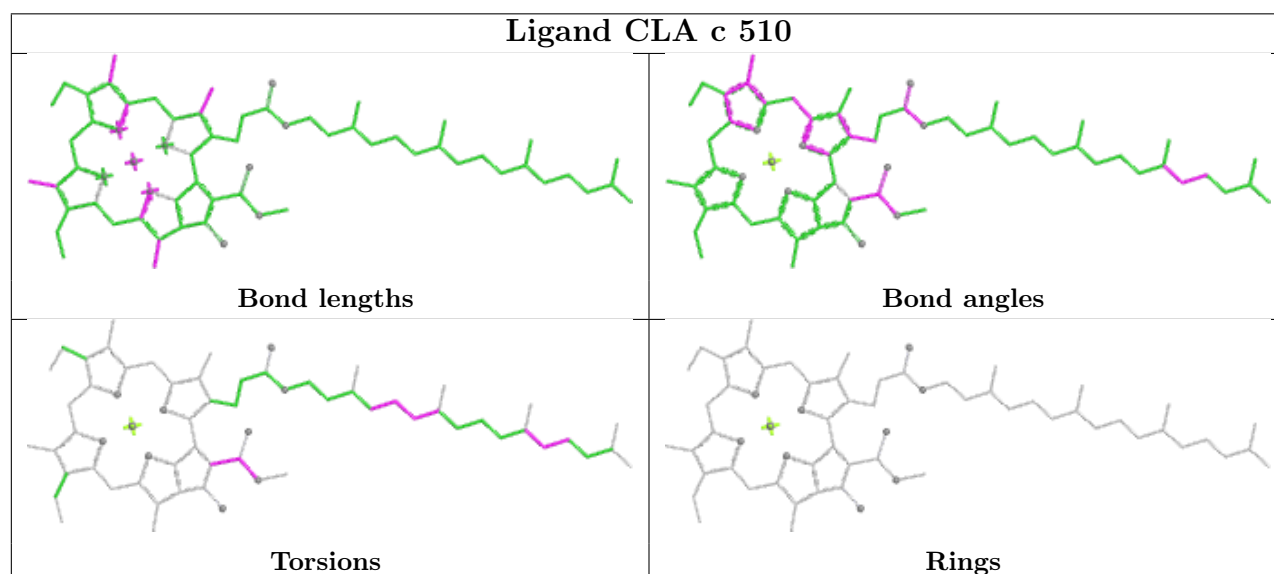
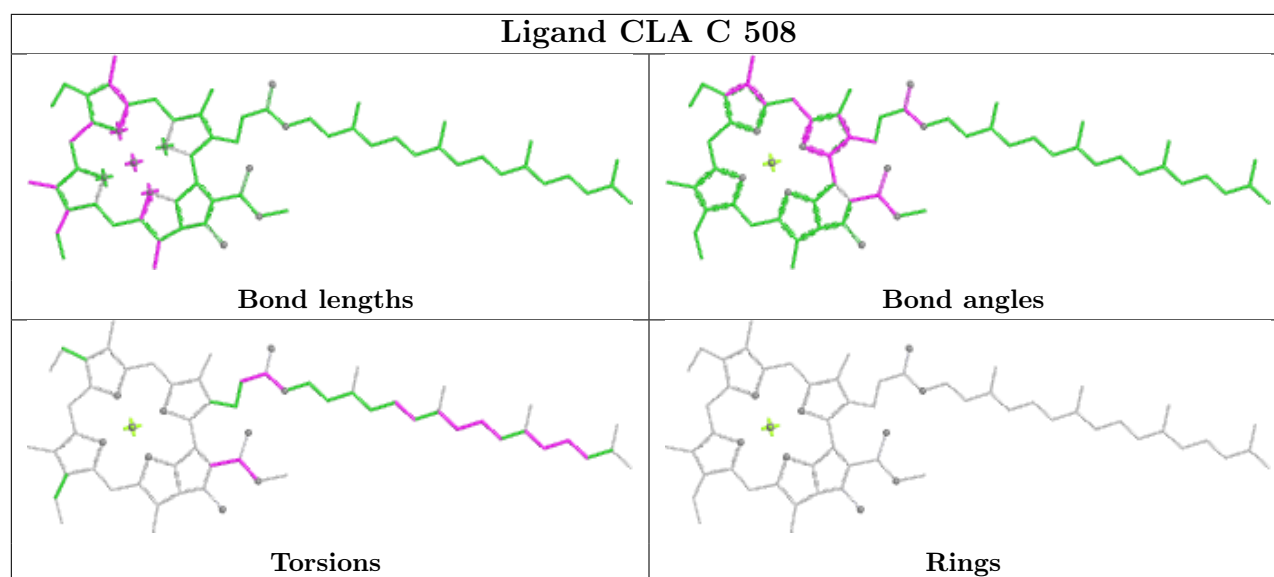


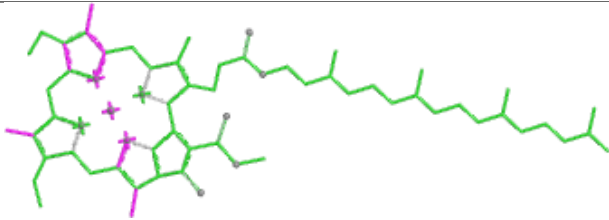
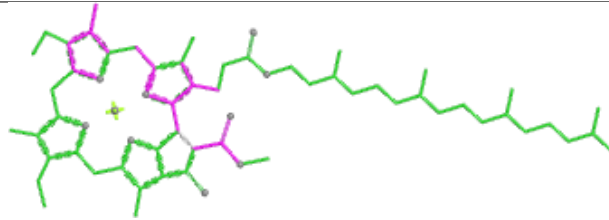
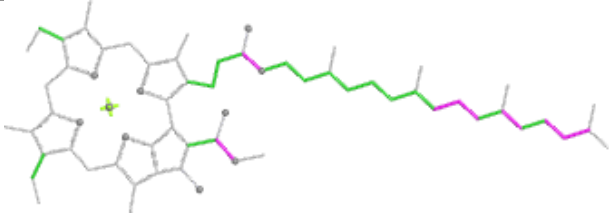
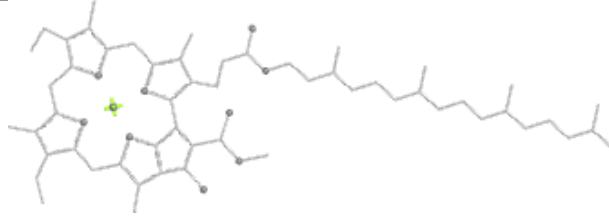
Ligand A86 32 316

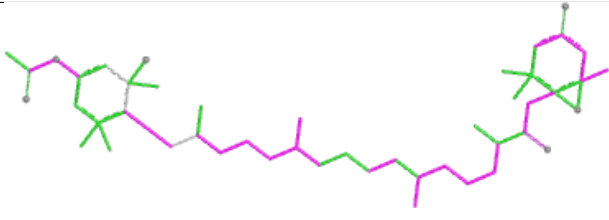
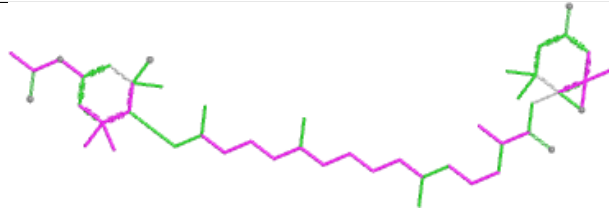
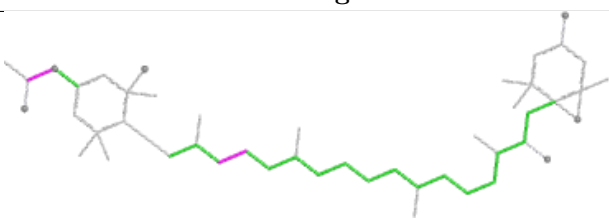
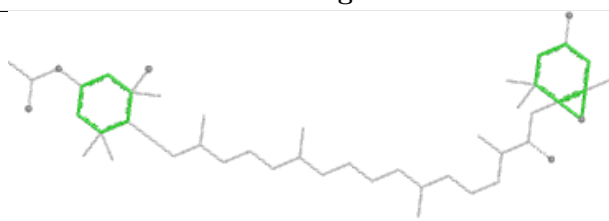


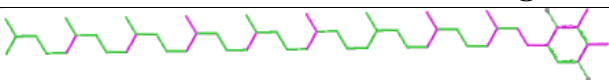
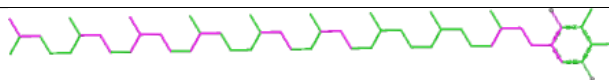
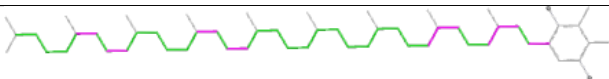
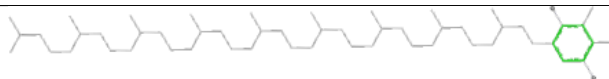


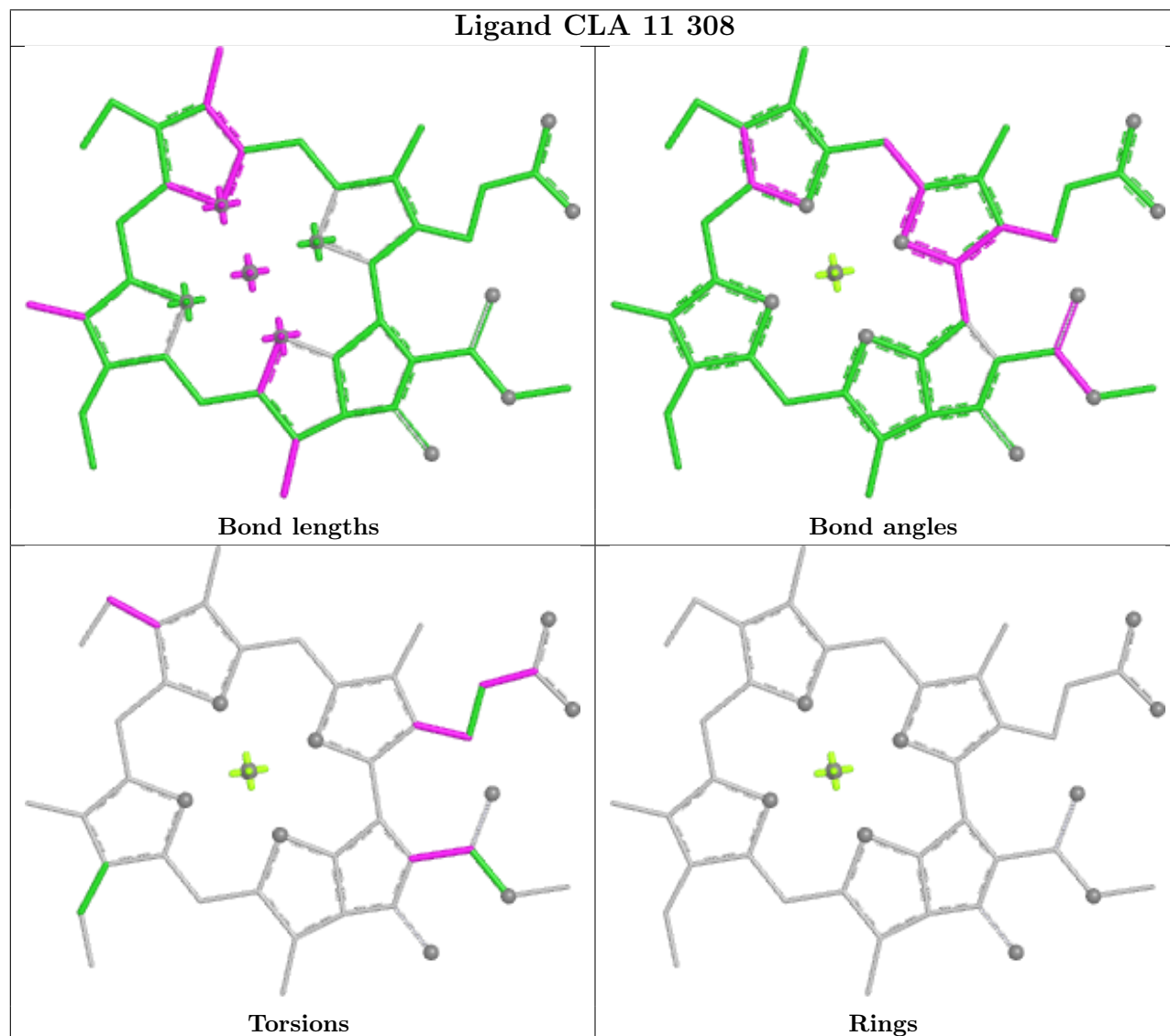
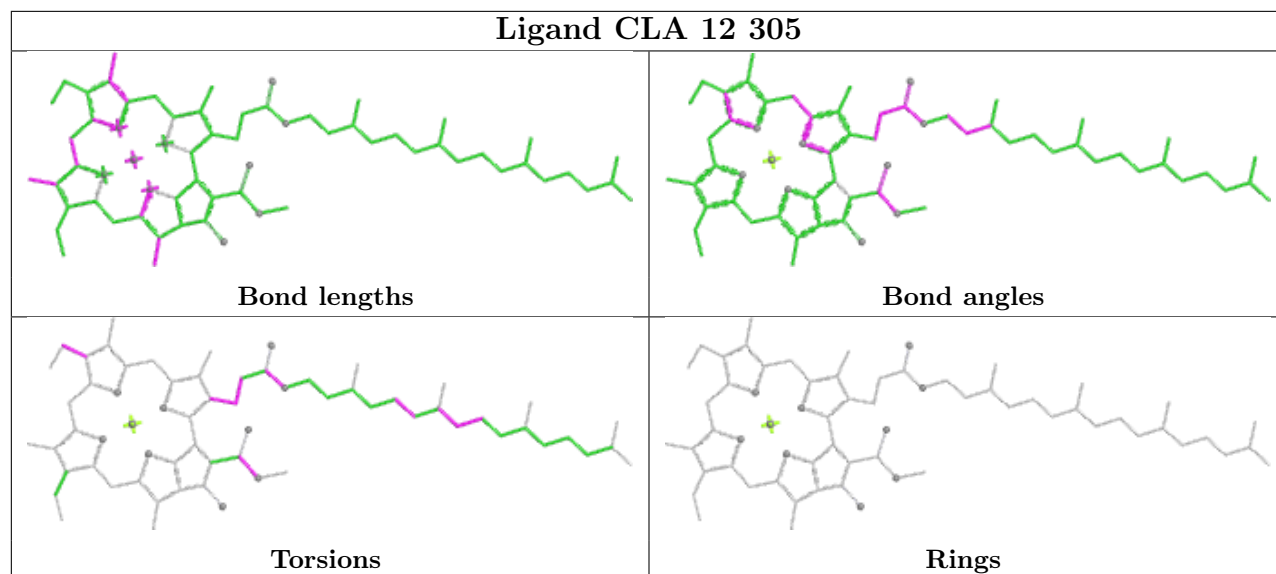


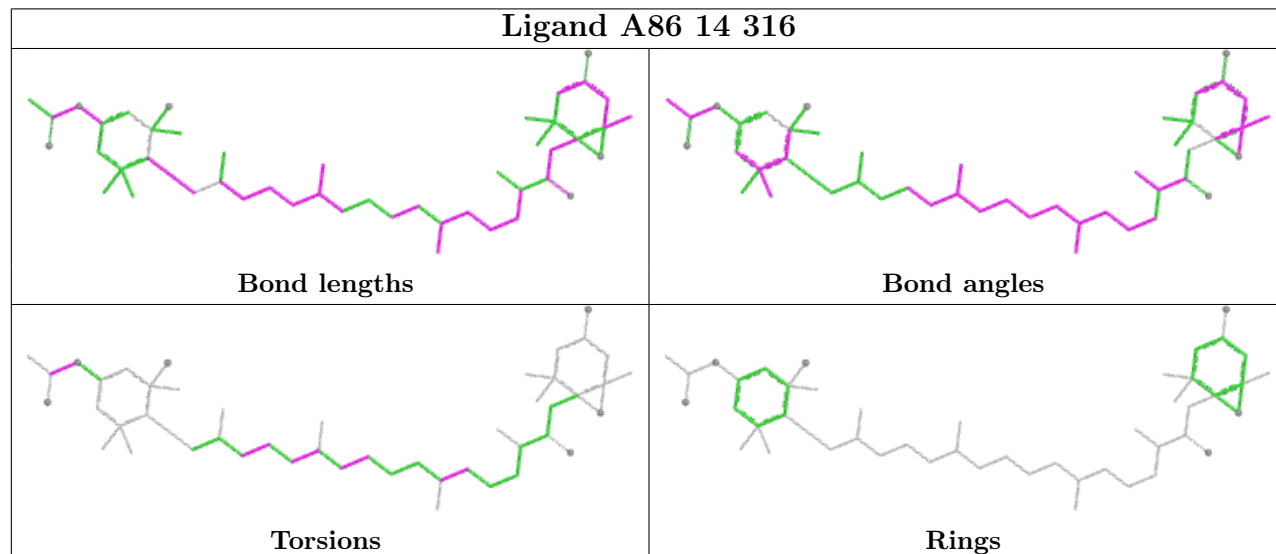
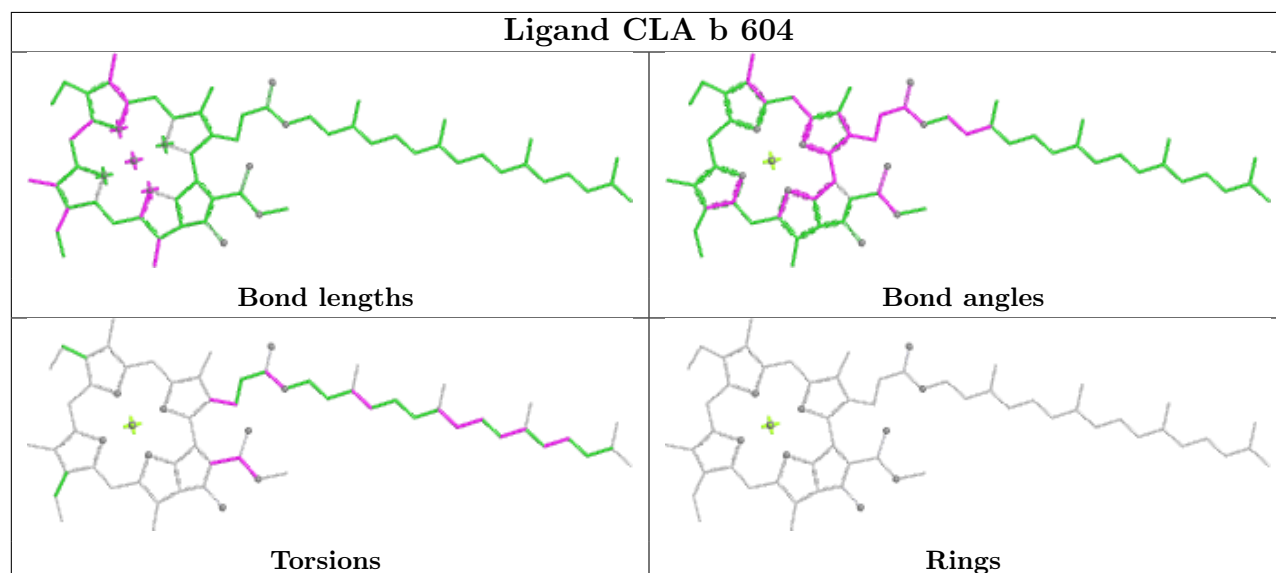
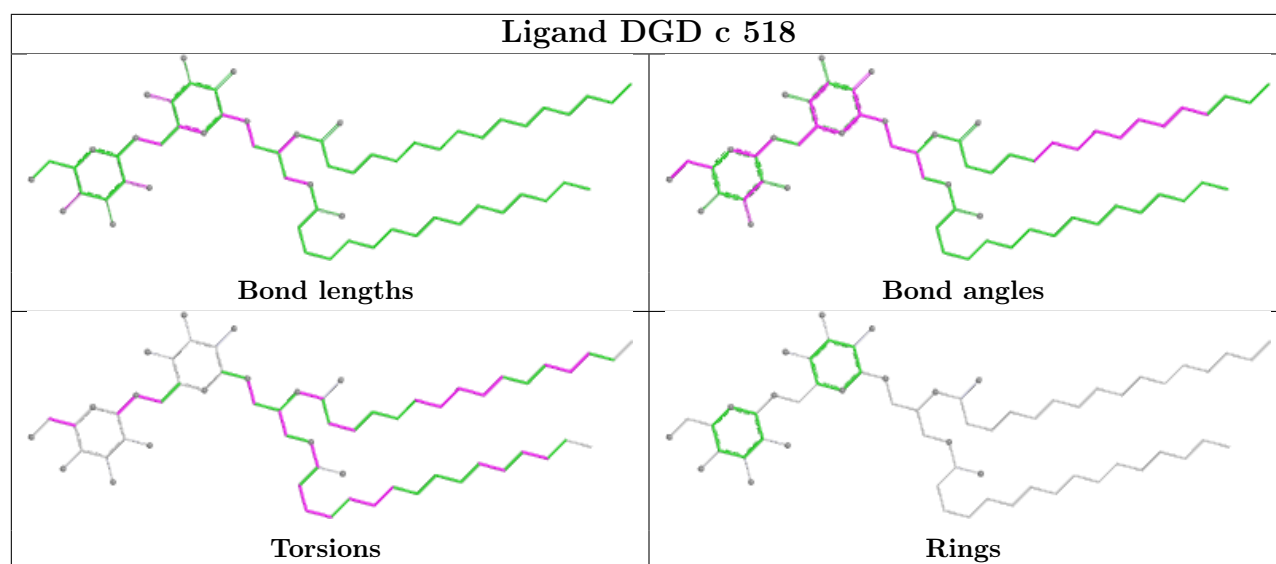


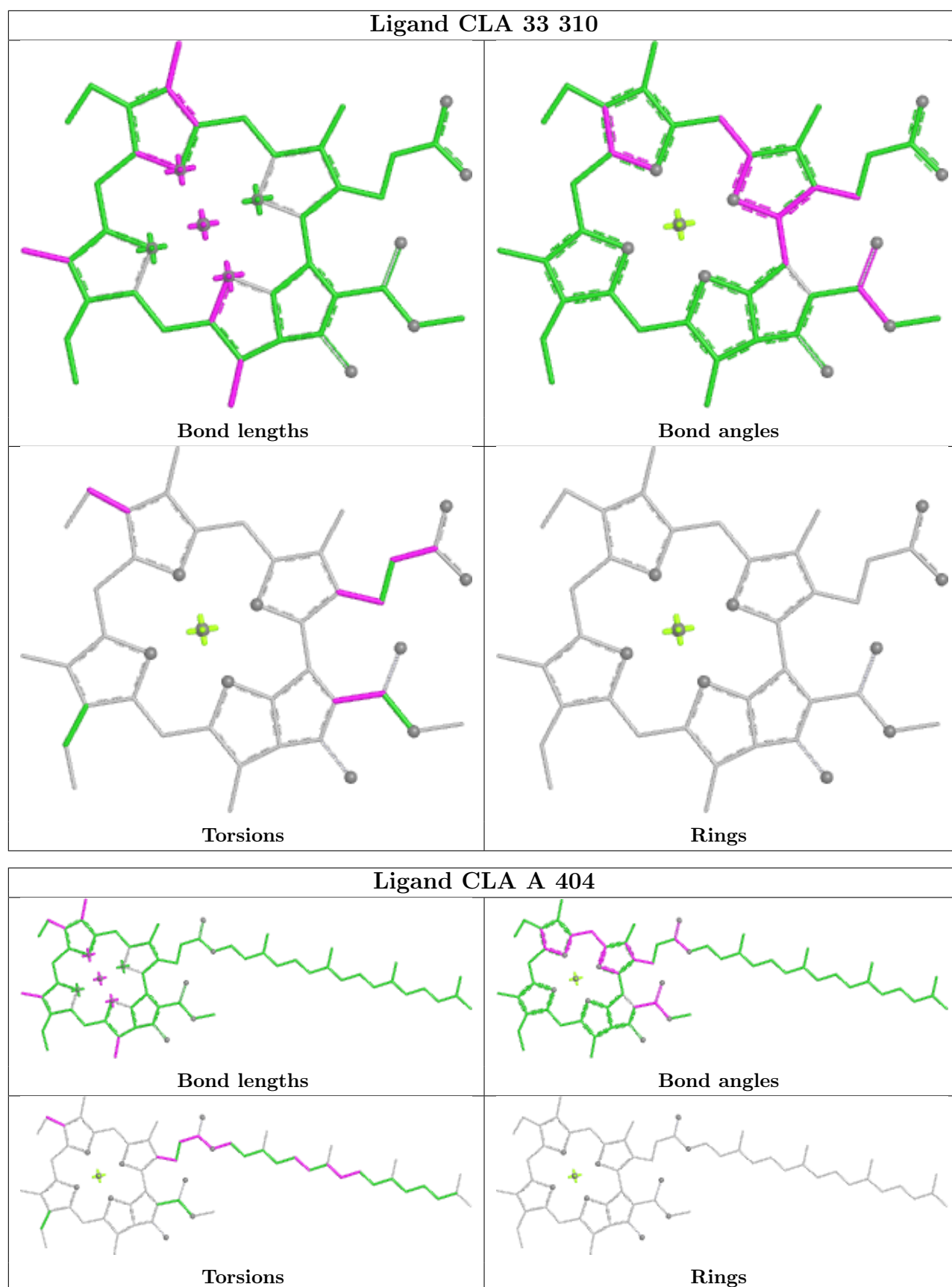
Ligand CLA C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

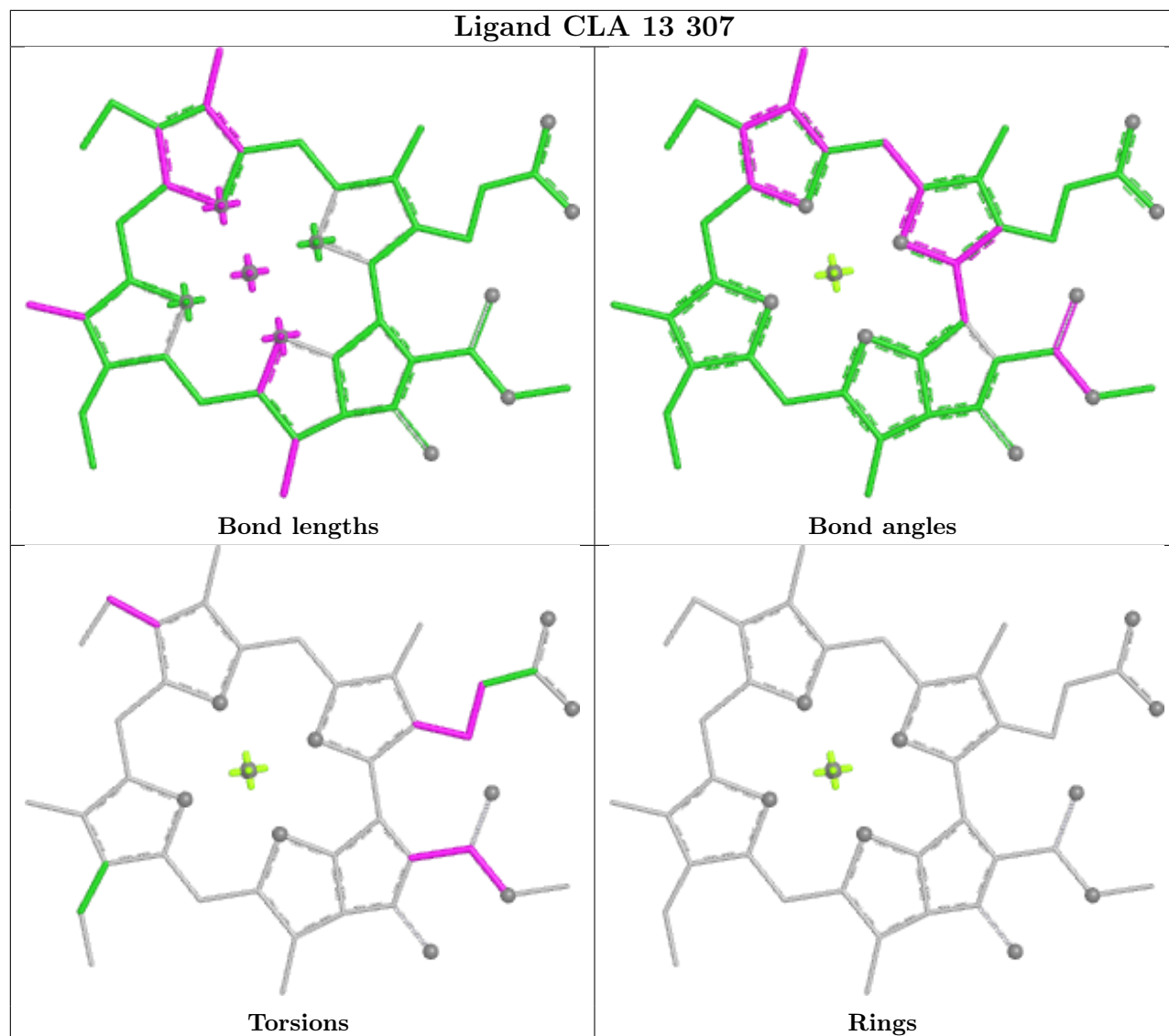
Ligand A86 12 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

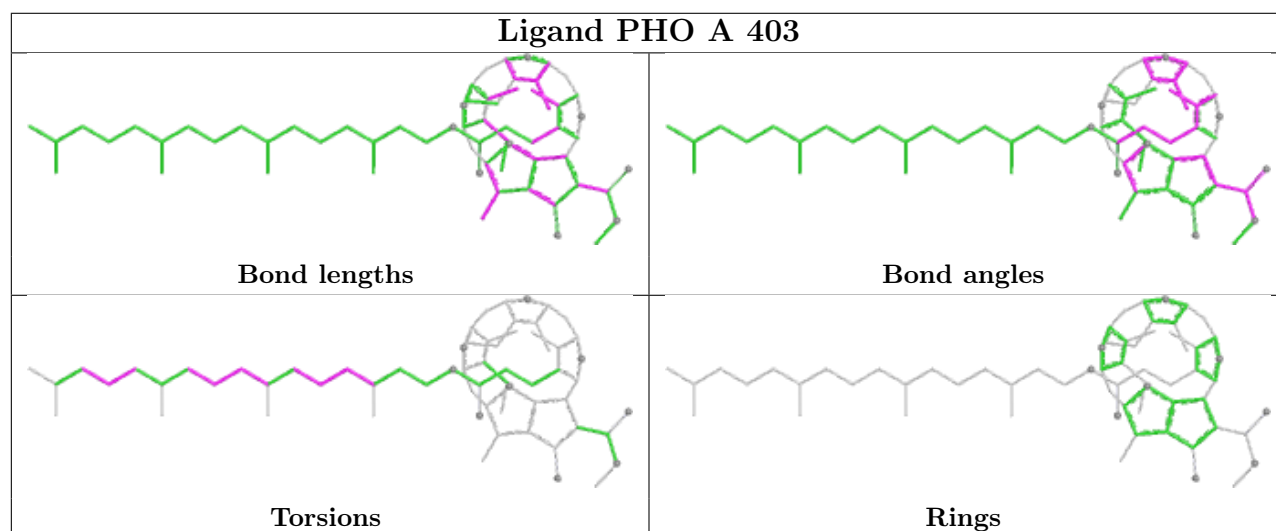
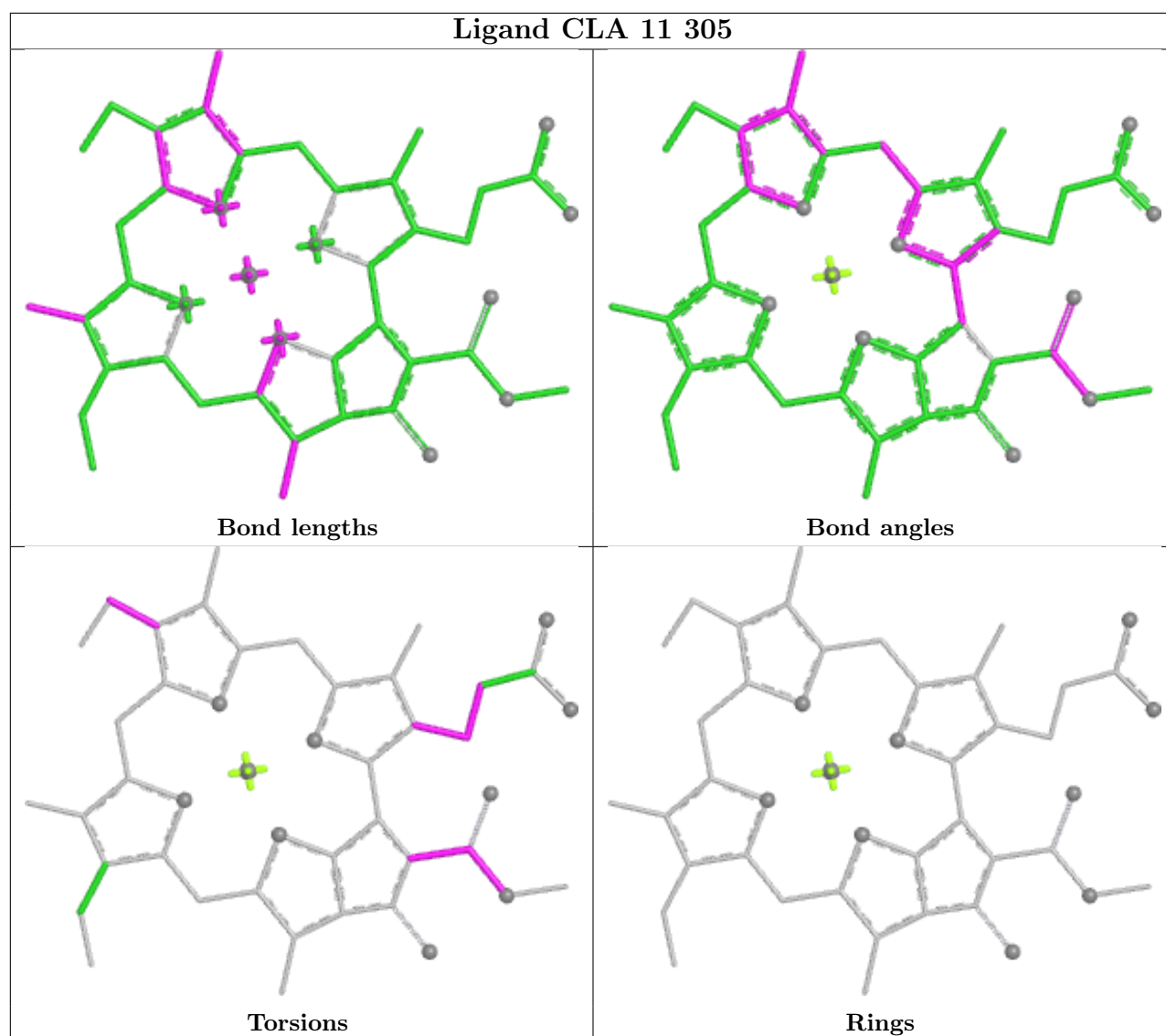
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Bond lengths	Bond angles
	
Torsions	Rings

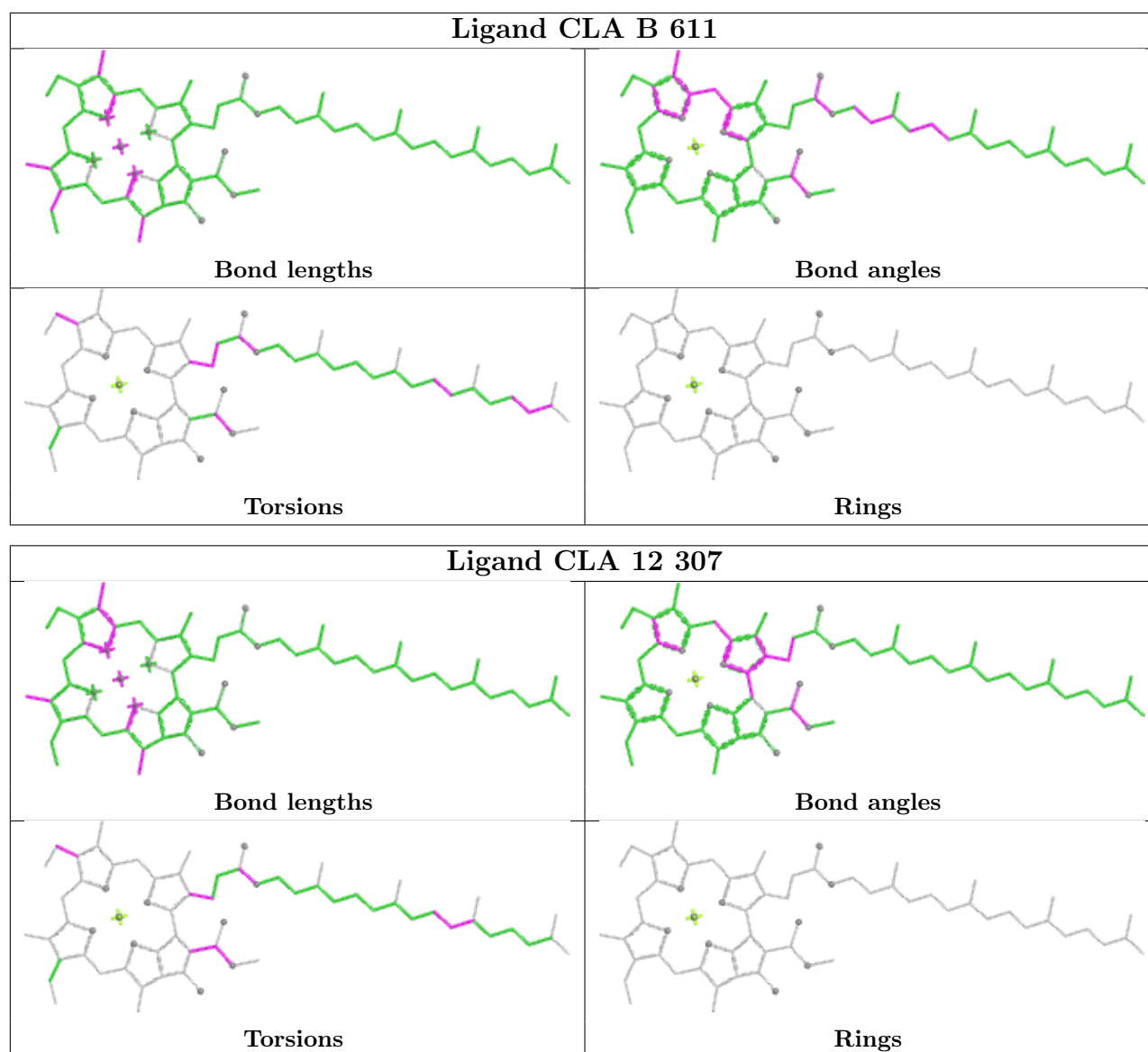


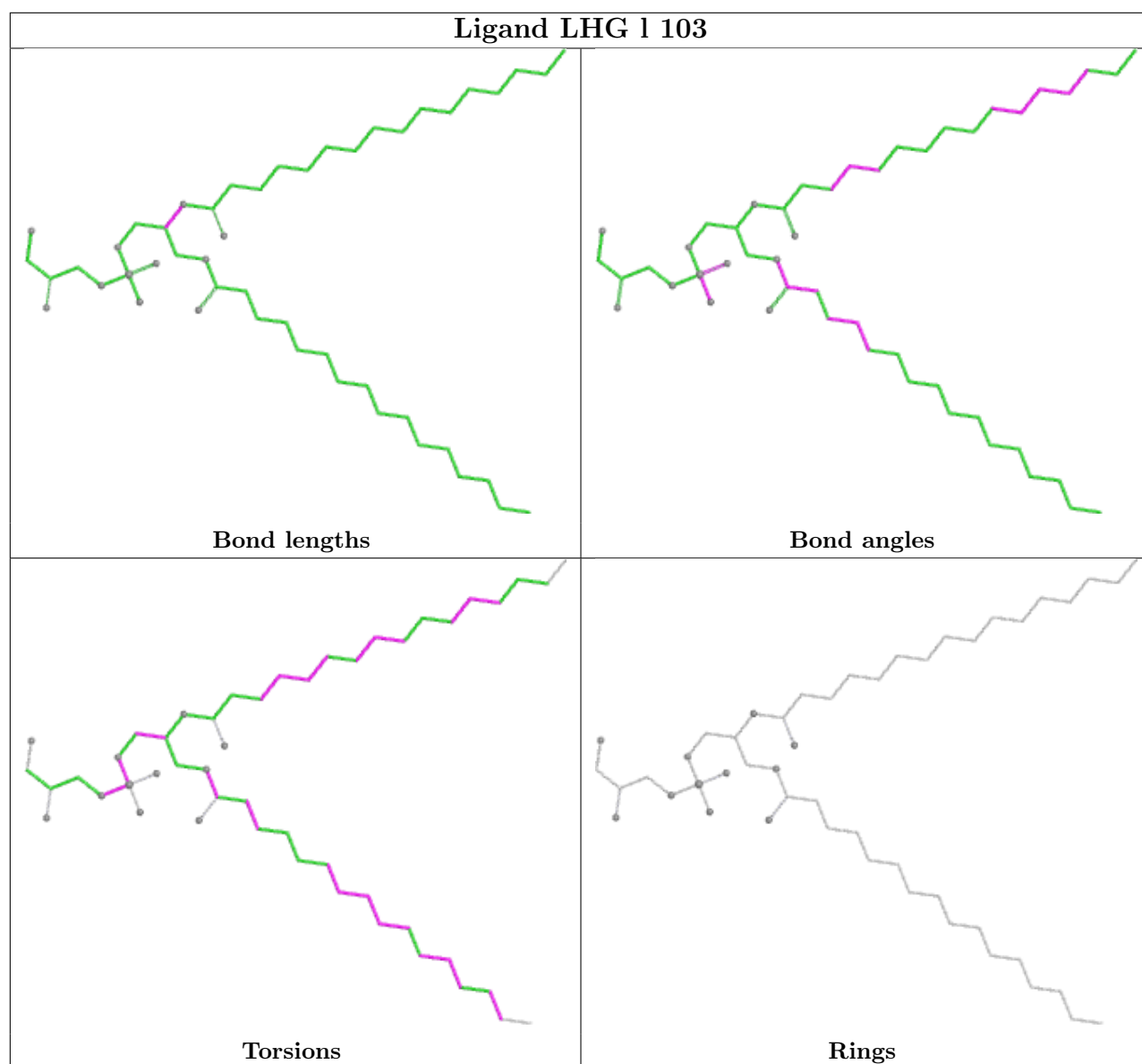




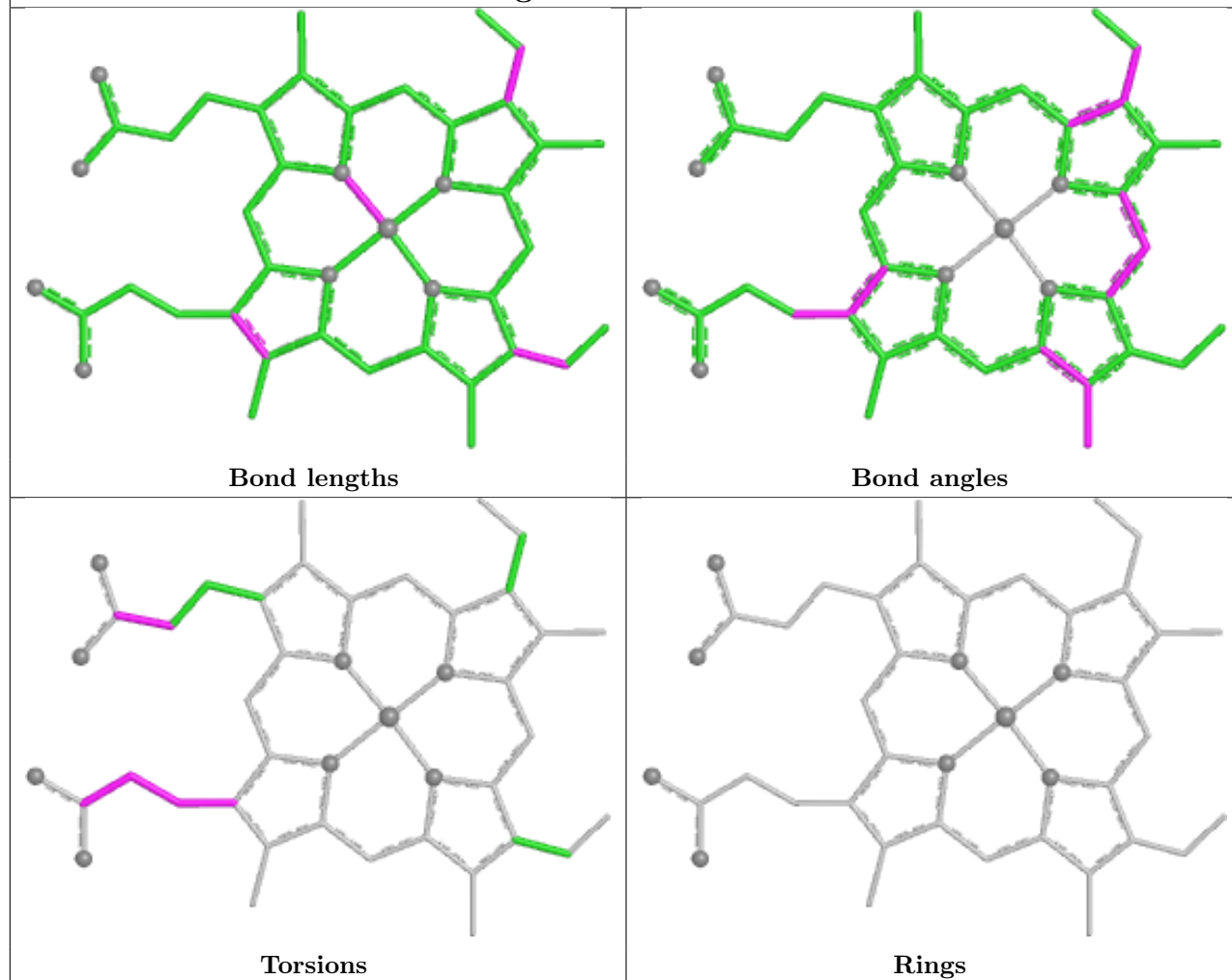




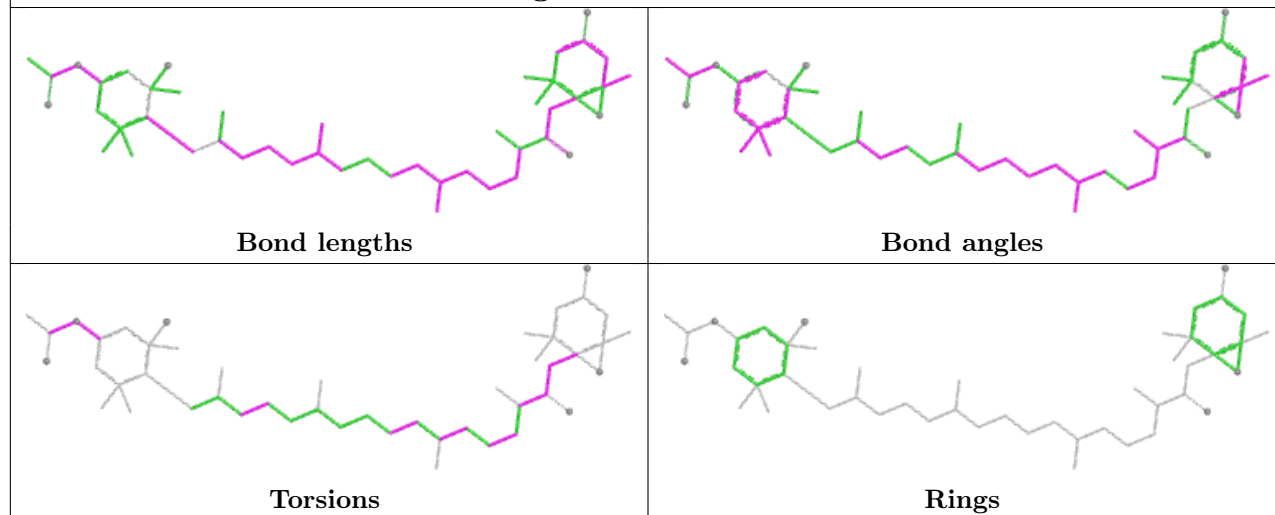


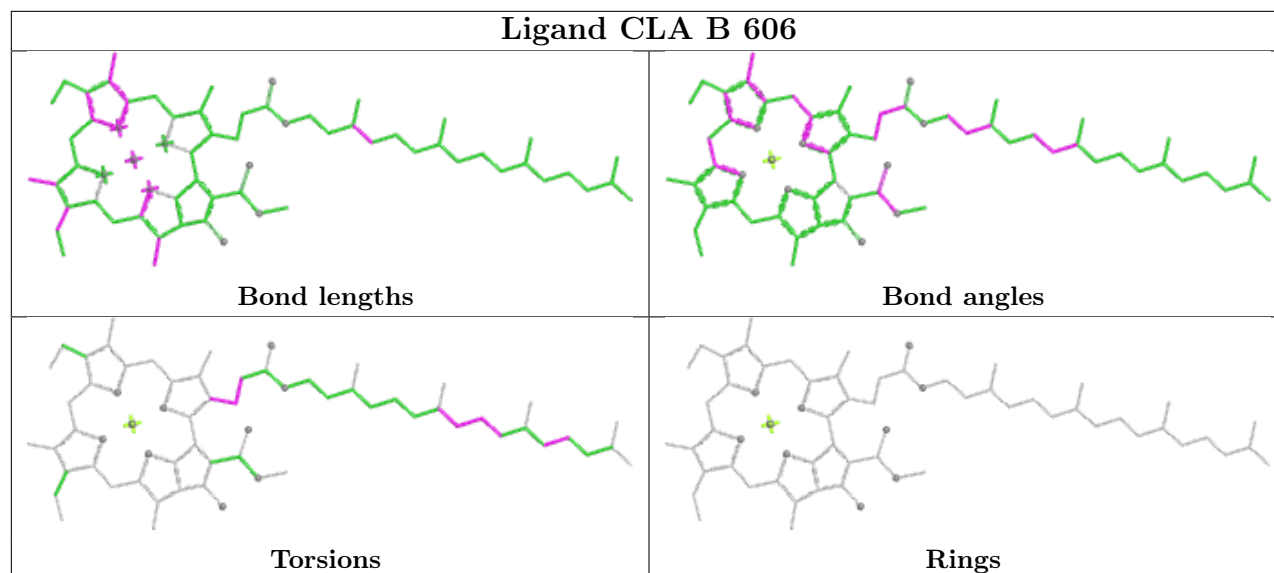
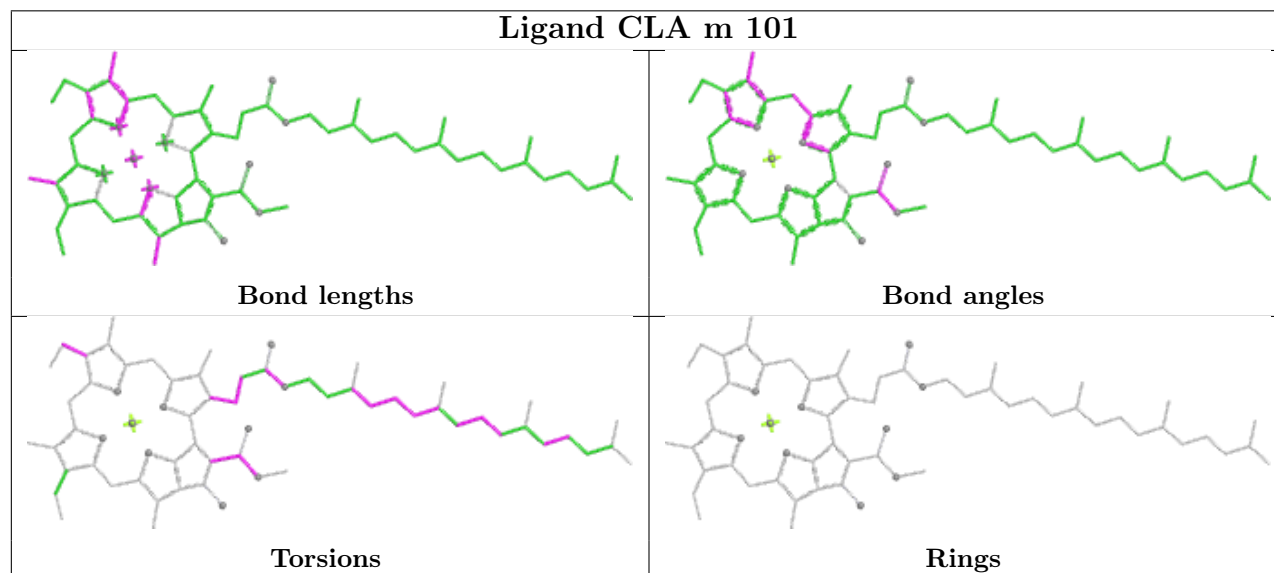
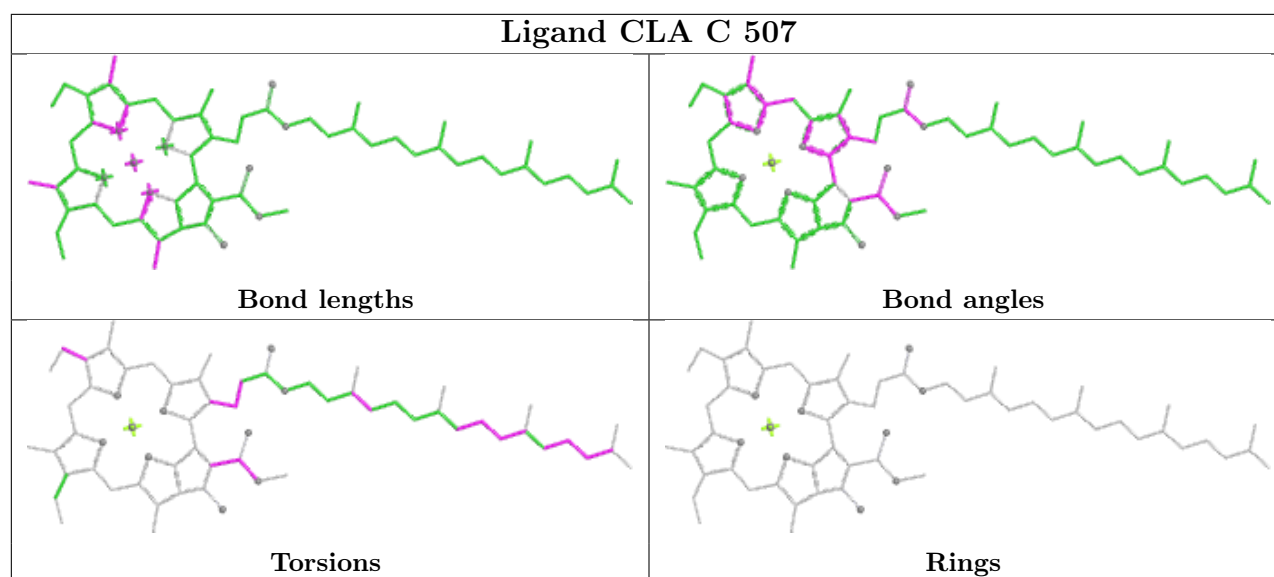


