



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 01:45 AM JST

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:

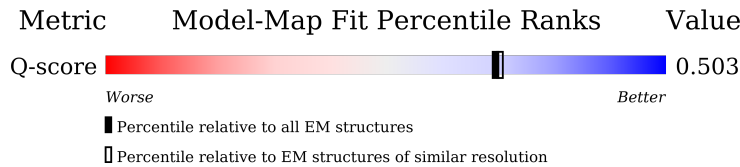
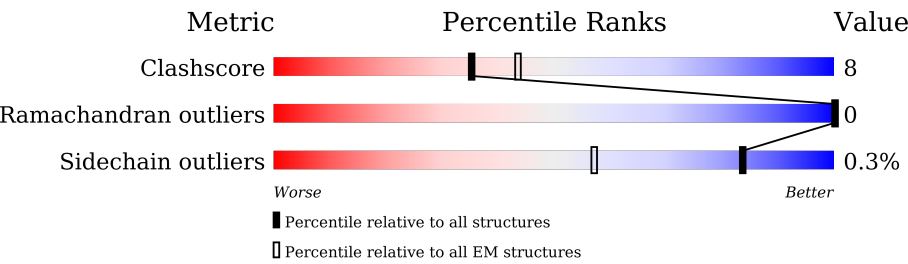
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 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.



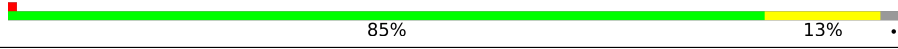
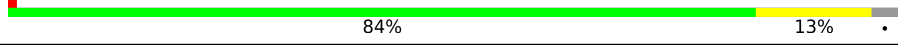
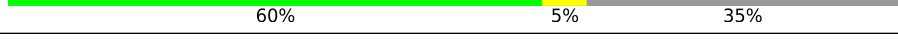
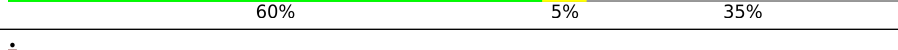
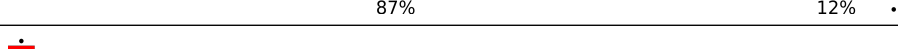
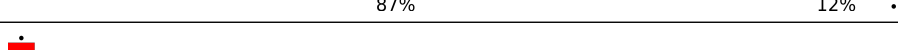
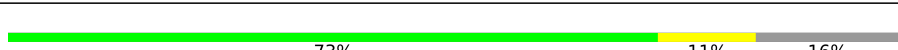
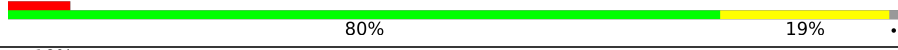
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	84% 13% •
1	a	344	84% 13% •
2	B	509	83% 13% 5%
2	b	509	83% 13% 5%

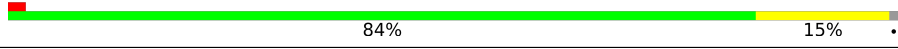
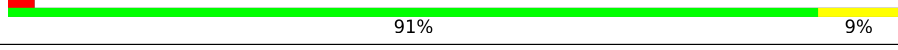
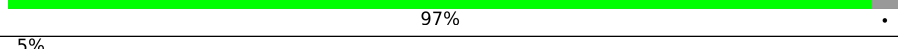
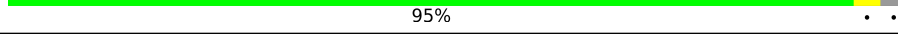
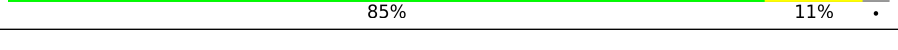
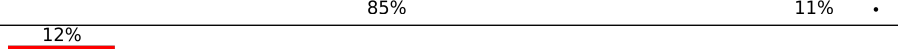
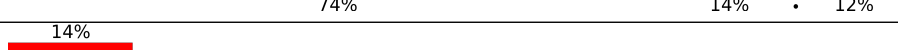
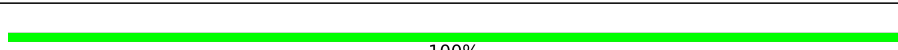
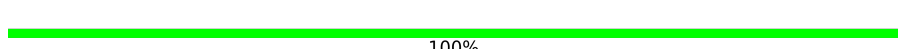
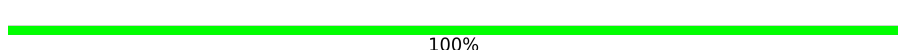
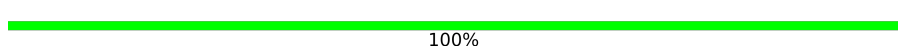
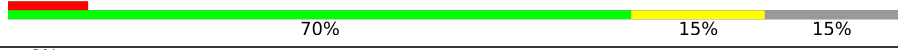
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Mol	Chain	Length	Quality of chain
3	C	471	
3	c	471	
4	D	351	
4	d	351	
5	E	84	
5	e	84	
6	F	43	
6	f	43	
7	H	67	
7	h	67	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	44	
10	k	44	
11	L	38	
11	l	38	
12	M	131	
12	m	131	
13	O	248	
13	o	248	
14	T	31	
14	t	31	
15	U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