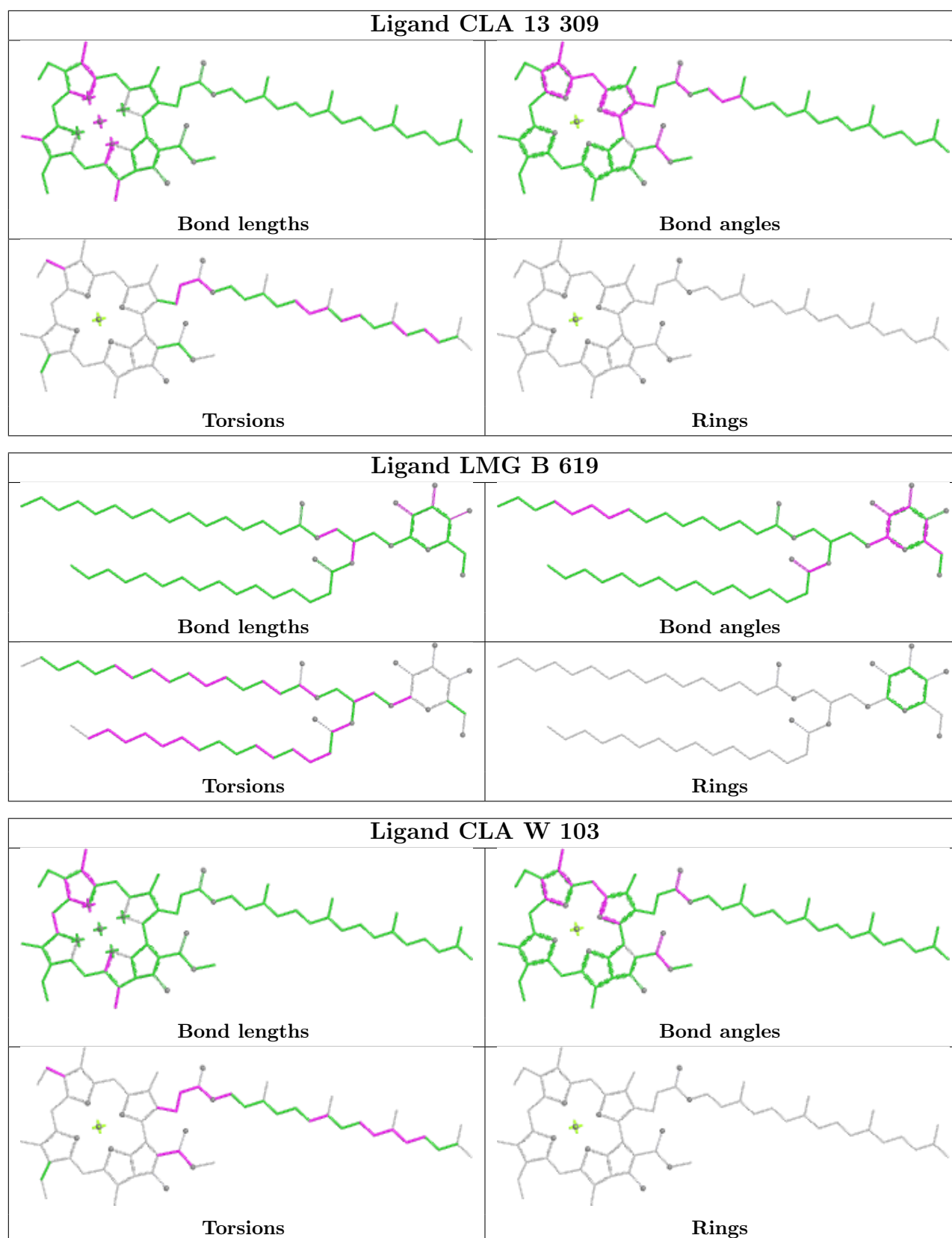
Ligand HEM f 102

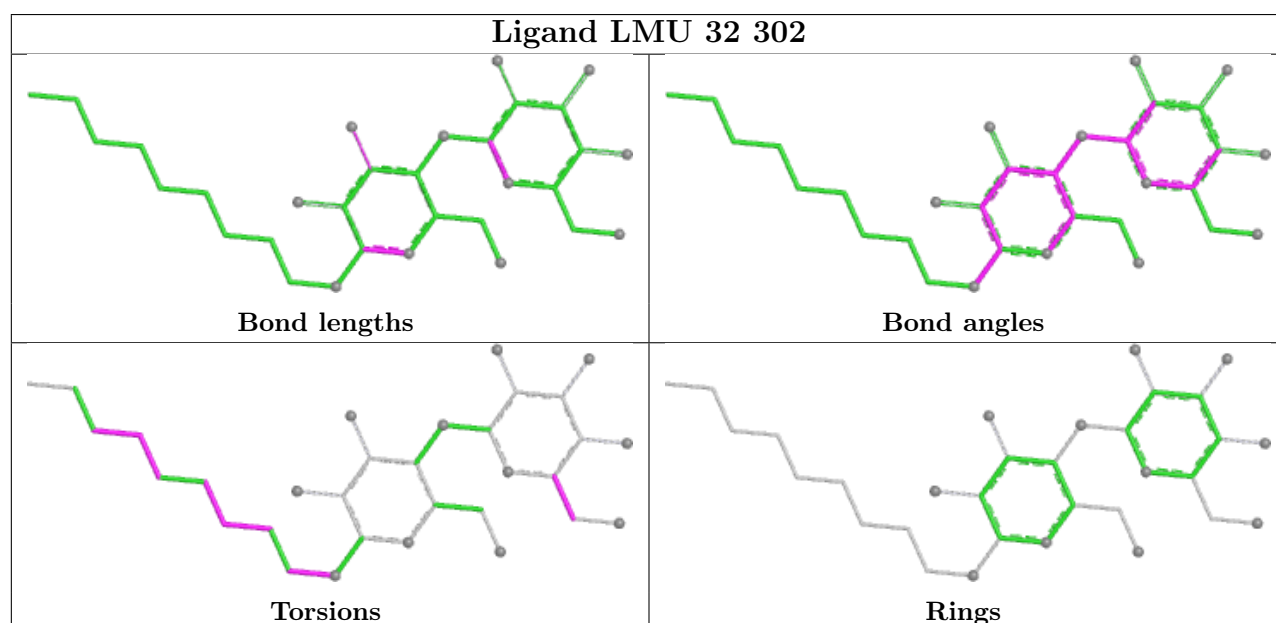
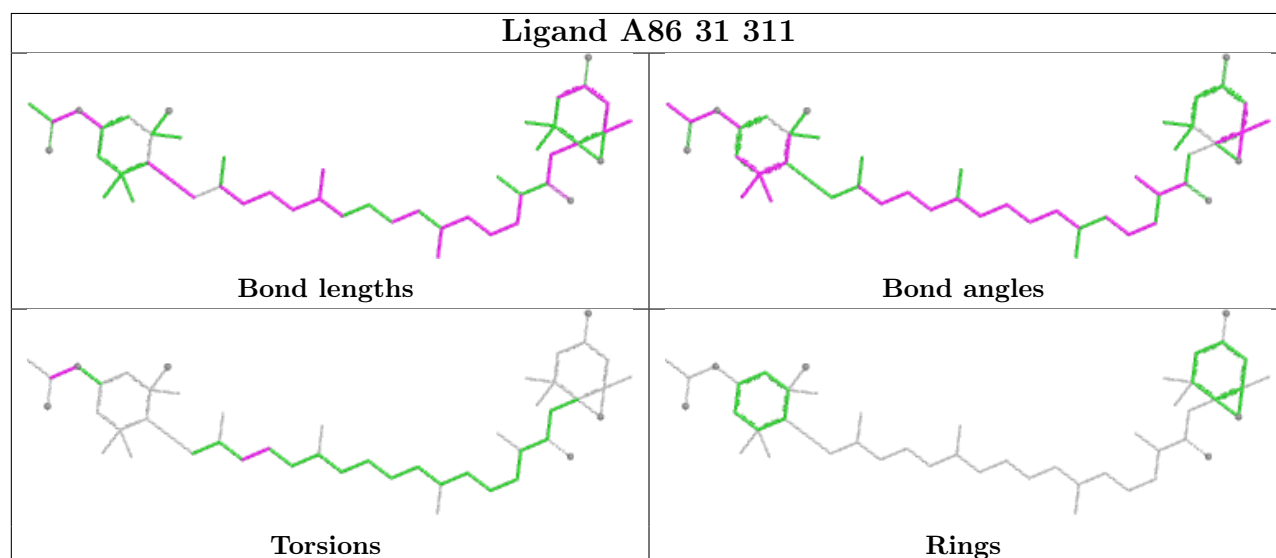
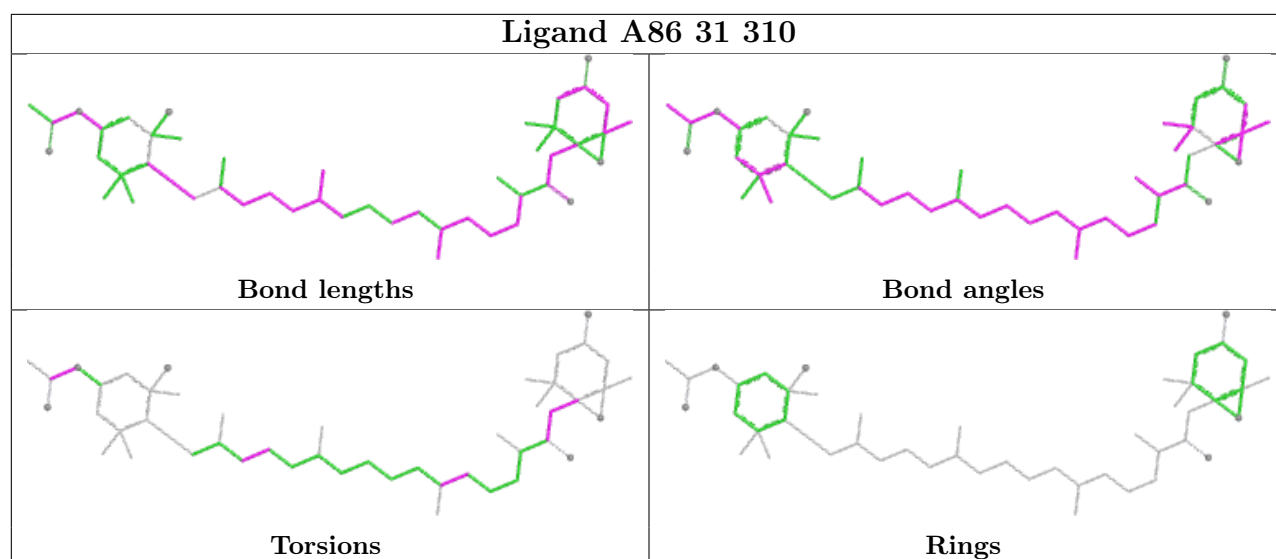


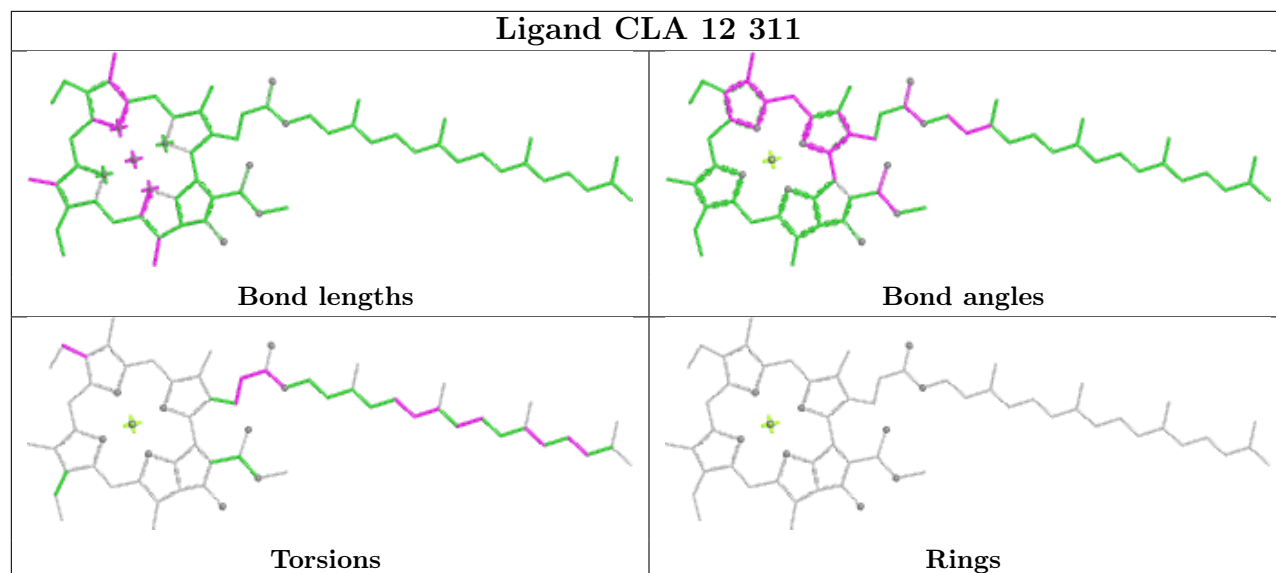
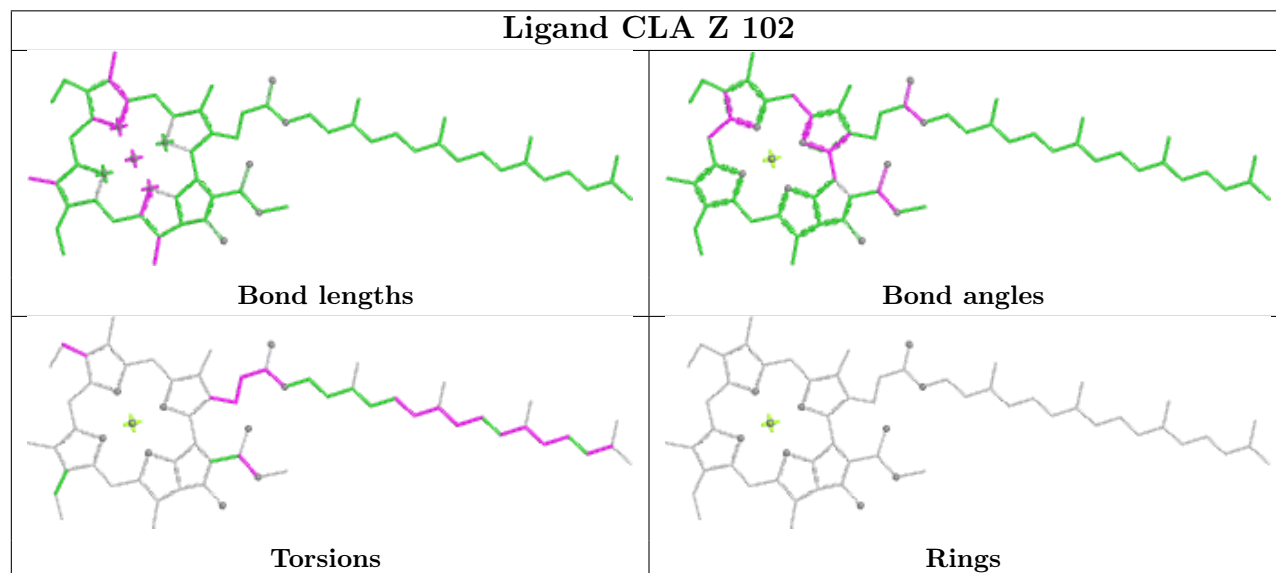
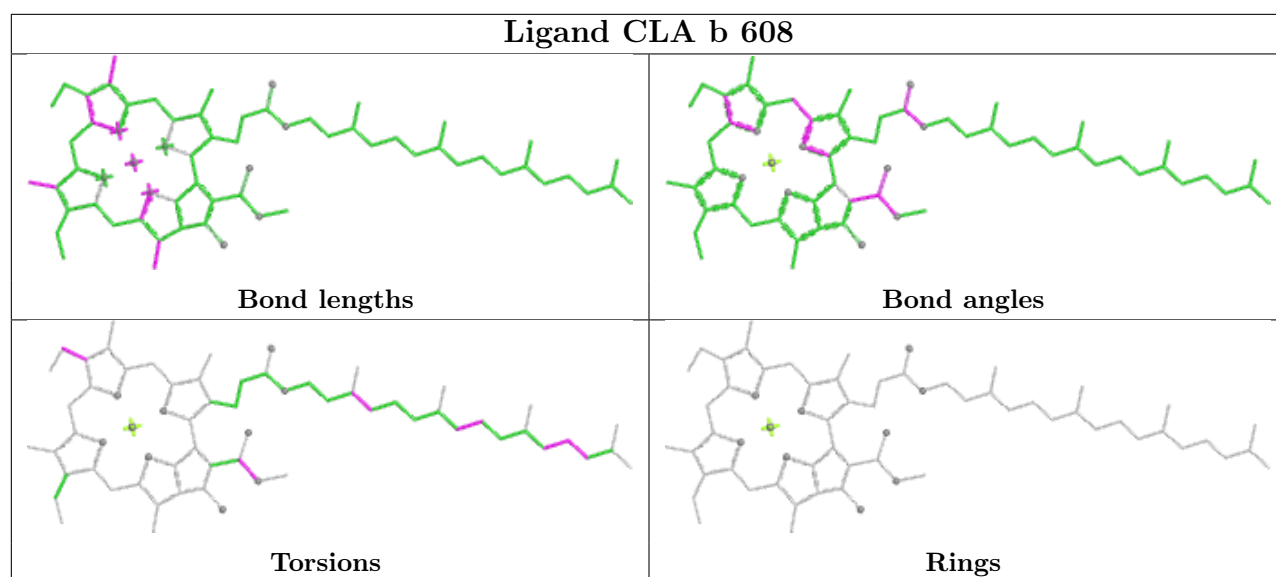
Ligand A86 31 316



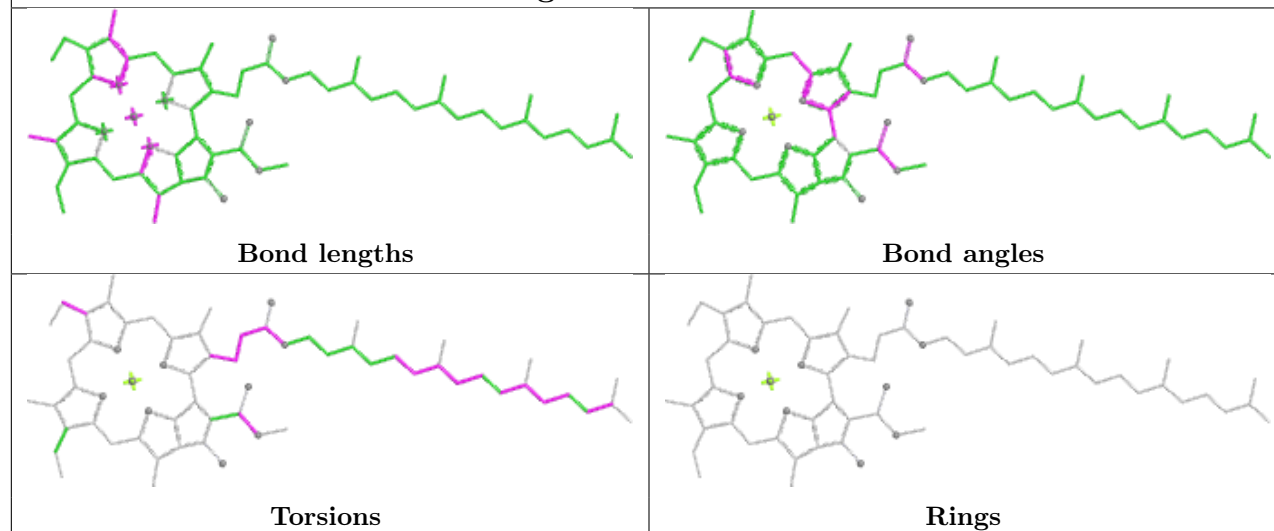




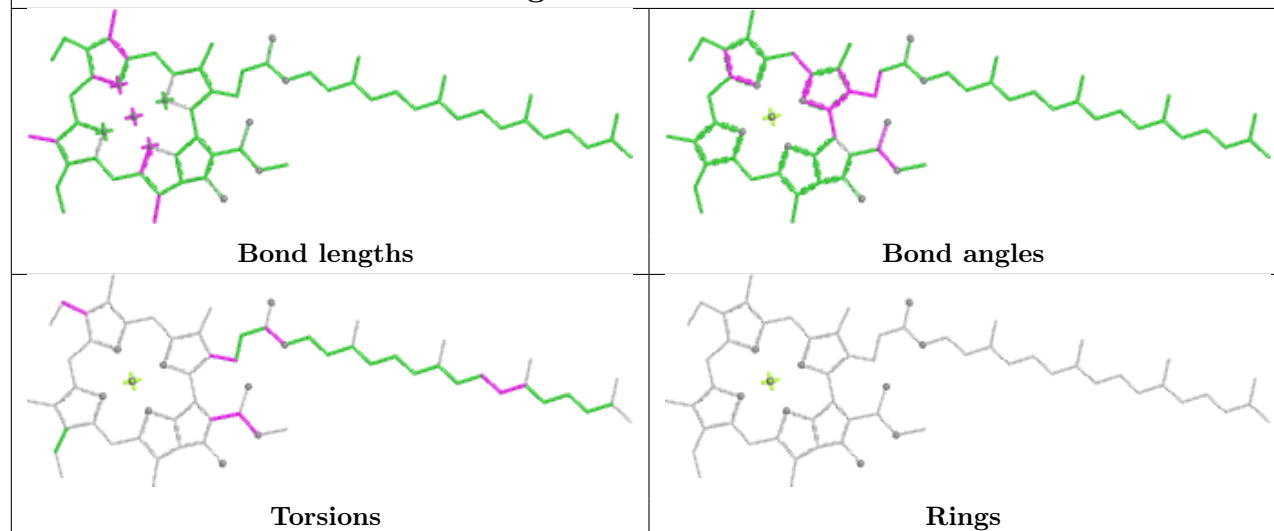




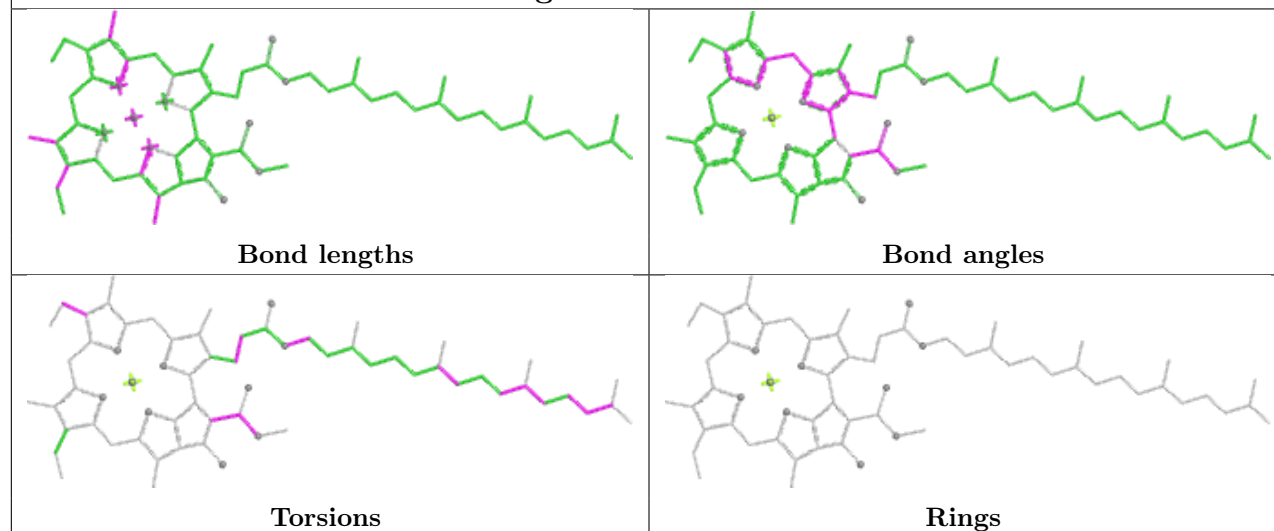
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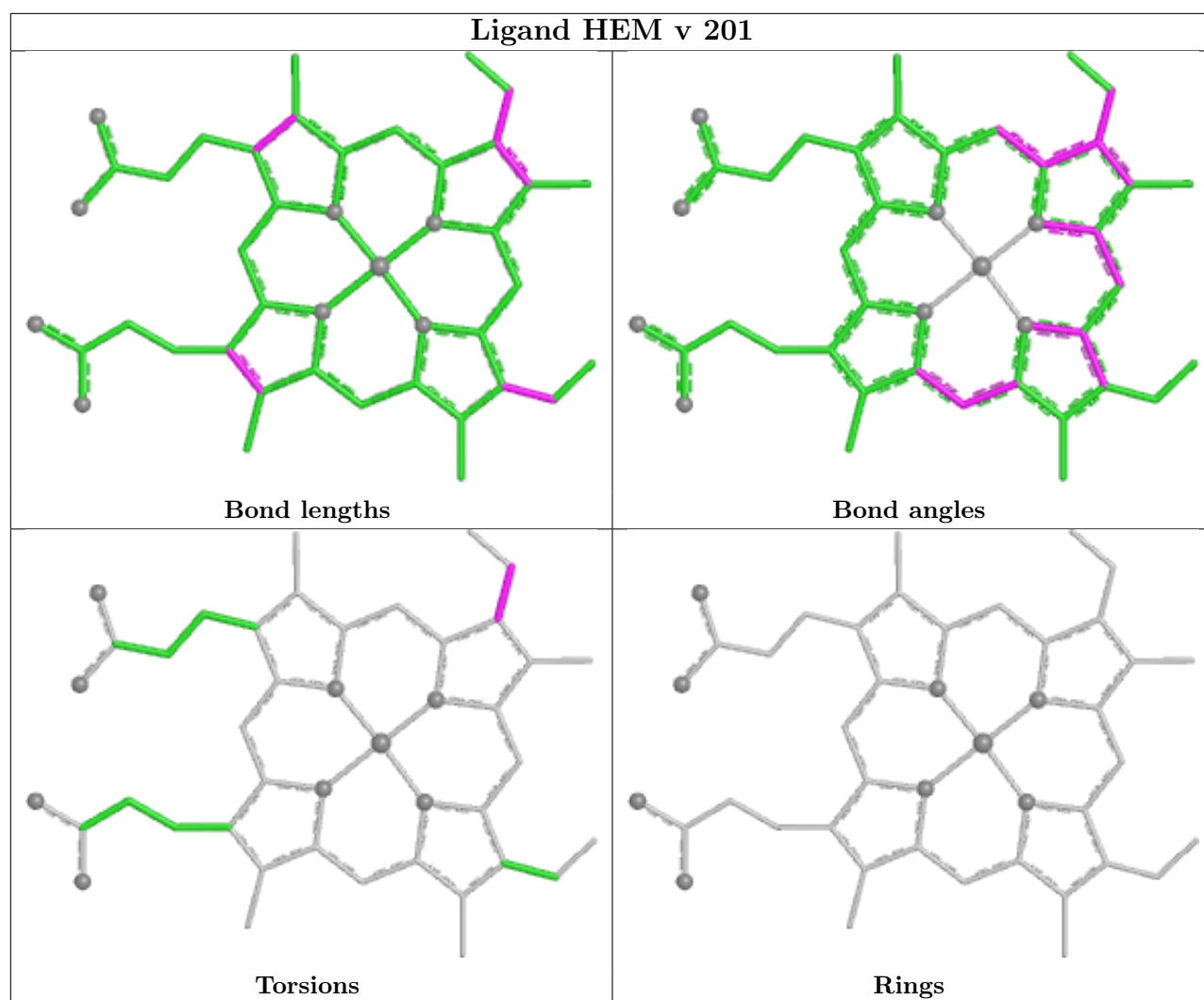


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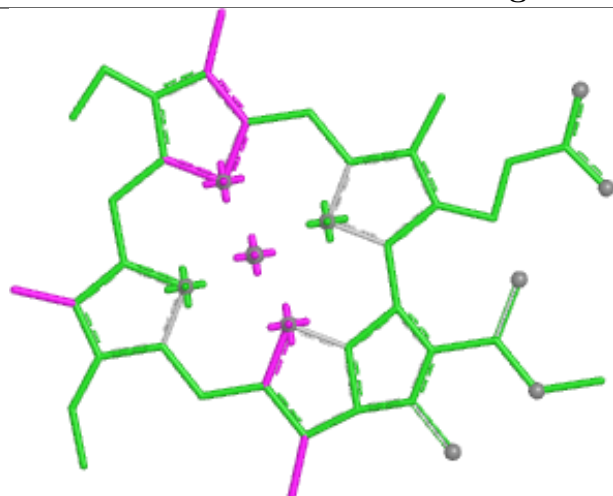


Ligand CLA b 610

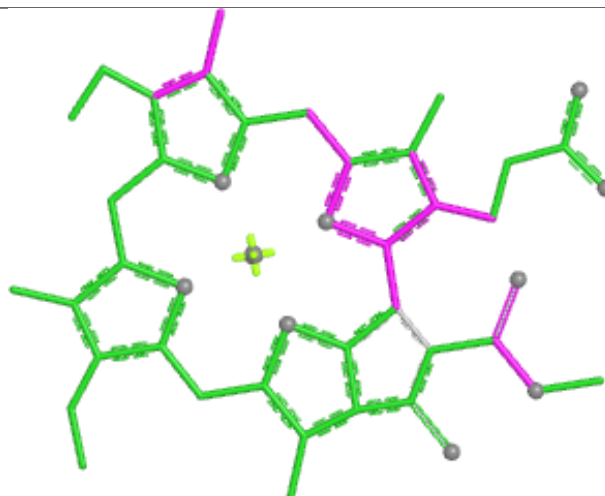




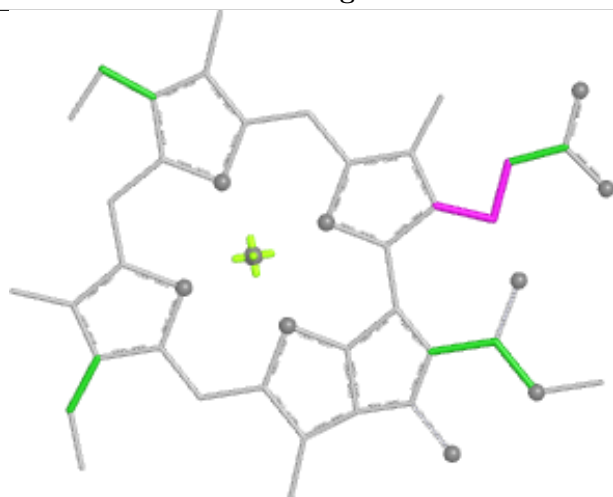
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Bond lengths



Bond angles

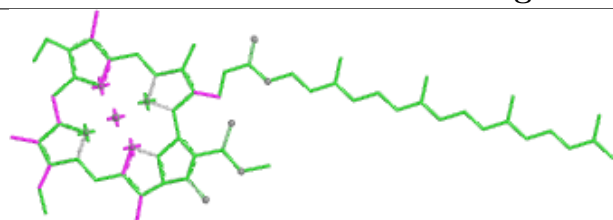


Torsions

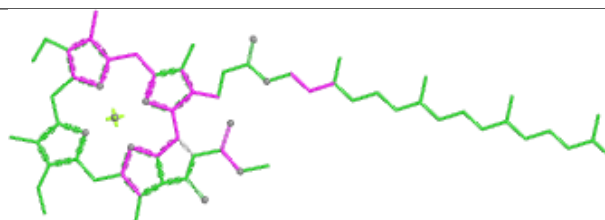


Rings

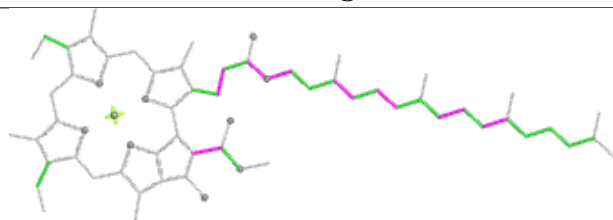
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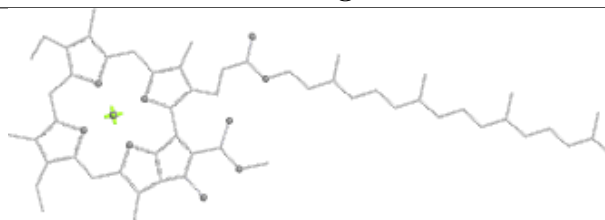
Bond lengths



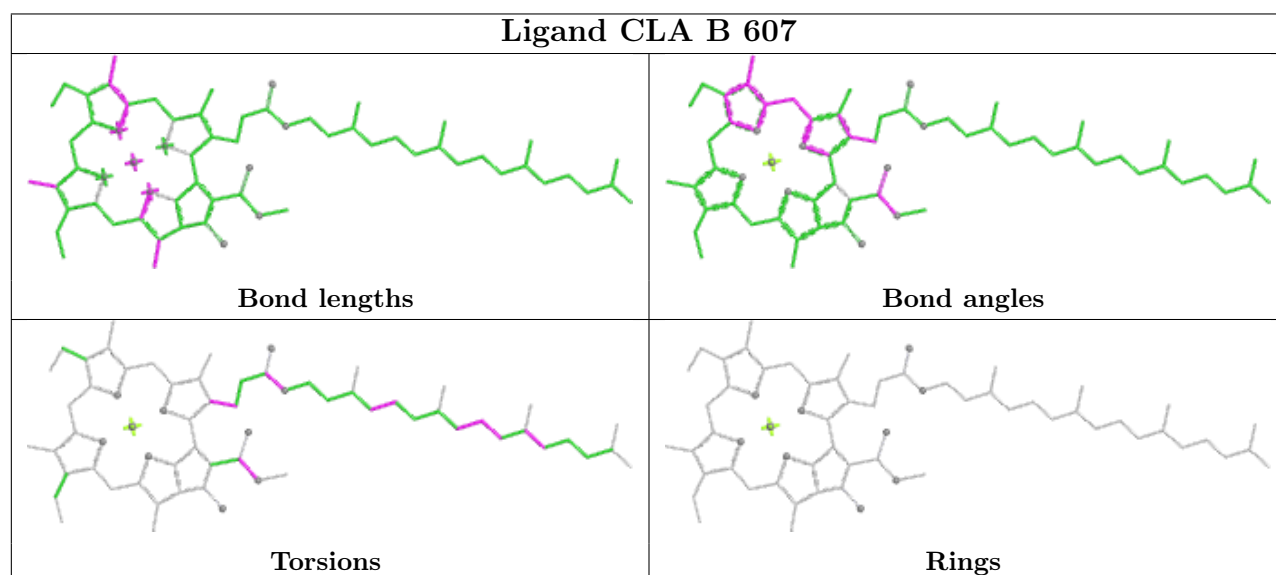
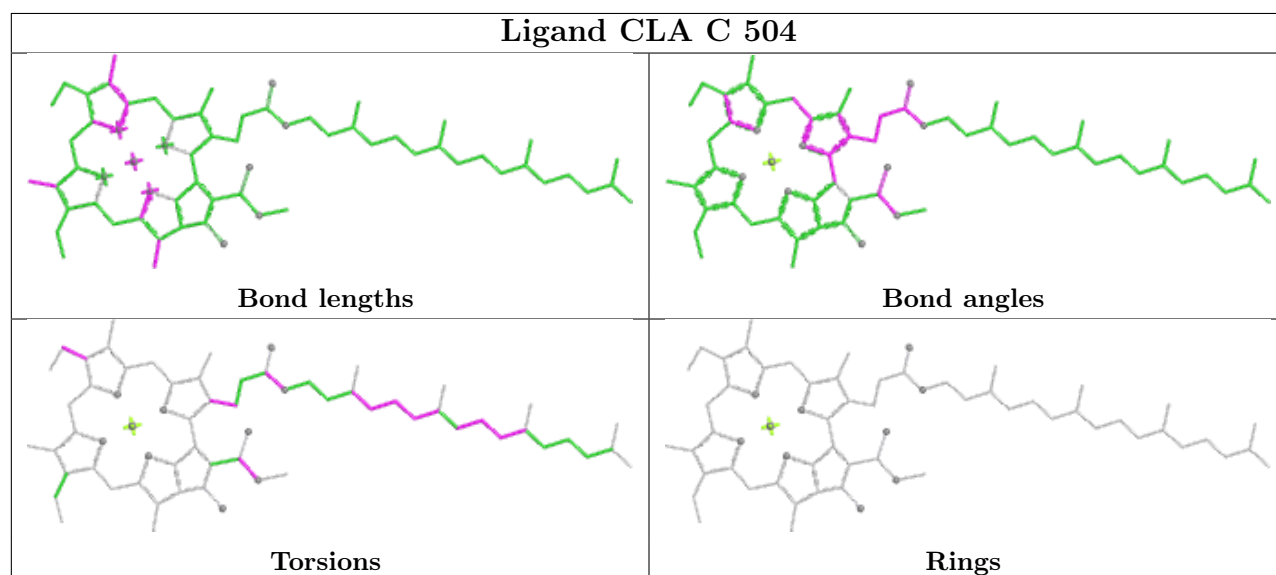
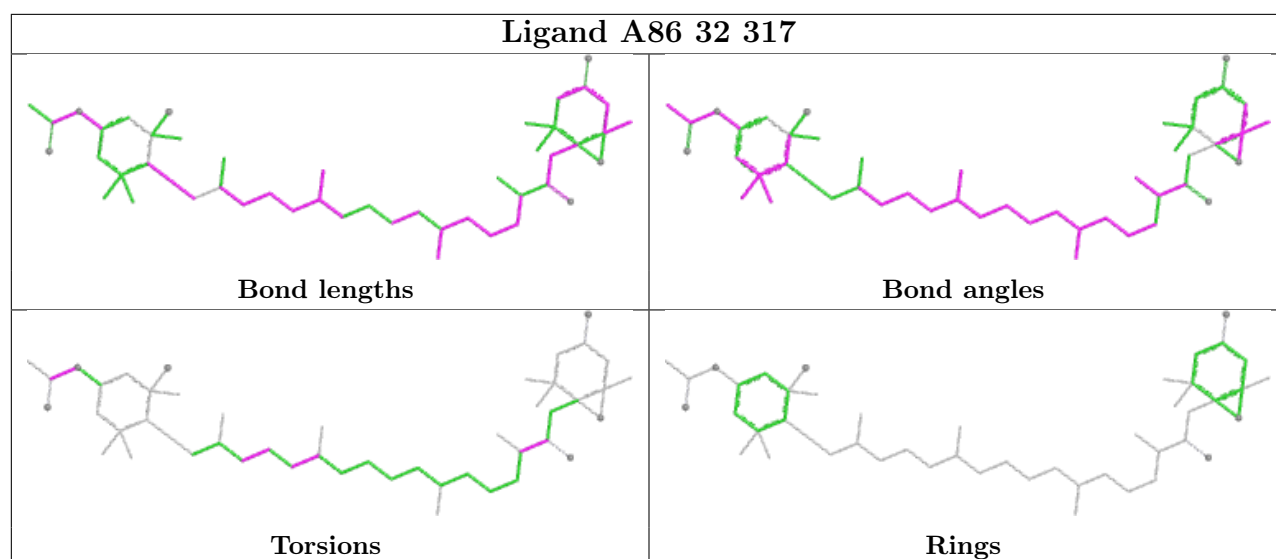
Bond angles

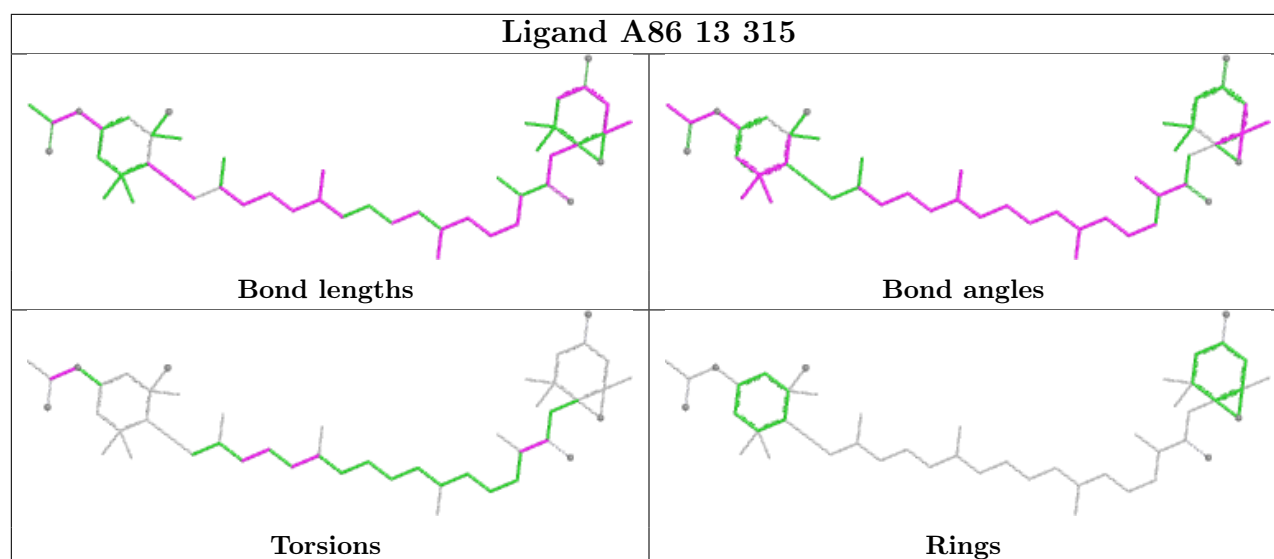
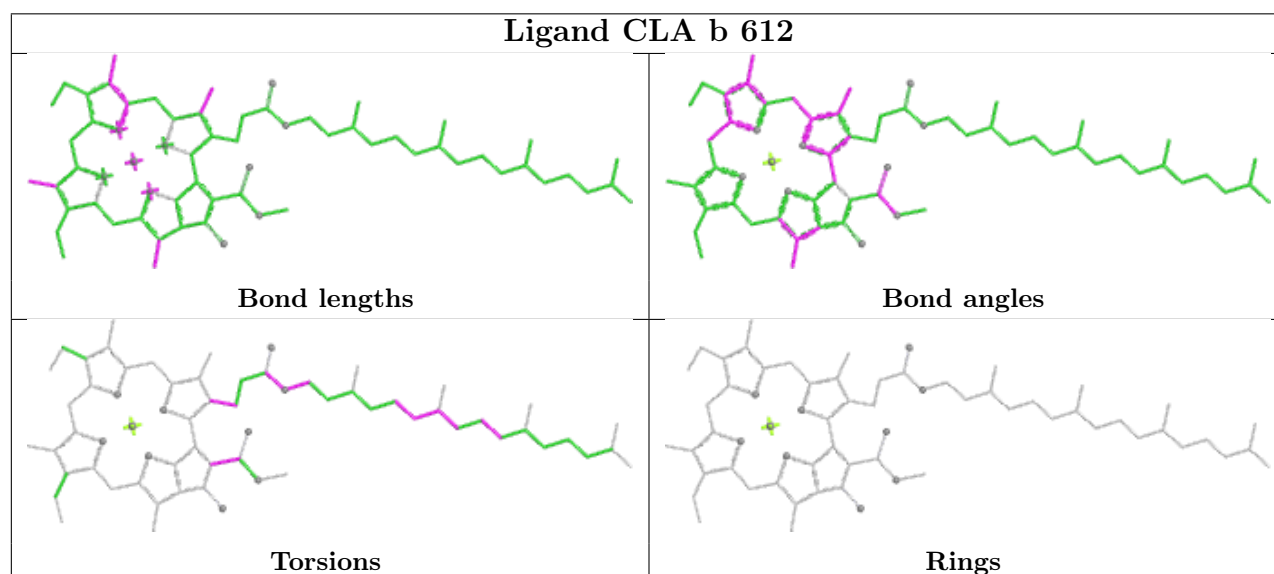
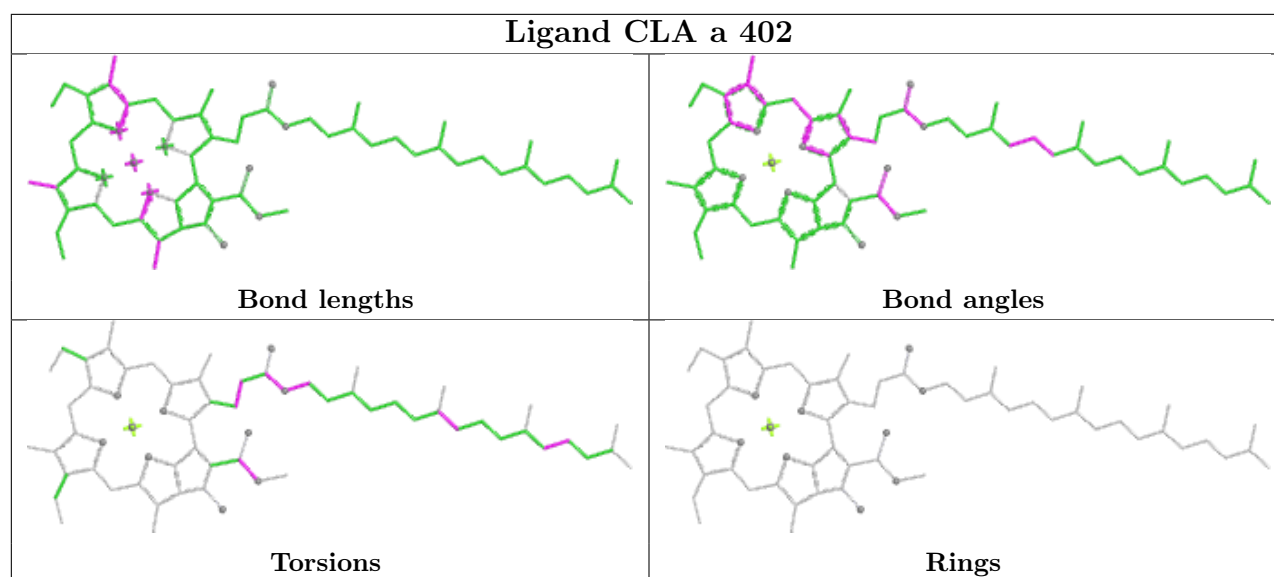


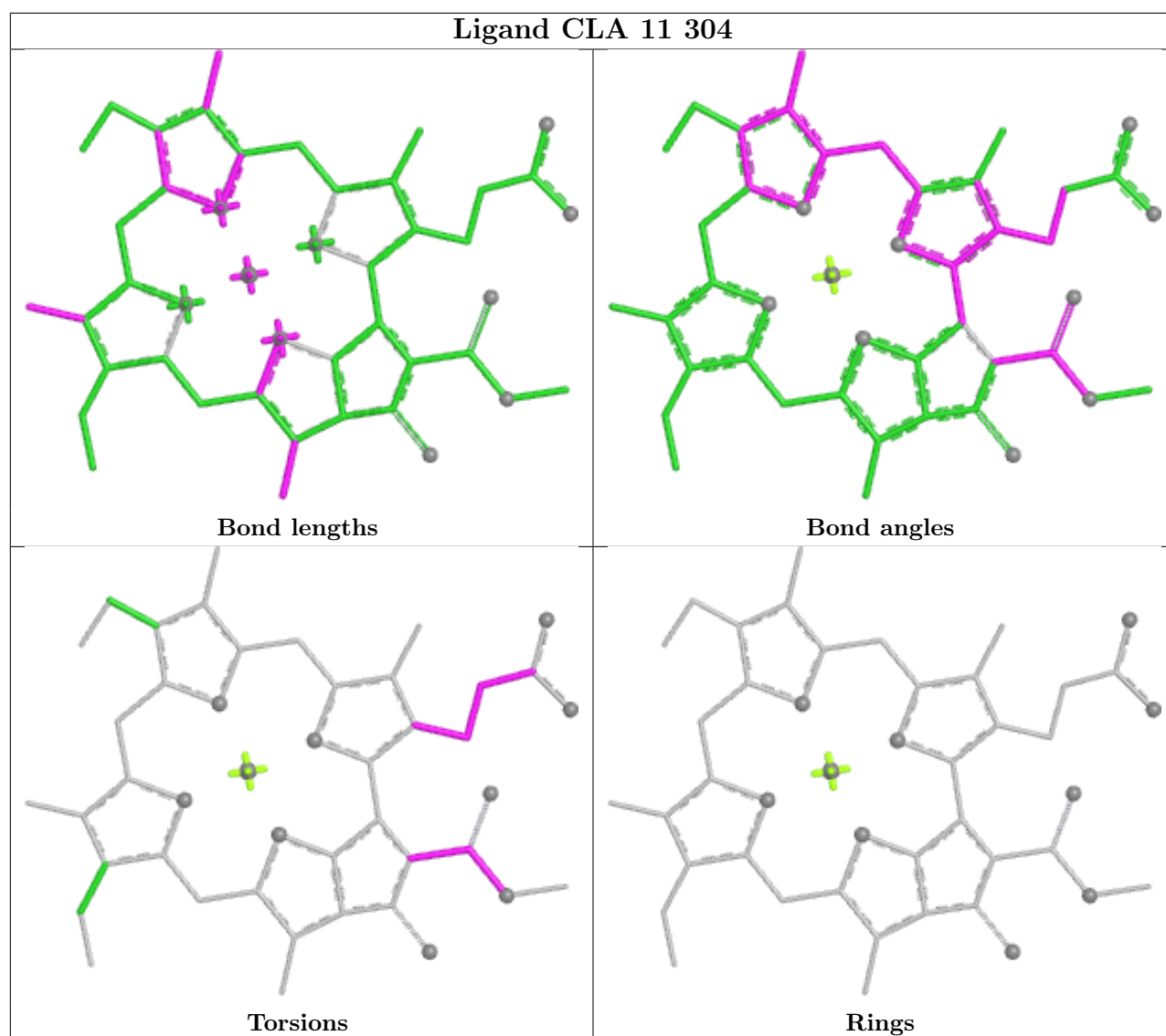
Torsions

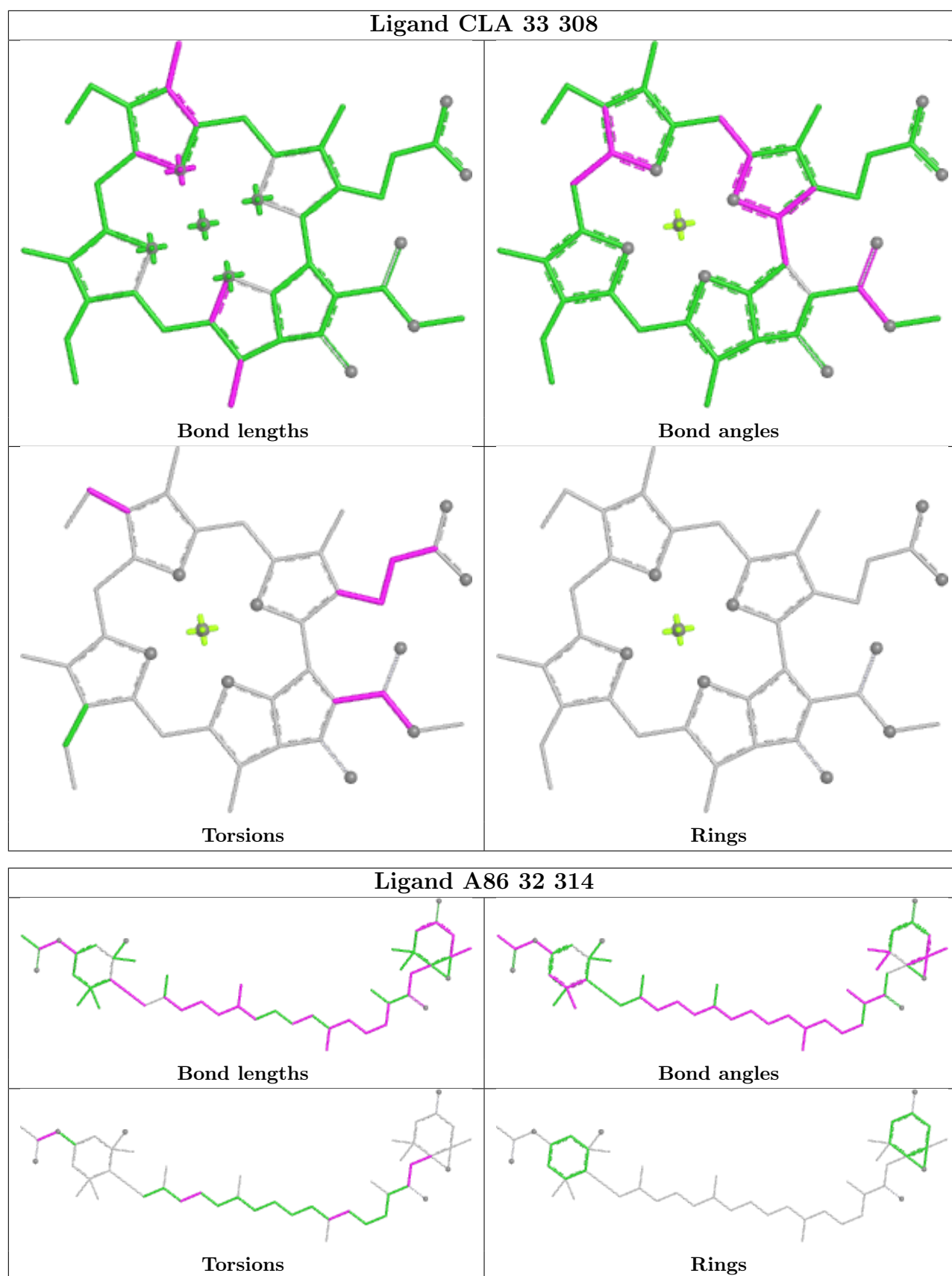


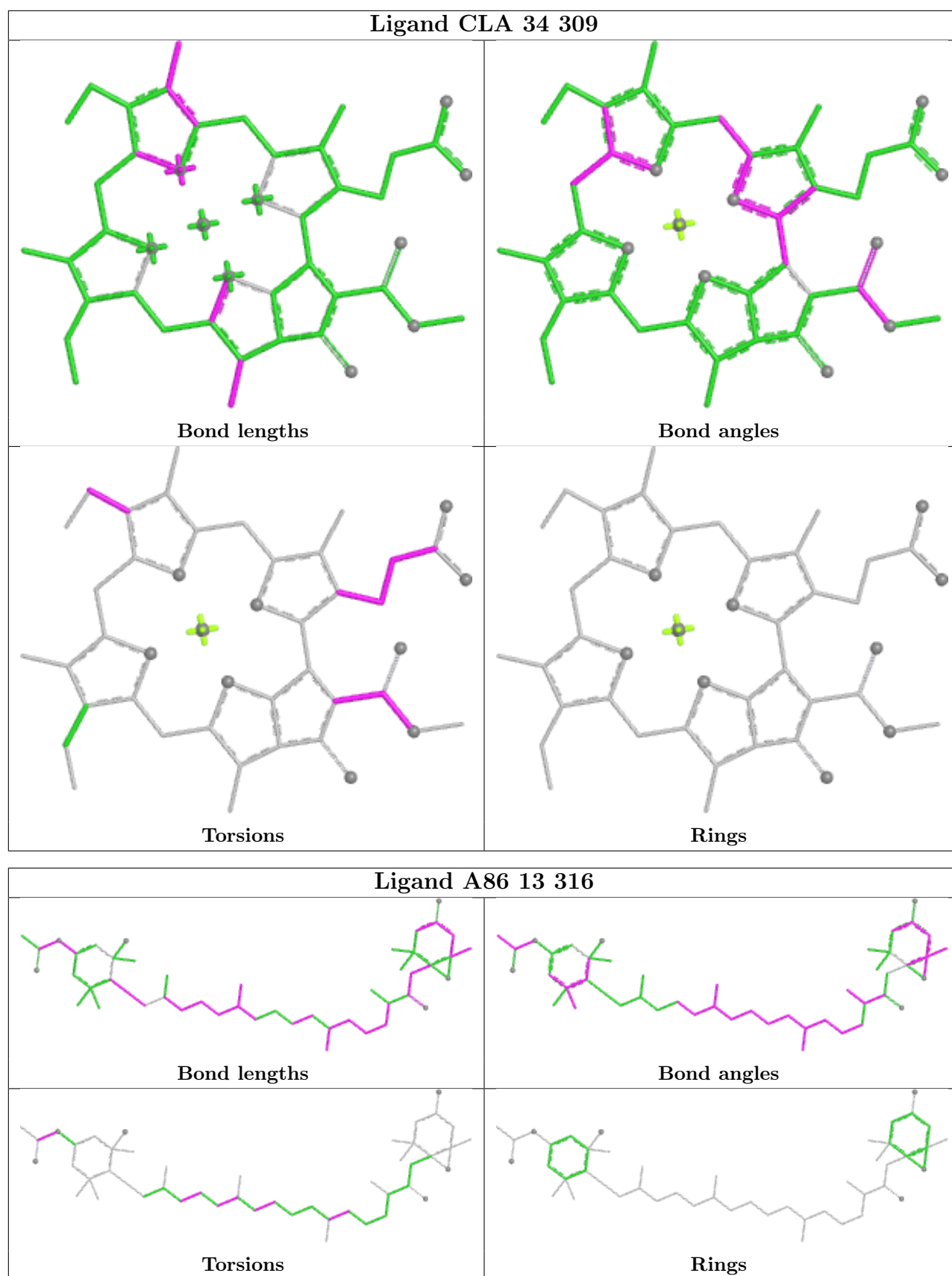
Rings

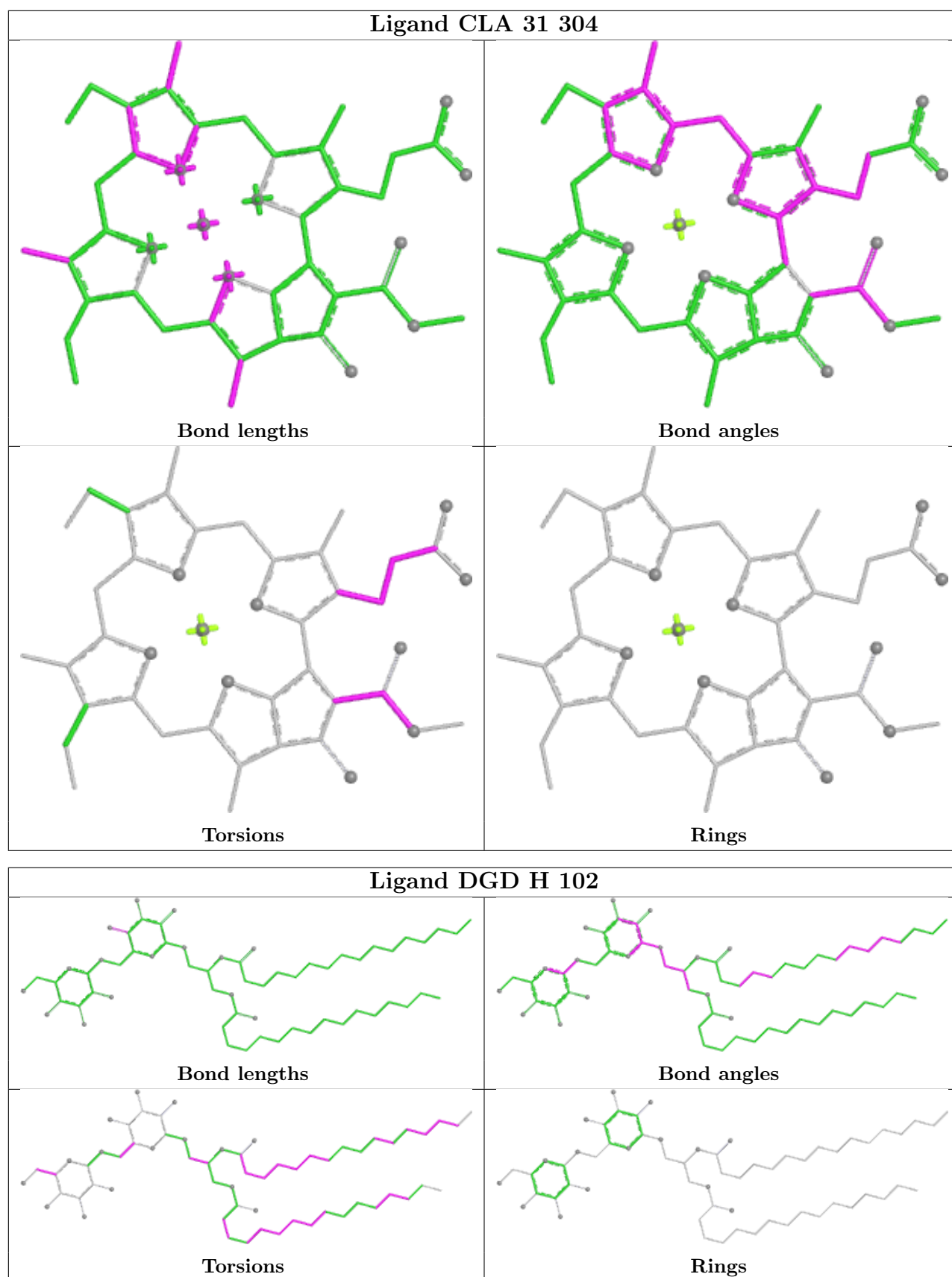


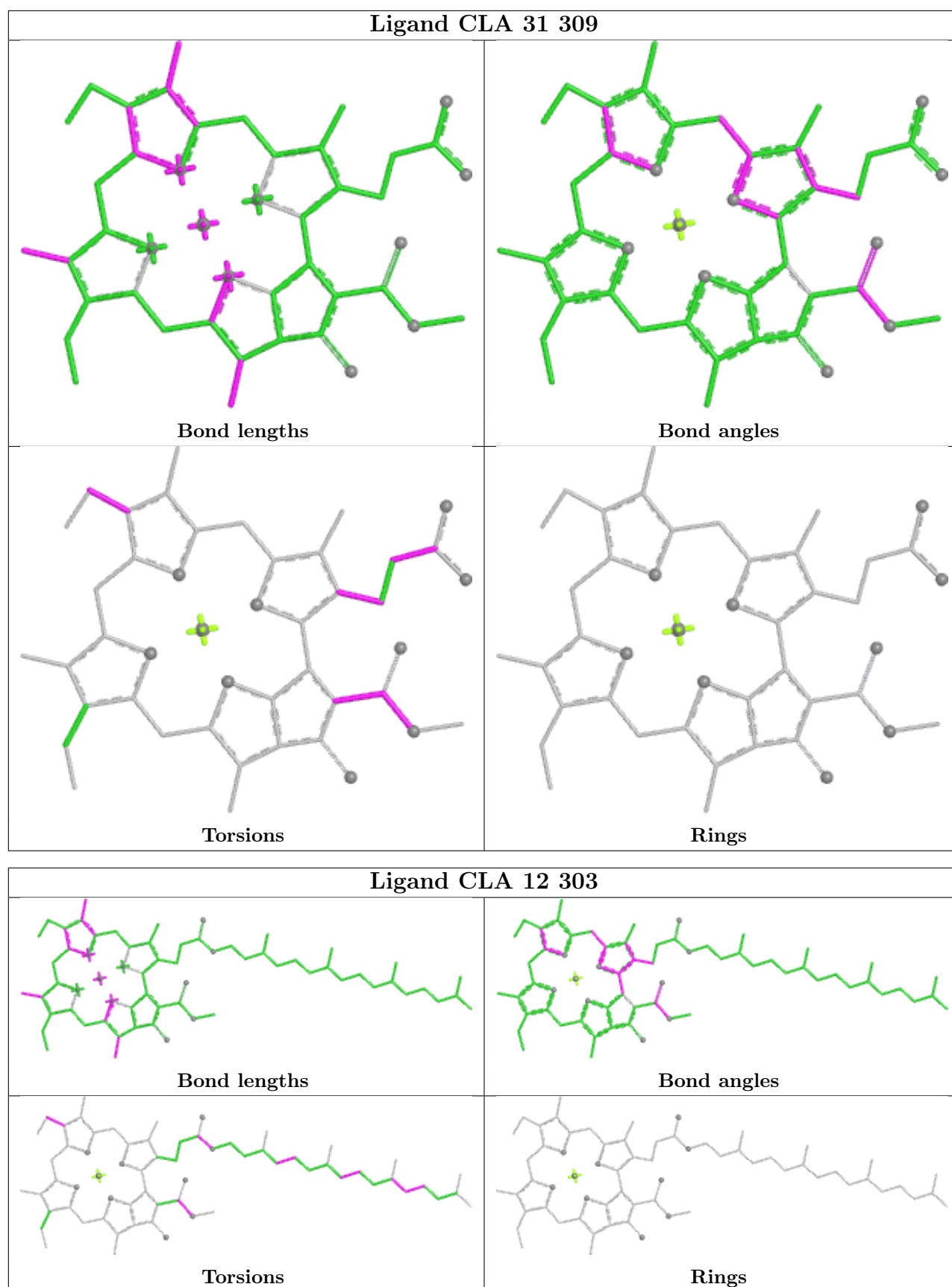


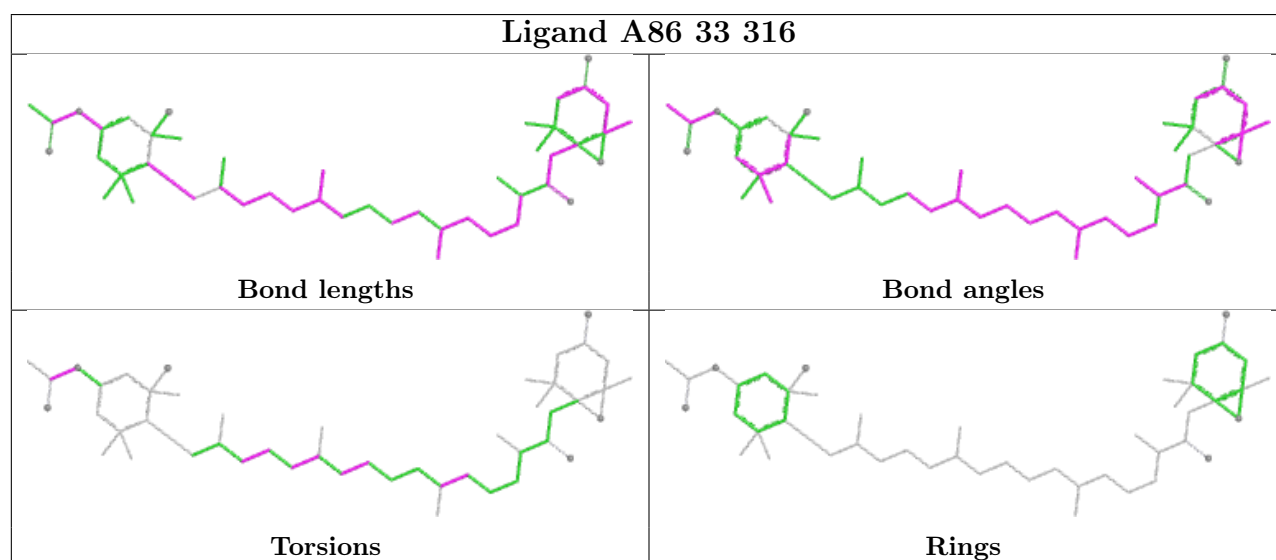
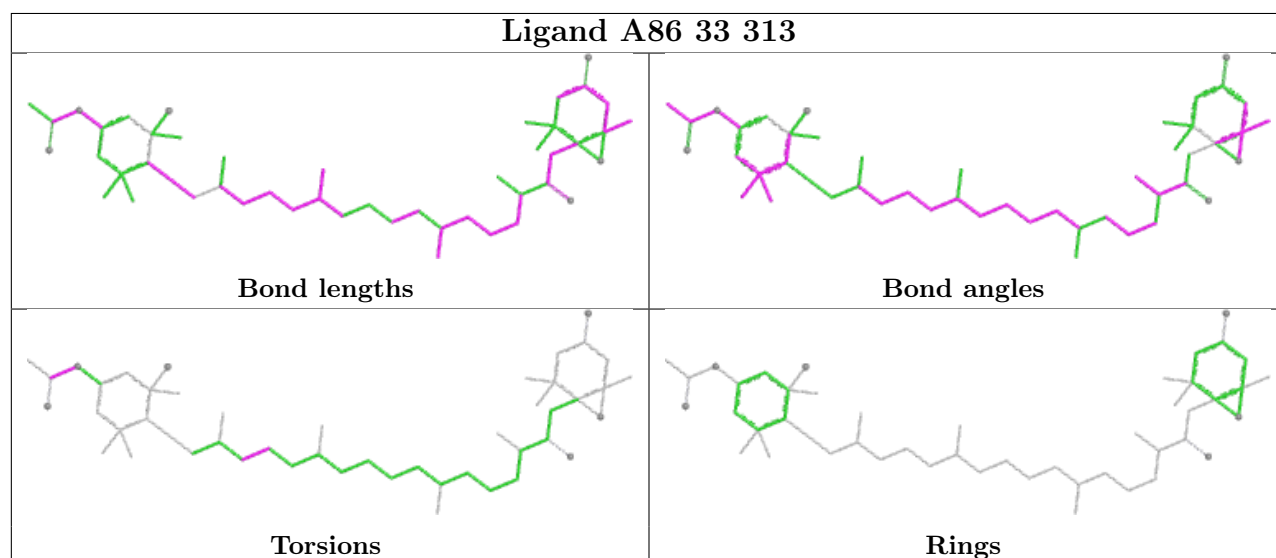
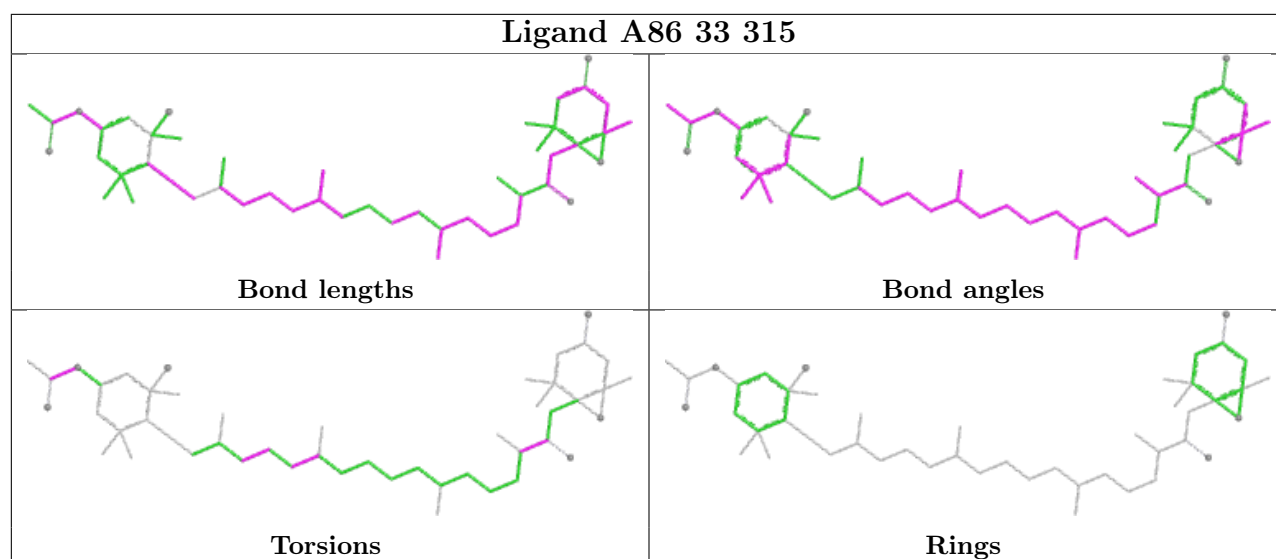


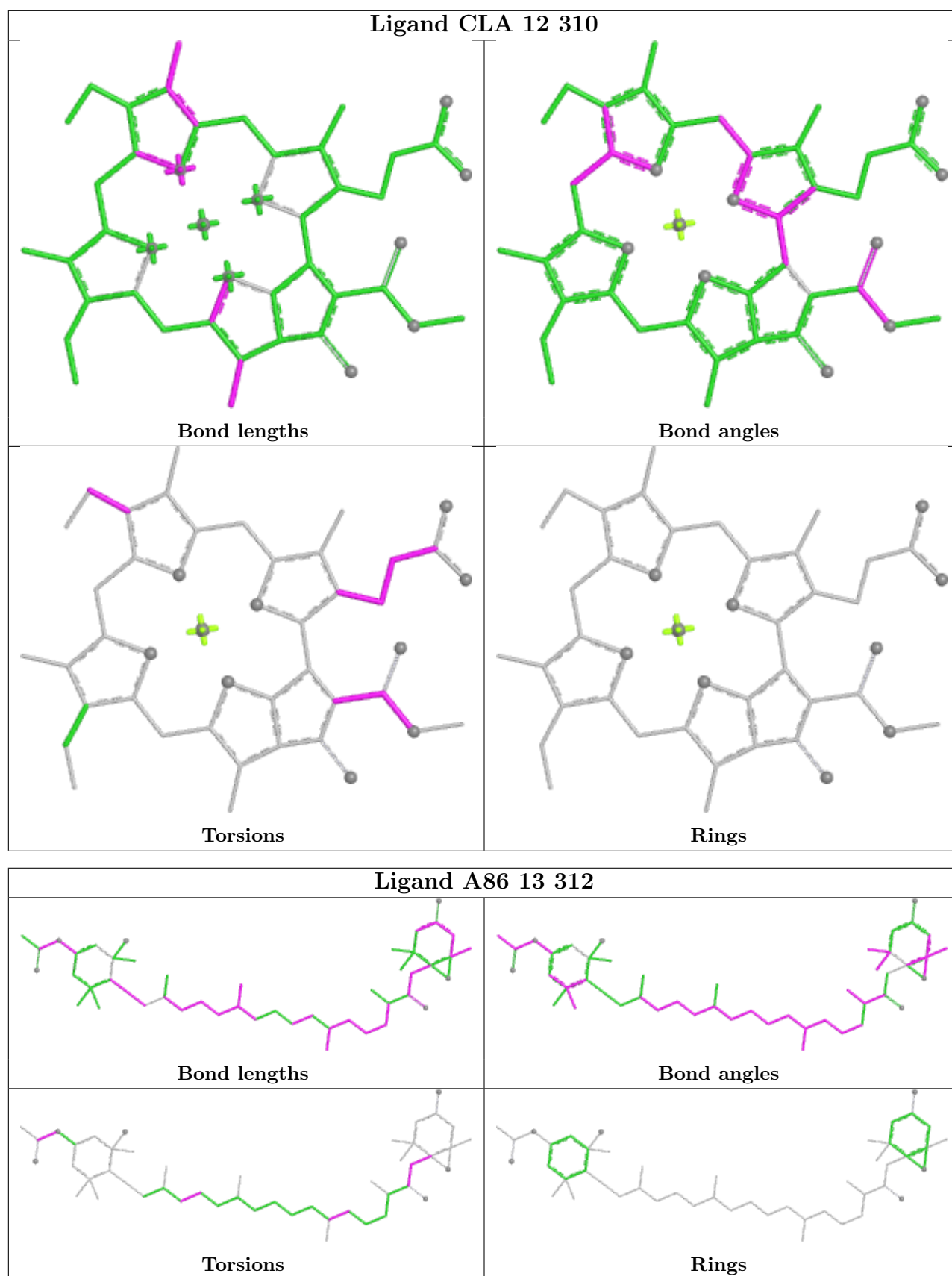


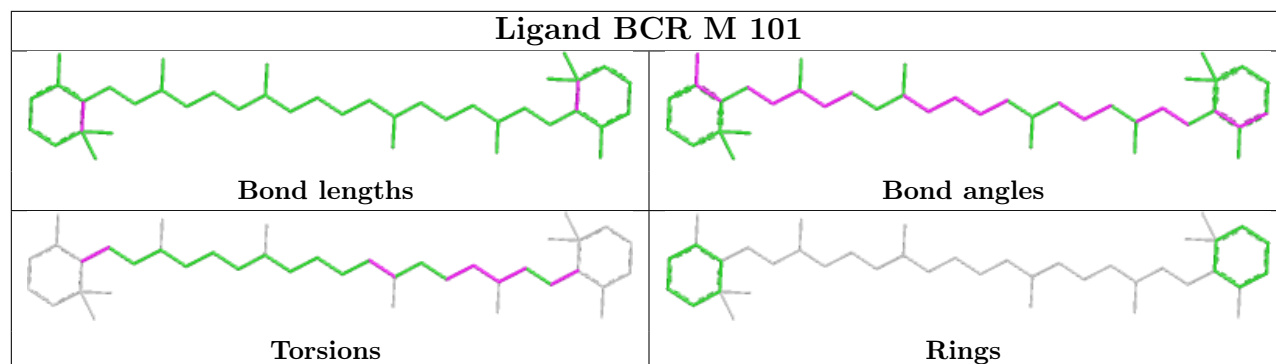
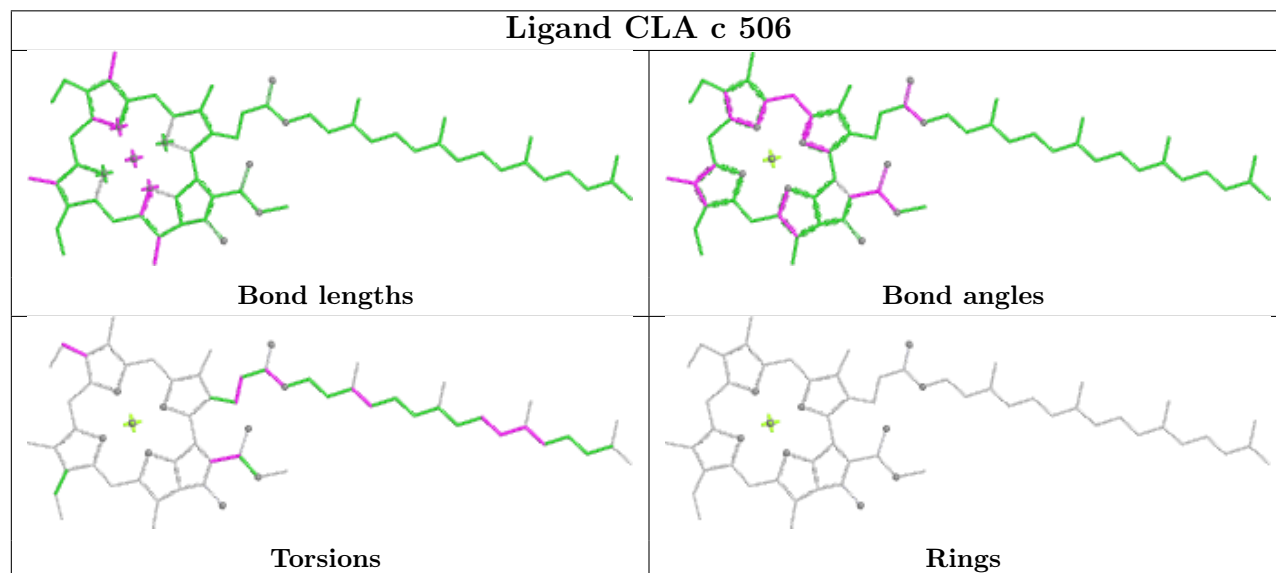
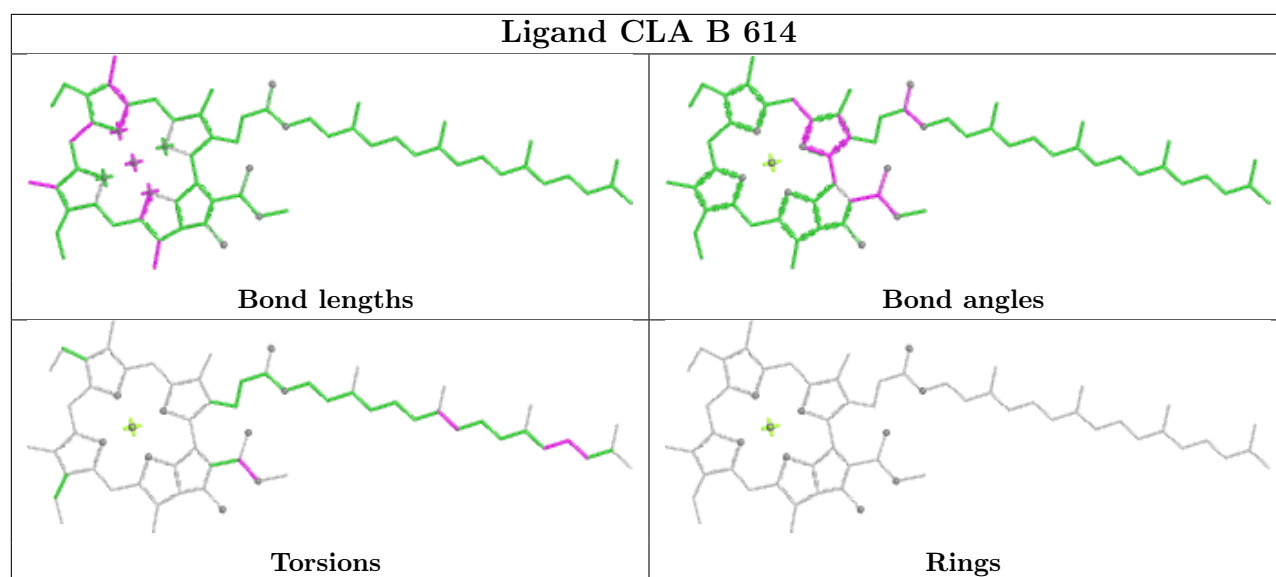


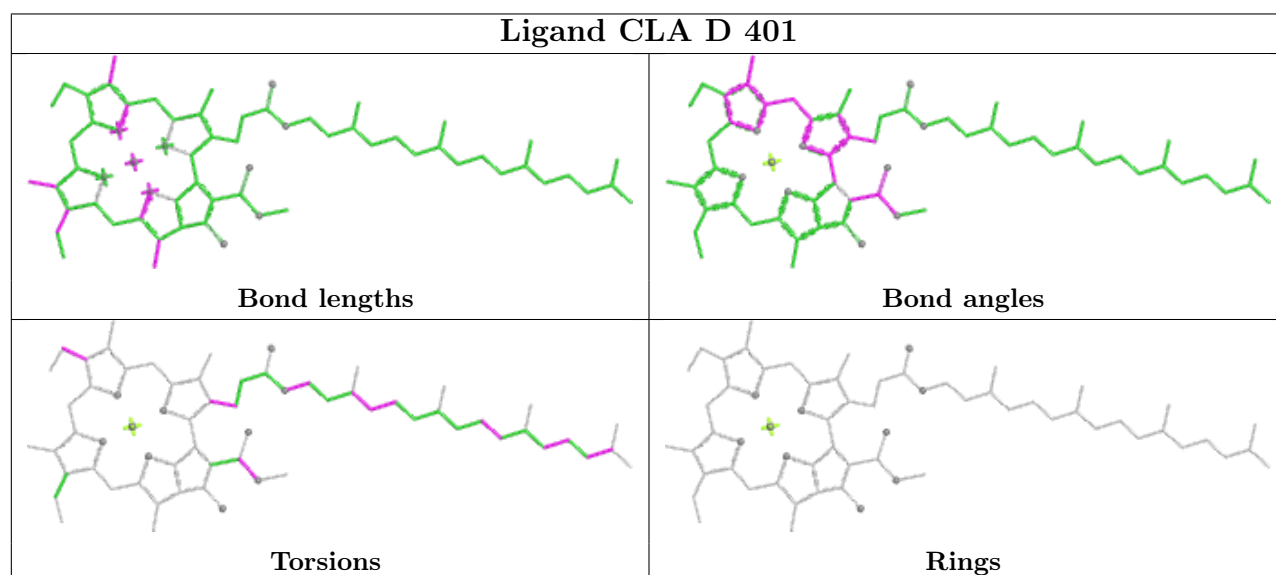
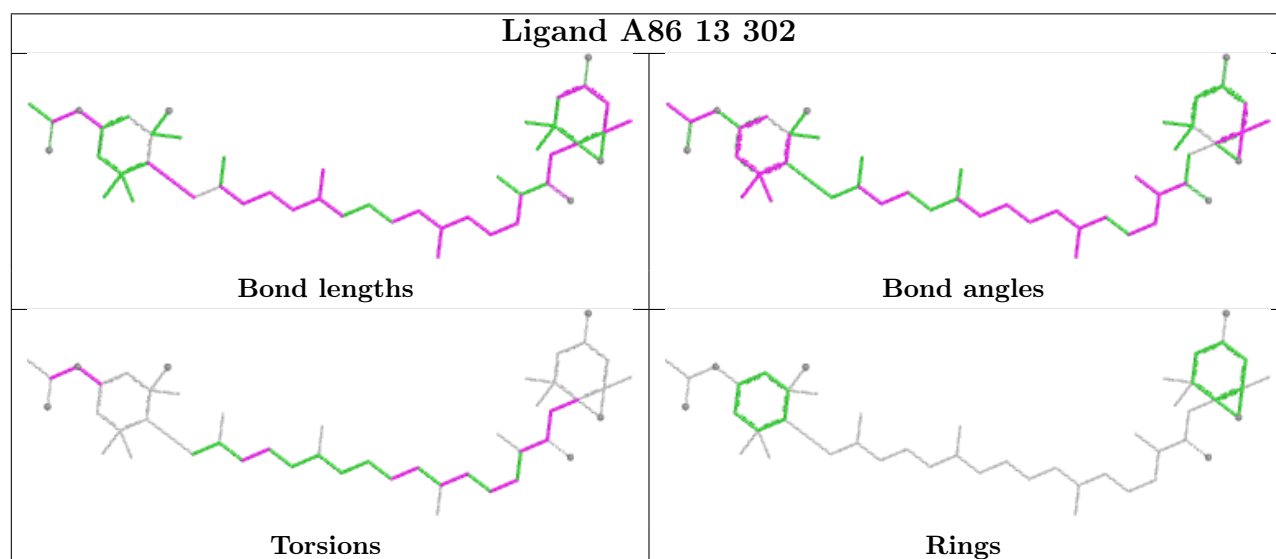
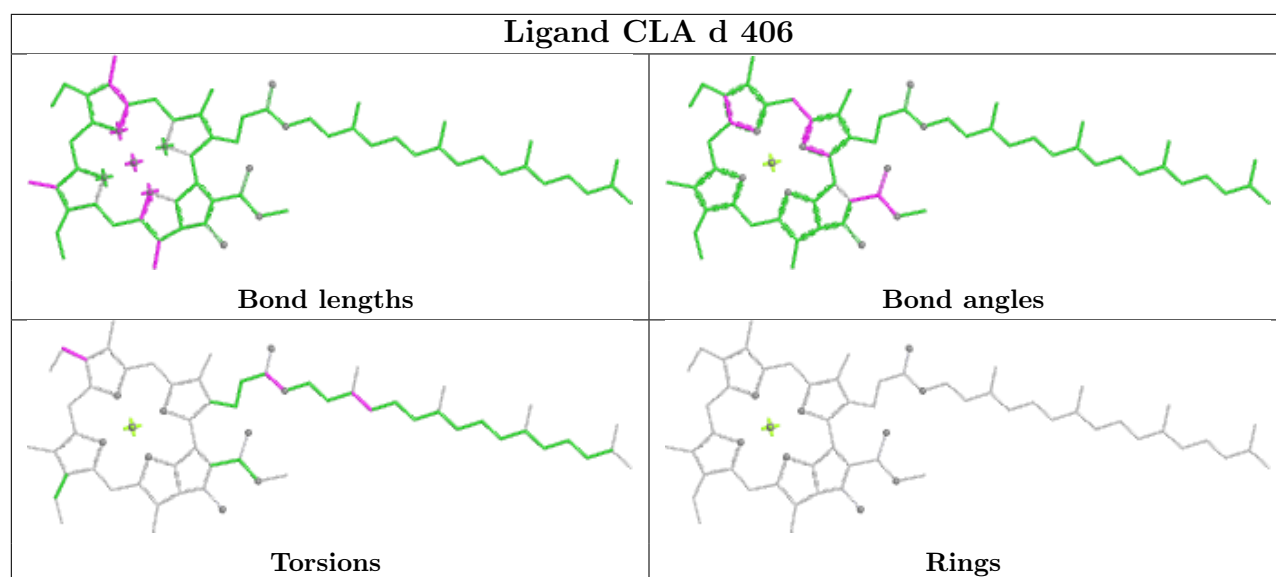


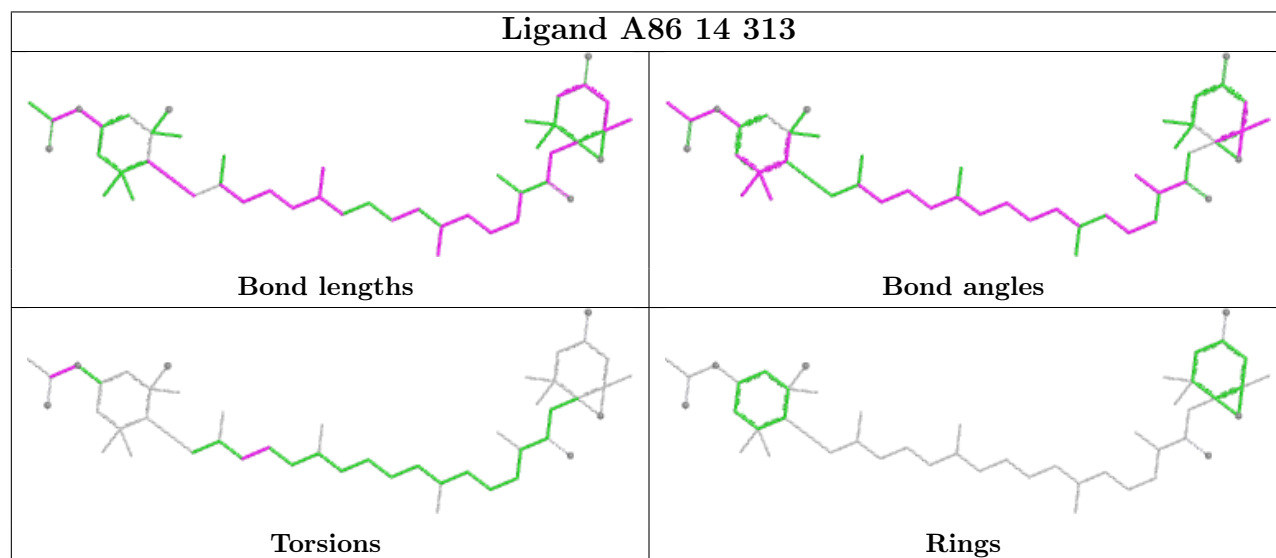
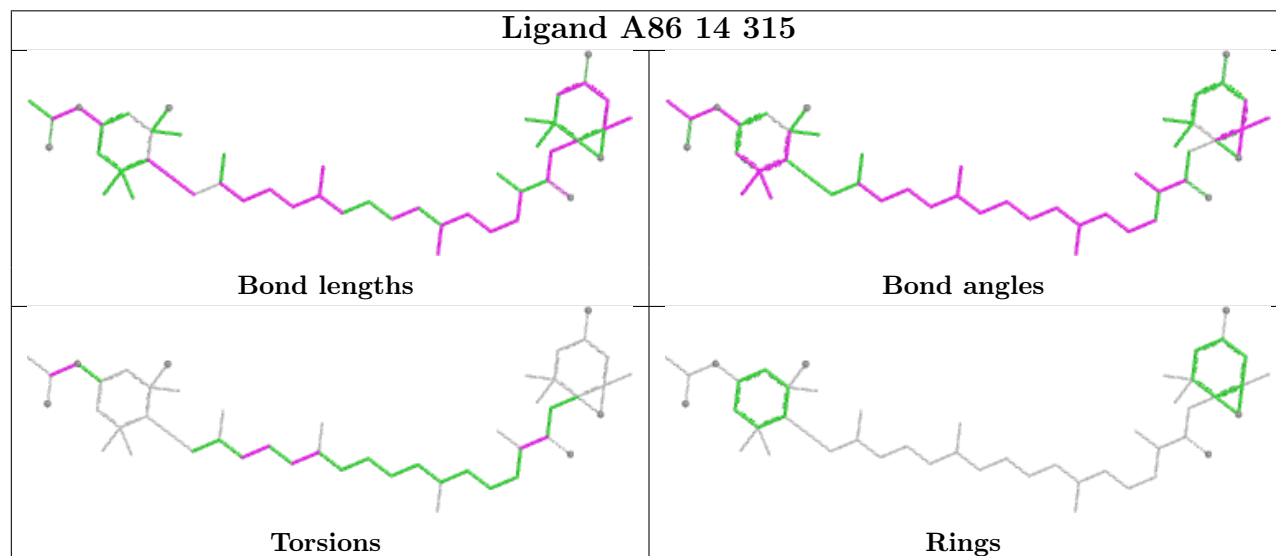
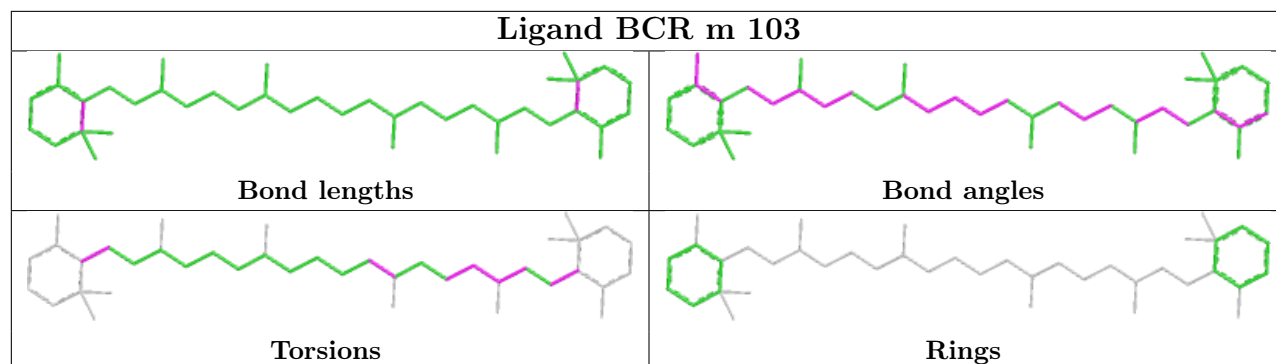


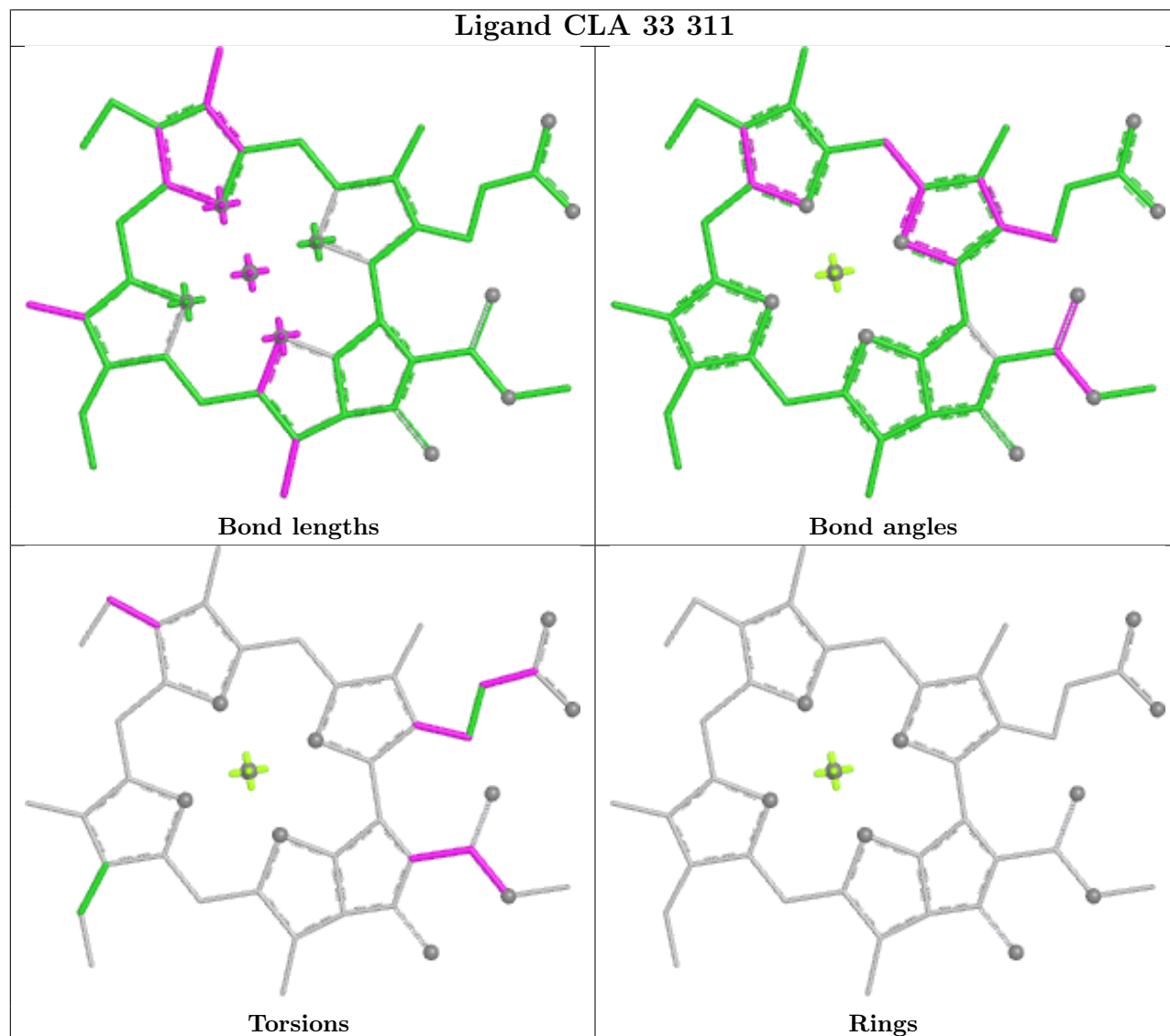
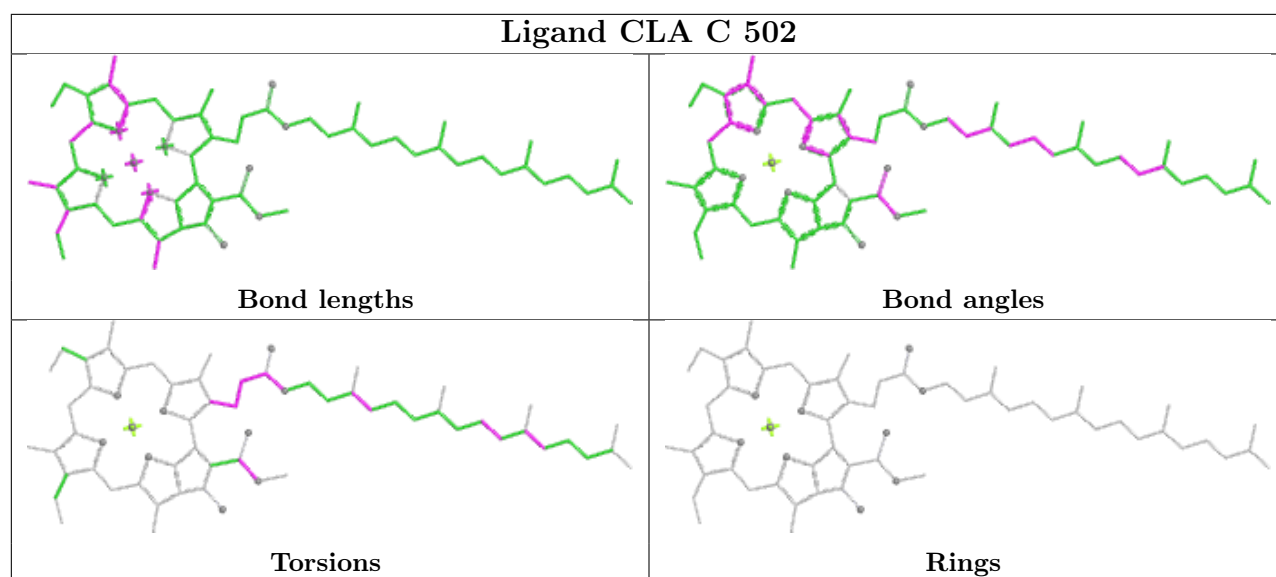