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Mol	Chain	Length	Quality of chain
15	u	93	 82%18%
16	V	137	 82%18%
16	v	137	 84%15%
17	Y	34	 91%9%
17	y	34	 88%12%
18	X	38	 5%97%
18	x	38	 5%95%
19	Z	61	 85%11%
19	z	61	 85%11%
20	Q	155	 12%74%14%
20	q	155	 14%73%15%
21	W	72	 8%62%10%
21	w	72	 7%61%11%
22	0	31	 100%
22	5	31	 100%
23	1	30	 100%
23	6	30	 100%
24	2	10	 100%
24	7	10	 100%
25	11	207	 69%16%
25	12	207	 5%69%16%
25	13	207	 9%70%15%
25	14	207	 8%69%16%
25	31	207	 68%17%
25	32	207	 5%67%18%

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Mol	Chain	Length	Quality of chain
25	33	207	10% 69% 16% 15%
25	34	207	10% 70% 15% 15%

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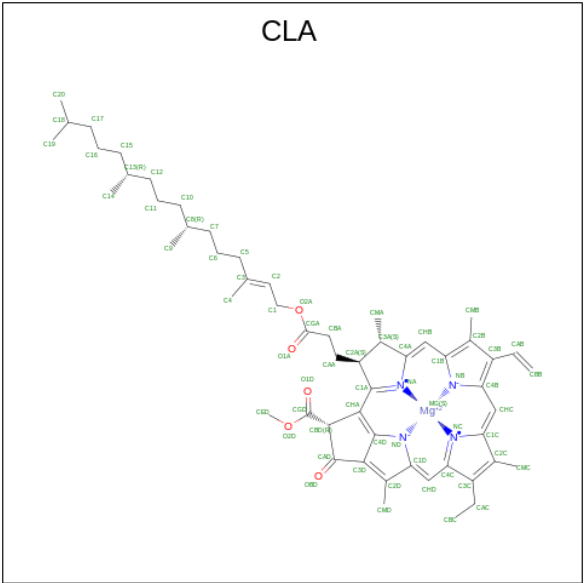
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Mol	Chain	Residues	Atoms					AltConf	Trace
25	32	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	33	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	34	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		

- 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
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 65	C 55	Mg 1	N 4	O 5	0
27	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	13	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

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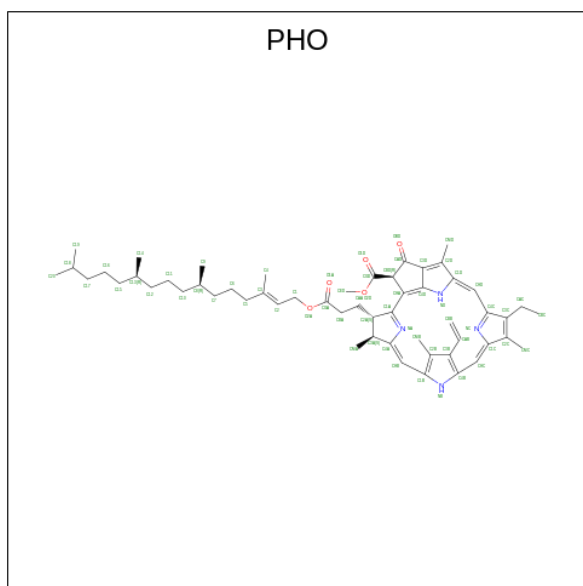
Mol	Chain	Residues	Atoms					AltConf
27	32	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	32	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	32	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	32	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	32	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	32	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	32	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	32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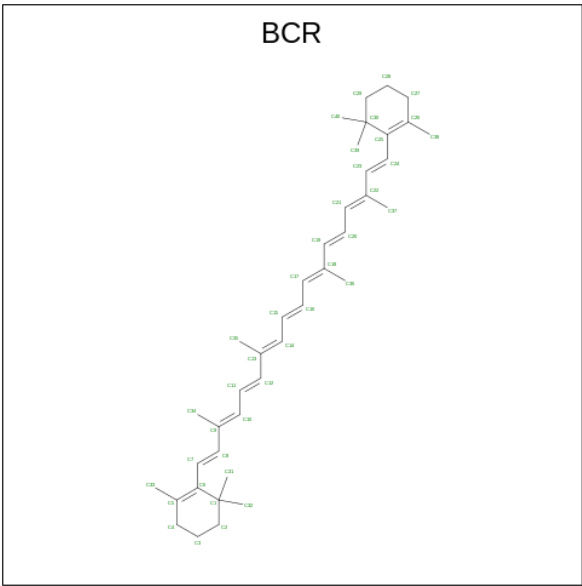
Mol	Chain	Residues	Atoms					AltConf
27	34	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	34	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	34	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	34	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	34	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	34	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	34	1	Total	C	Mg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

- Molecule 28 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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).