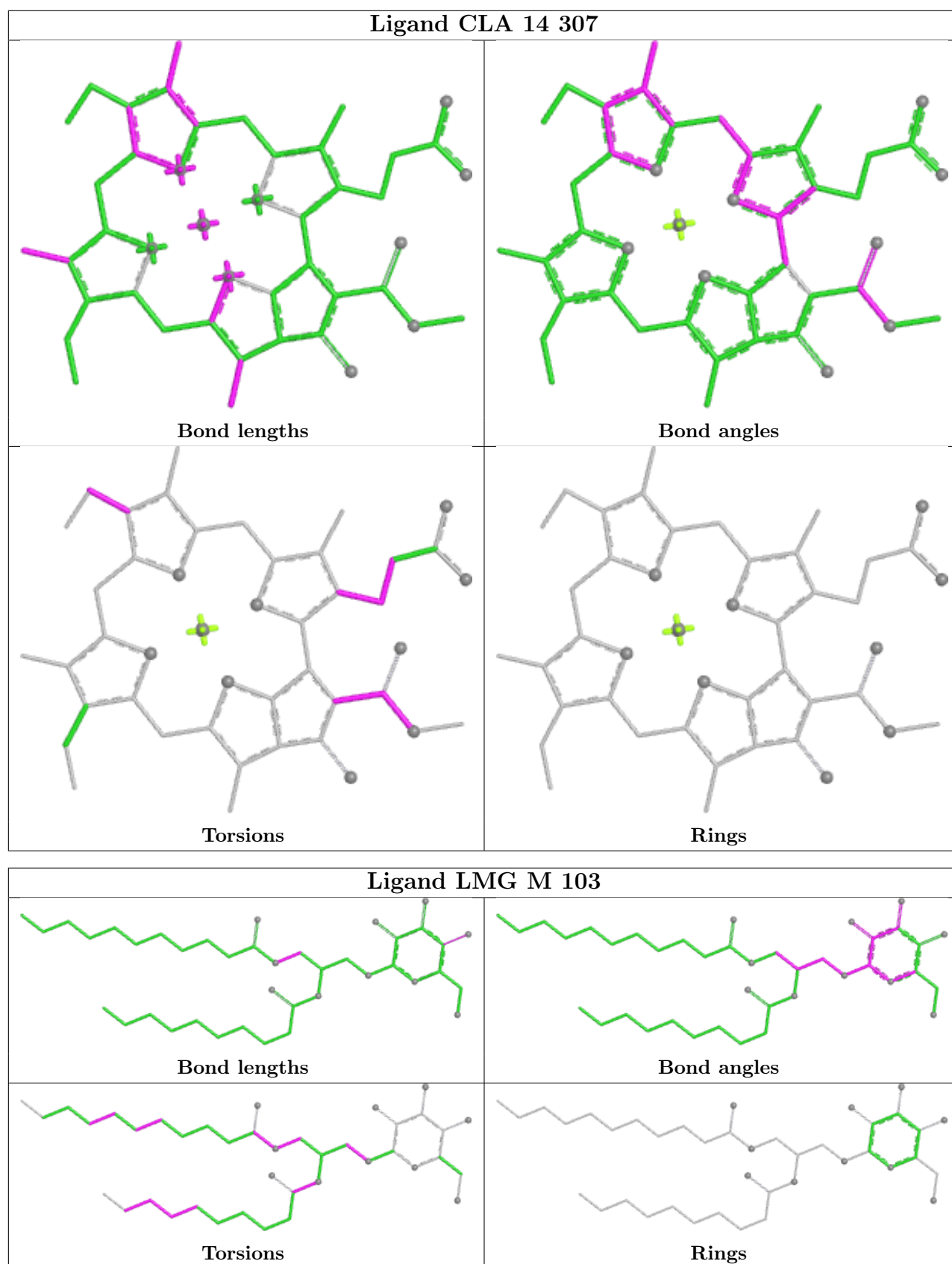




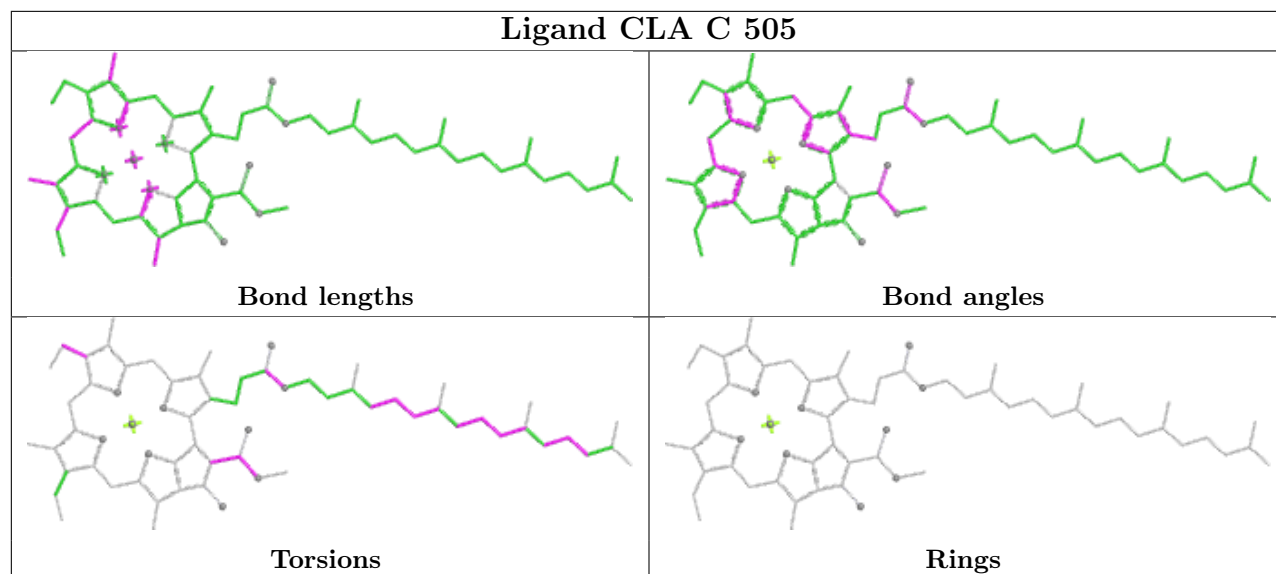




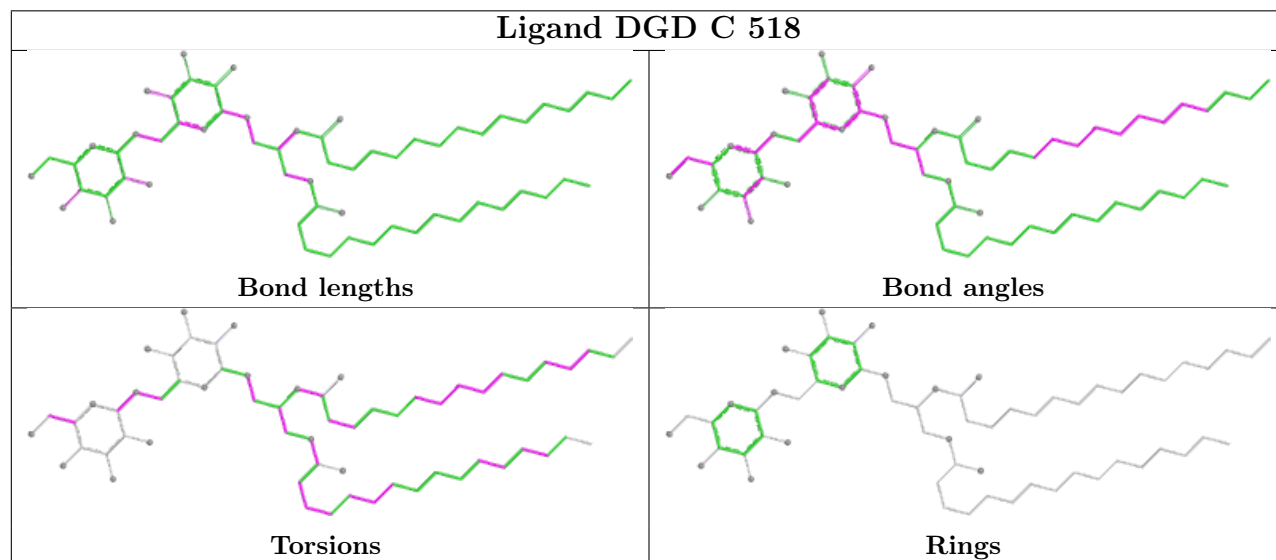


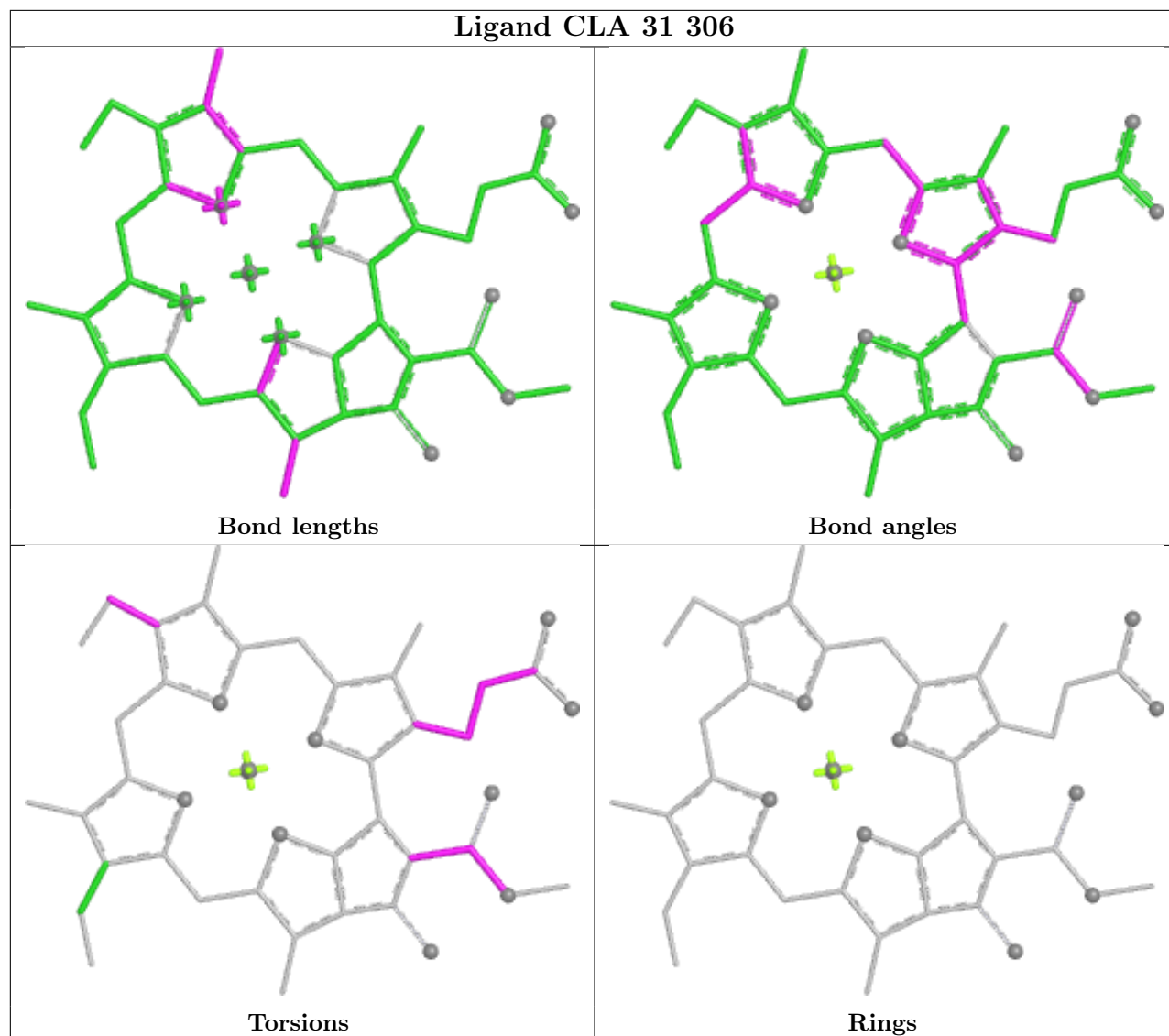


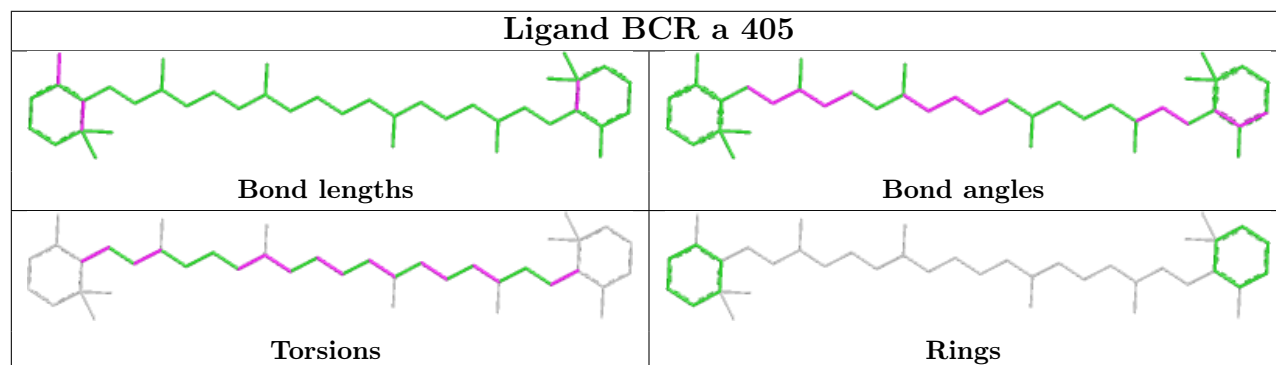
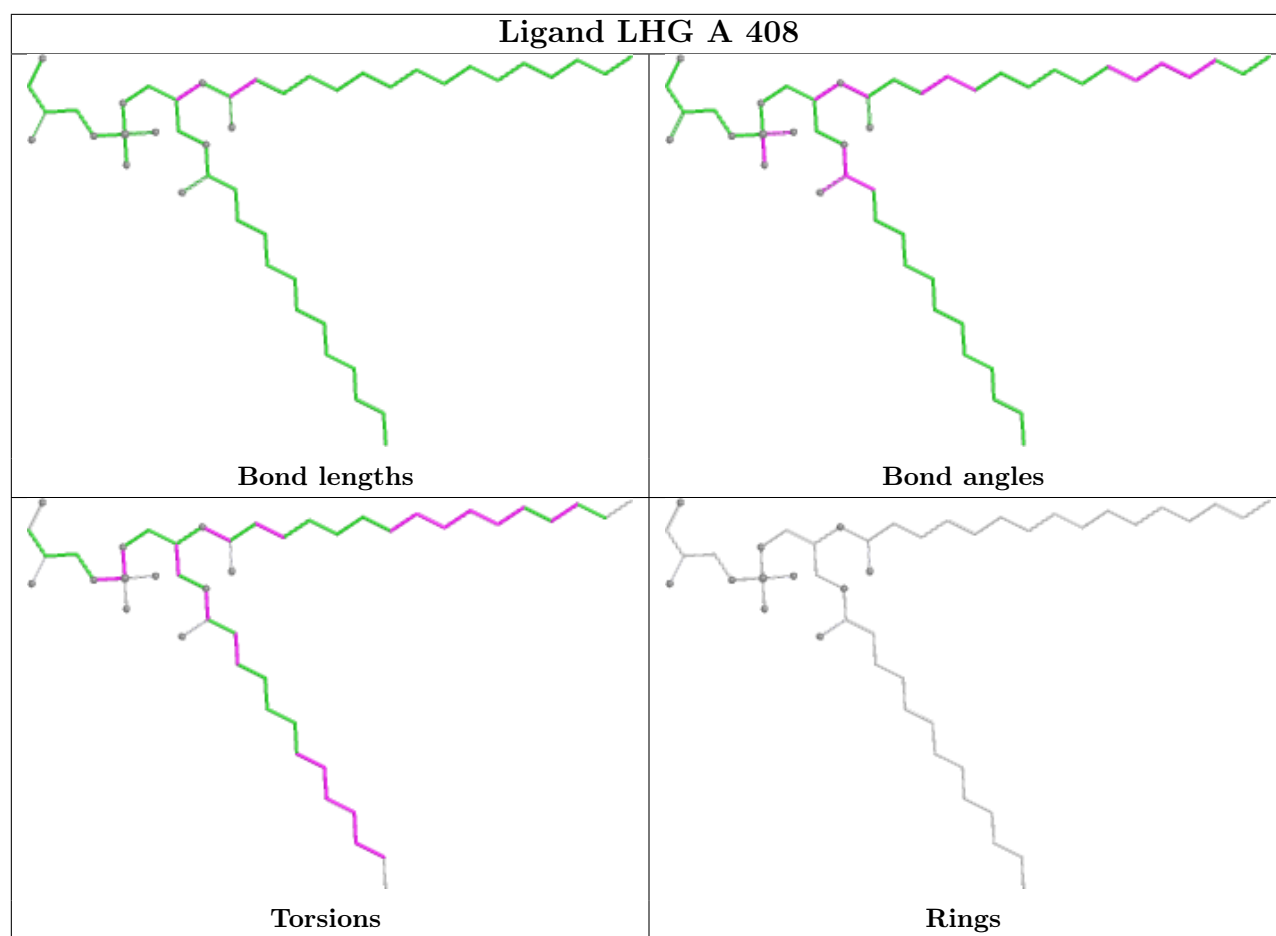
Ligand CLA C 505

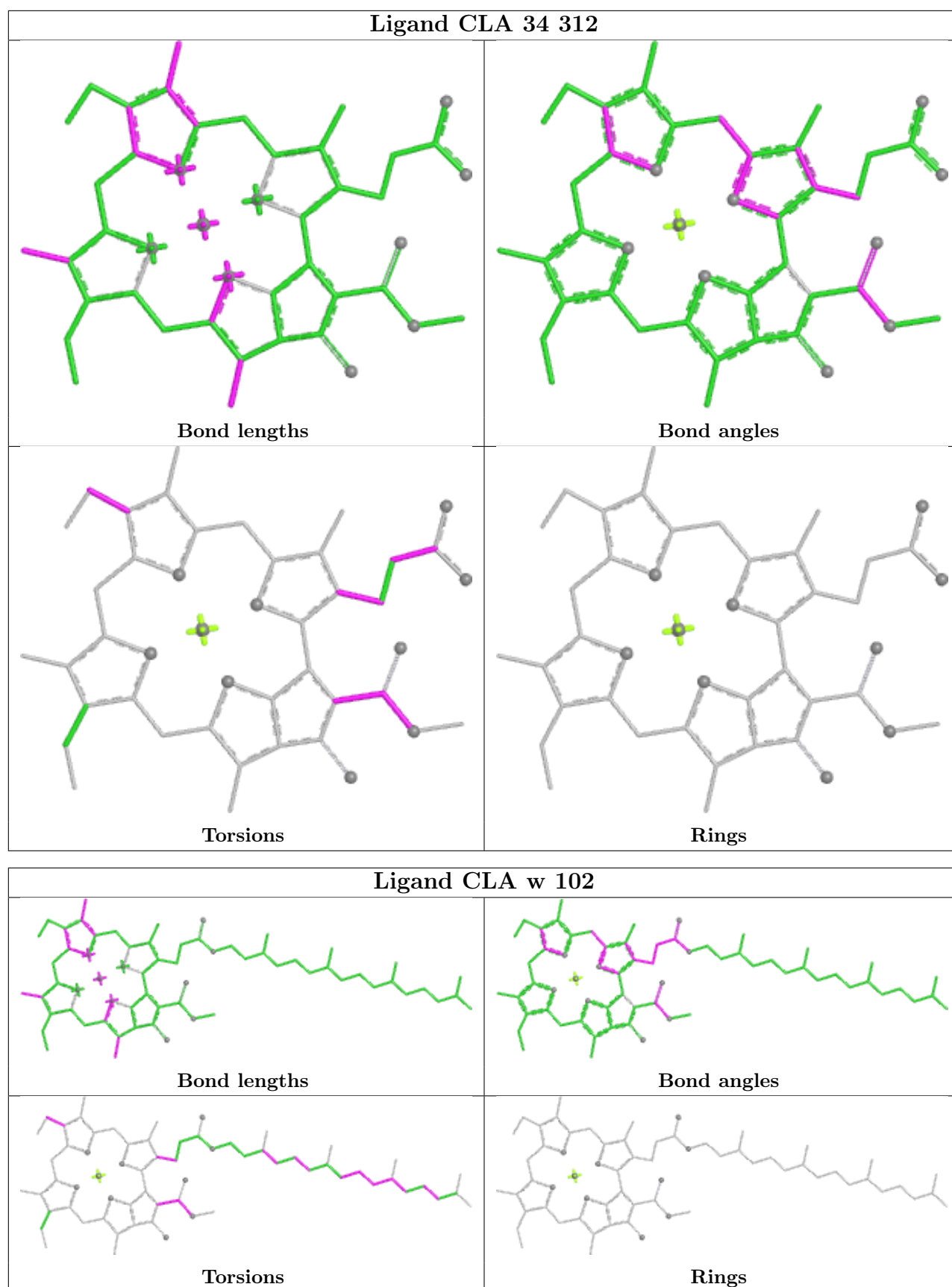


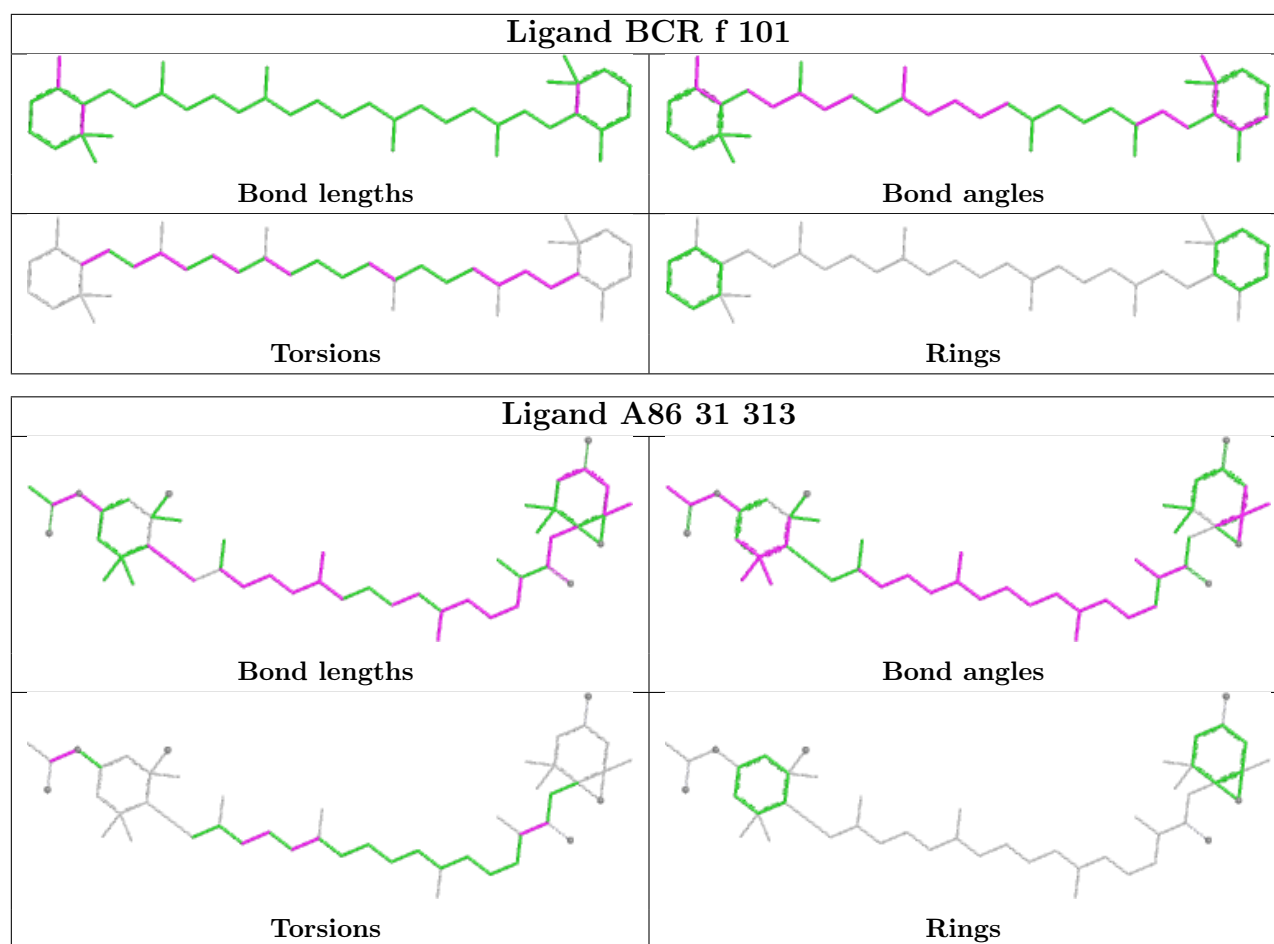
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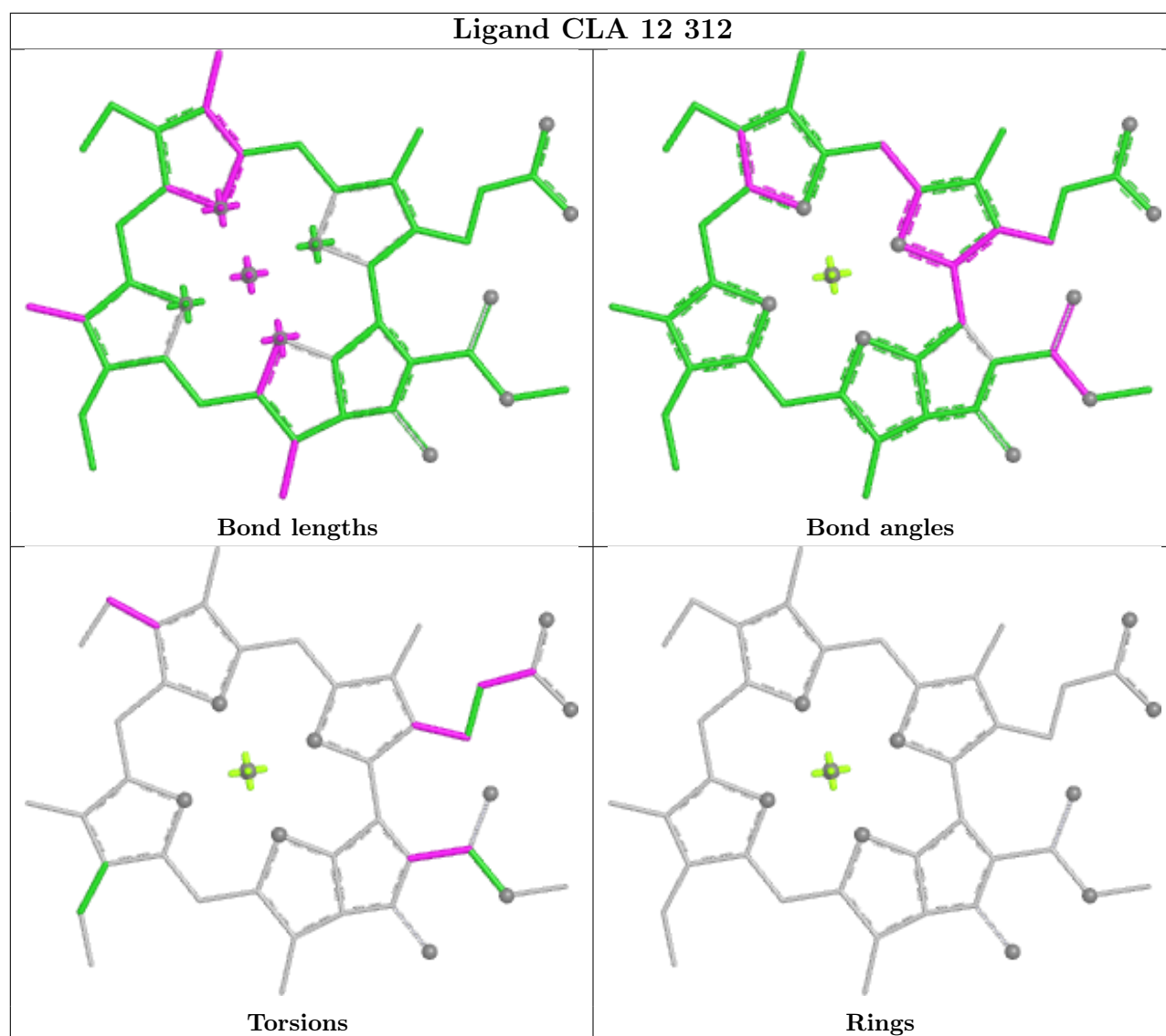


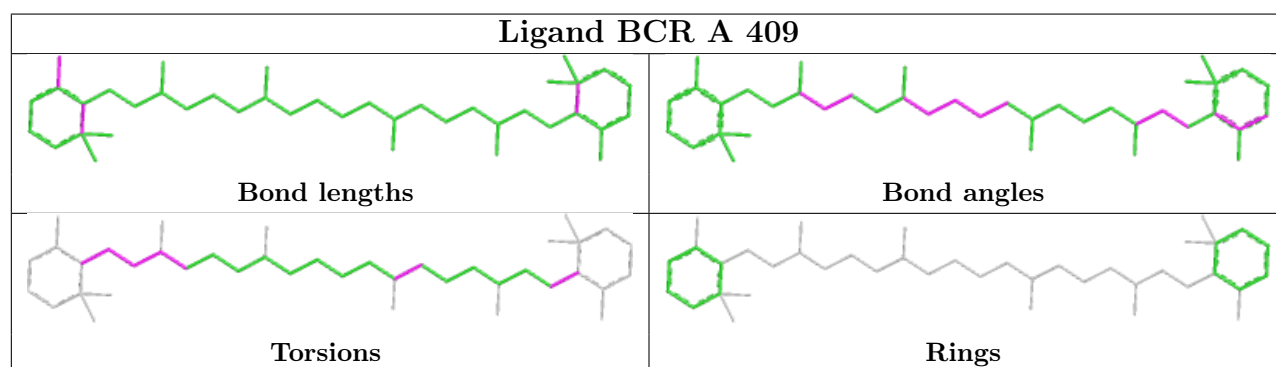
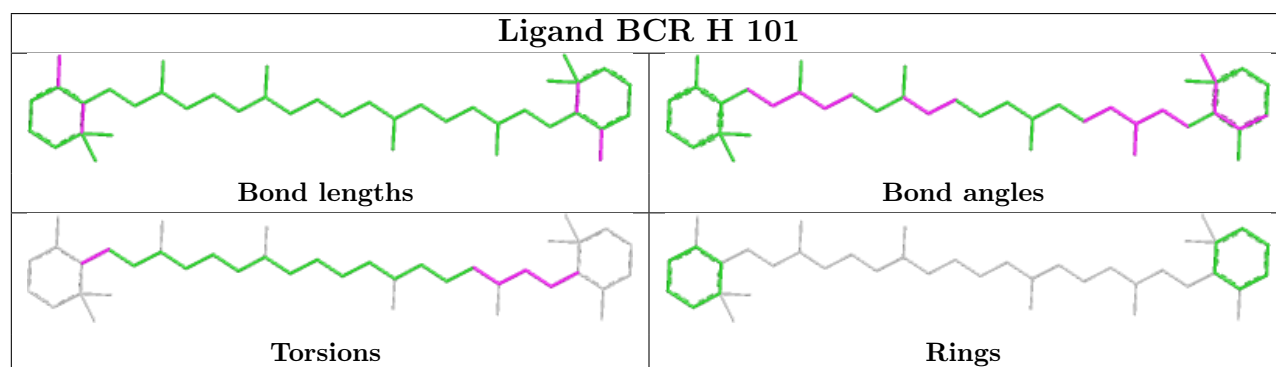
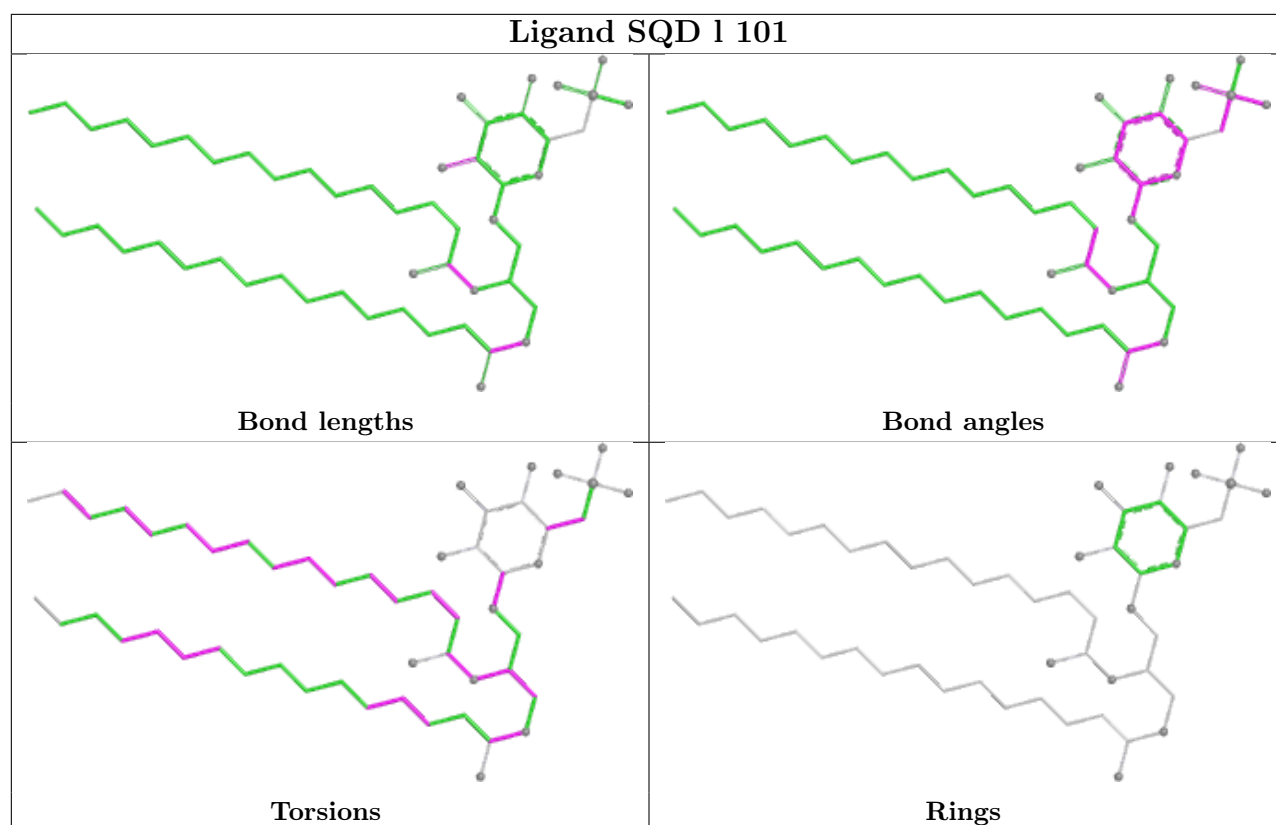


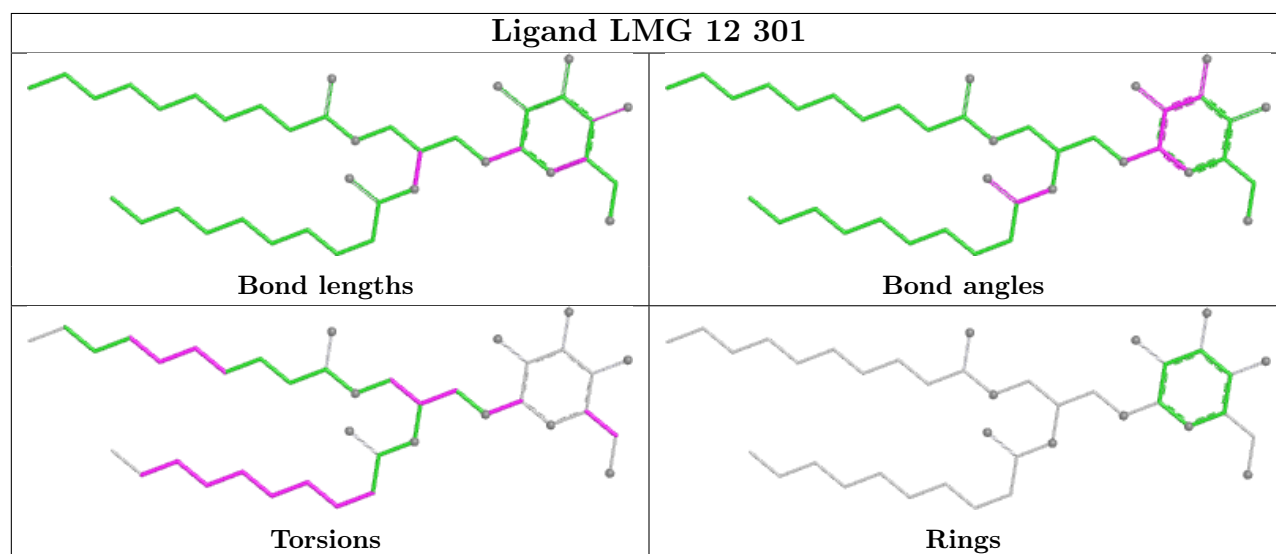
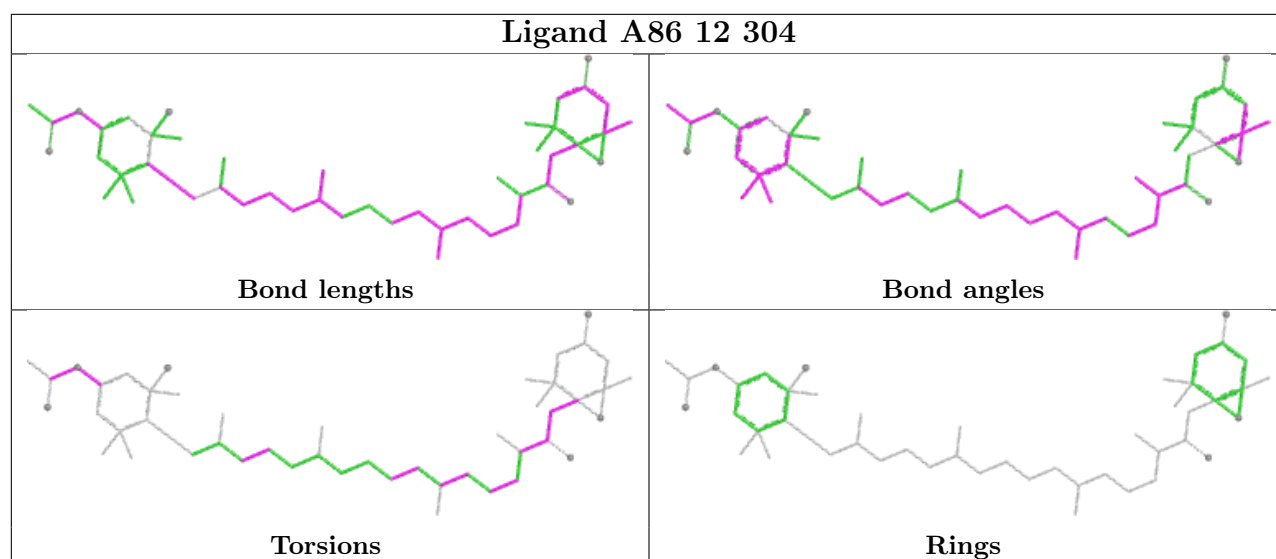


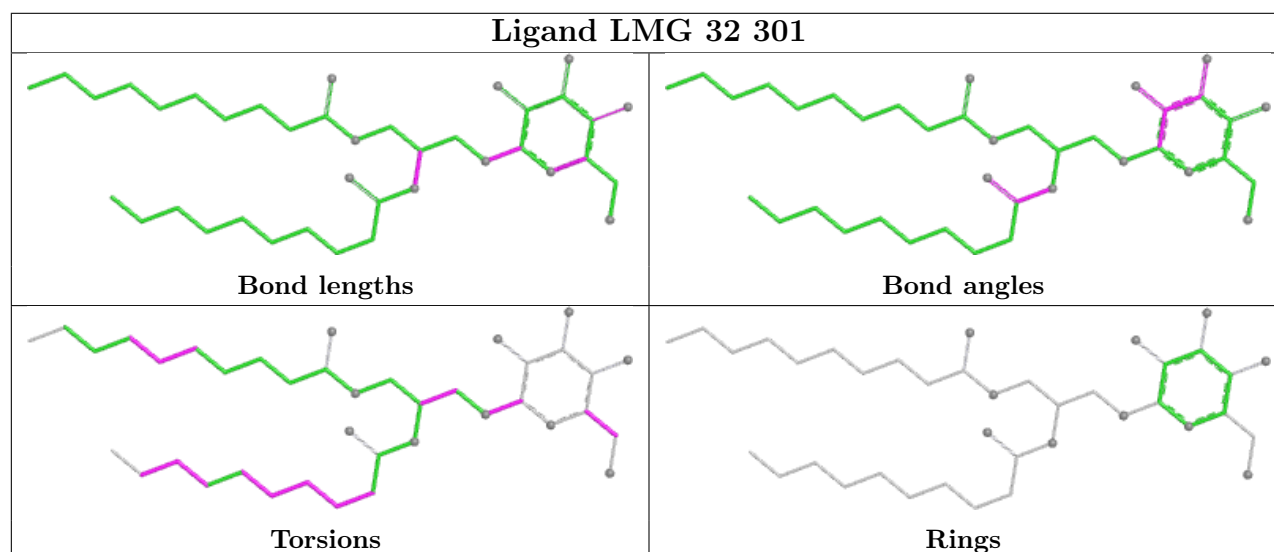
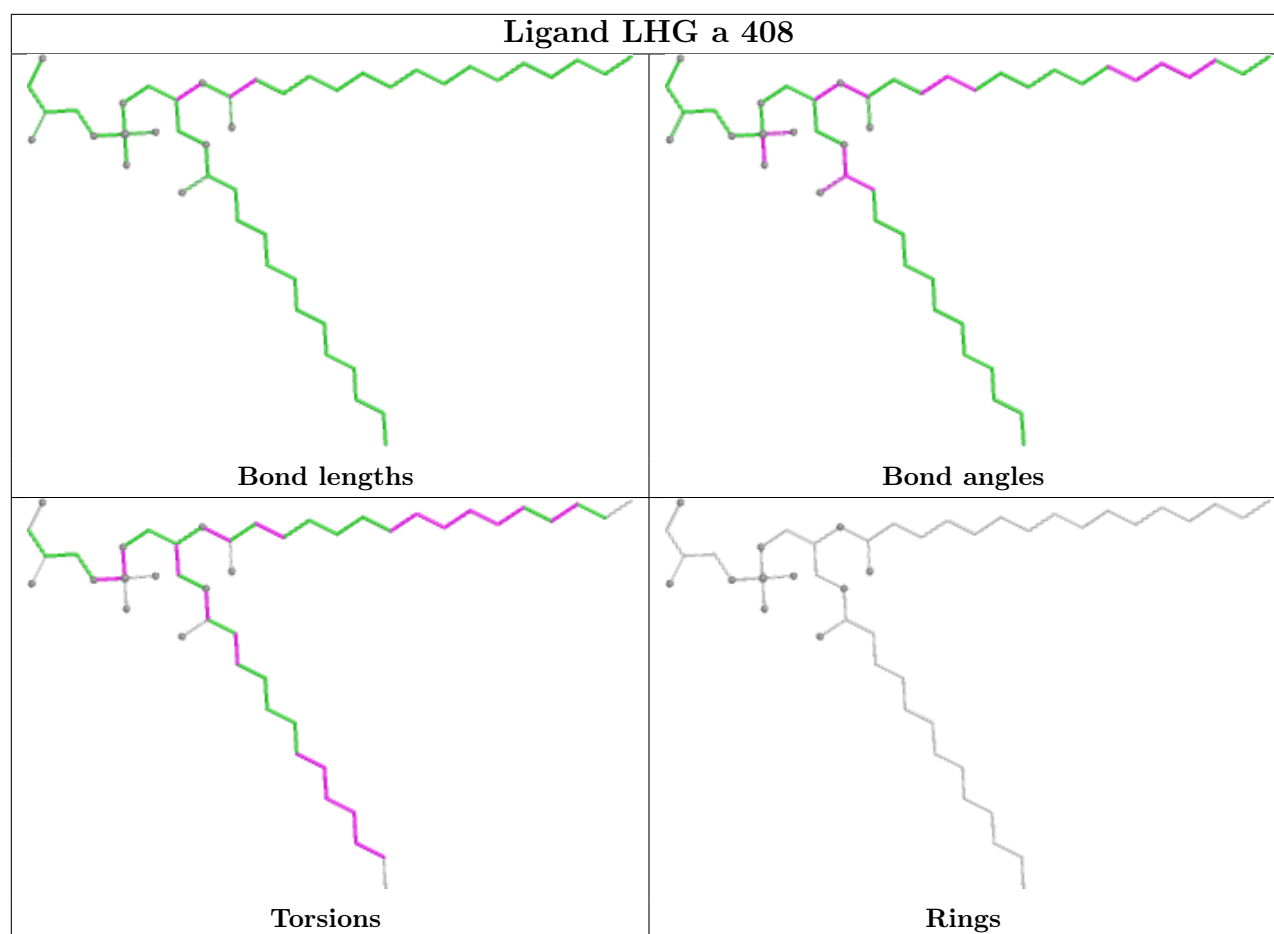


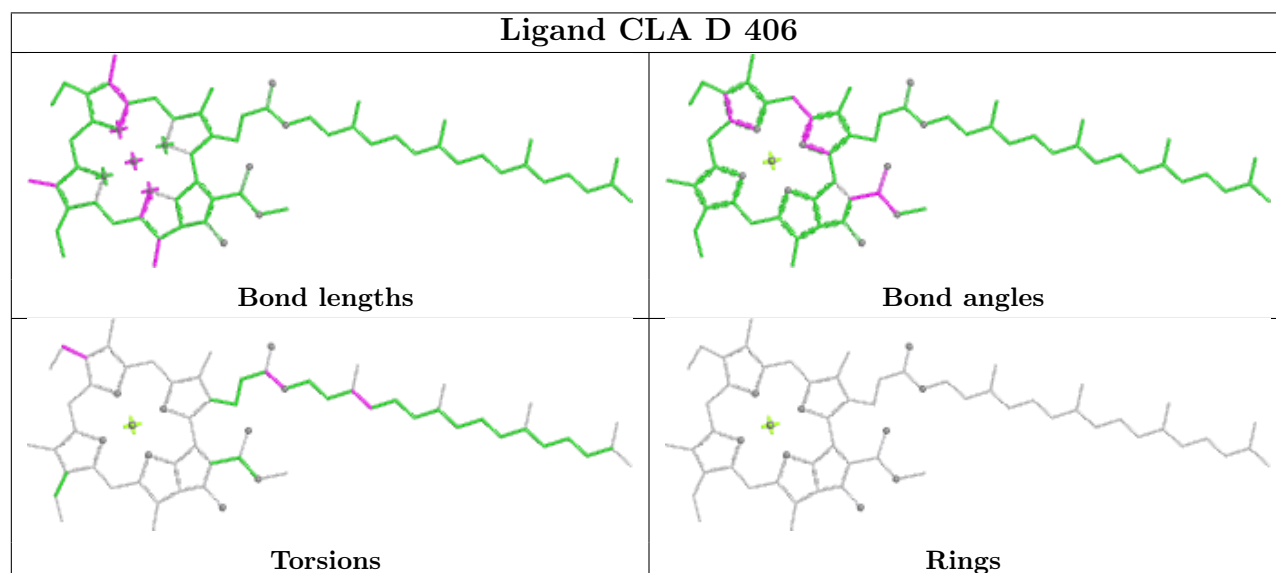
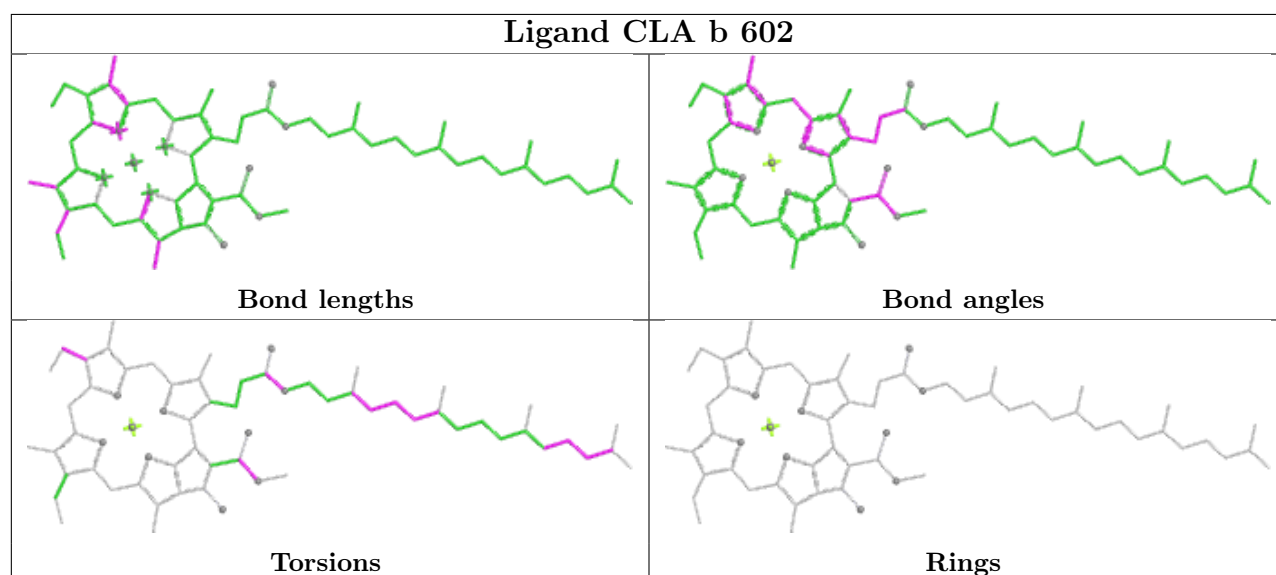
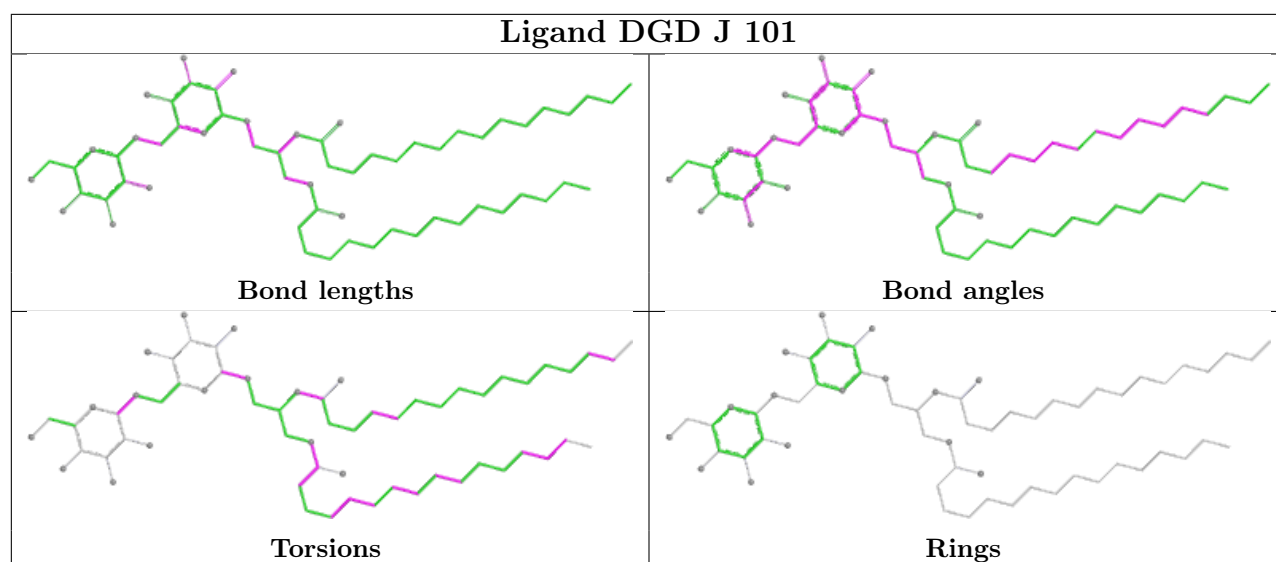


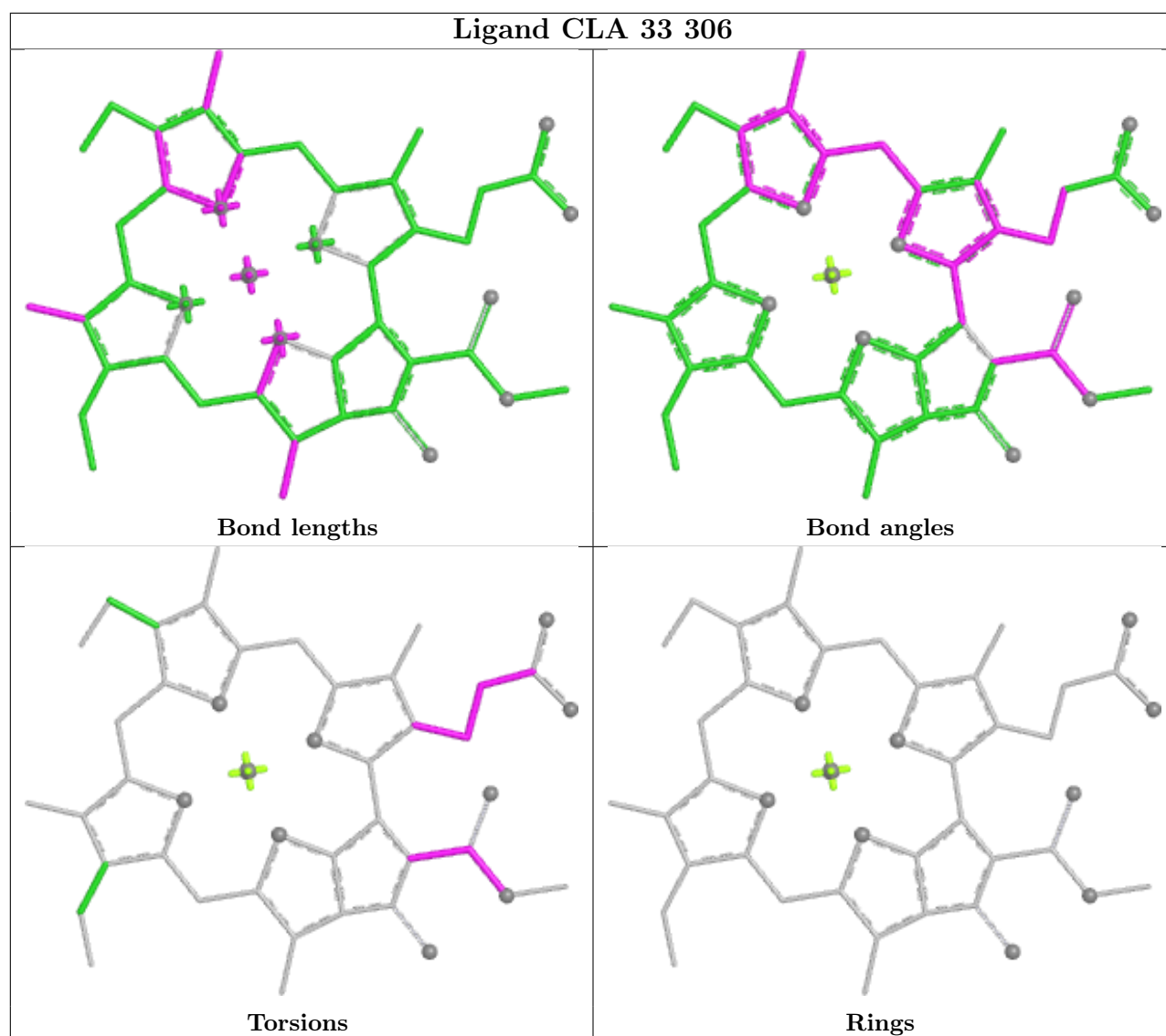


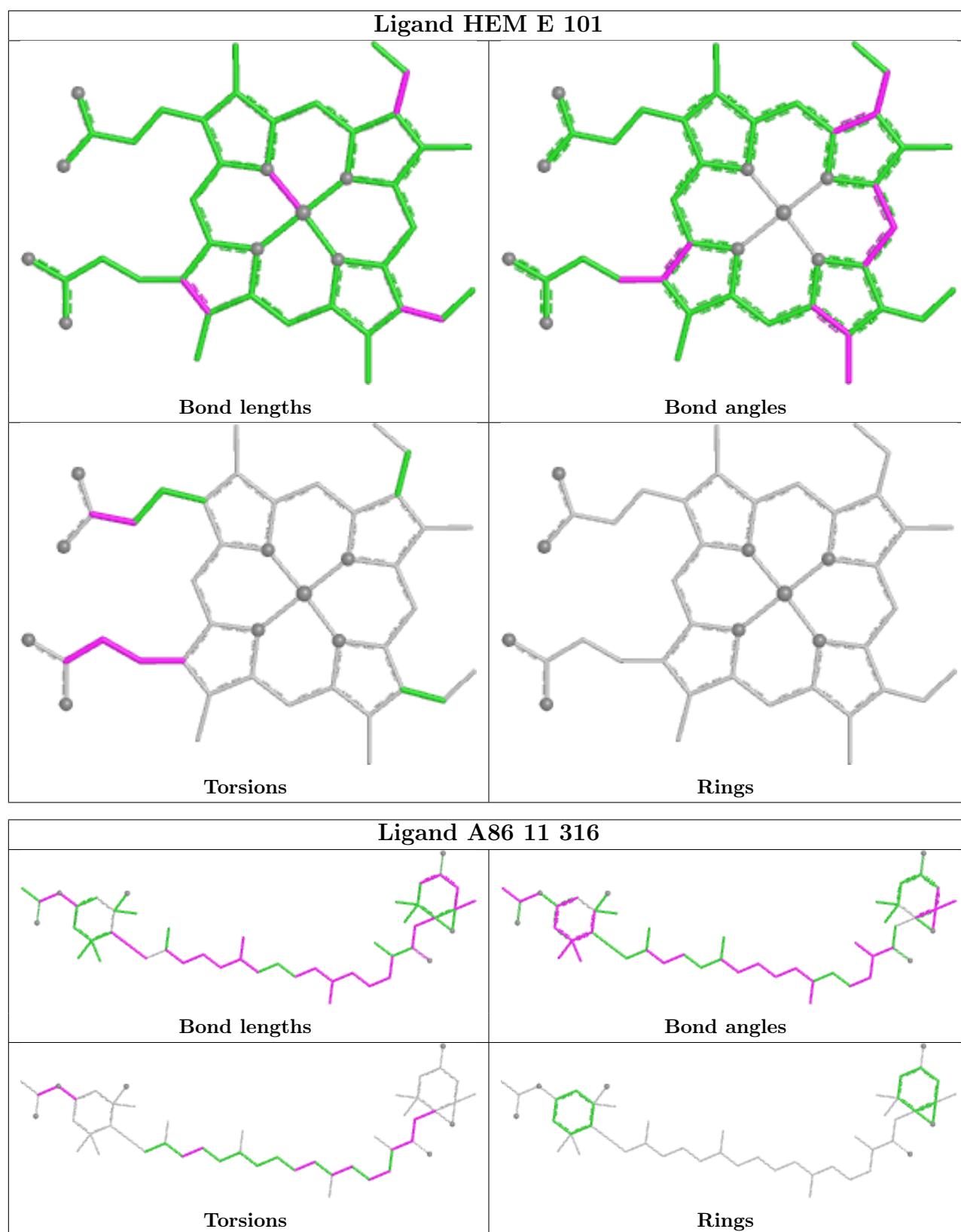


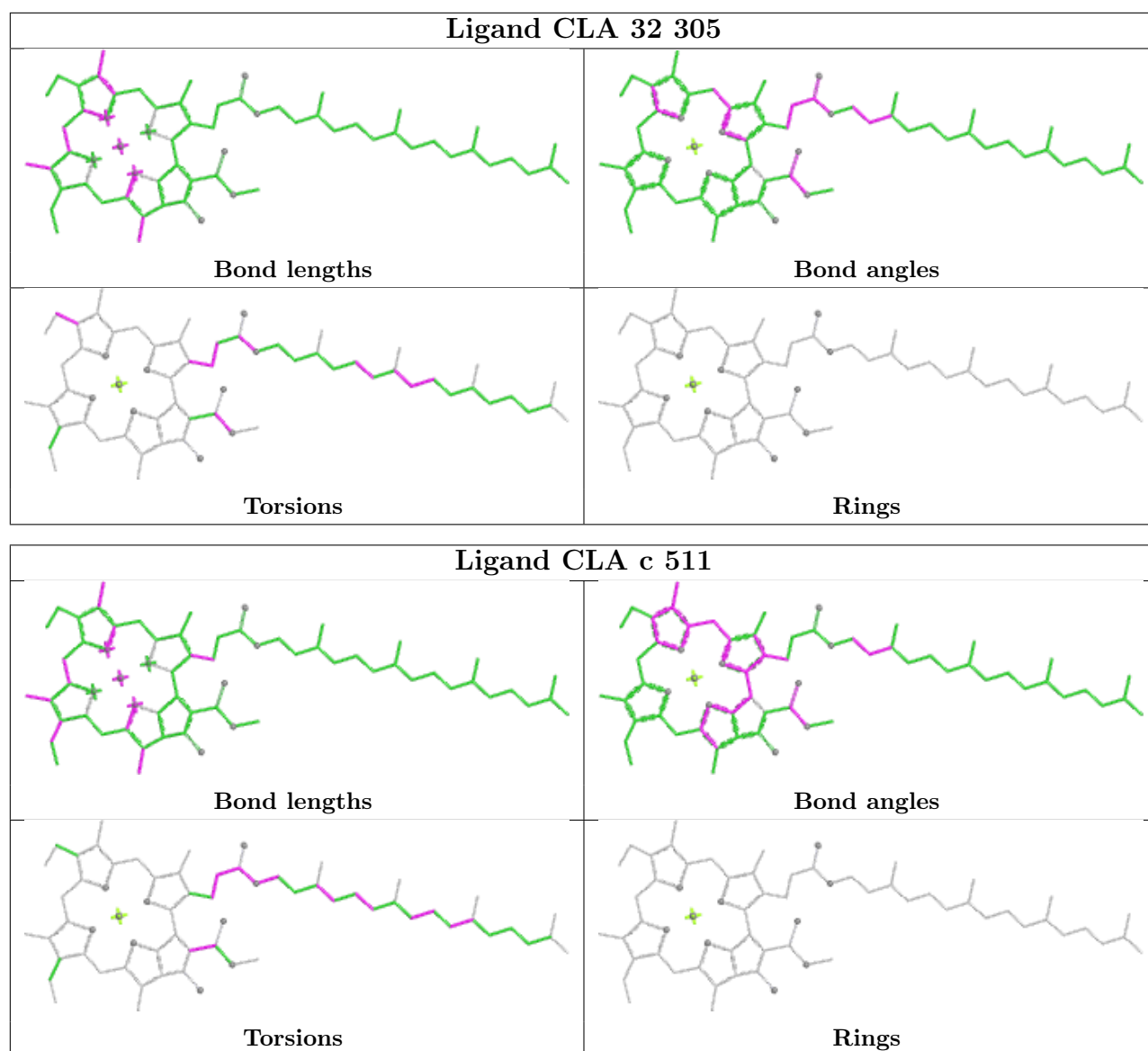


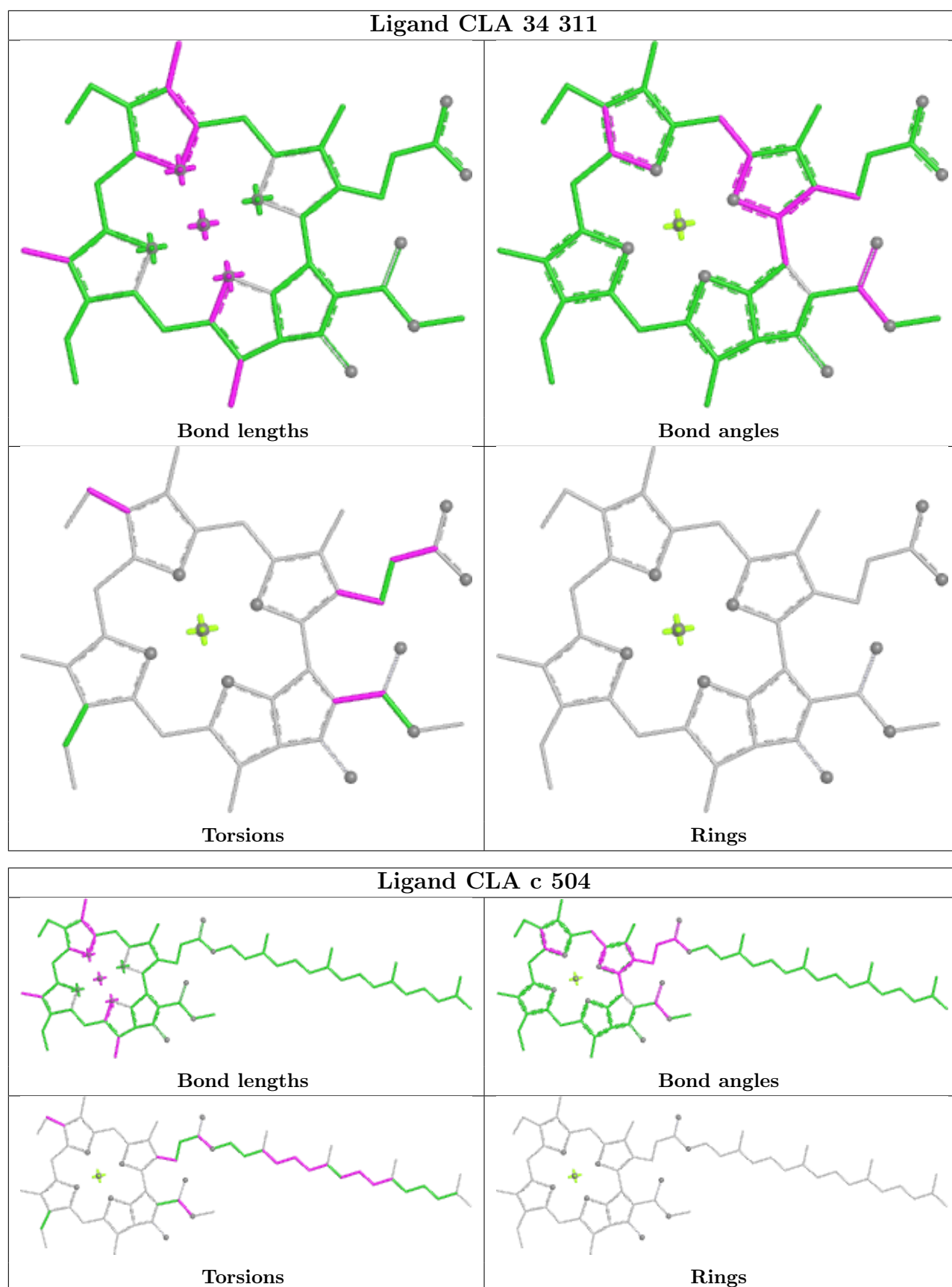


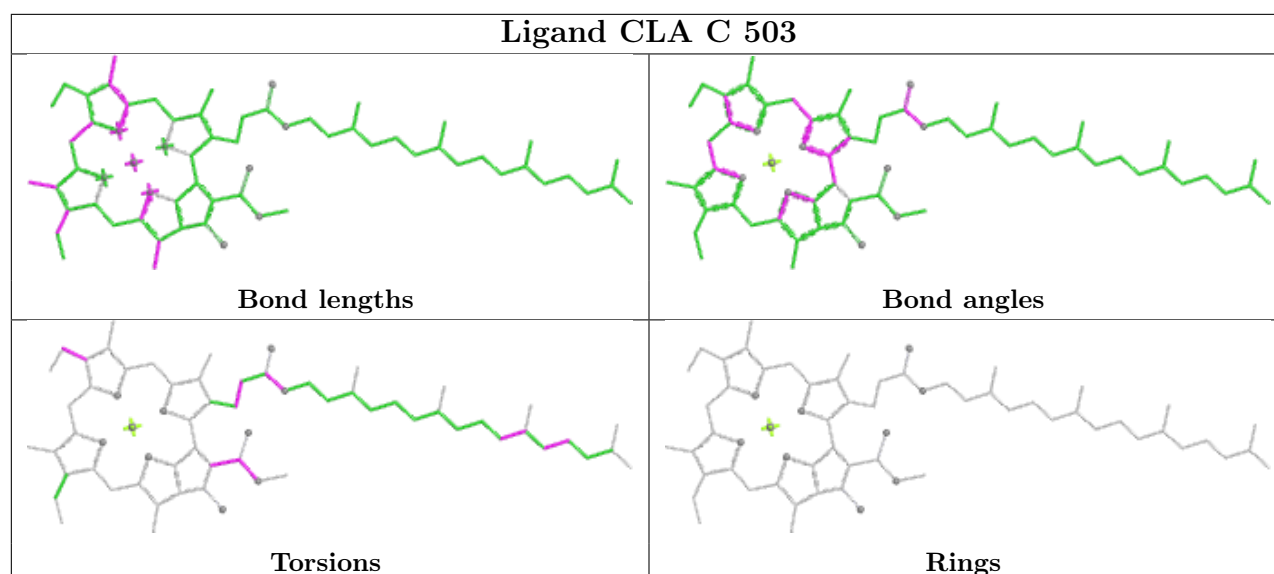
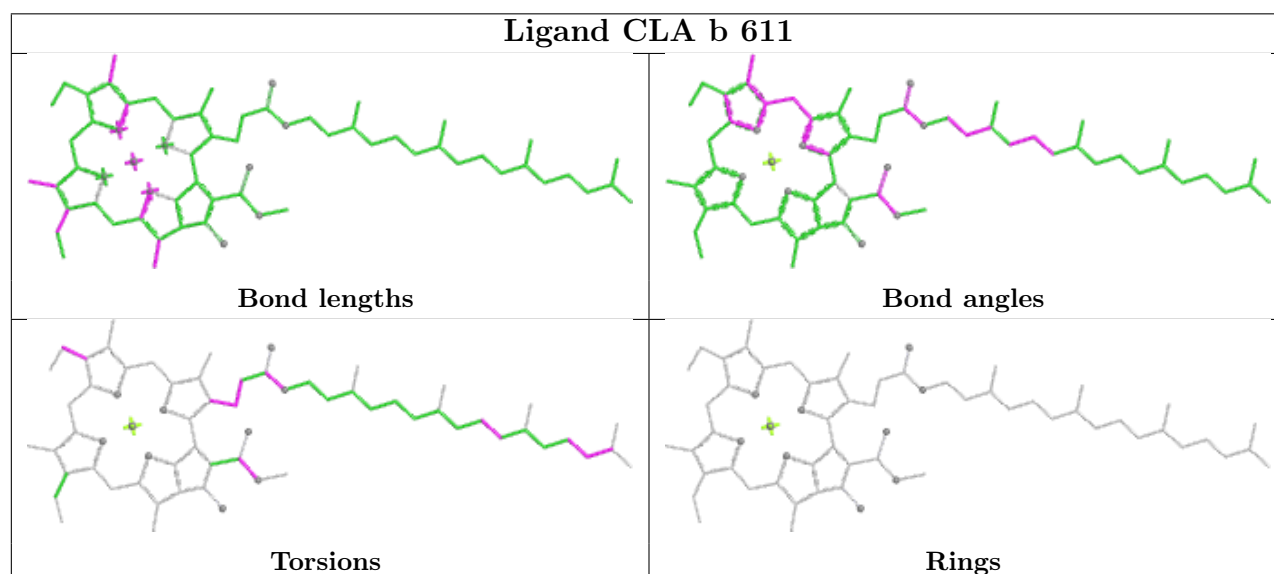
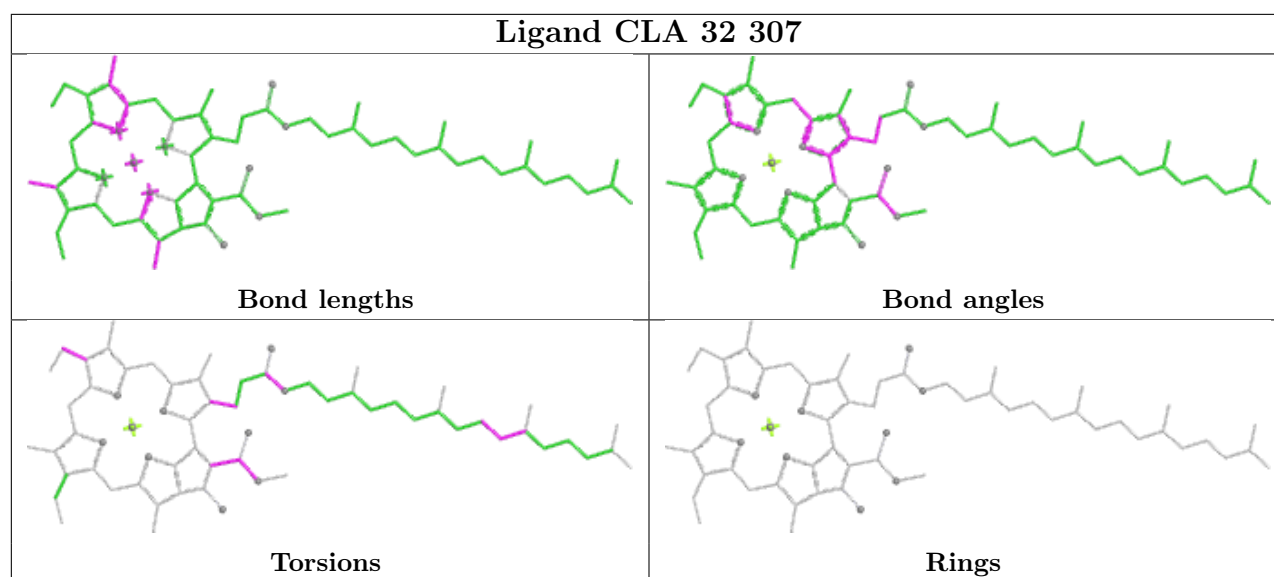


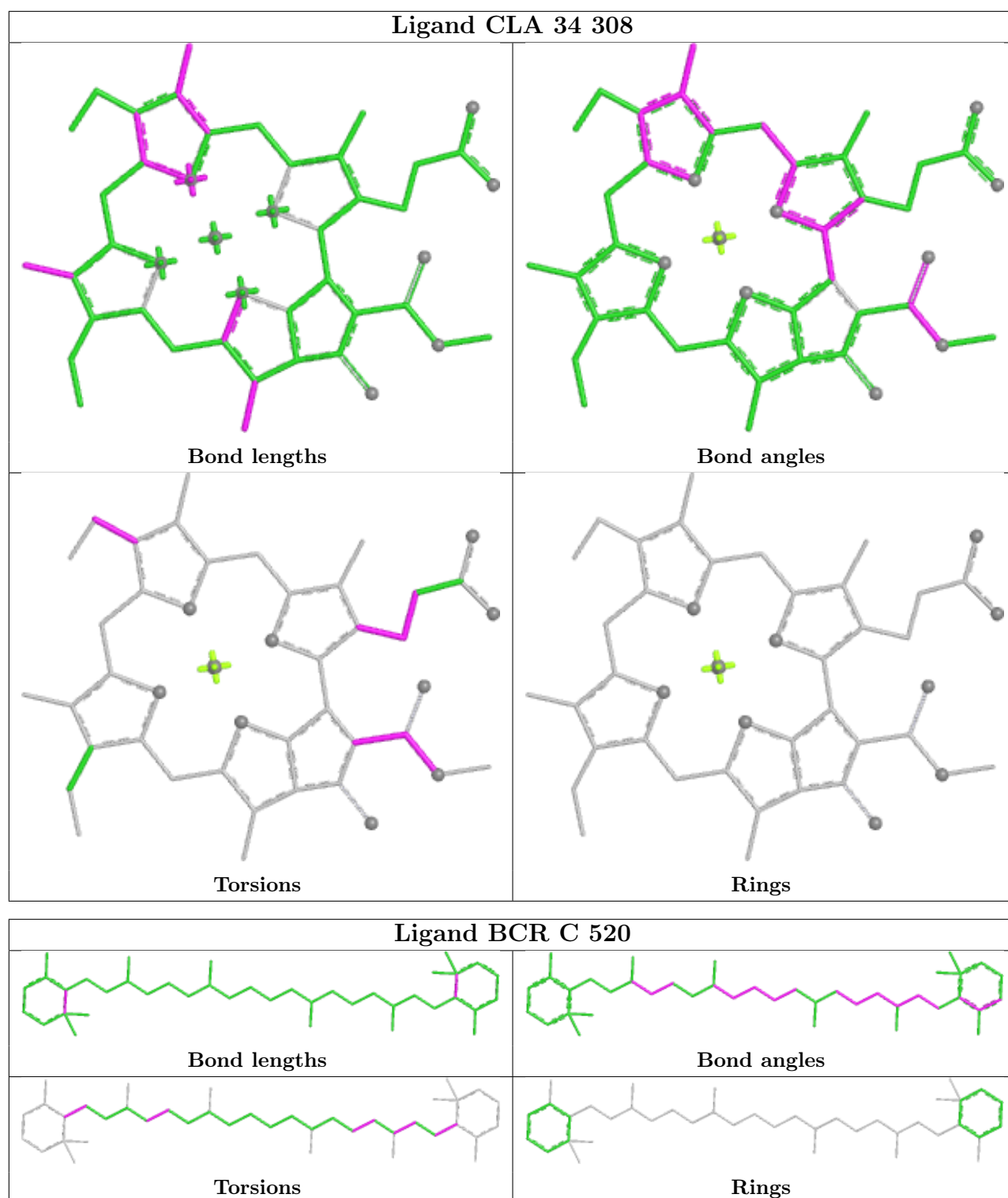


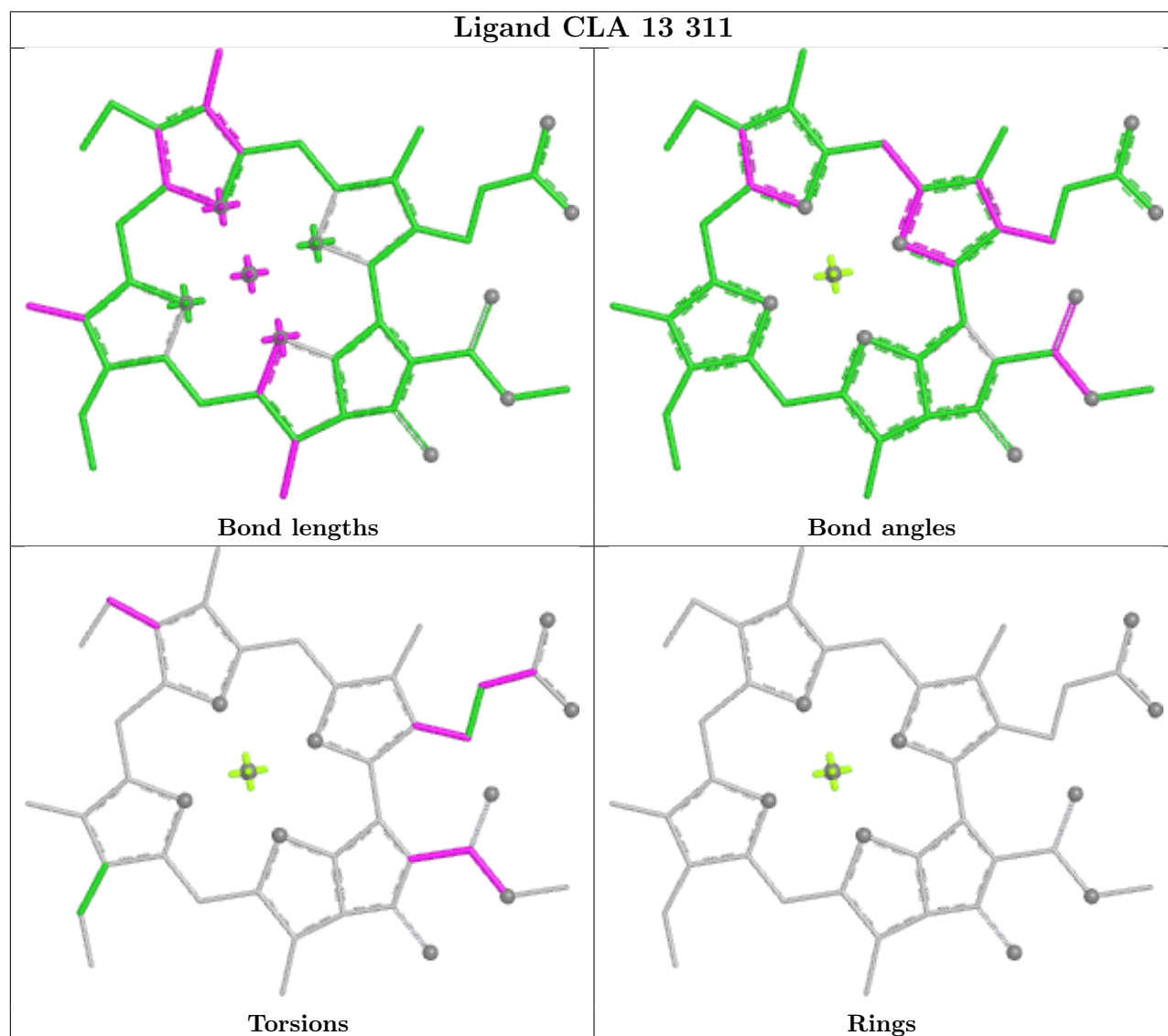
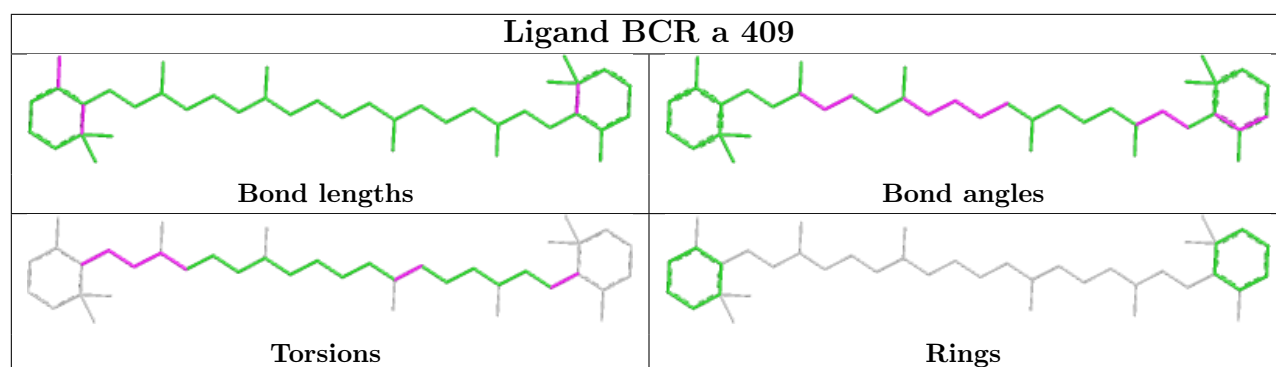


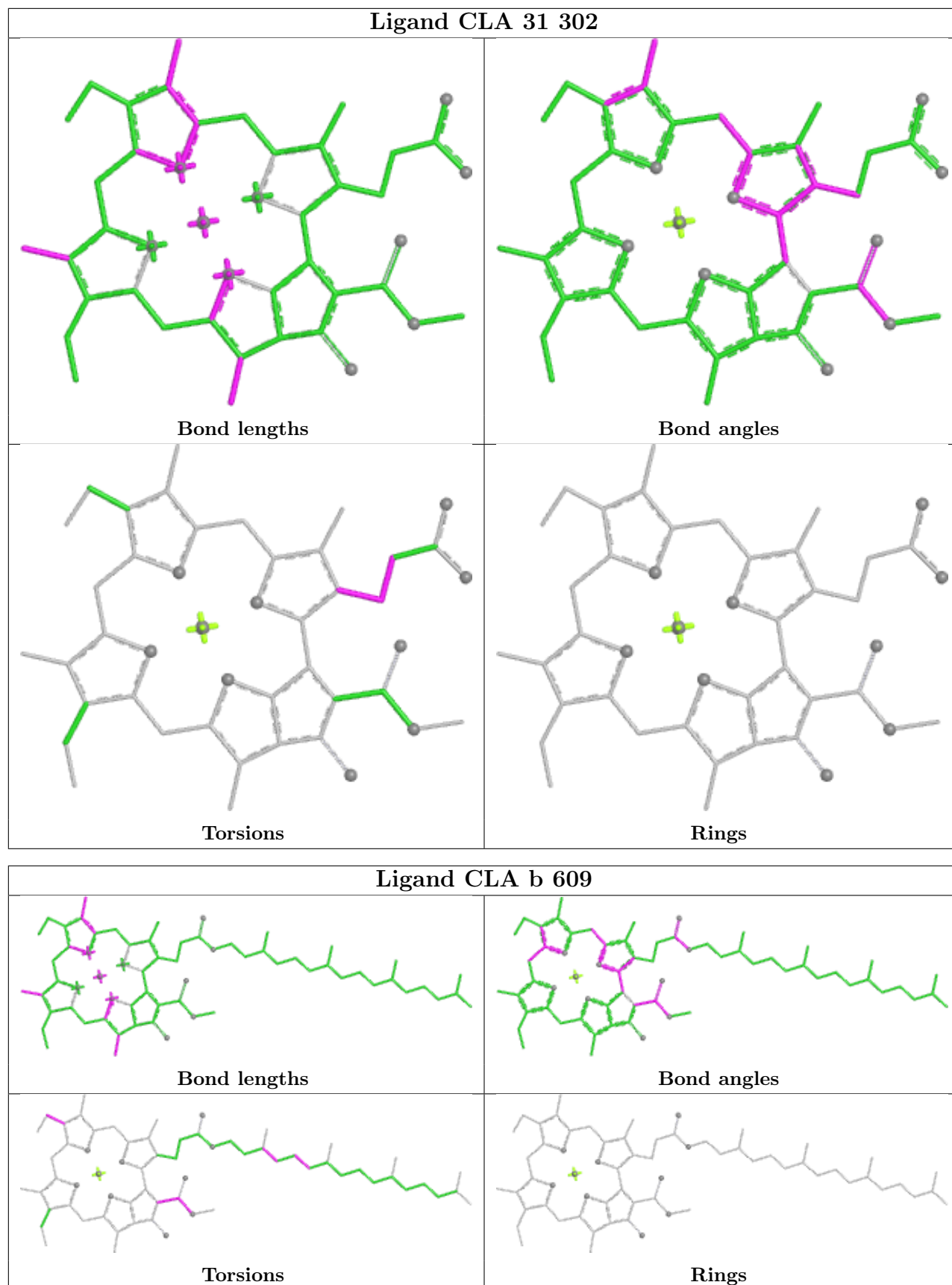


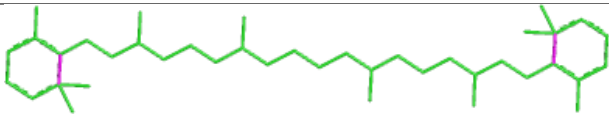
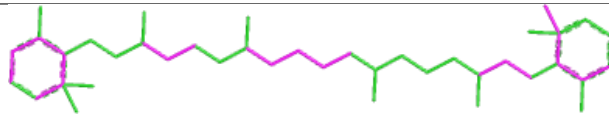
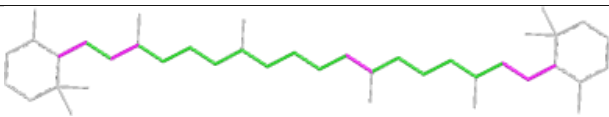
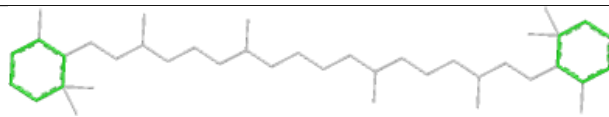


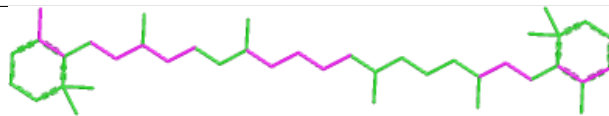
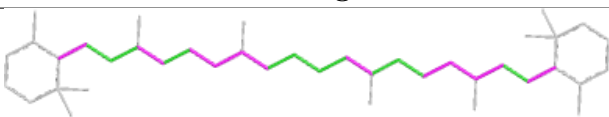
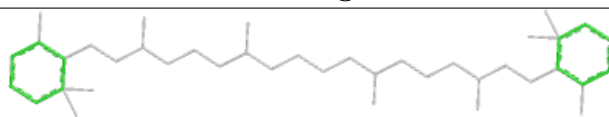


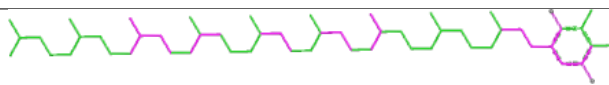
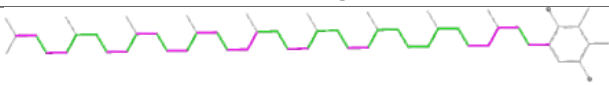
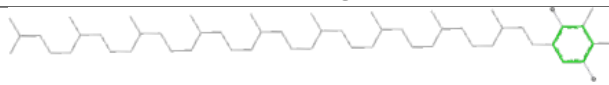


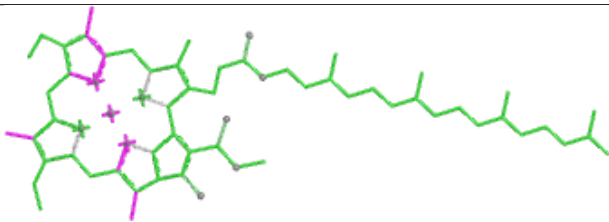
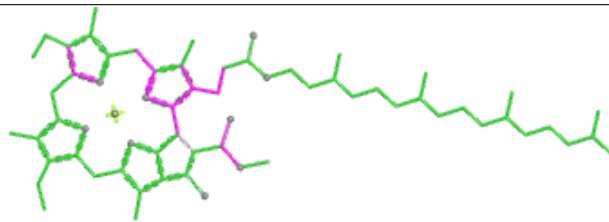
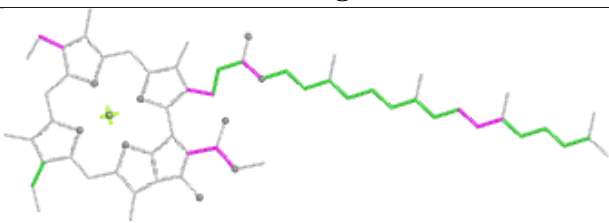
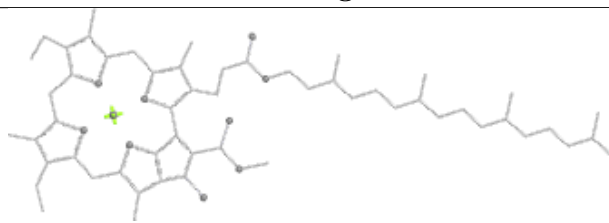




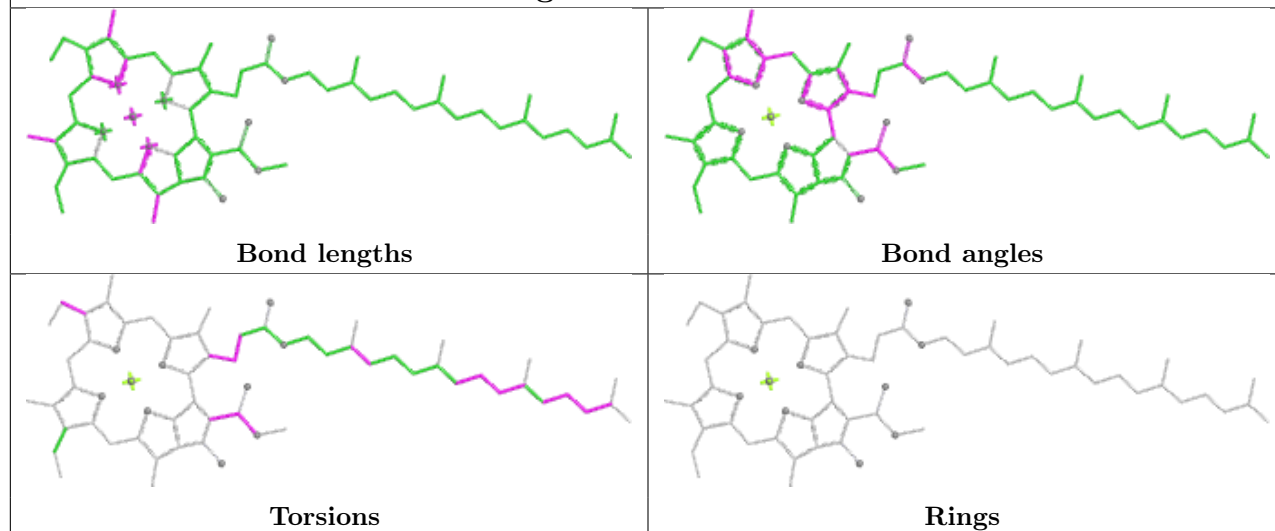
Ligand BCR b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR c 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

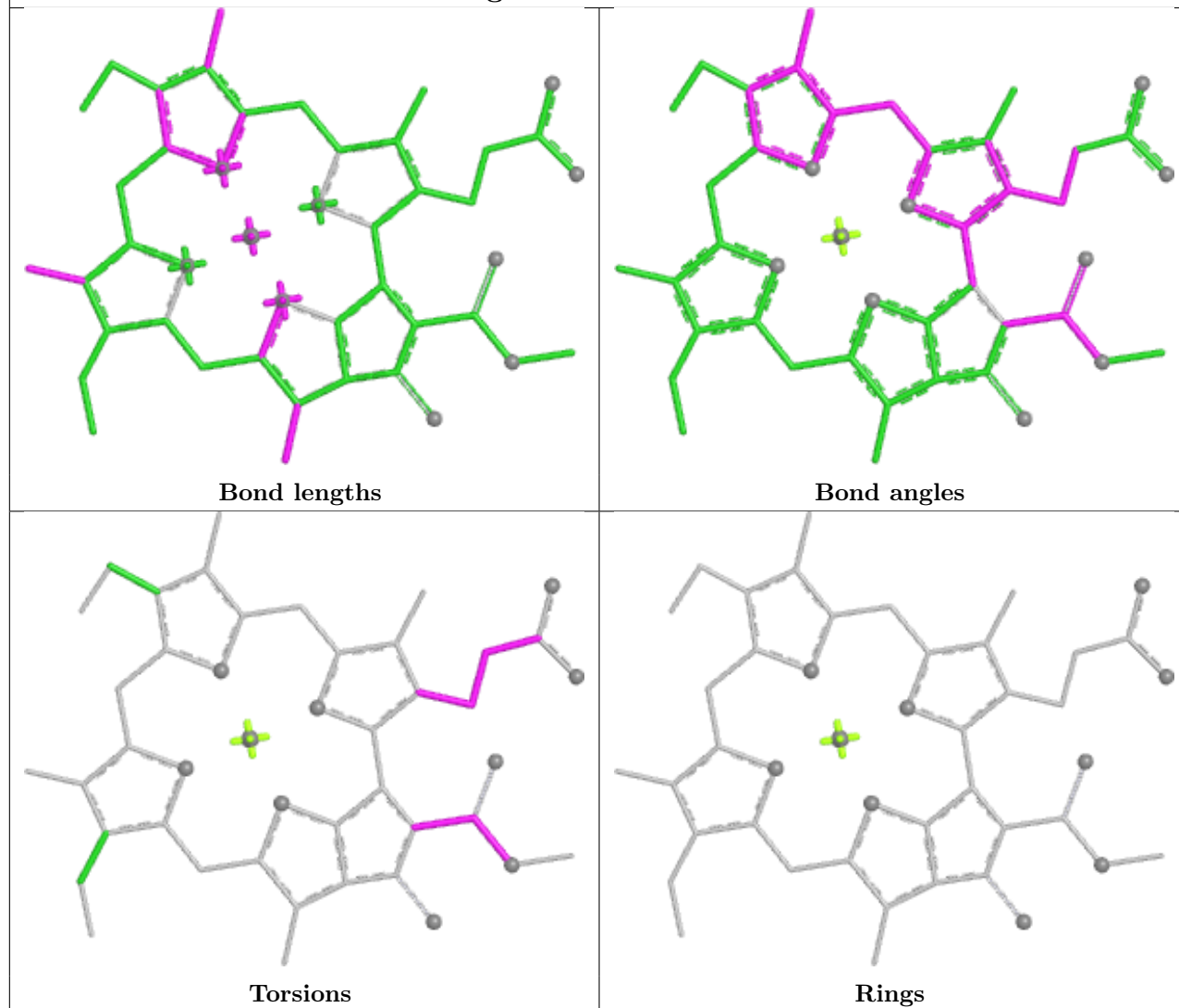
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Bond lengths	Bond angles
	
Torsions	Rings

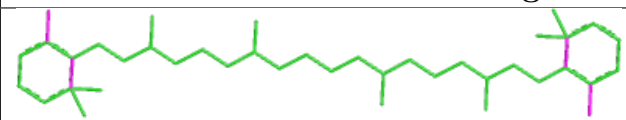
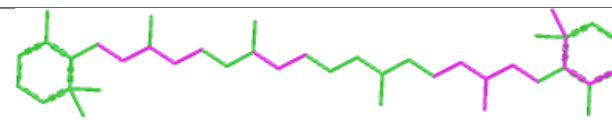
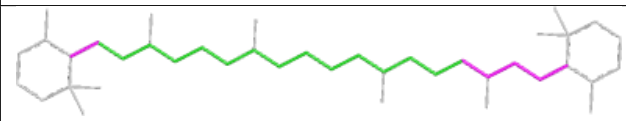
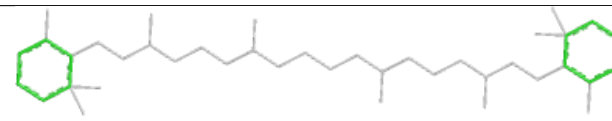
Ligand CLA 31 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

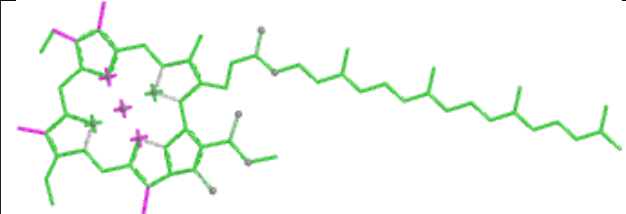
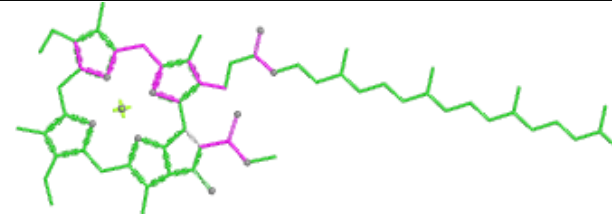
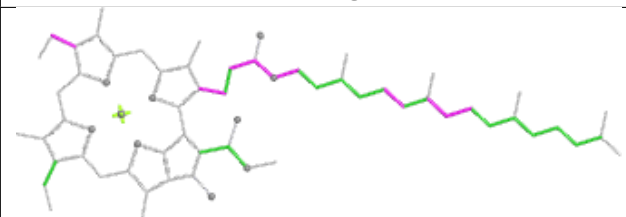
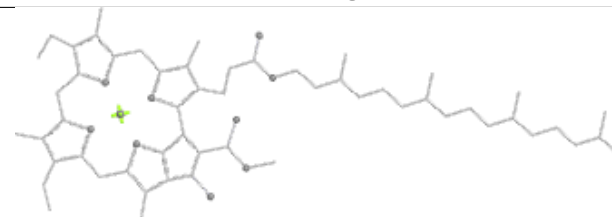
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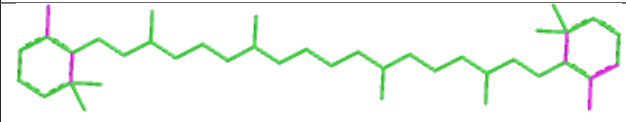
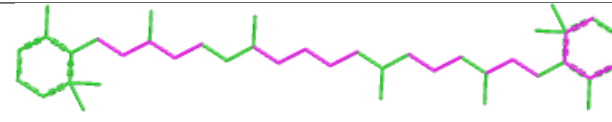
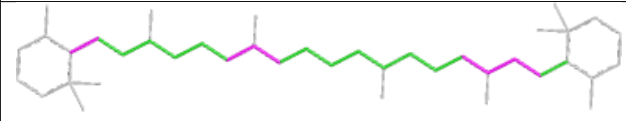
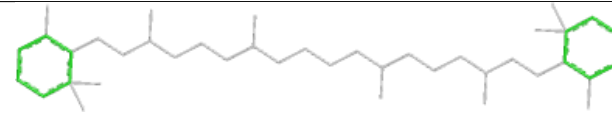


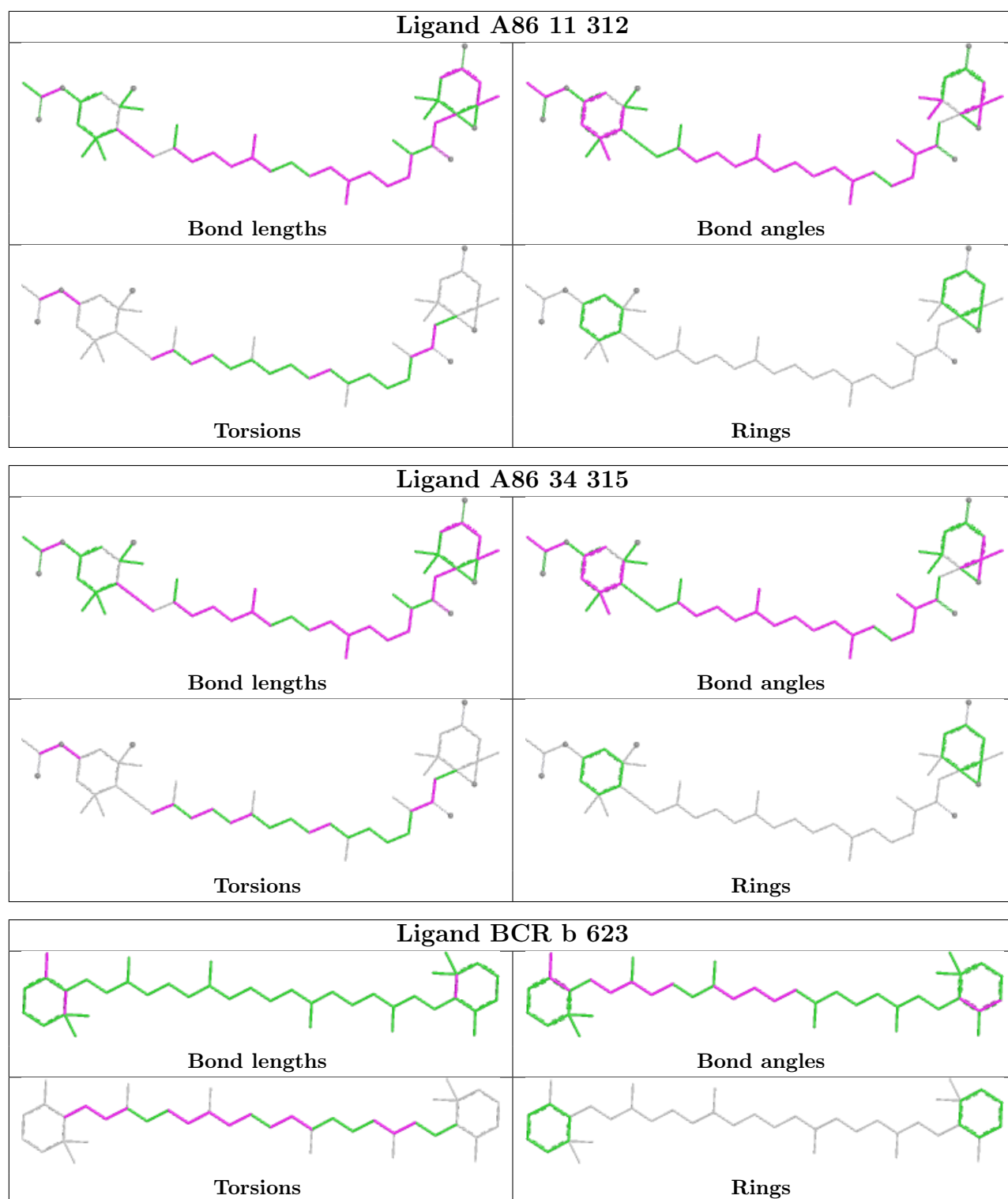
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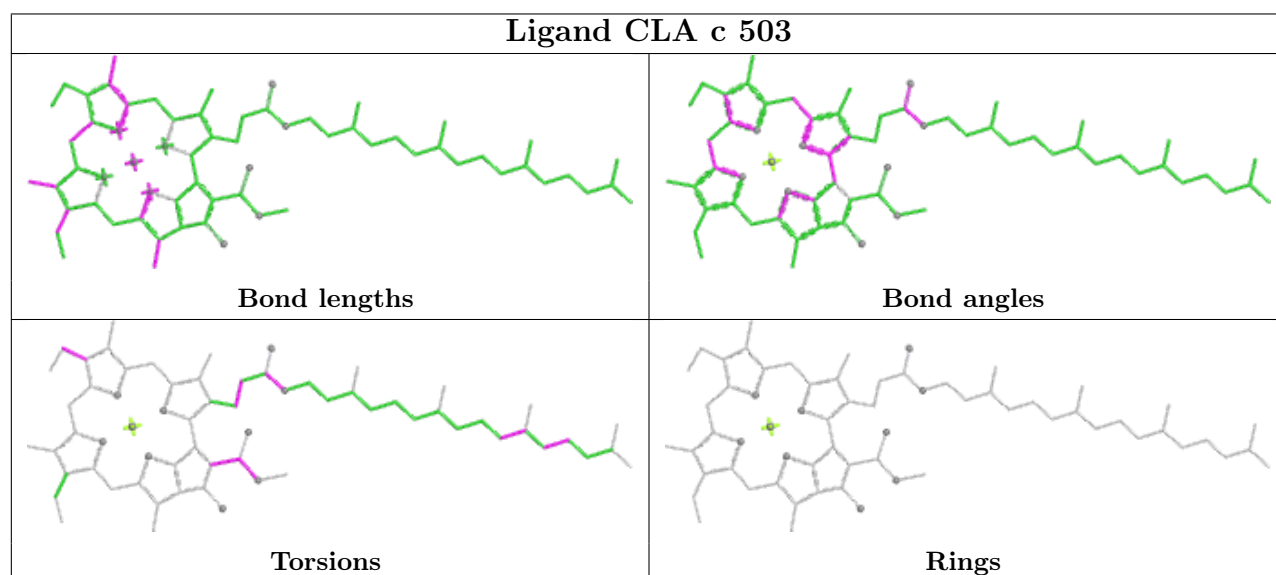
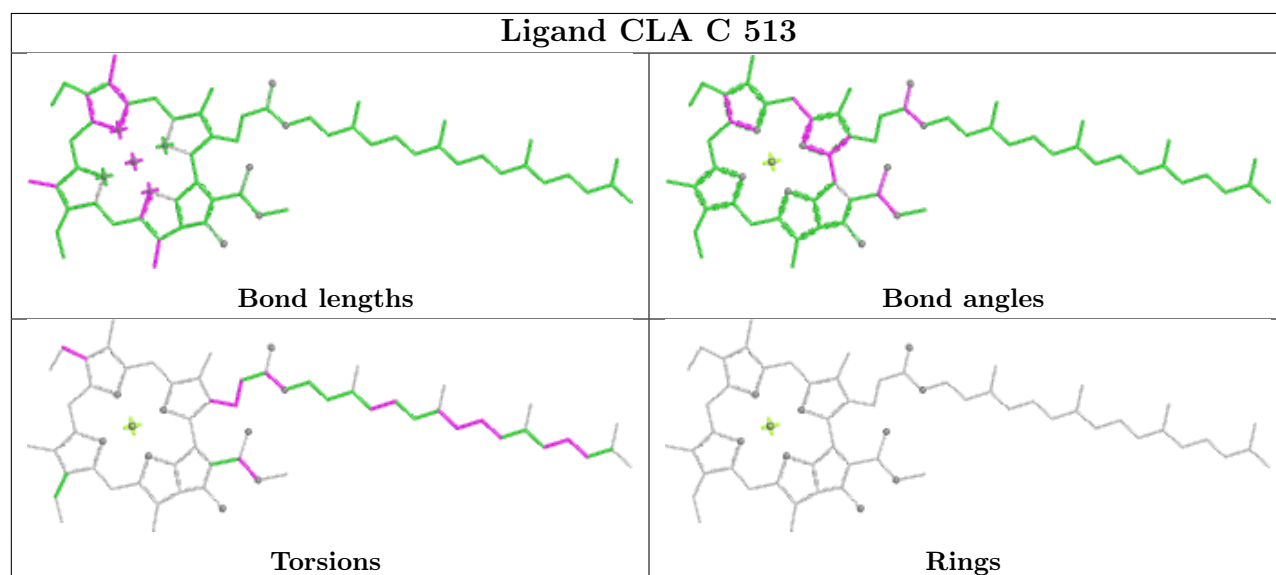
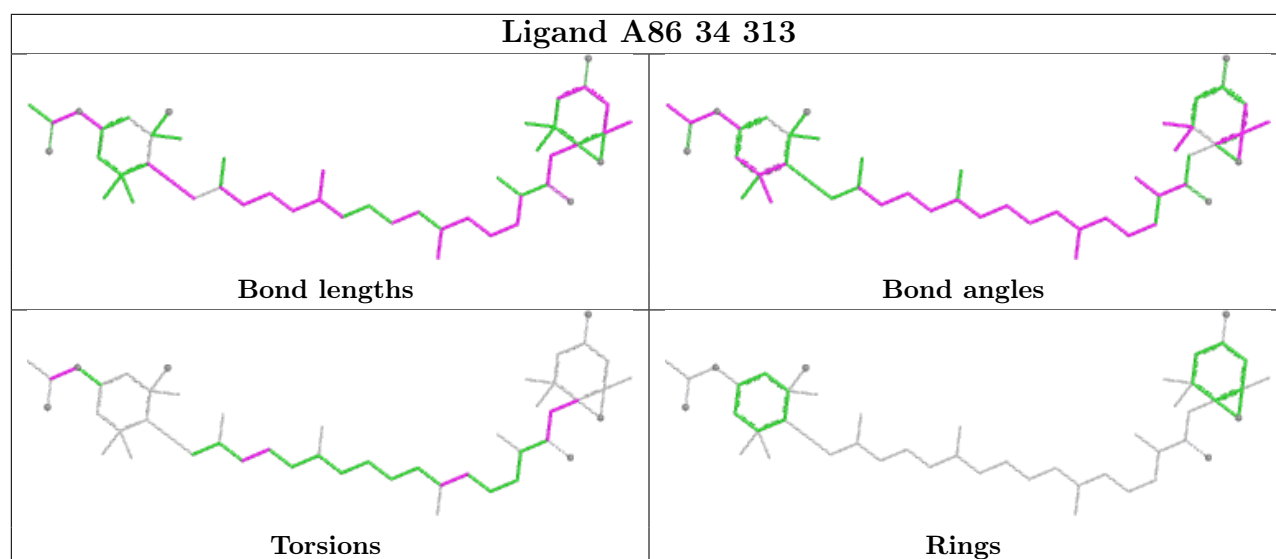


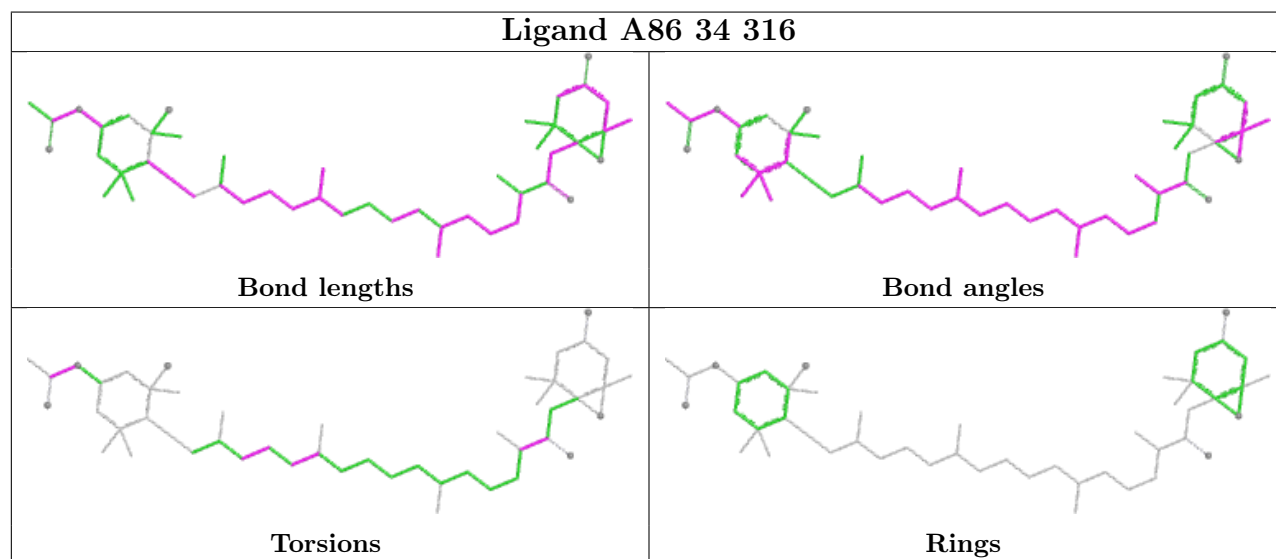
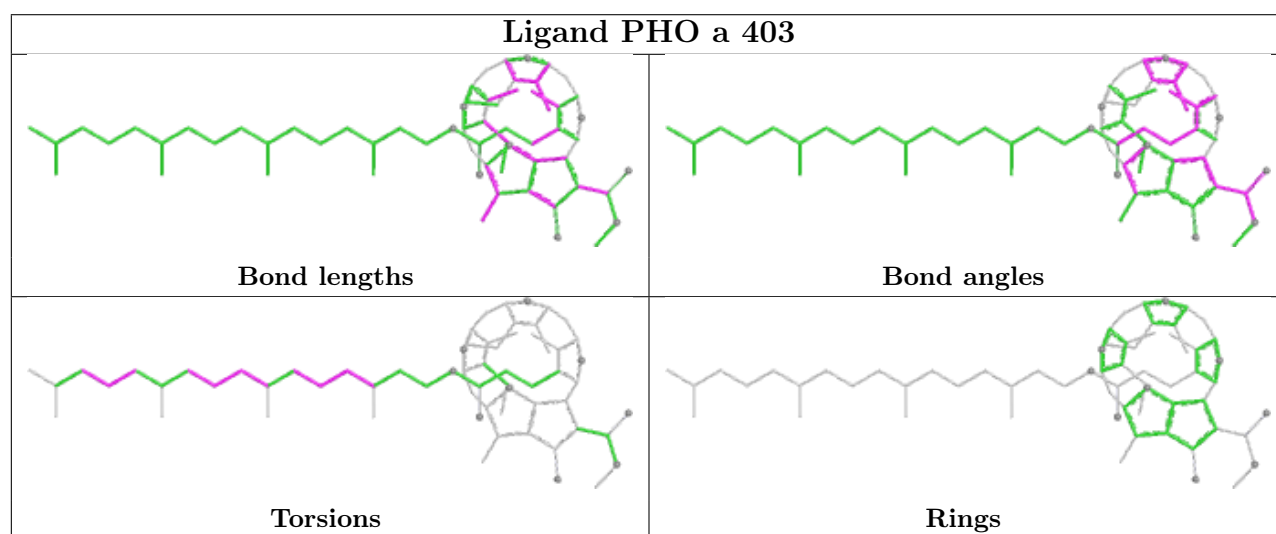
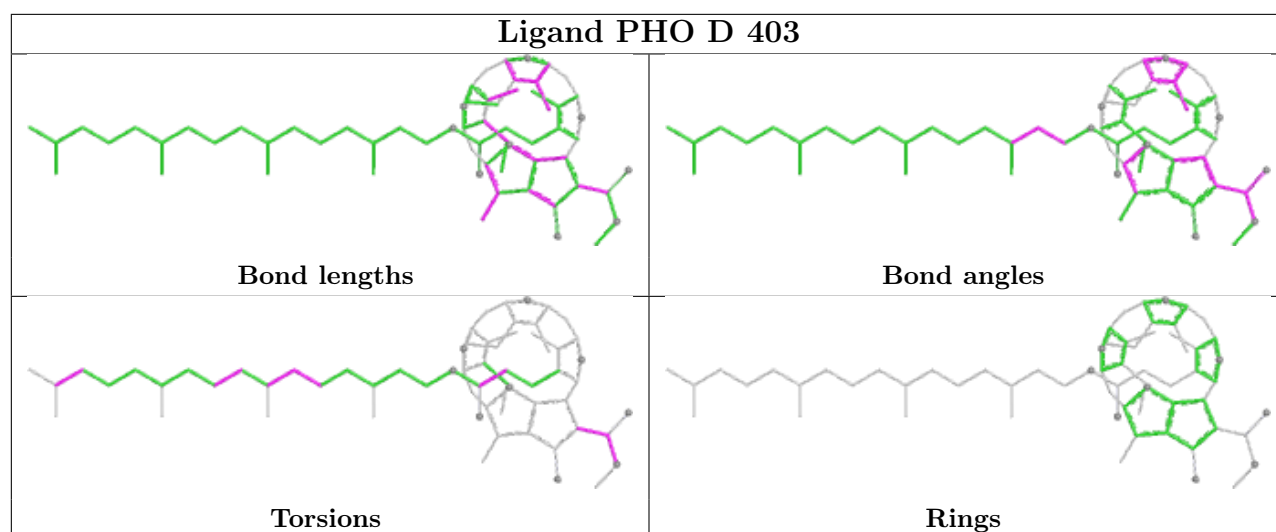
Ligand BCR h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

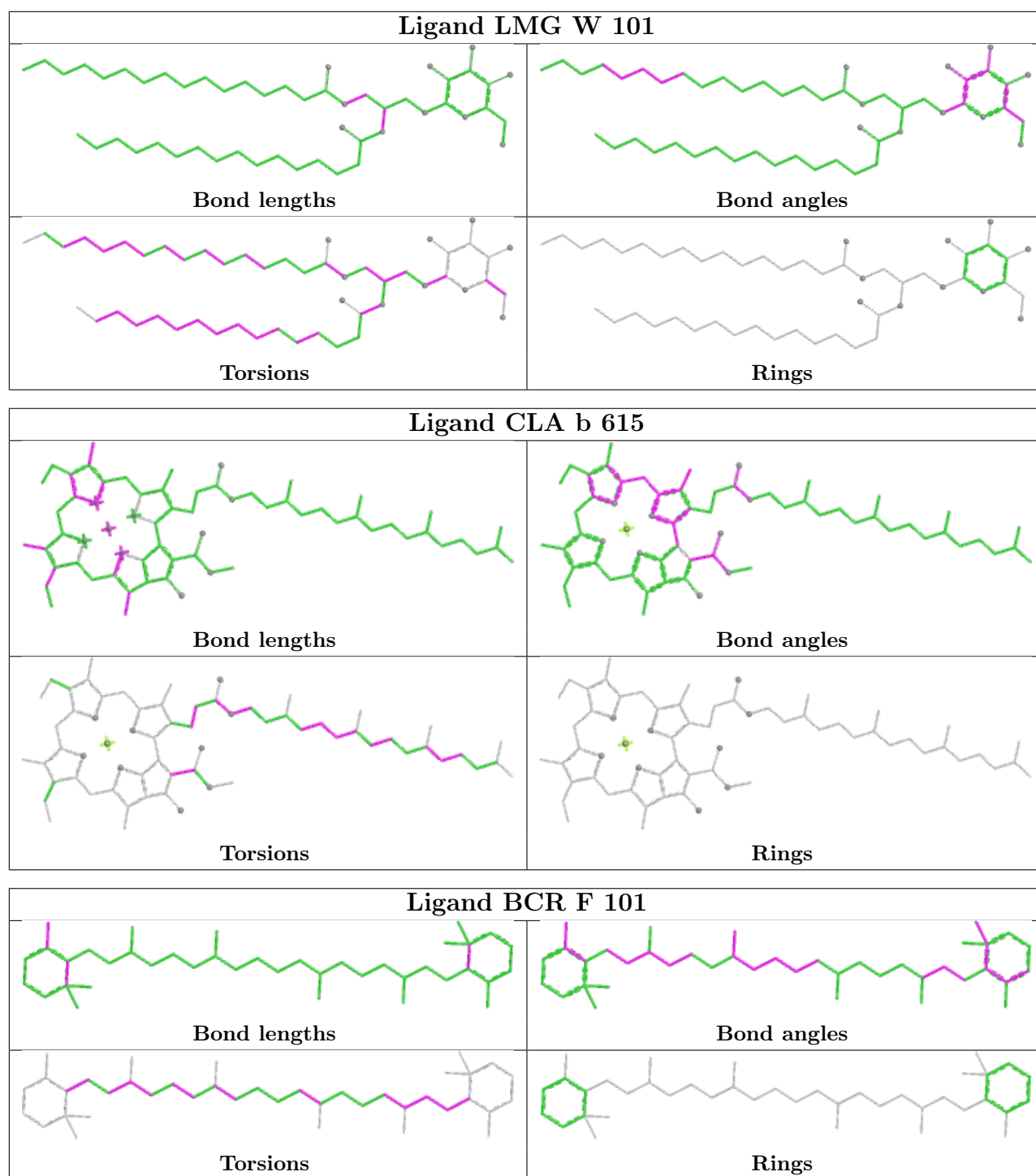
Ligand CLA a 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

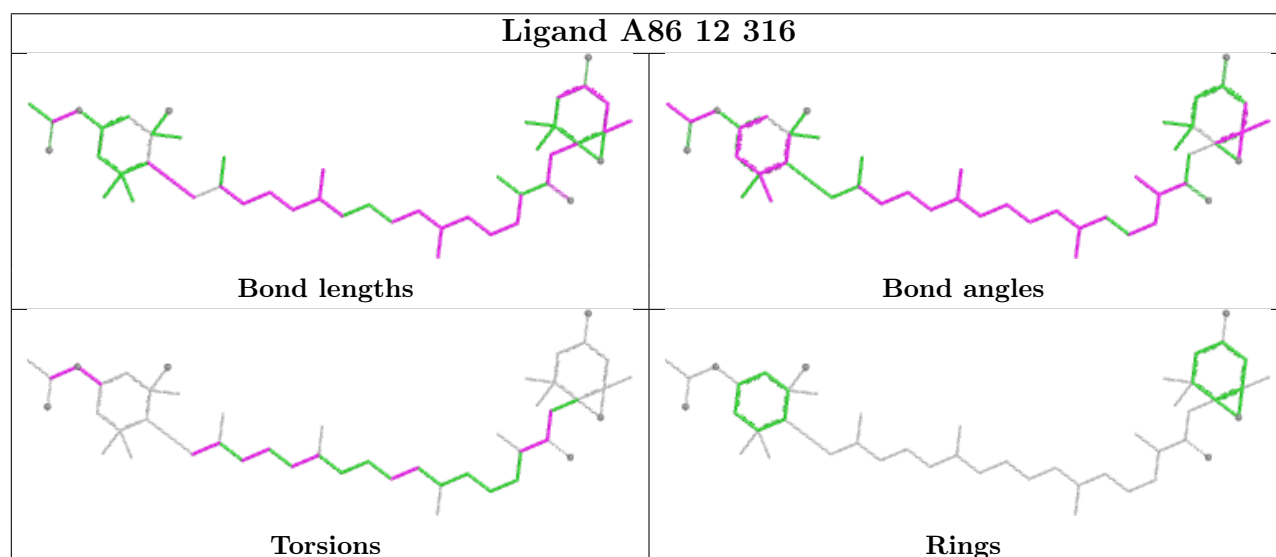
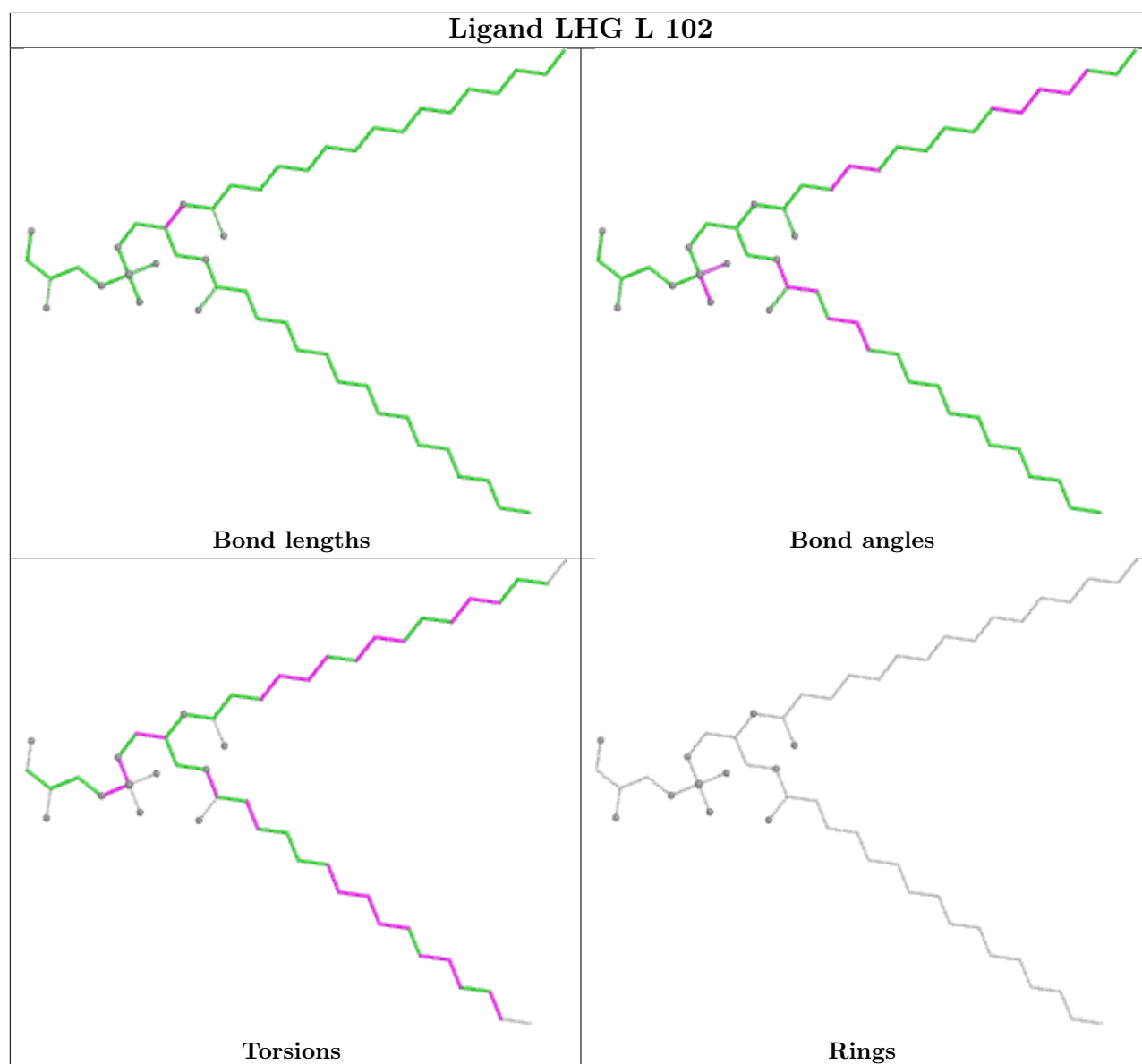
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Bond lengths	Bond angles
	
Torsions	Rings

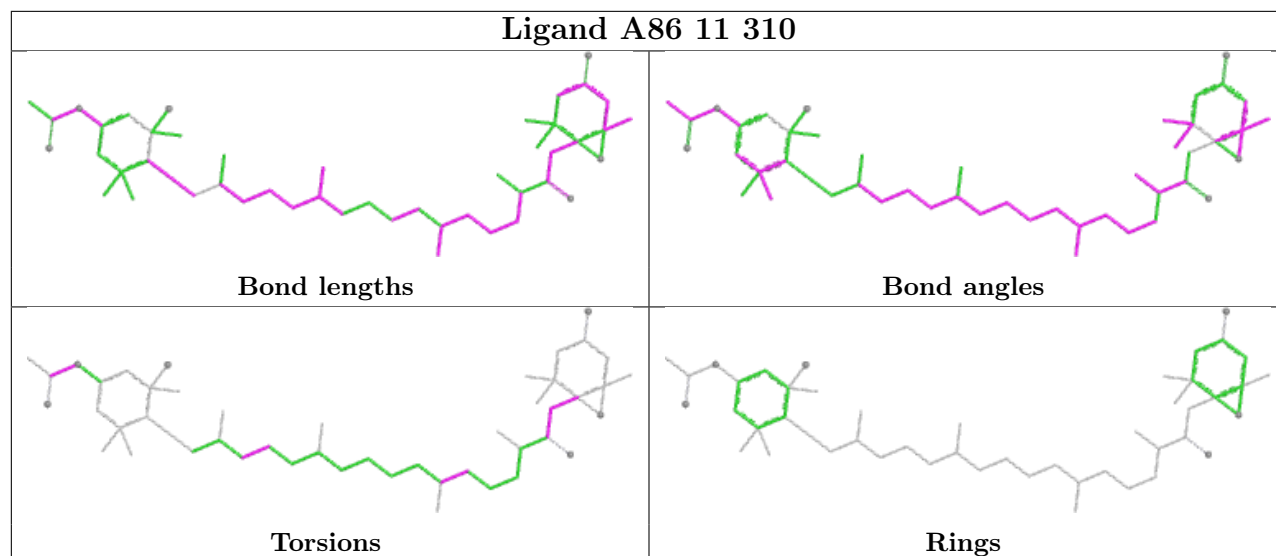
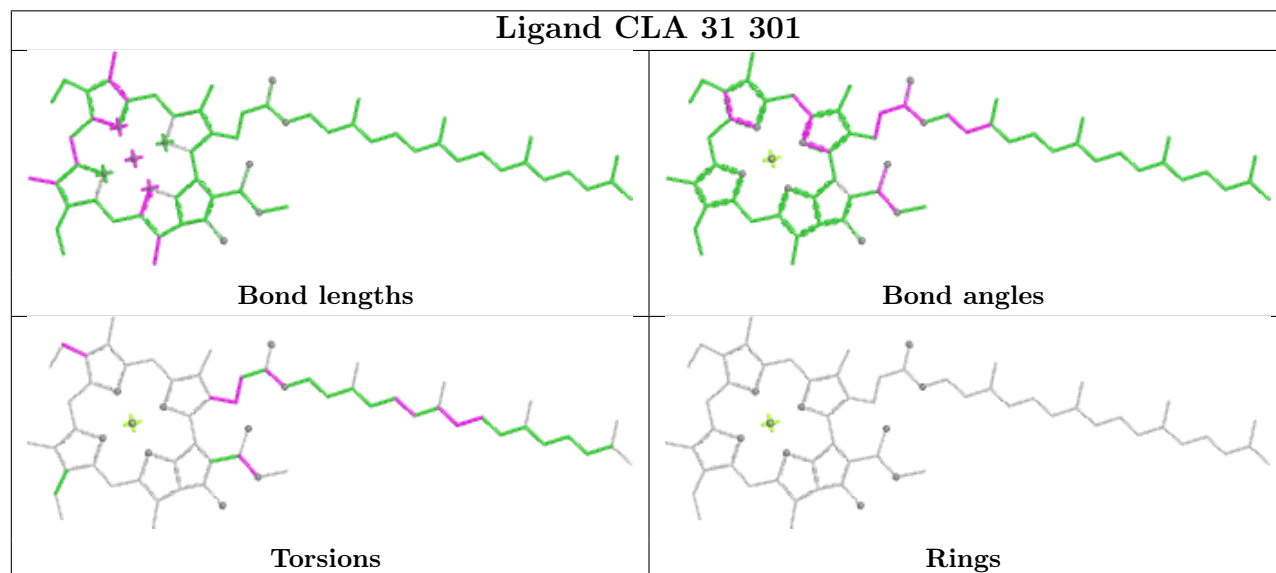
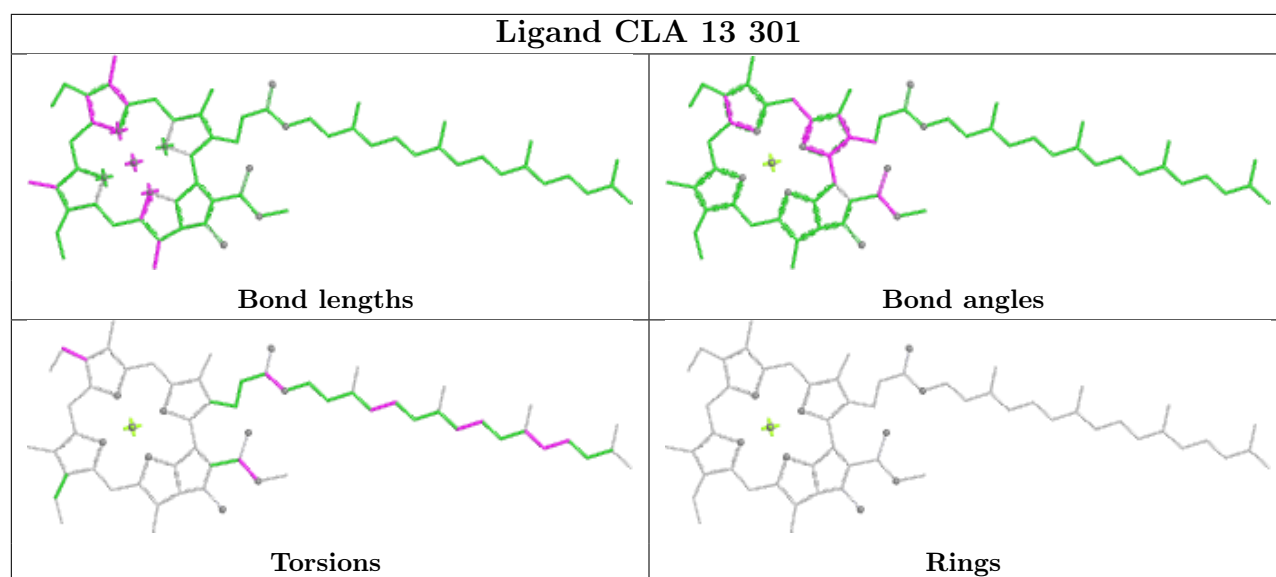


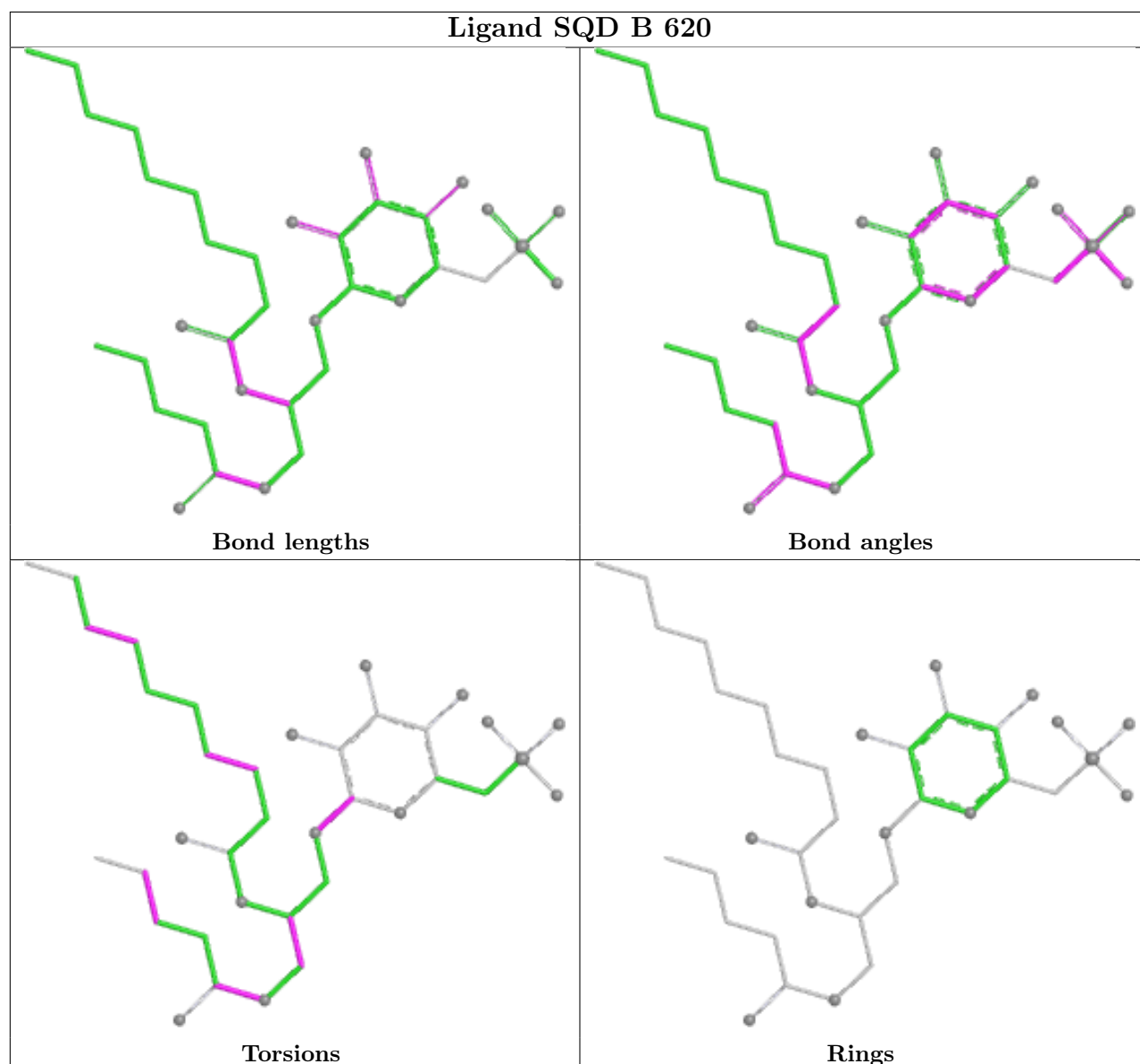
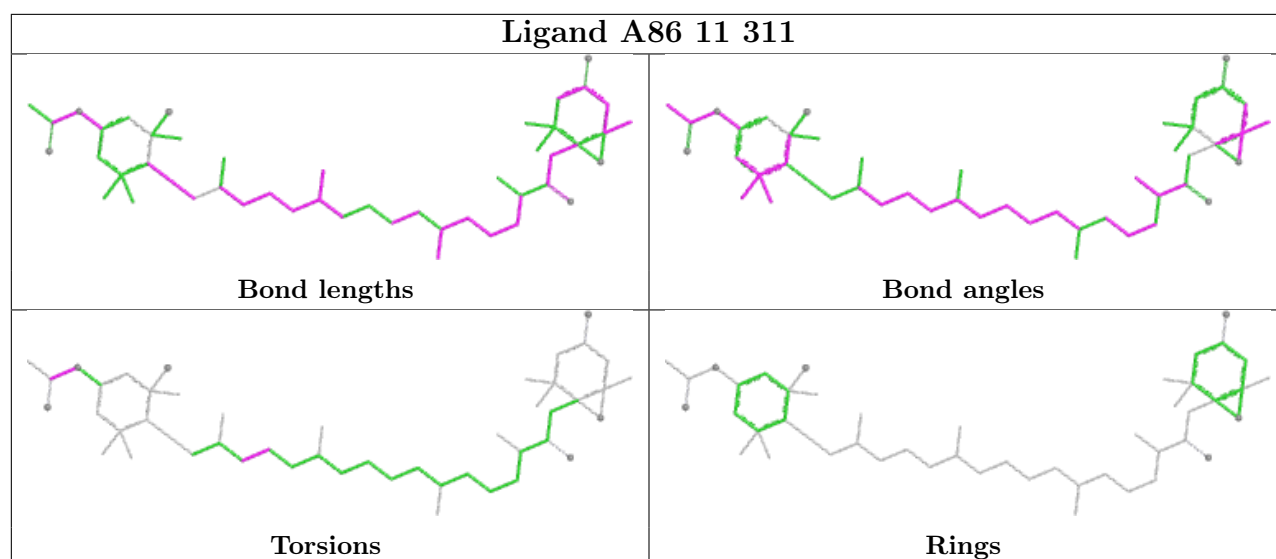


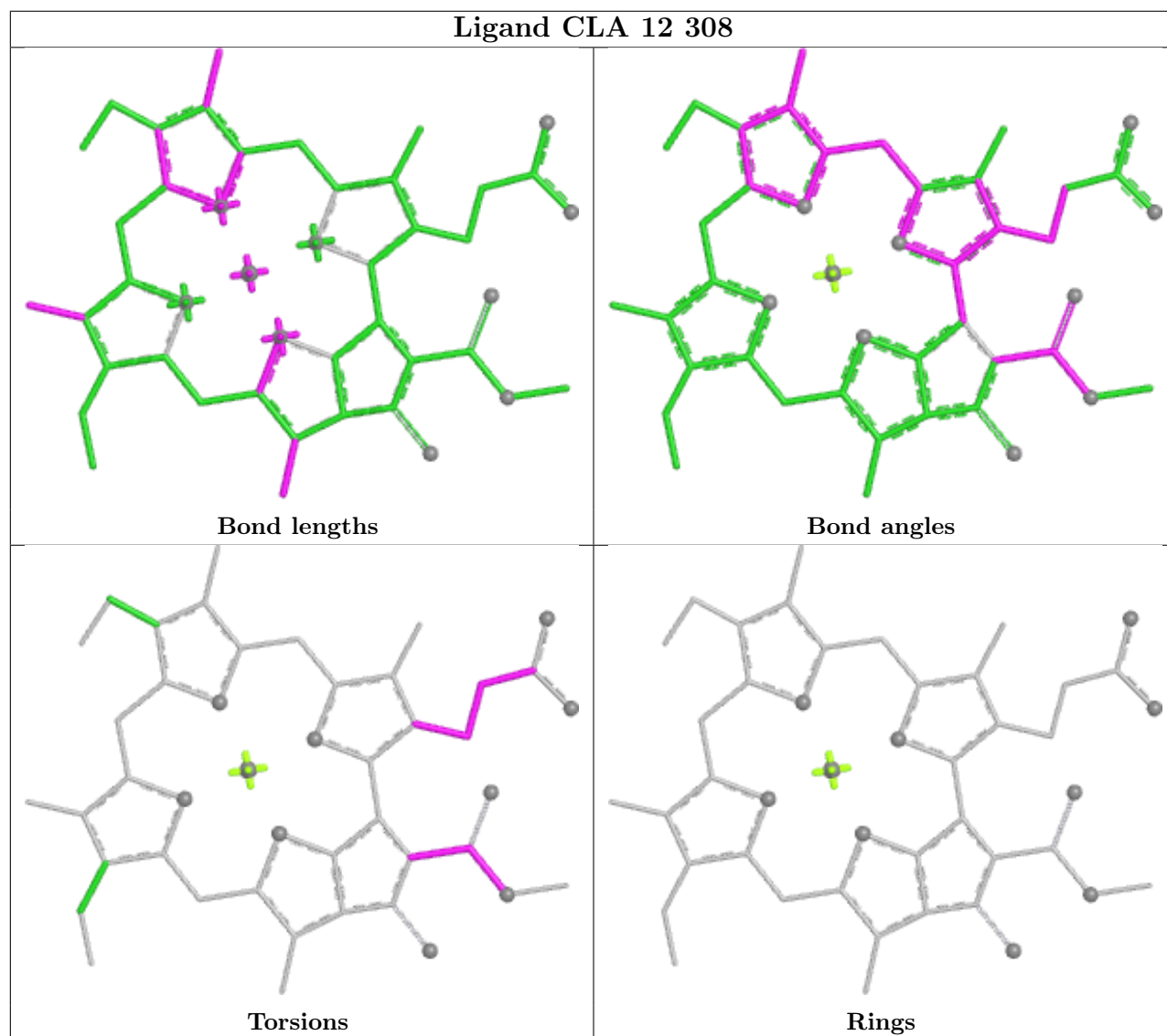
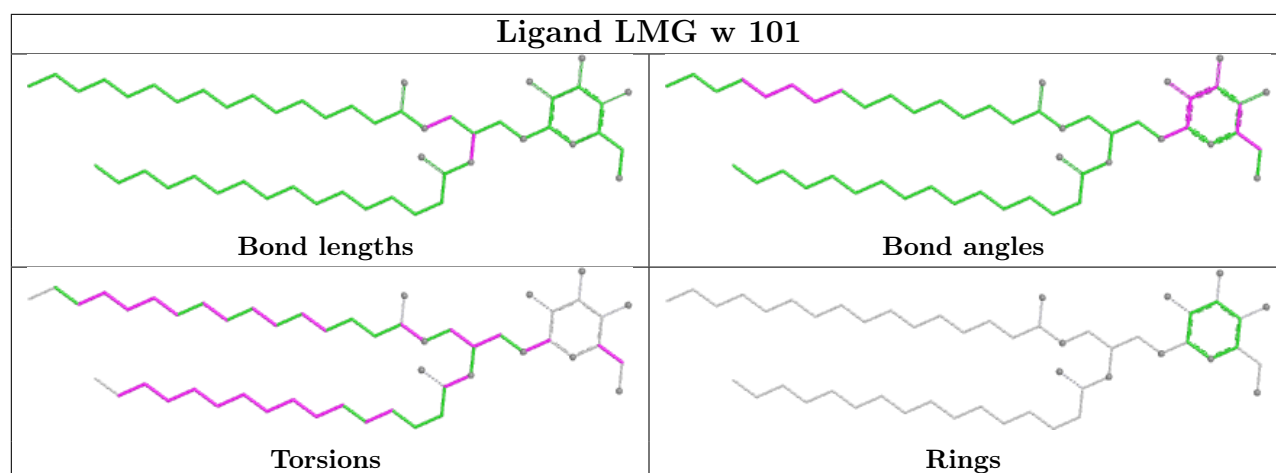


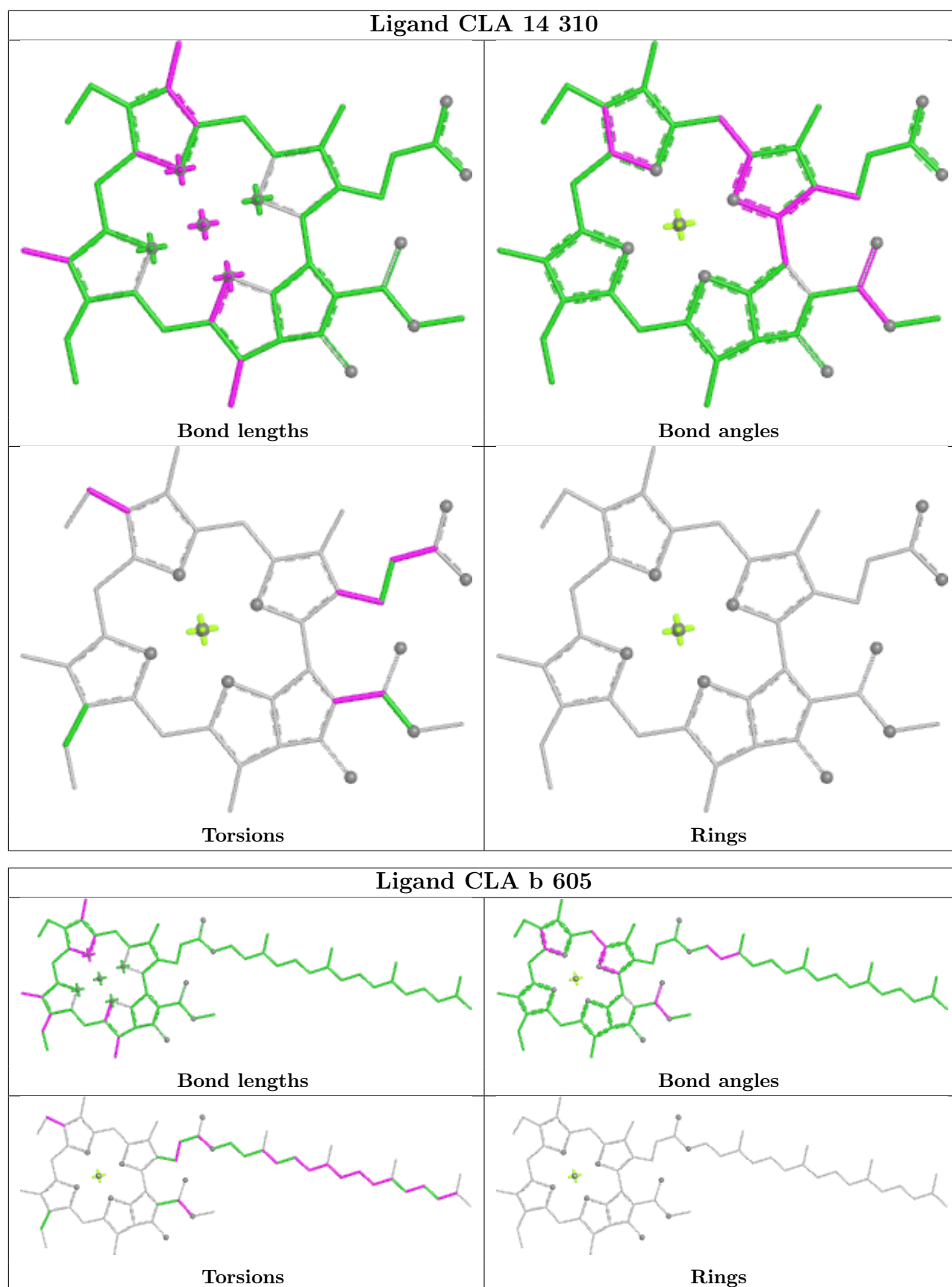


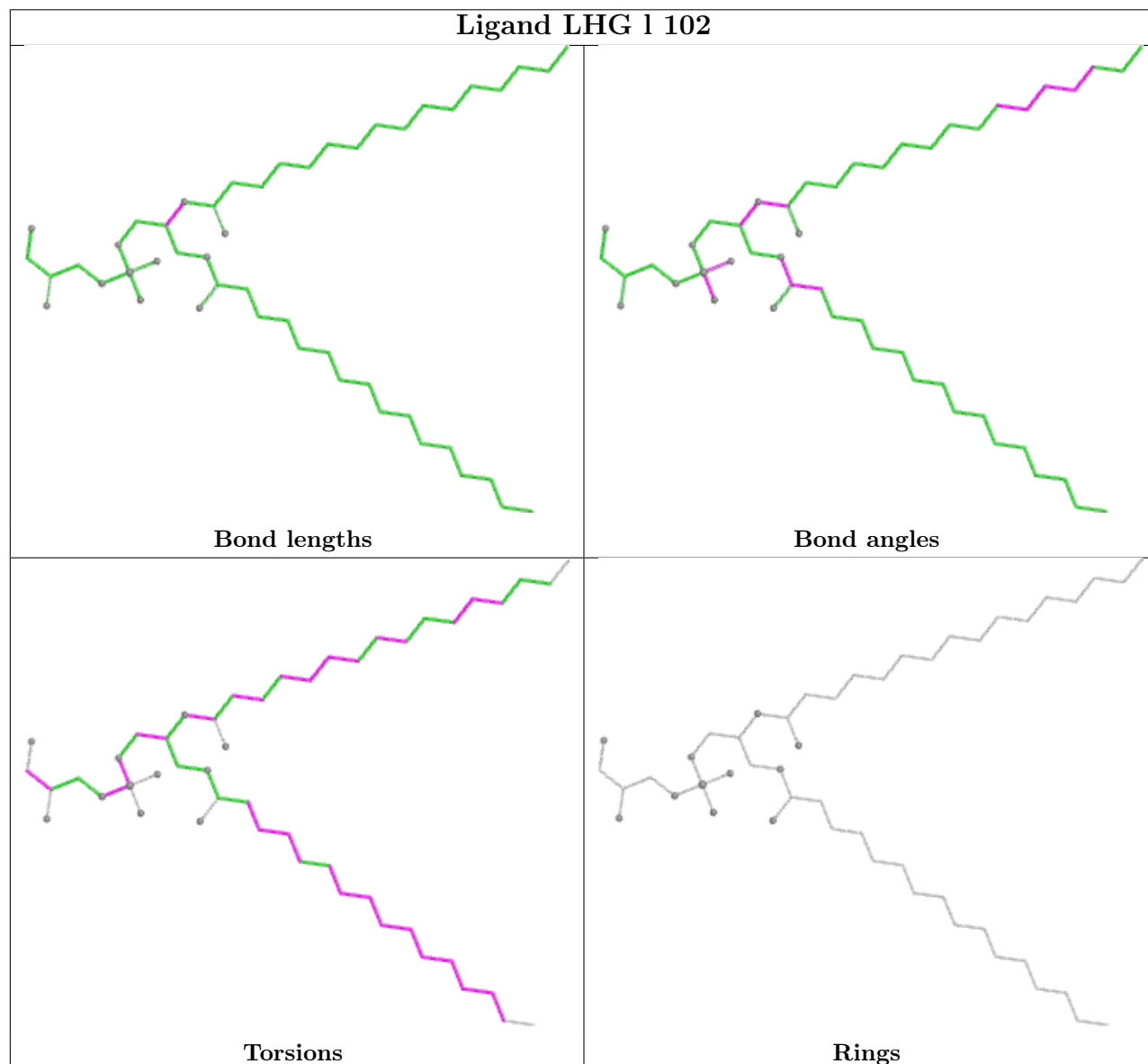
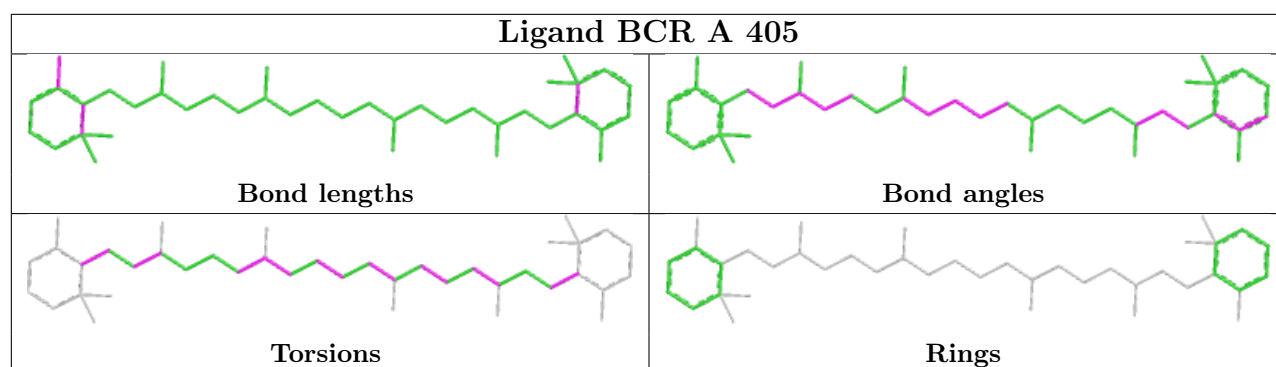


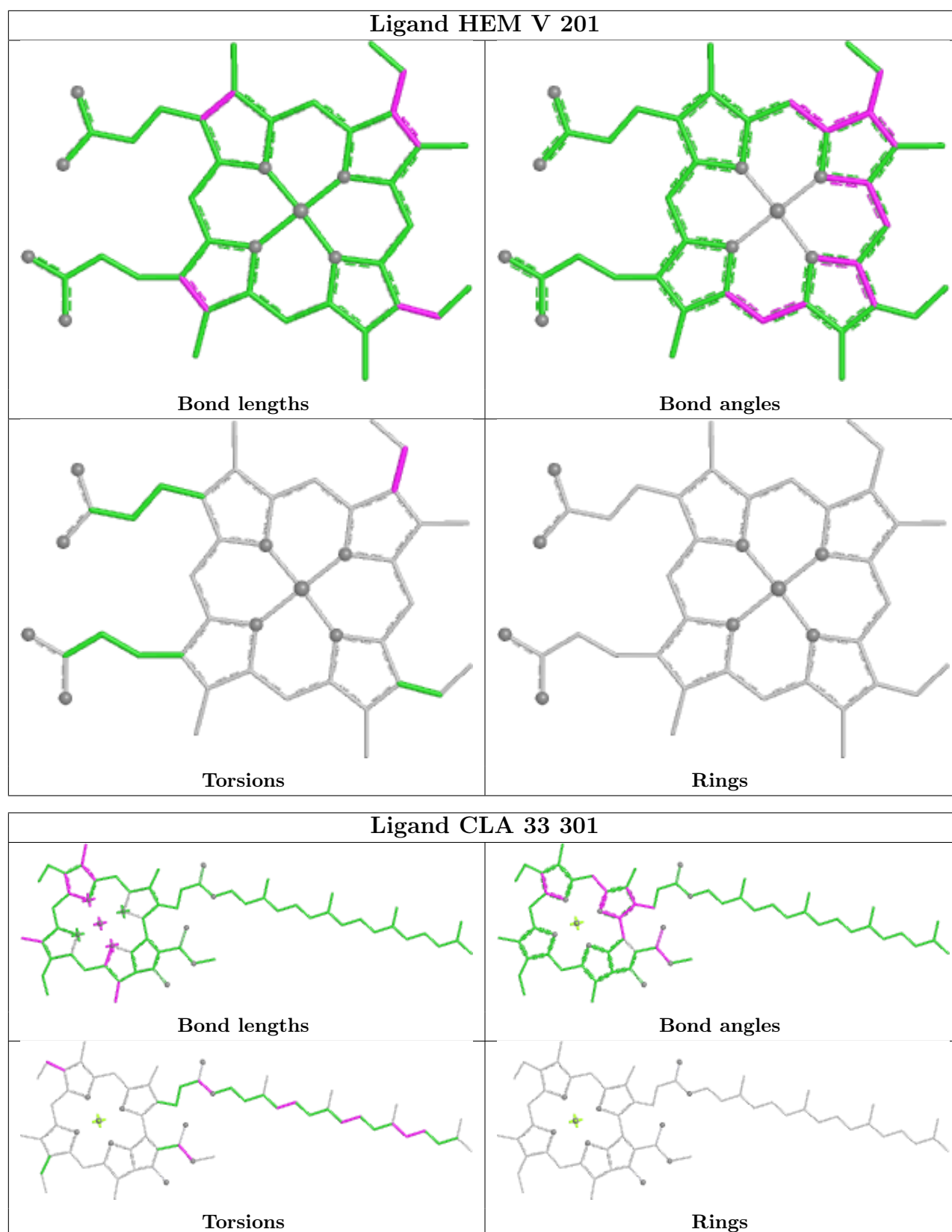


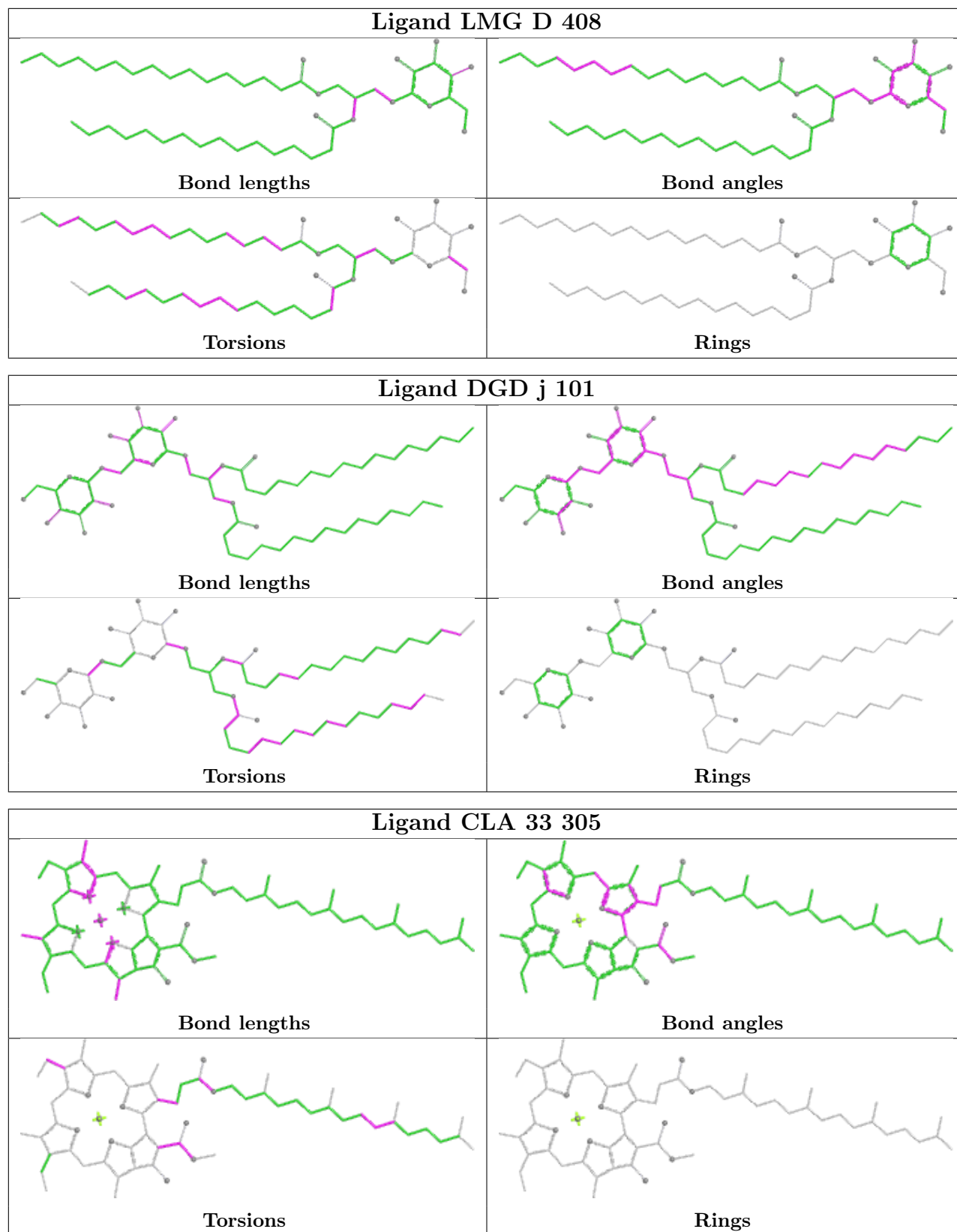


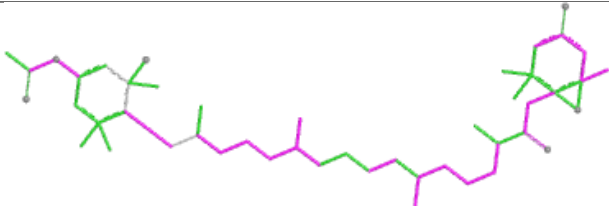
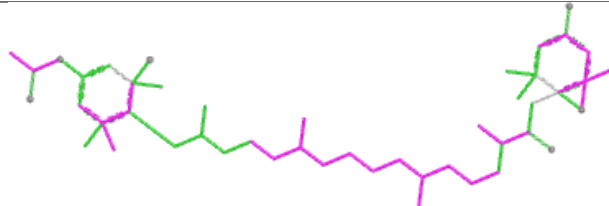
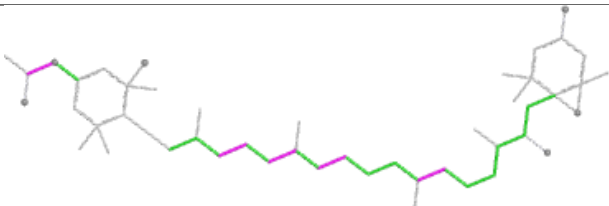
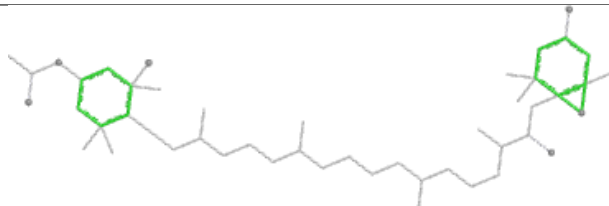
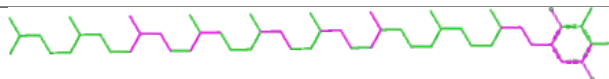
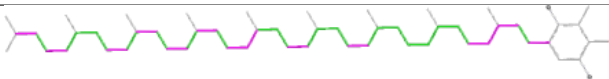
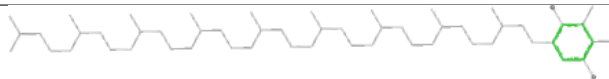
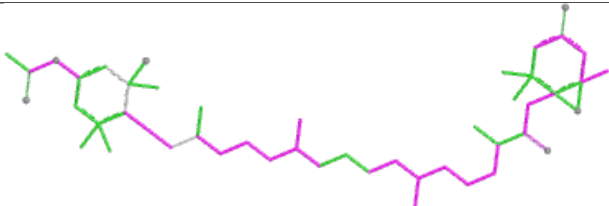
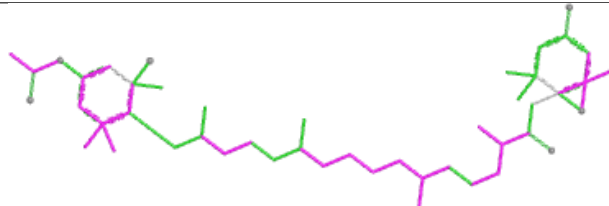
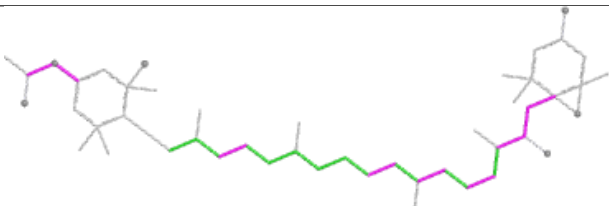
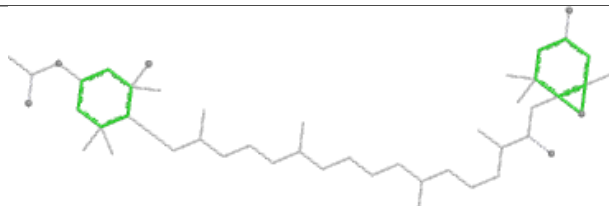


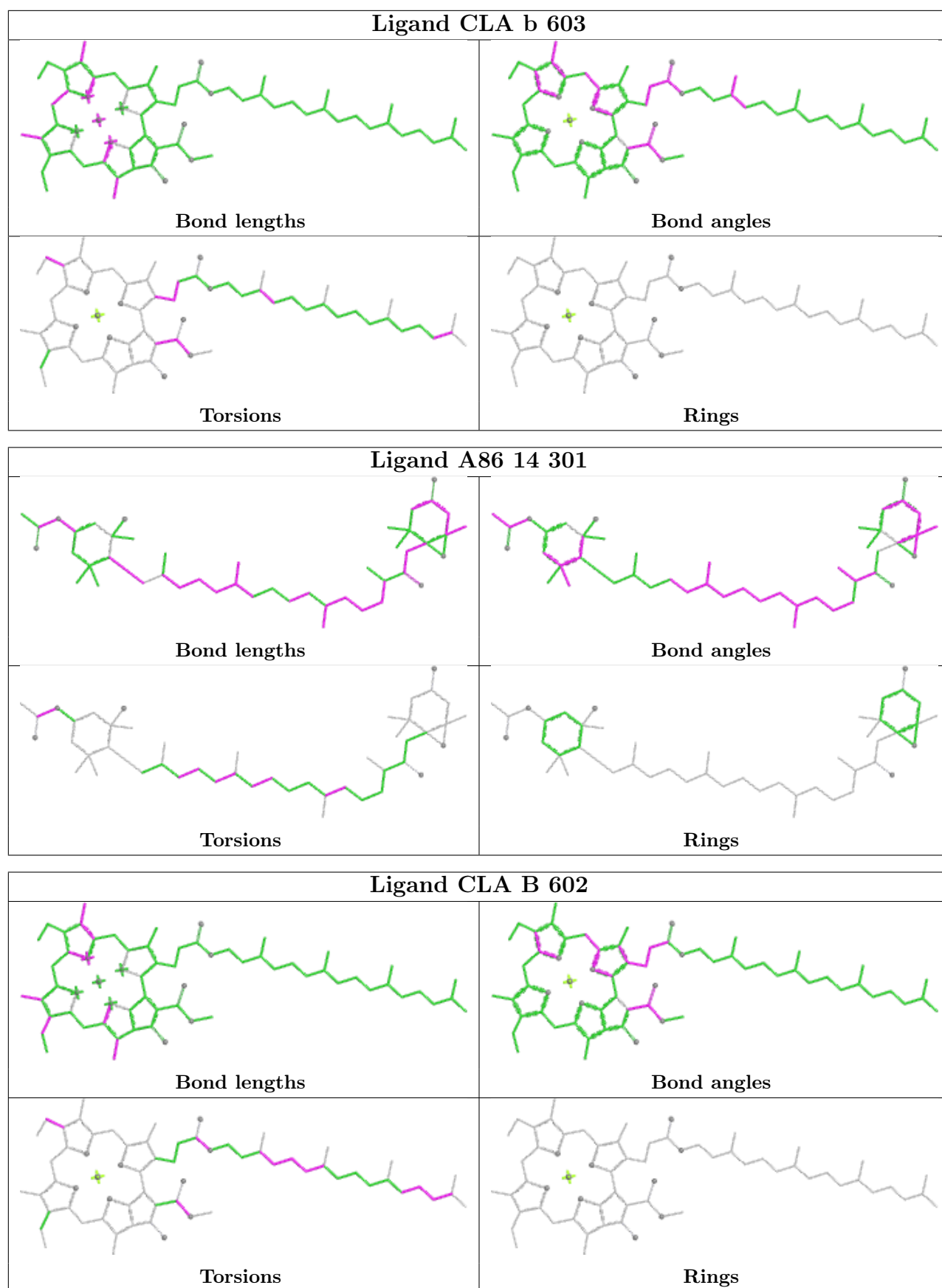


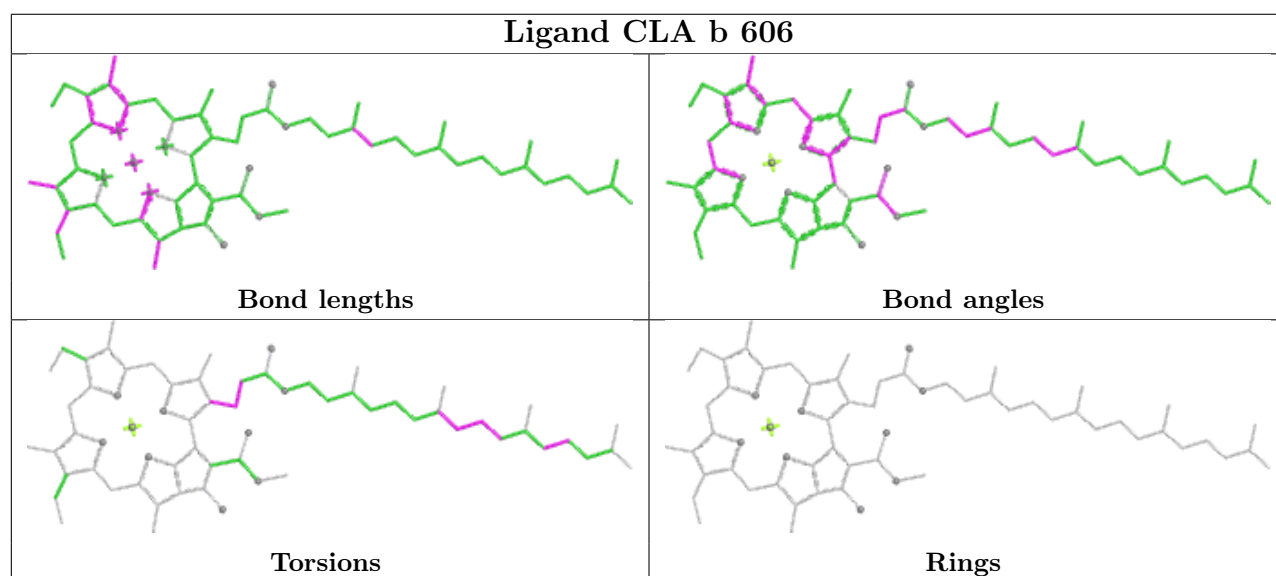
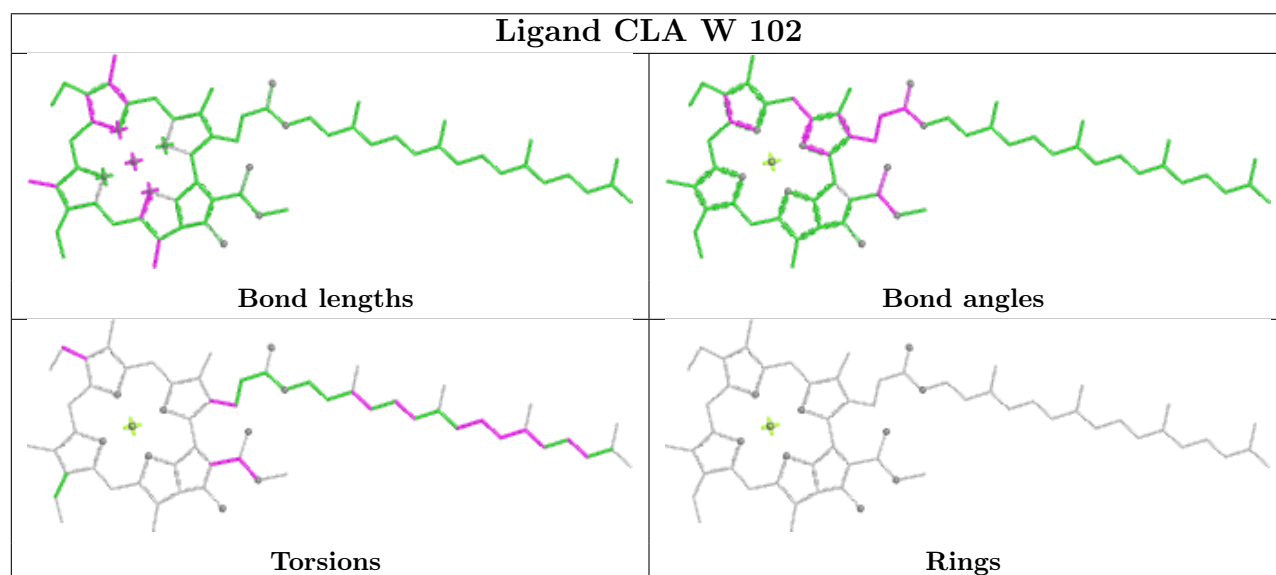
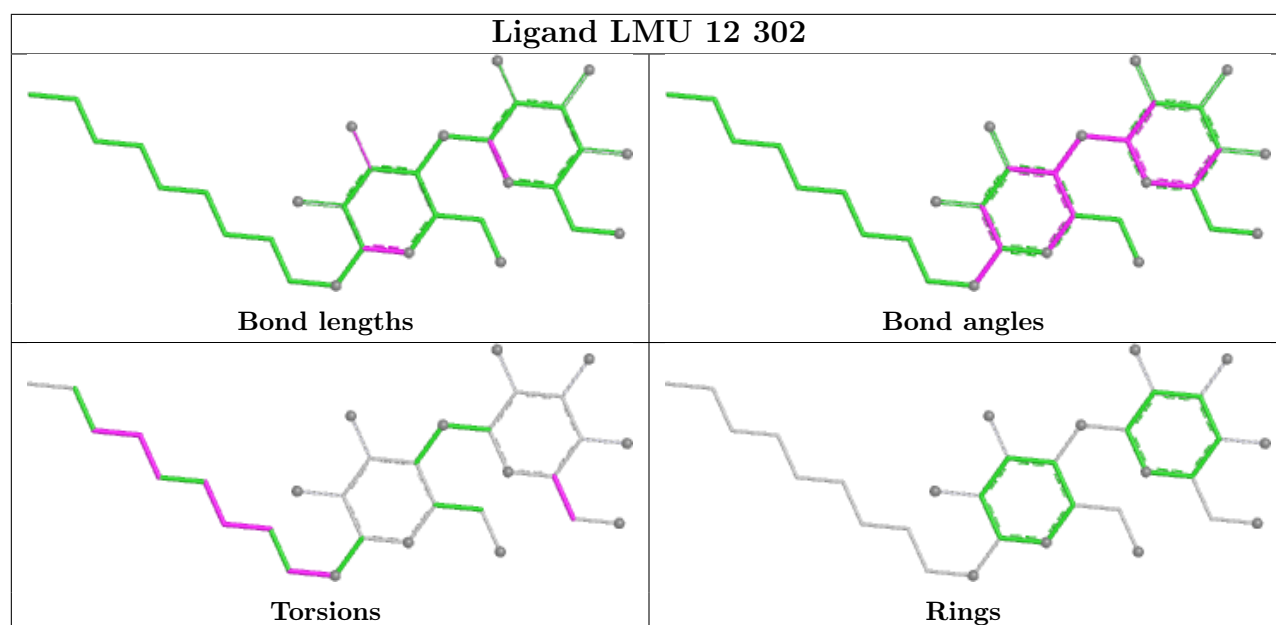


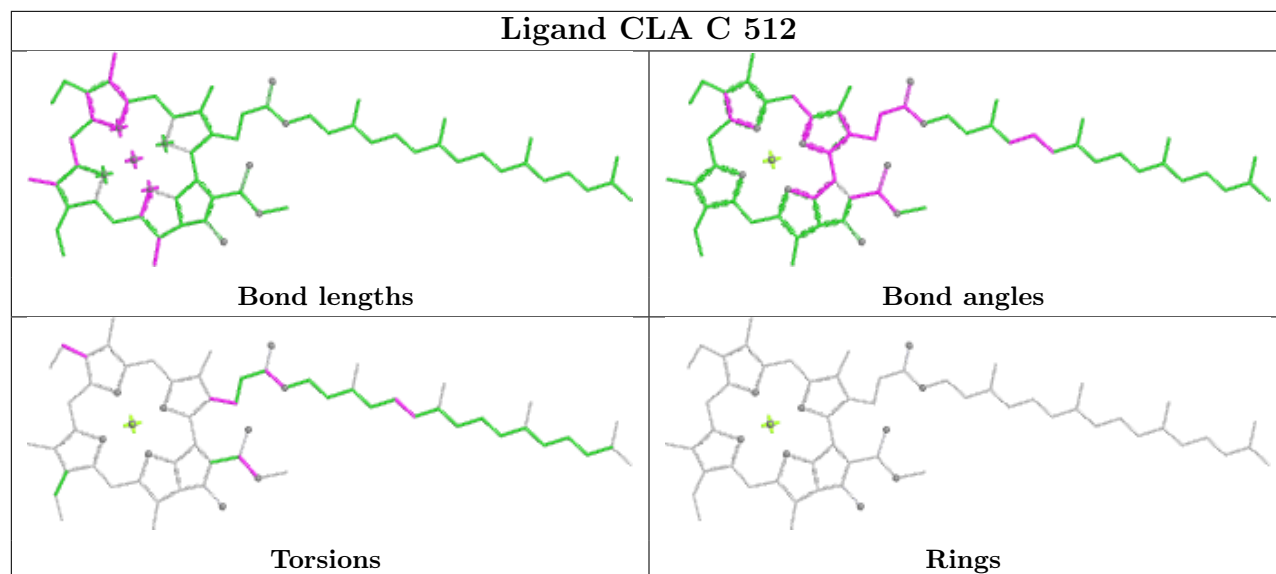
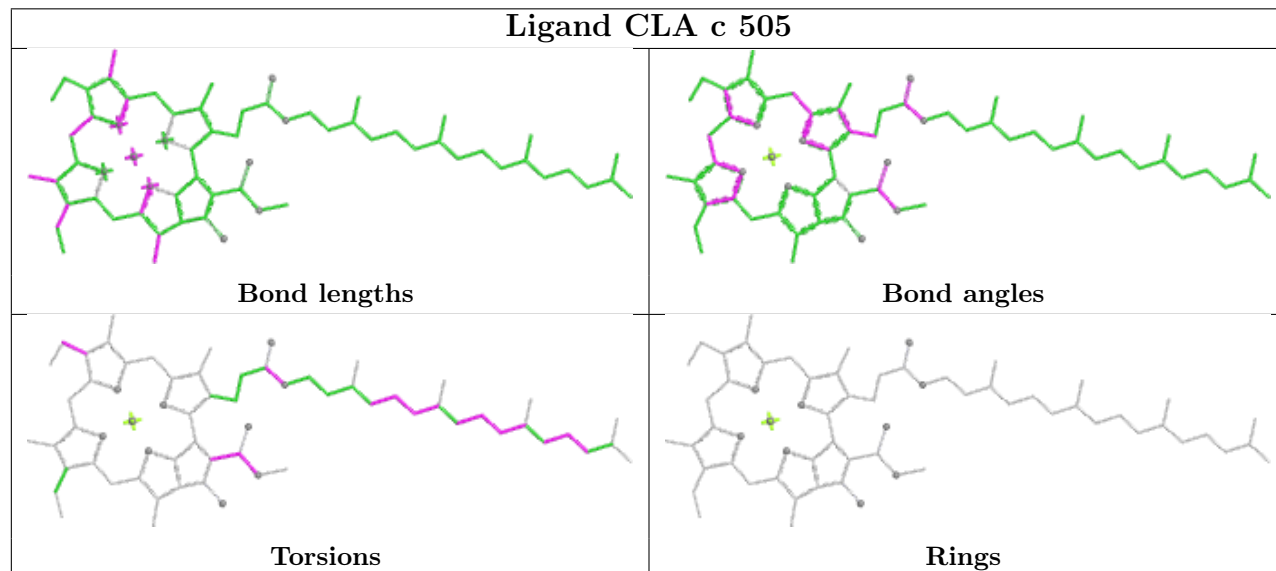


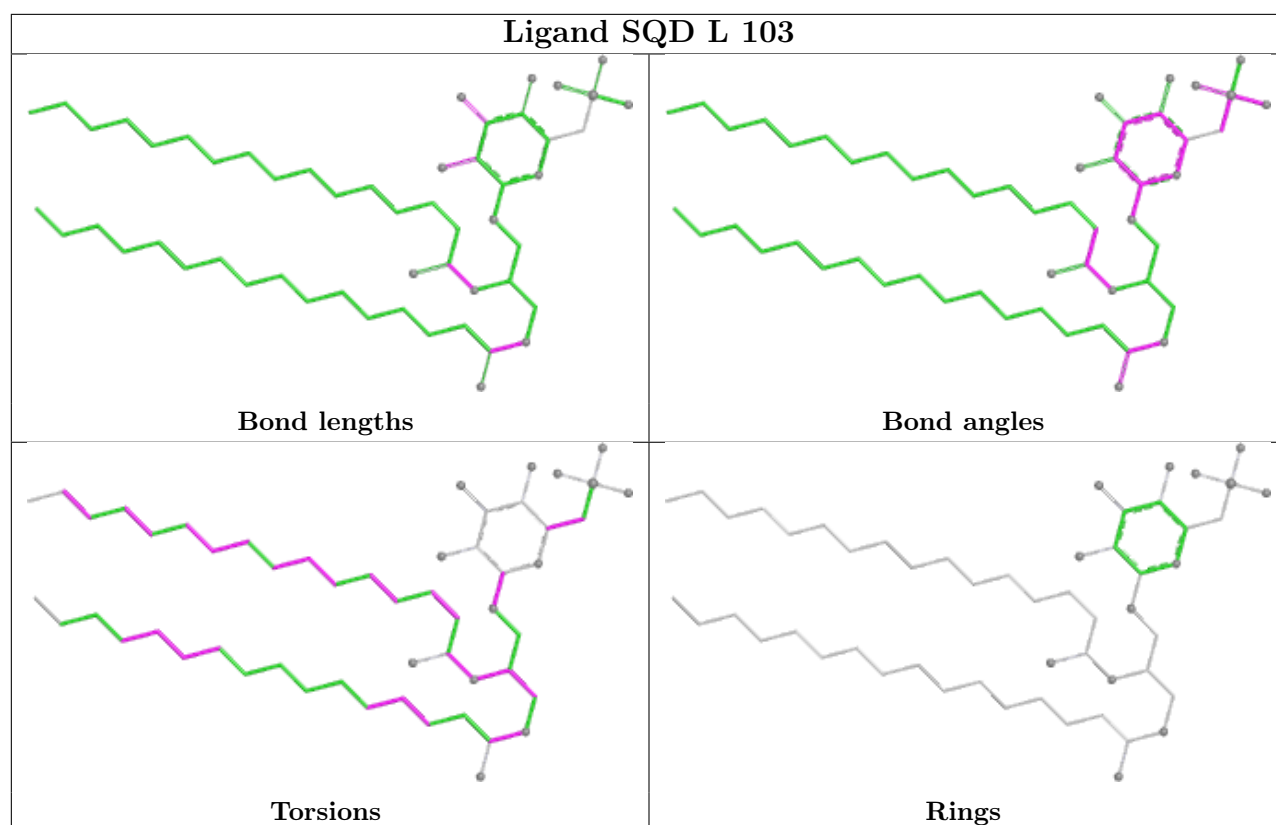


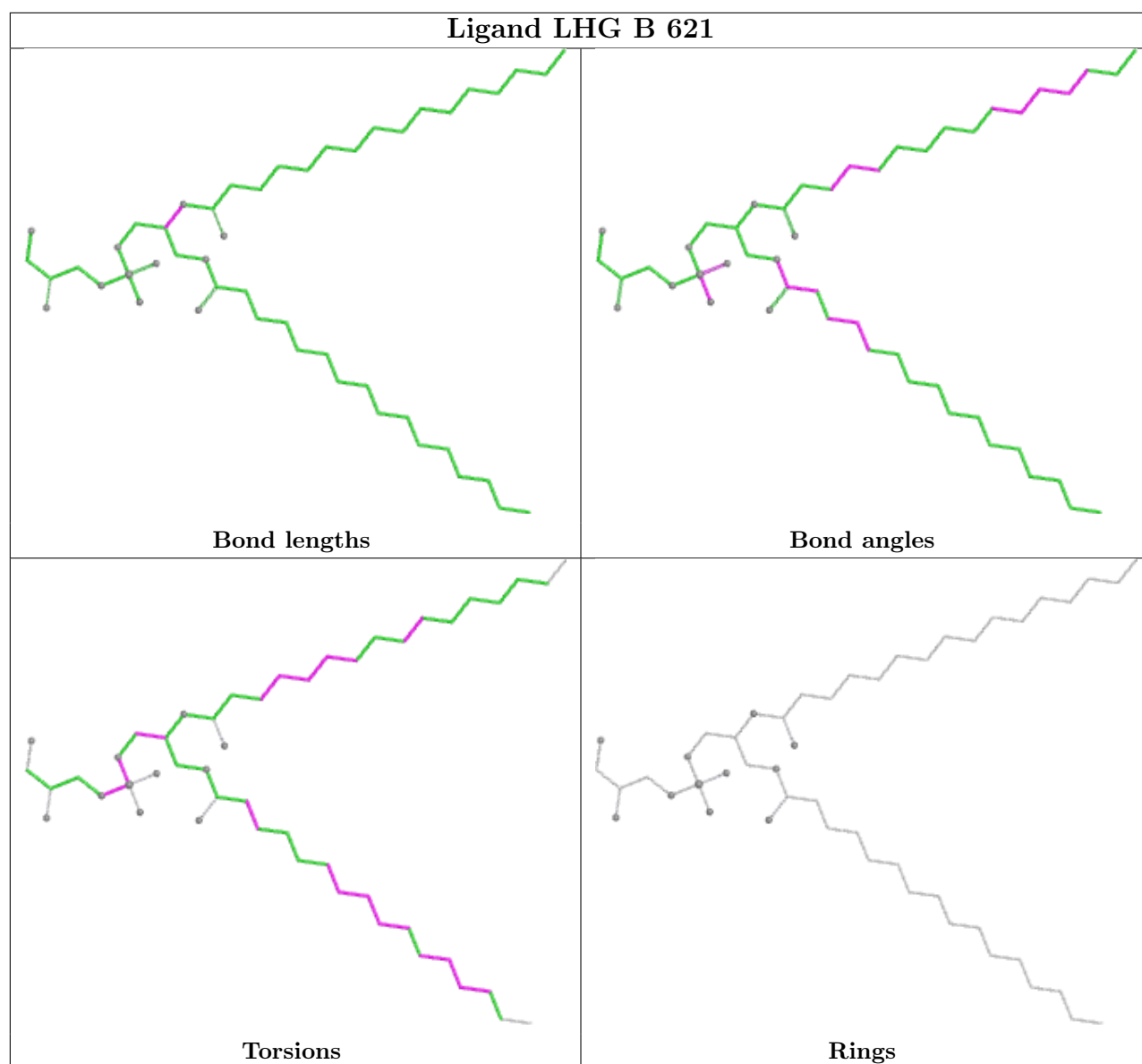
Ligand A86 11 314	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 d 404	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand A86 34 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

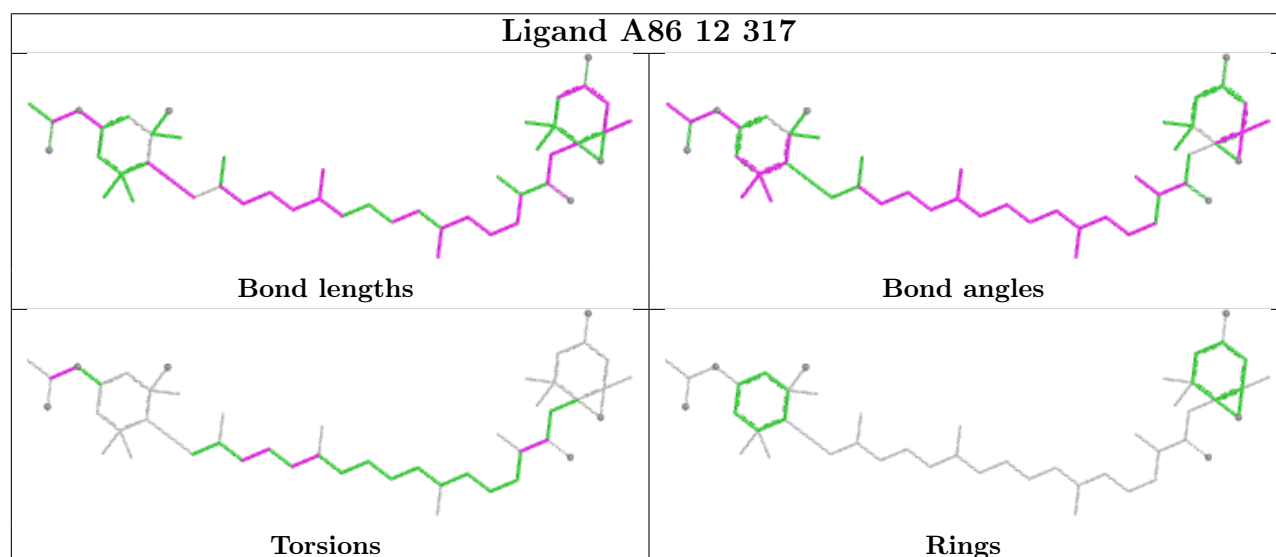
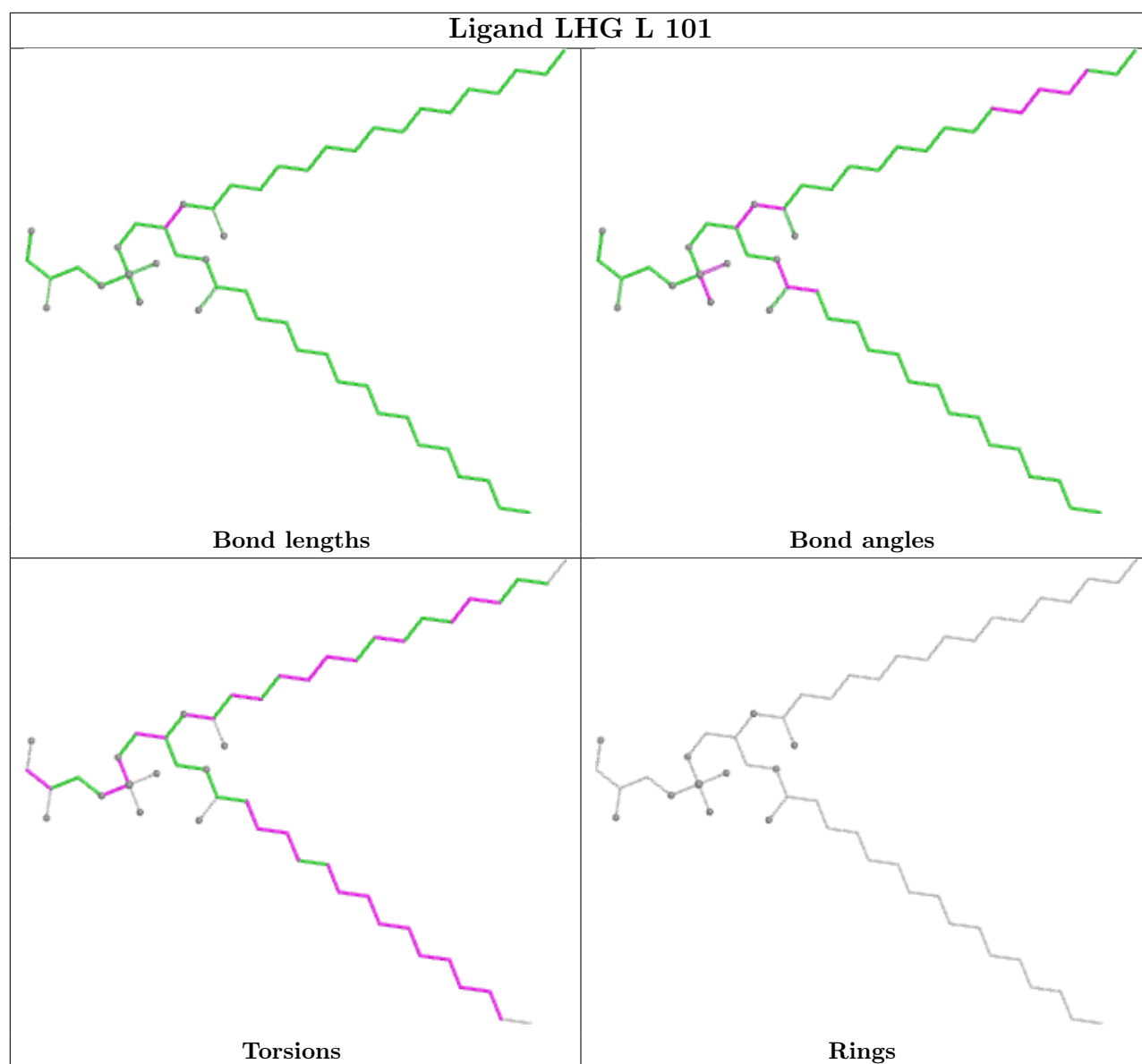


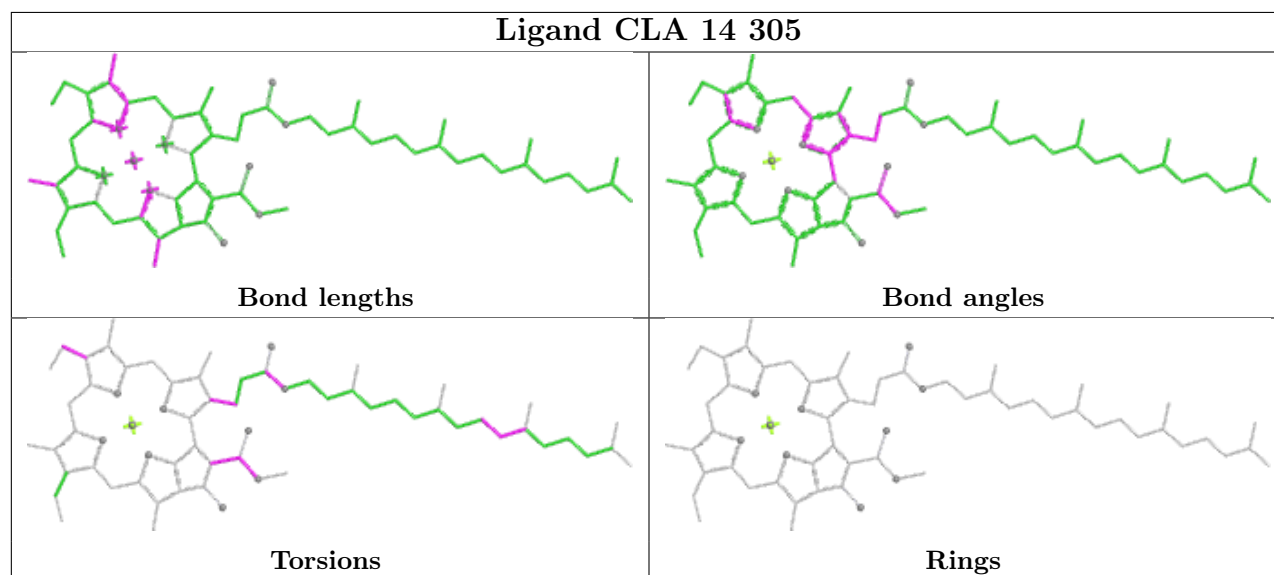
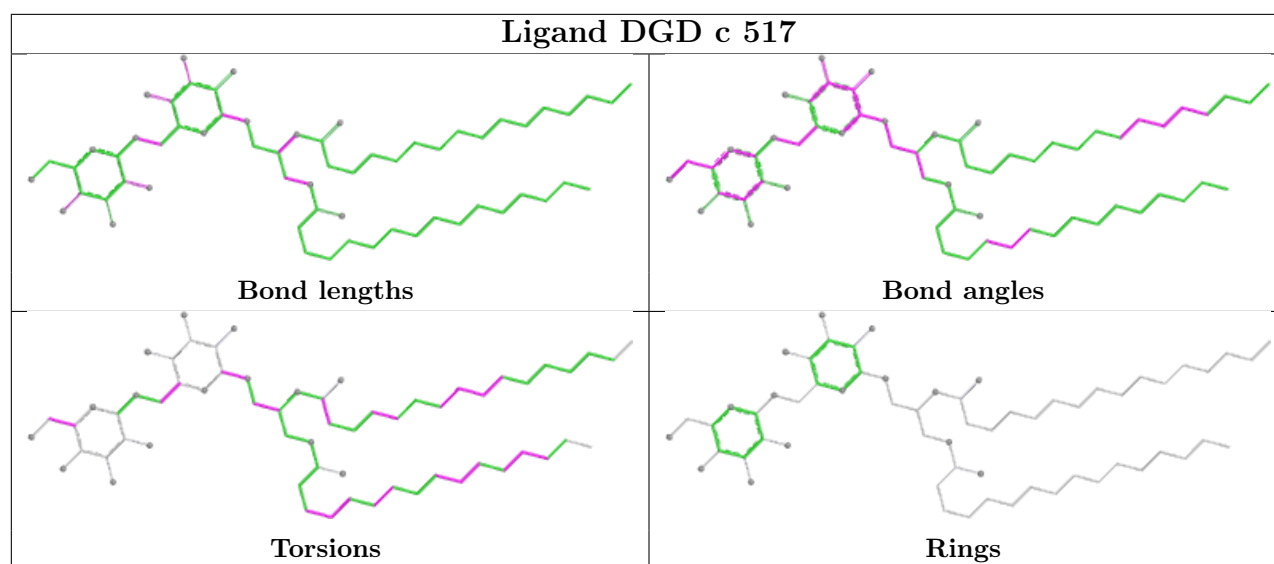


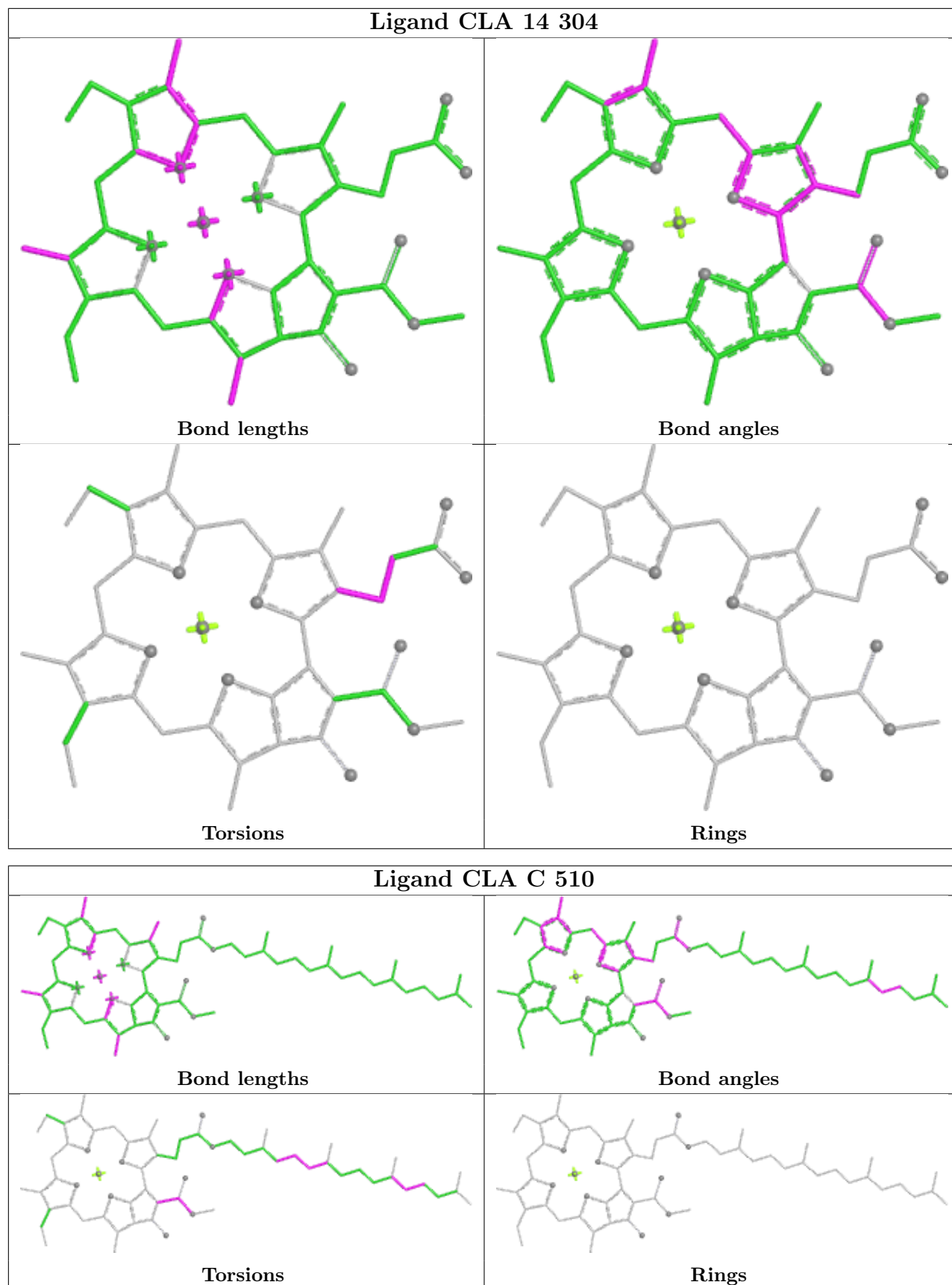
Ligand CLA C 512**Ligand CLA c 505**

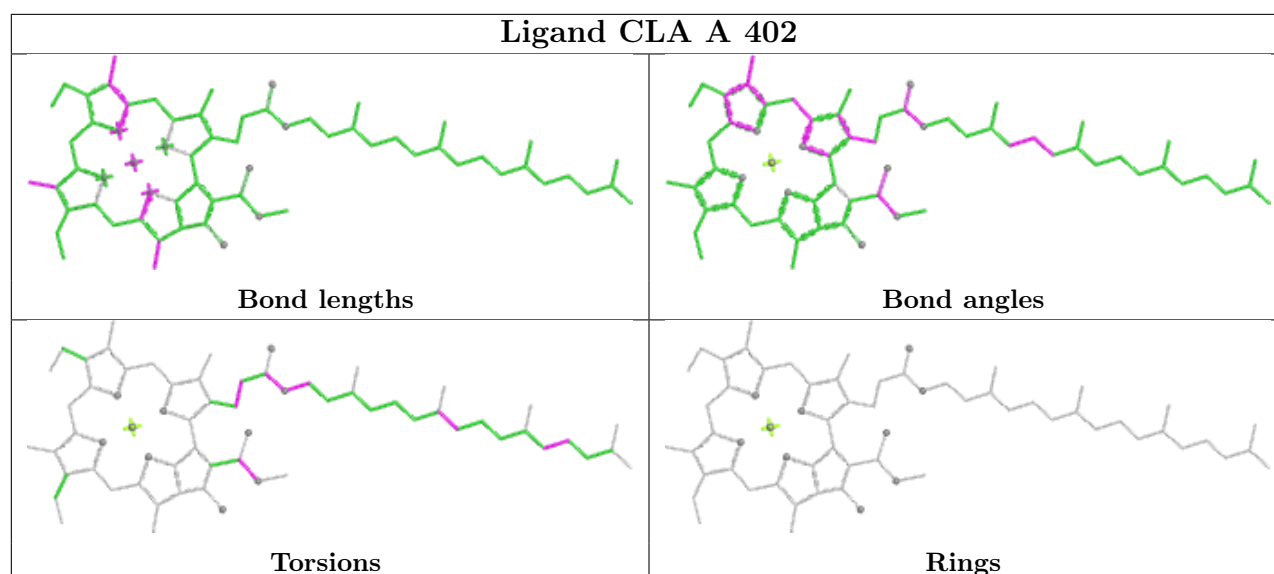
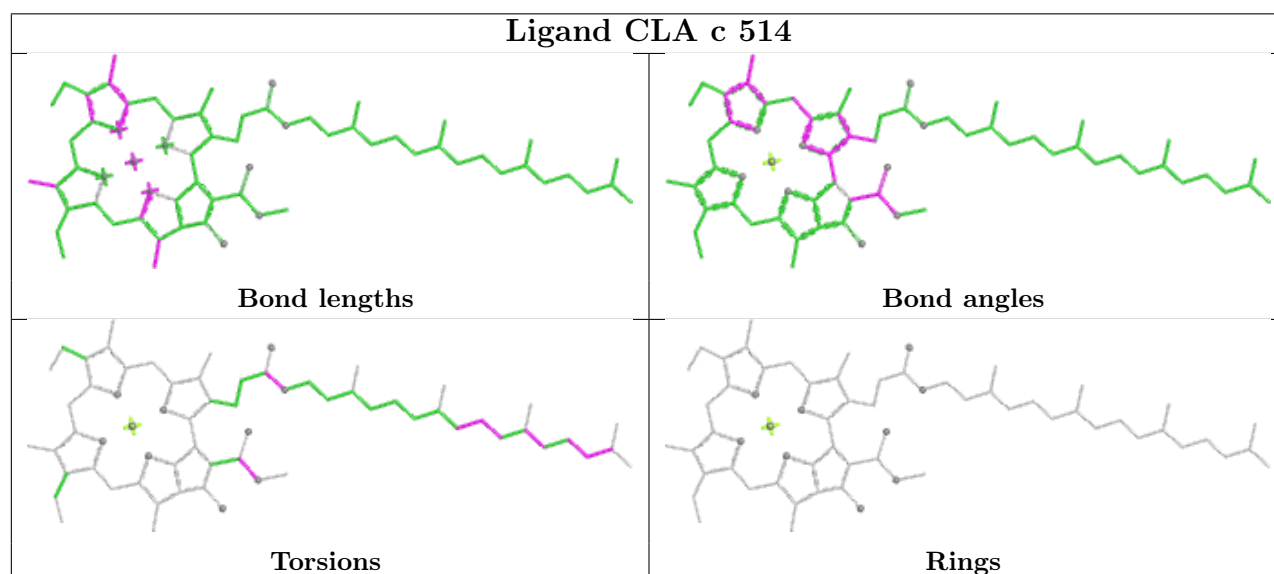
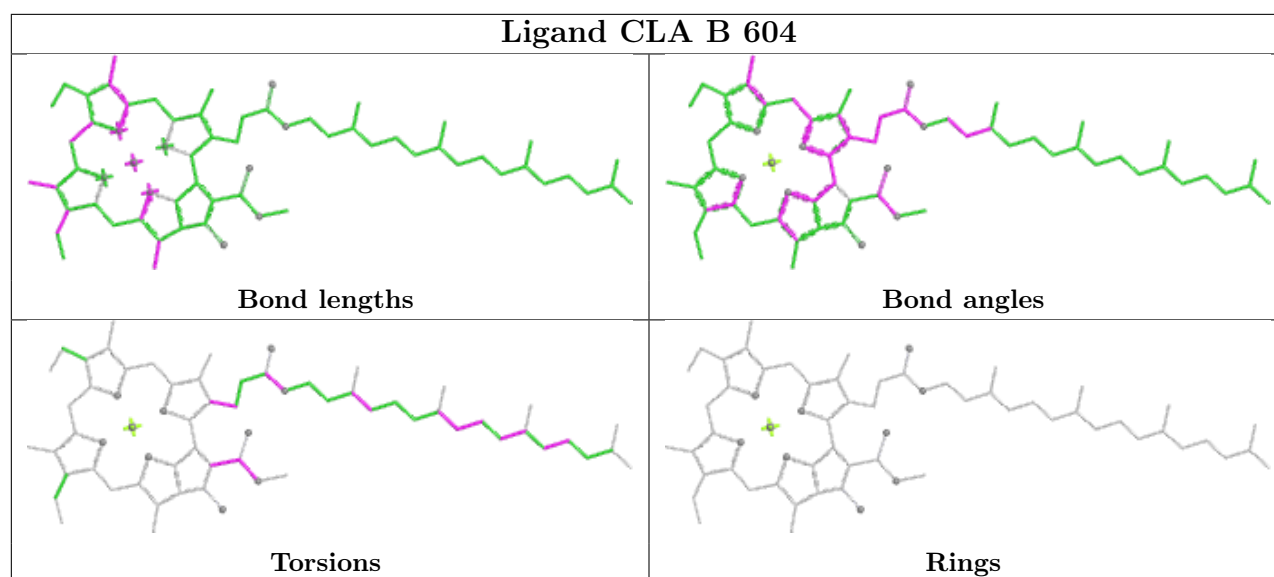


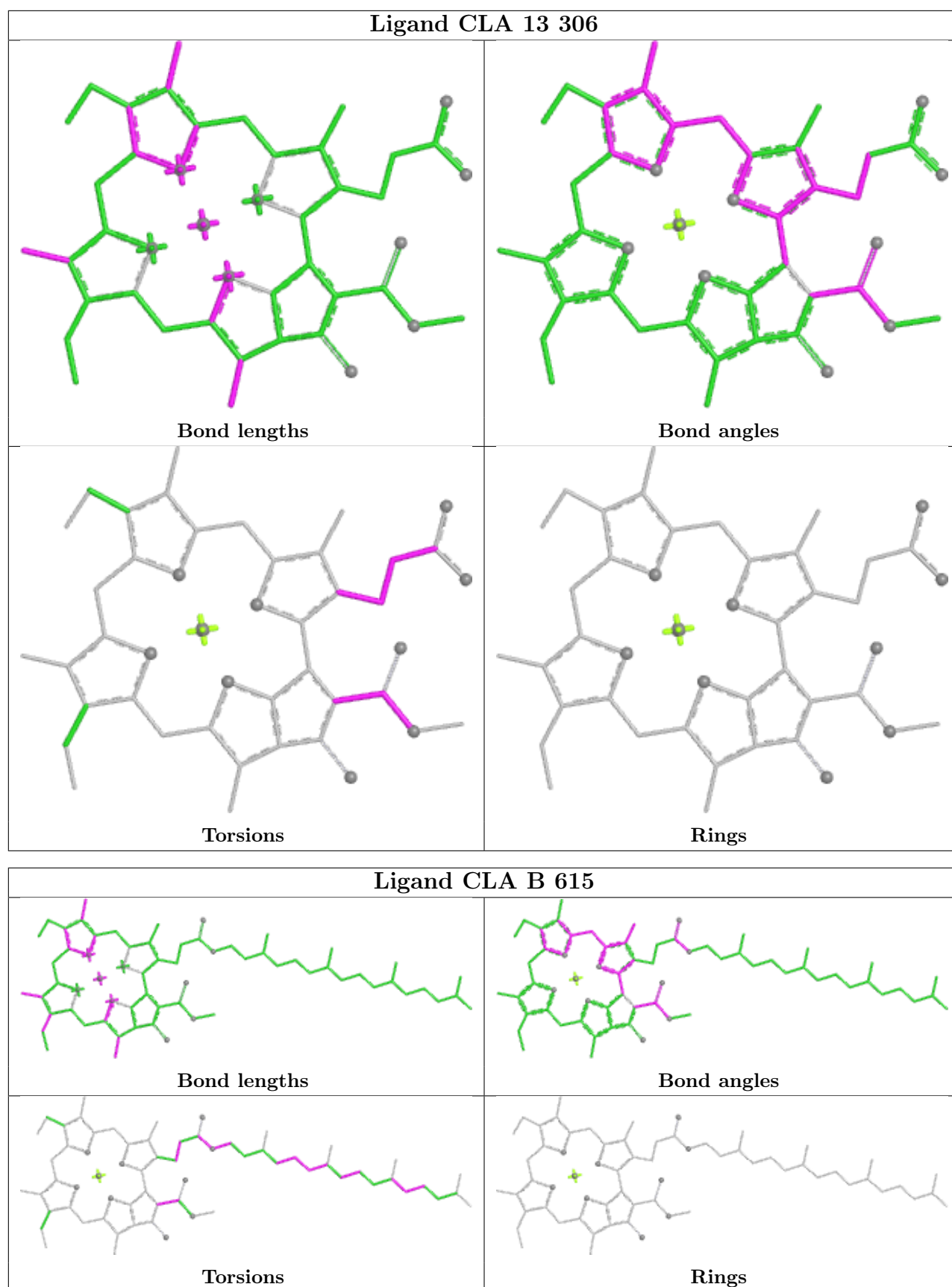


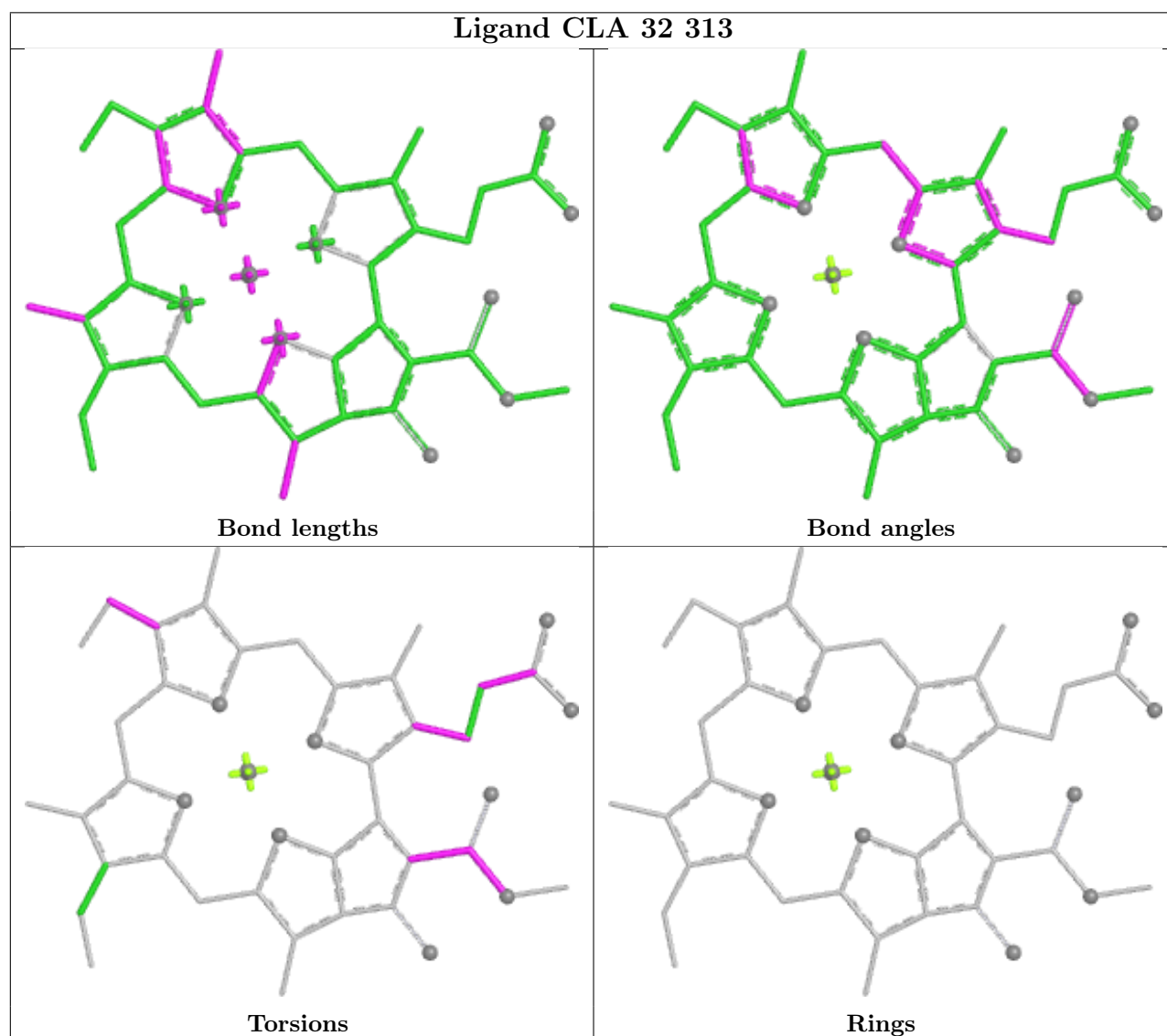
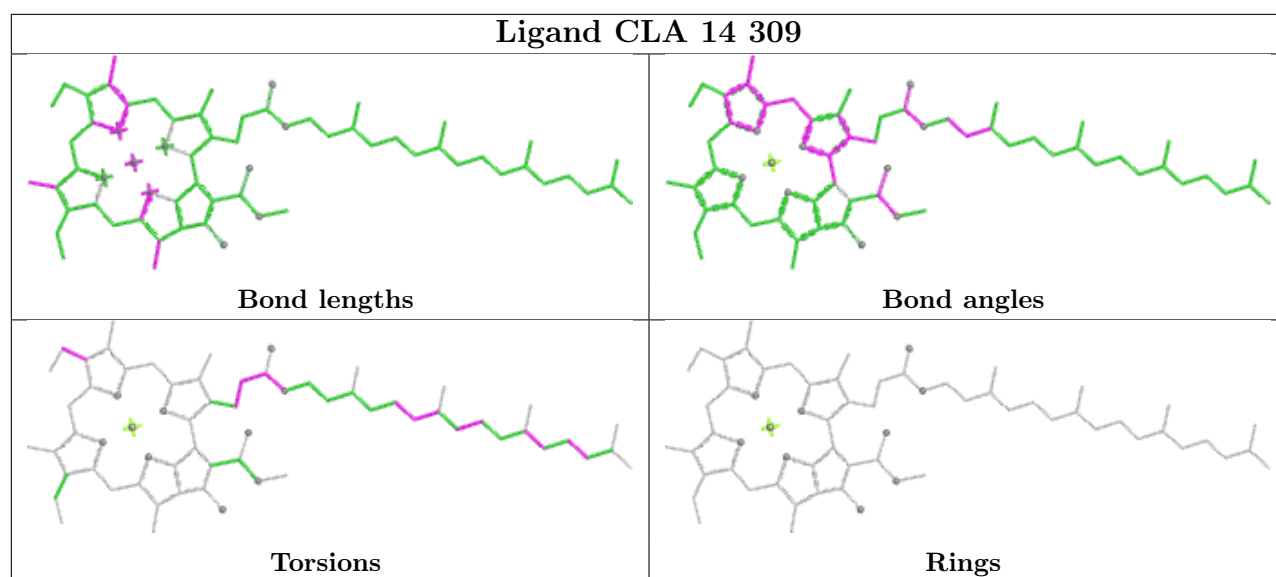


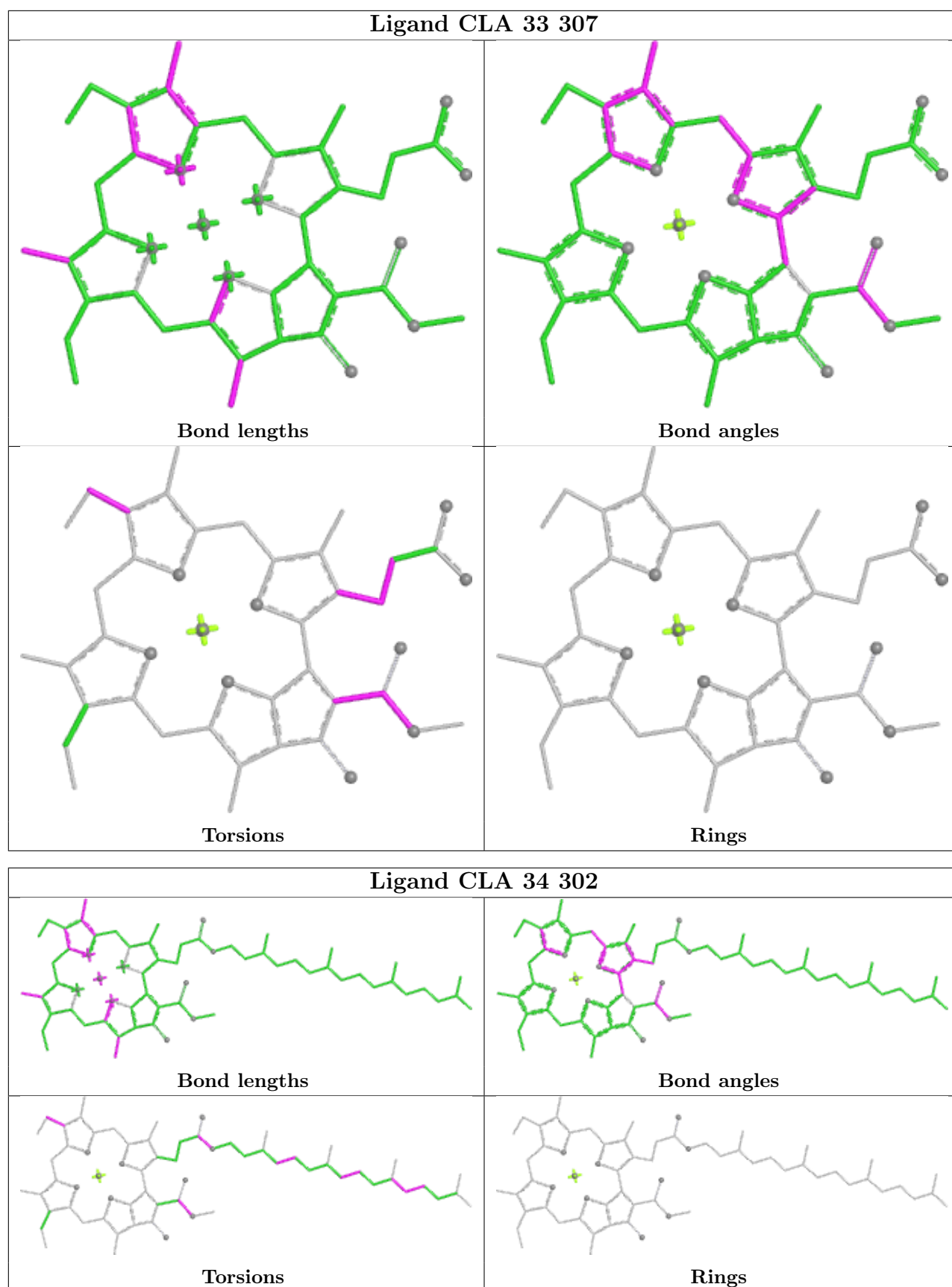


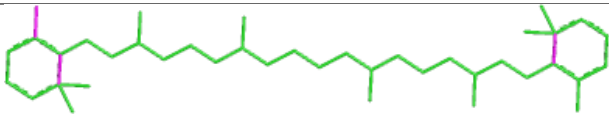
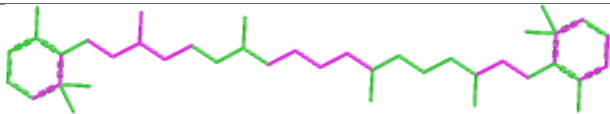
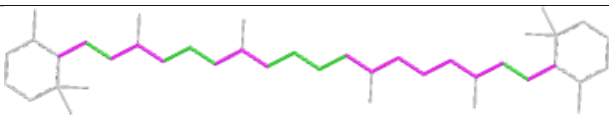
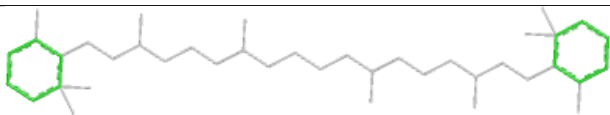




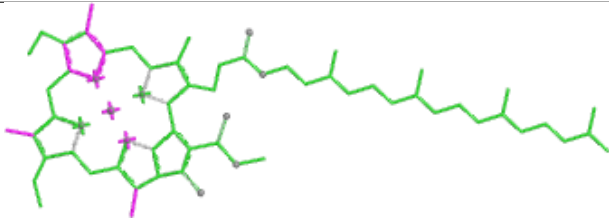
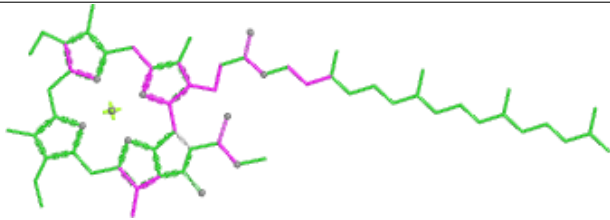
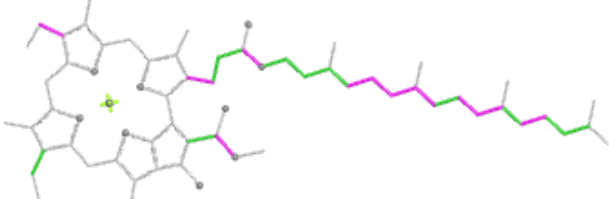
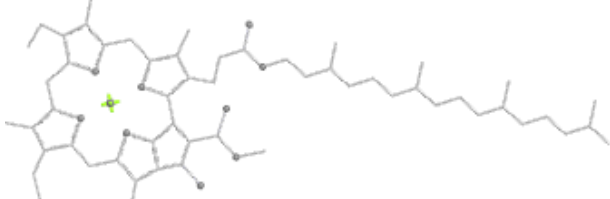


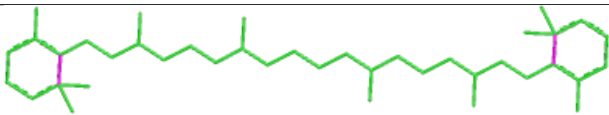
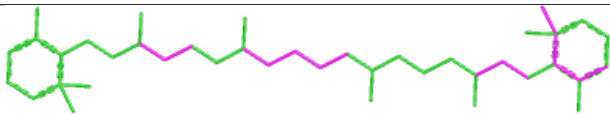
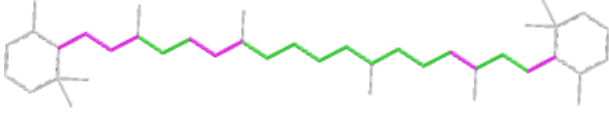
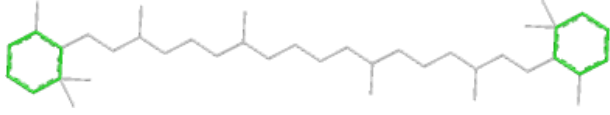


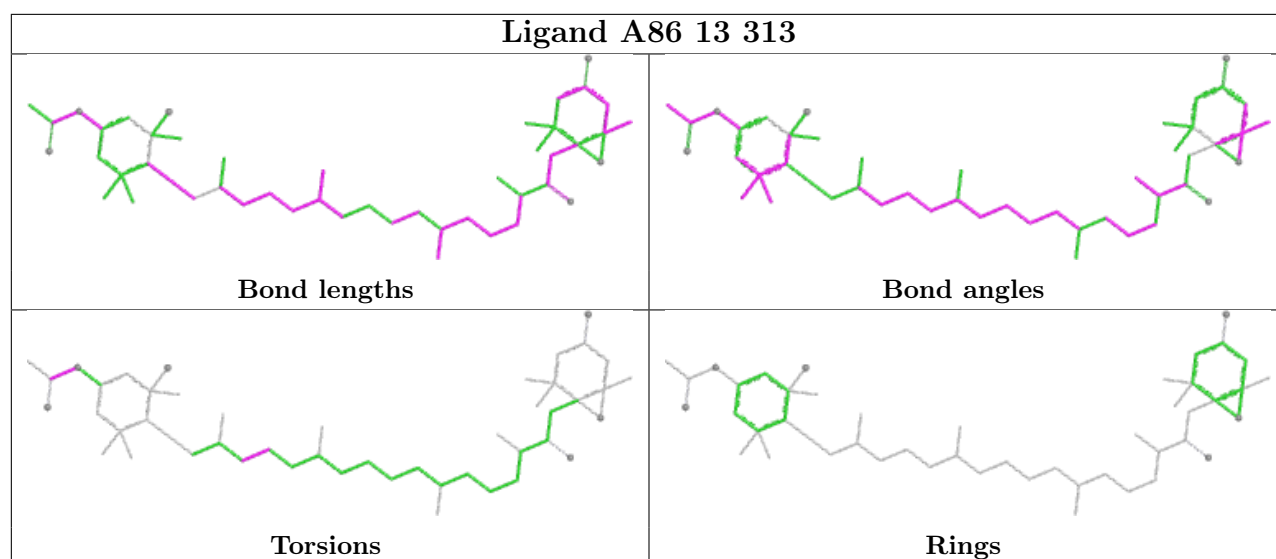


Ligand BCR z 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 D 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 616	
	
Bond lengths	Bond angles
	
Torsions	Rings



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-9775. These allow visual inspection of the internal detail of the map and identification of artifacts.

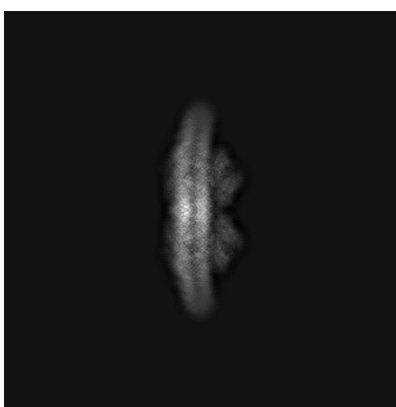
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

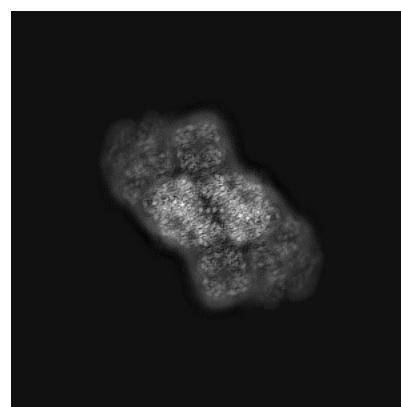
6.1.1 Primary map



X



Y

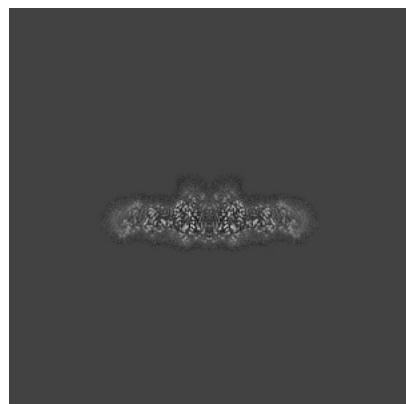


Z

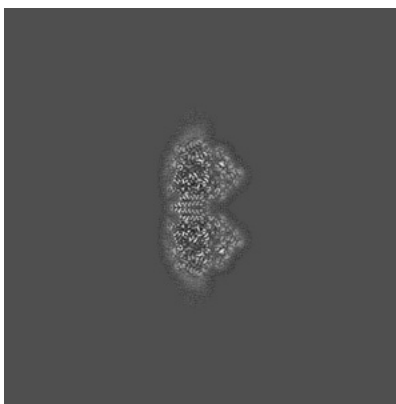
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

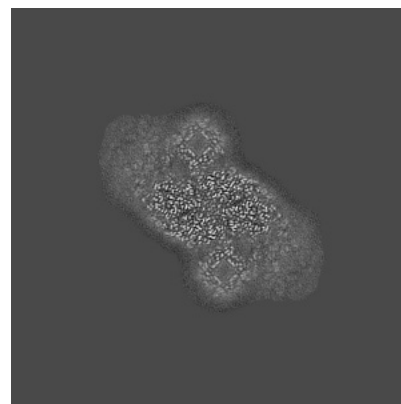
6.2.1 Primary map



X Index: 256



Y Index: 256

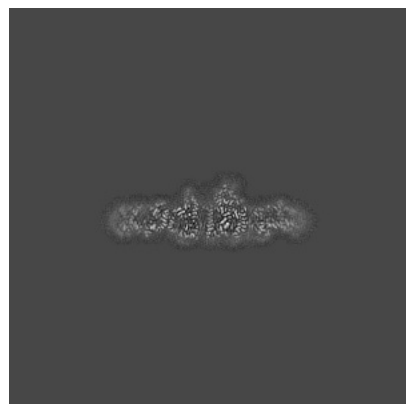


Z Index: 256

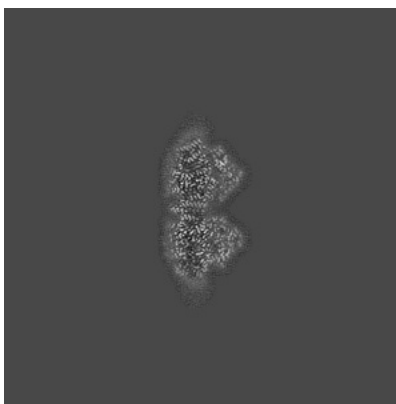
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

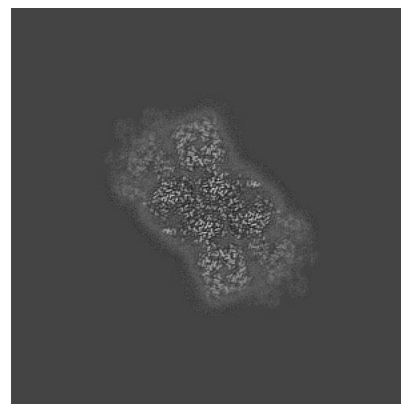
6.3.1 Primary map



X Index: 261



Y Index: 258

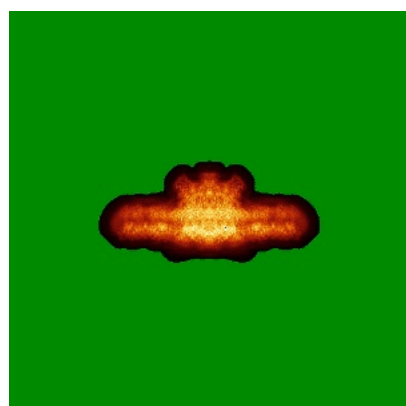


Z Index: 232

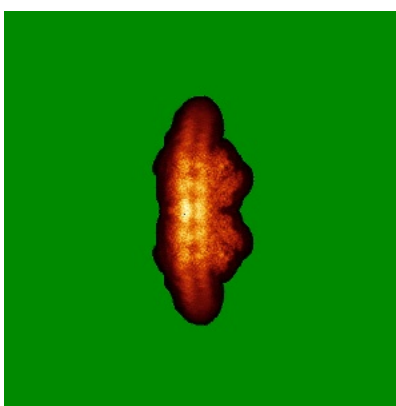
The images above show the largest variance slices of the map in three orthogonal directions.

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

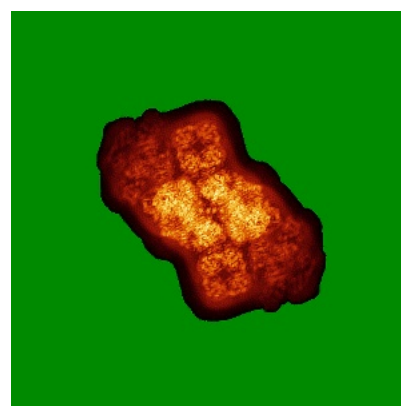
6.4.1 Primary map



X



Y

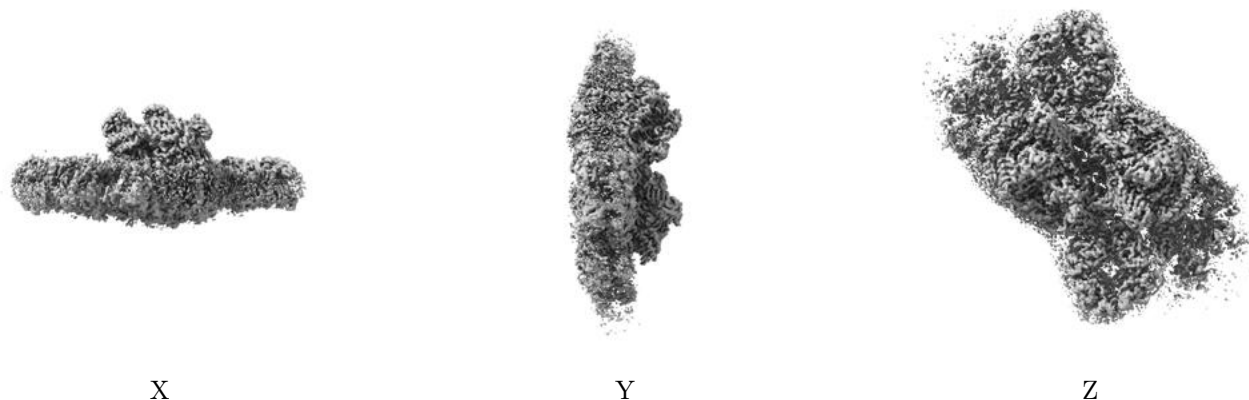


Z

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 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

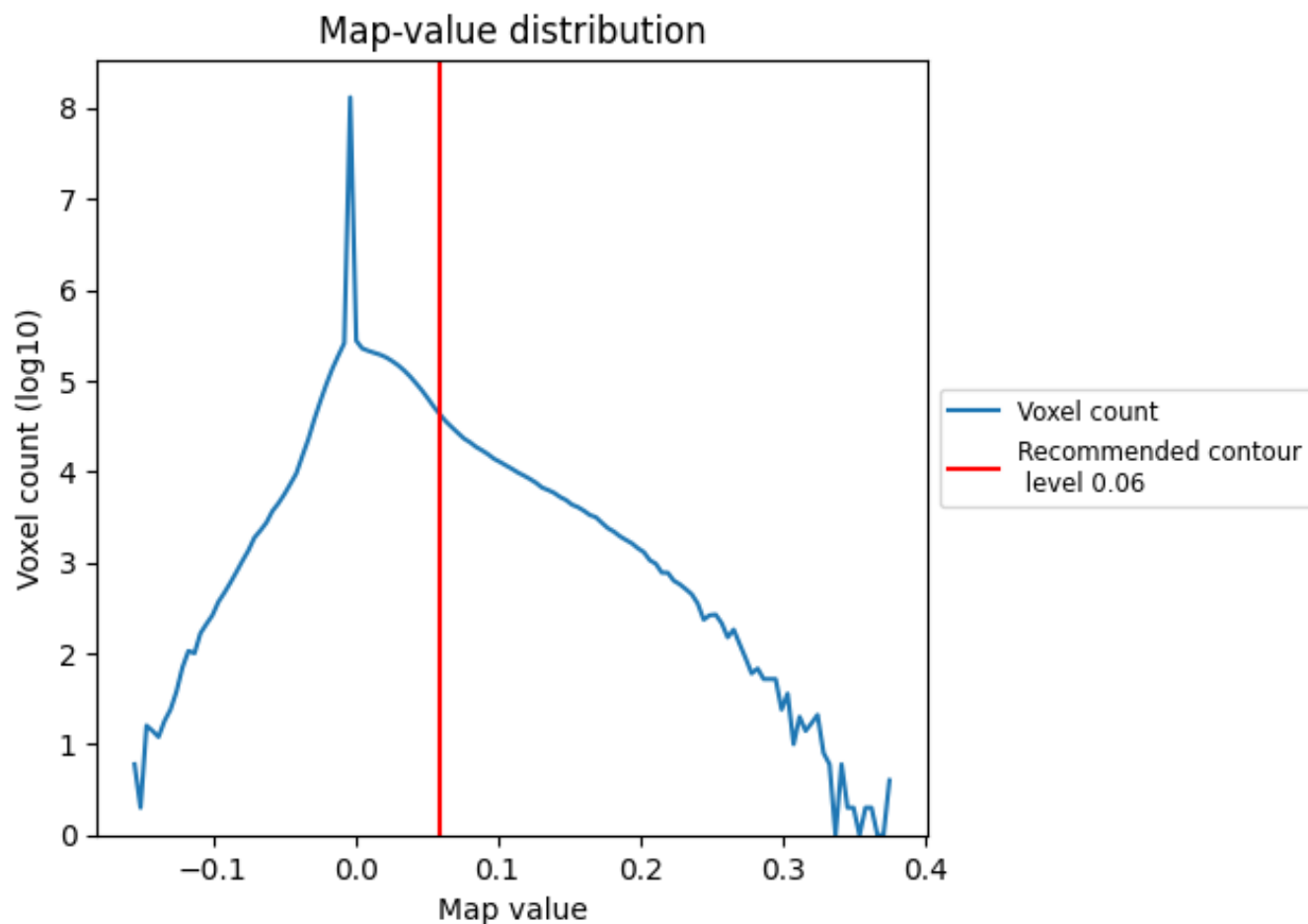
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

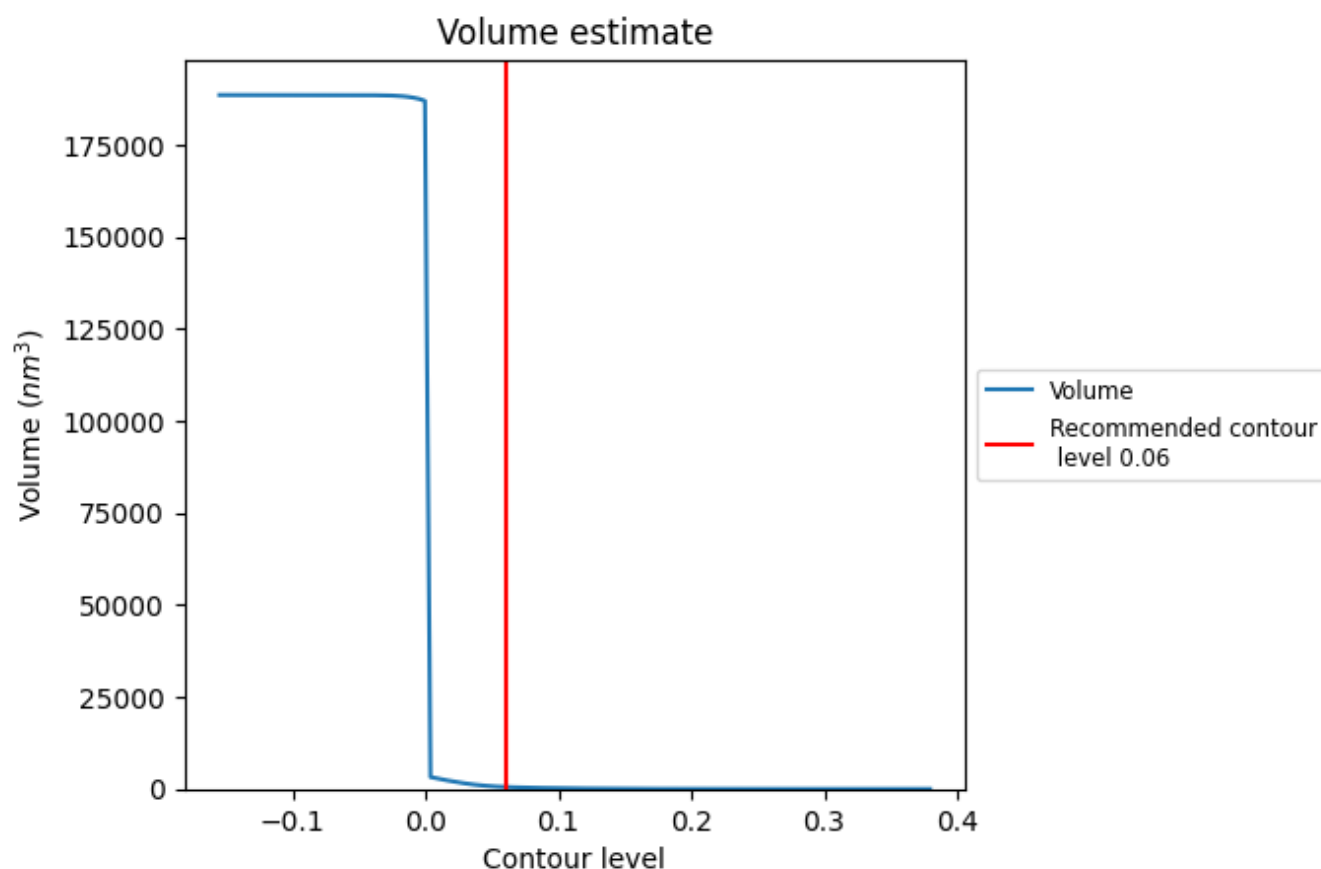
This section contains the results of statistical analysis of the map.

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.

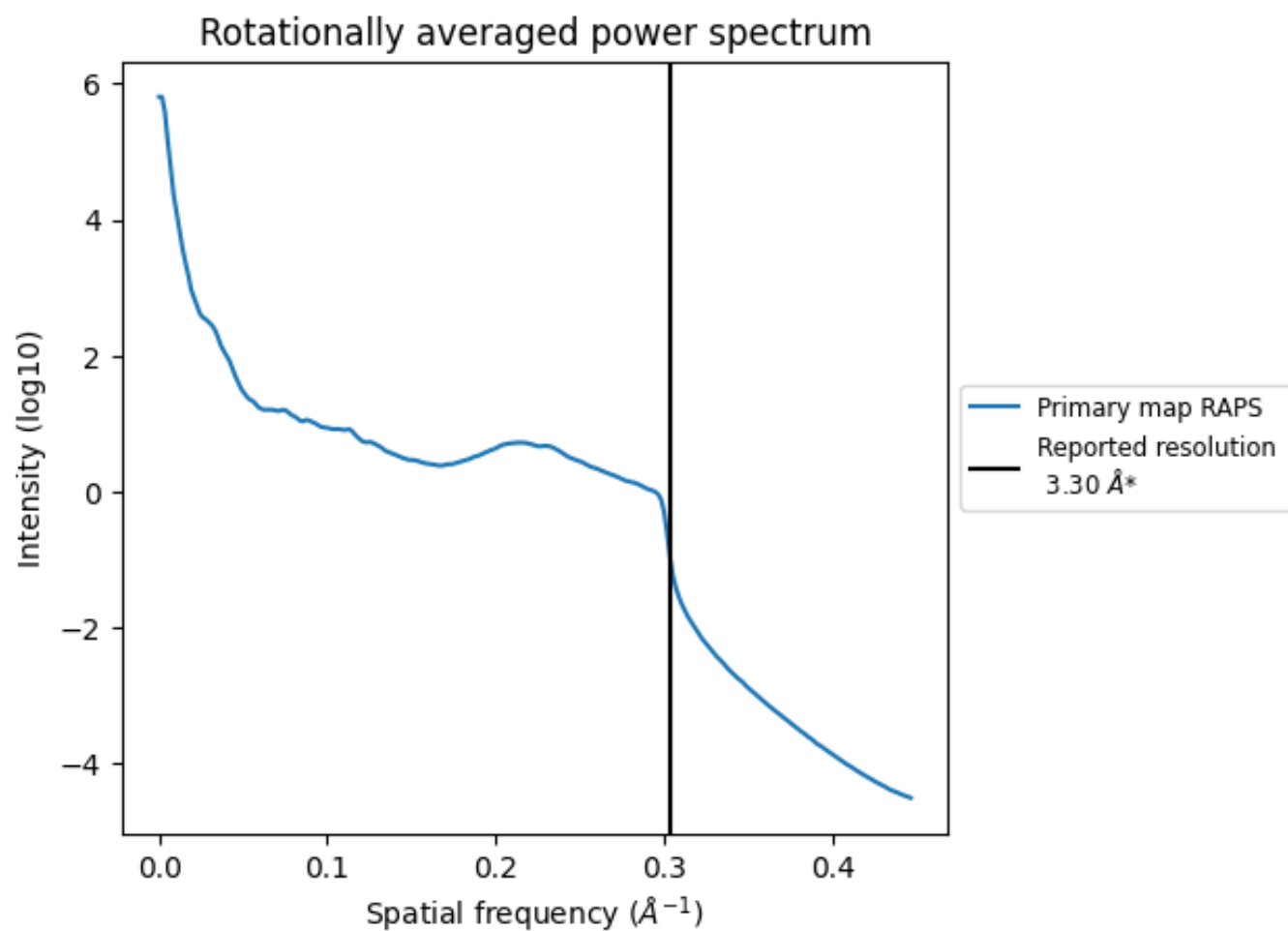
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 536 nm^3 ; this corresponds to an approximate mass of 484 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 ⓘ

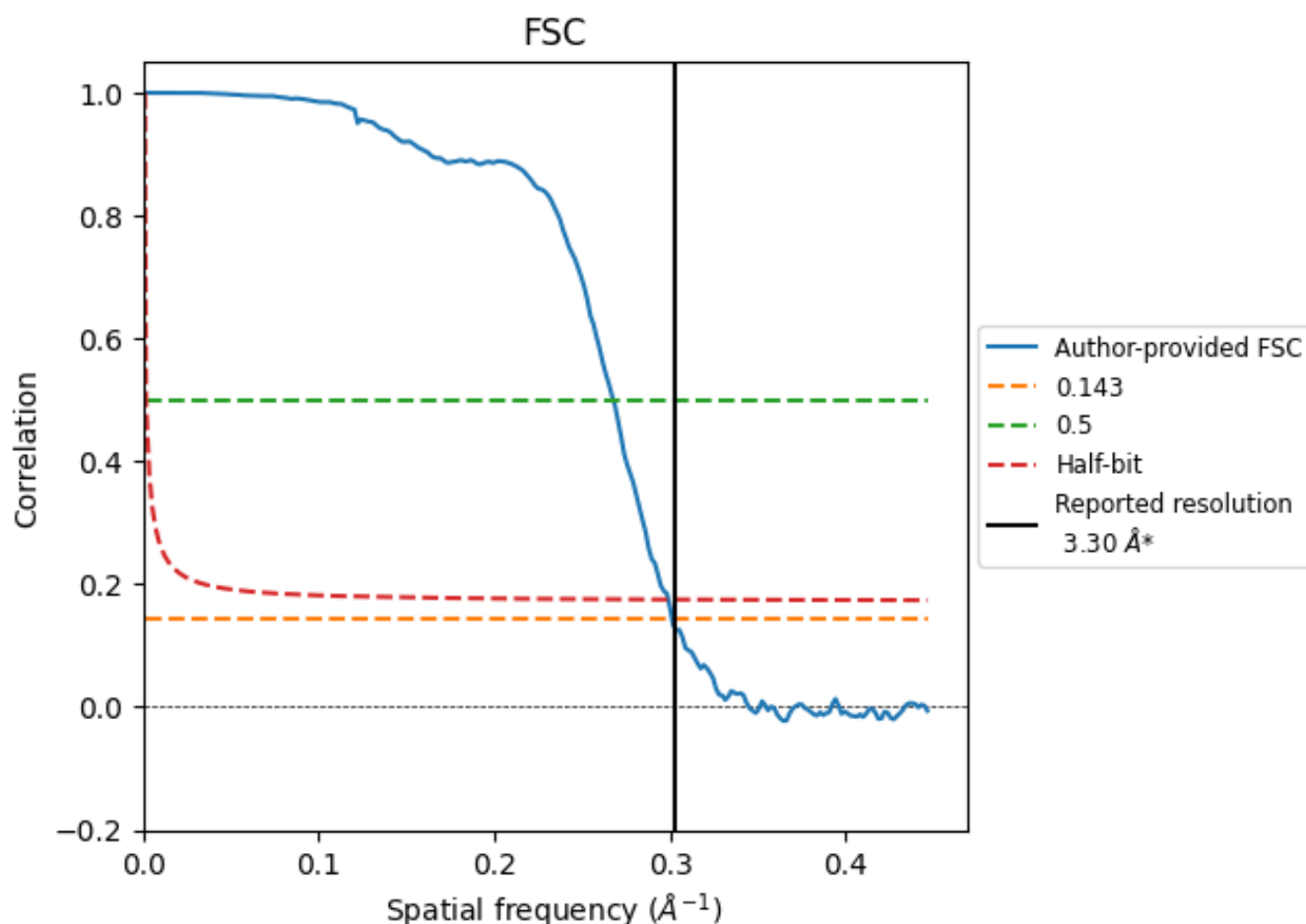


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.74	3.35
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

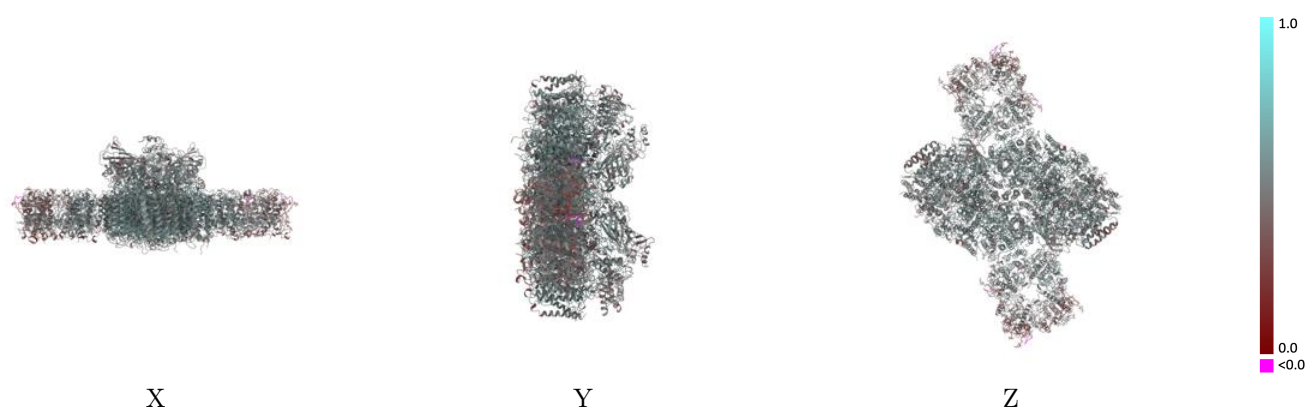
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9775 and PDB model 6J3Y. Per-residue inclusion information can be found in section 3 on page 35.

9.1 Map-model overlay [i](#)

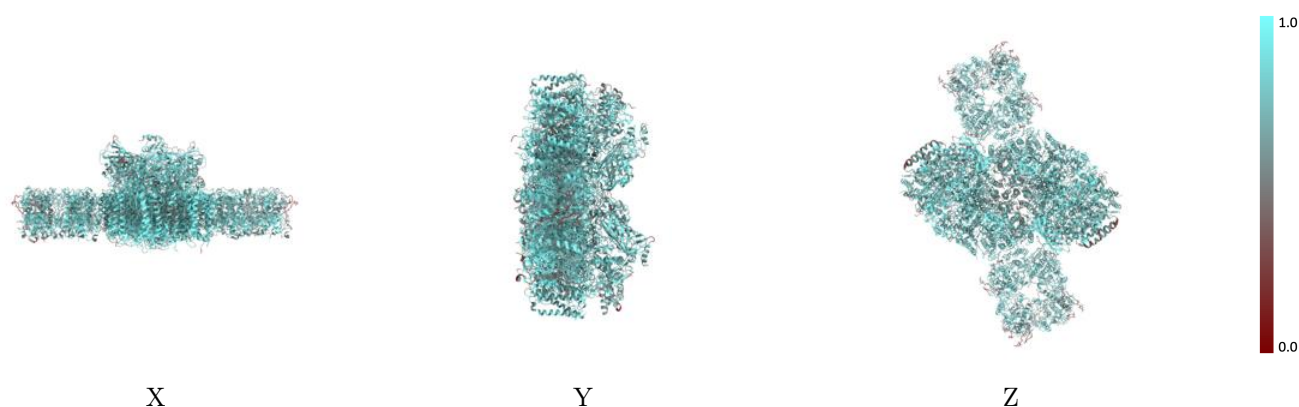
This section was not generated.

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



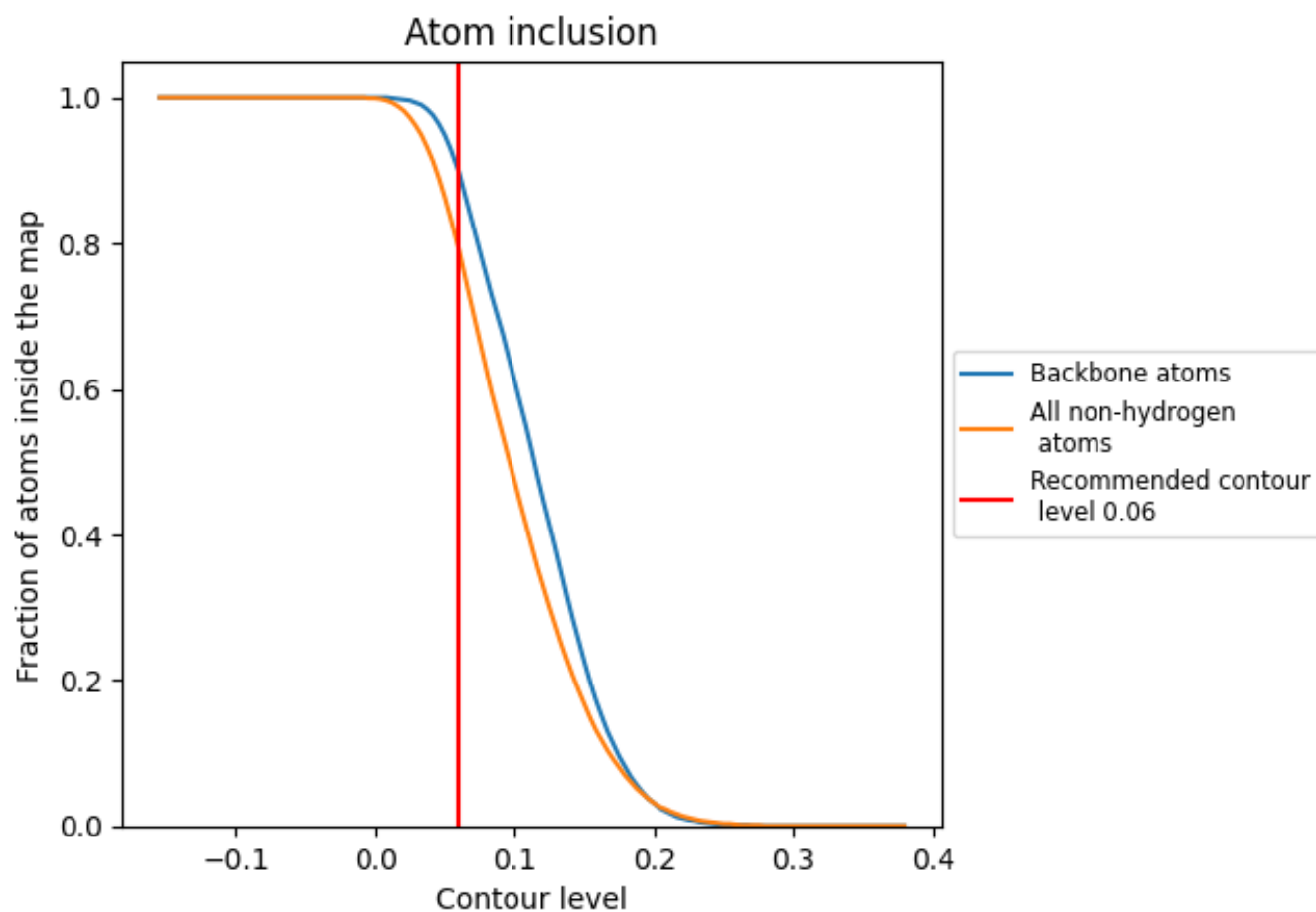
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 79% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7900	 0.5030
0	 0.8770	 0.5350
1	 0.9000	 0.5450
11	 0.7800	 0.4900
12	 0.7730	 0.4650
13	 0.6790	 0.3890
14	 0.6830	 0.4020
2	 0.8800	 0.4930
31	 0.7780	 0.4910
32	 0.7720	 0.4620
33	 0.6820	 0.3870
34	 0.6820	 0.4030
5	 0.8710	 0.5470
6	 0.9000	 0.5440
7	 0.9000	 0.4950
A	 0.8560	 0.5520
B	 0.8410	 0.5500
C	 0.8420	 0.5410
D	 0.8280	 0.5470
E	 0.8170	 0.4860
F	 0.8140	 0.5040
H	 0.8130	 0.5260
I	 0.8260	 0.5270
J	 0.7590	 0.5260
K	 0.8310	 0.5130
L	 0.7310	 0.5450
M	 0.6850	 0.5230
O	 0.7480	 0.4760
Q	 0.6640	 0.4470
T	 0.7390	 0.5130
U	 0.7860	 0.4820
V	 0.8160	 0.4900
W	 0.6860	 0.4810
X	 0.7300	 0.4660
Y	 0.7150	 0.4790



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Chain	Atom inclusion	Q-score
Z	 0.7520	 0.4780
a	 0.8550	 0.5510
b	 0.8410	 0.5490
c	 0.8450	 0.5420
d	 0.8280	 0.5470
e	 0.8200	 0.4850
f	 0.8010	 0.5060
h	 0.8150	 0.5260
i	 0.8440	 0.5300
j	 0.7650	 0.5250
k	 0.8550	 0.5110
l	 0.7270	 0.5450
m	 0.6850	 0.5210
o	 0.7440	 0.4780
q	 0.6570	 0.4530
t	 0.7470	 0.5180
u	 0.7840	 0.4810
v	 0.8170	 0.4940
w	 0.7070	 0.4830
x	 0.7300	 0.4700
y	 0.7150	 0.4880
z	 0.7590	 0.4810