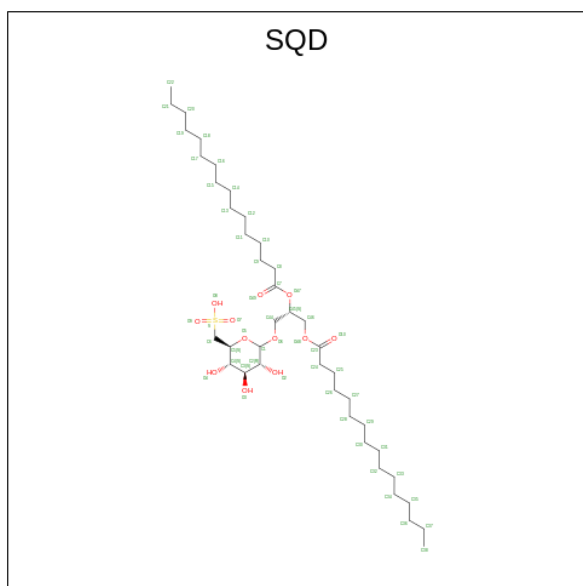
Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	C	1	Total C 40 40	0
29	C	1	Total C 40 40	0
29	C	1	Total C 40 40	0
29	F	1	Total C 40 40	0
29	H	1	Total C 40 40	0
29	M	1	Total C 40 40	0
29	Z	1	Total C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

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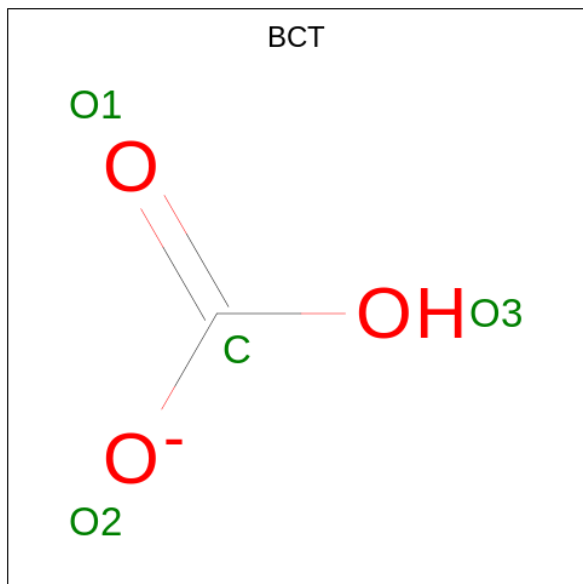
Mol	Chain	Residues	Atoms	AltConf
29	a	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	c	1	Total C 40 40	0
29	c	1	Total C 40 40	0
29	c	1	Total C 40 40	0
29	f	1	Total C 40 40	0
29	h	1	Total C 40 40	0
29	m	1	Total C 40 40	0
29	z	1	Total C 40 40	0

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



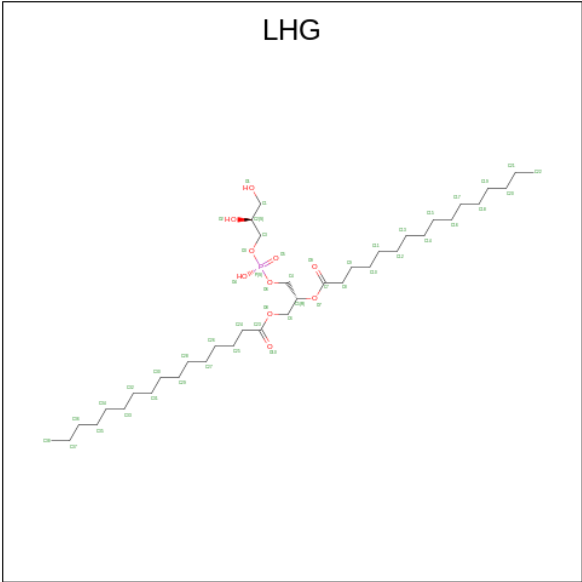
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	S	0
			54	41	12	1	
30	B	1	Total	C	O	S	0
			37	24	12	1	
30	L	1	Total	C	O	S	0
			54	41	12	1	
30	a	1	Total	C	O	S	0
			54	41	12	1	
30	b	1	Total	C	O	S	0
			37	24	12	1	
30	l	1	Total	C	O	S	0
			54	41	12	1	

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



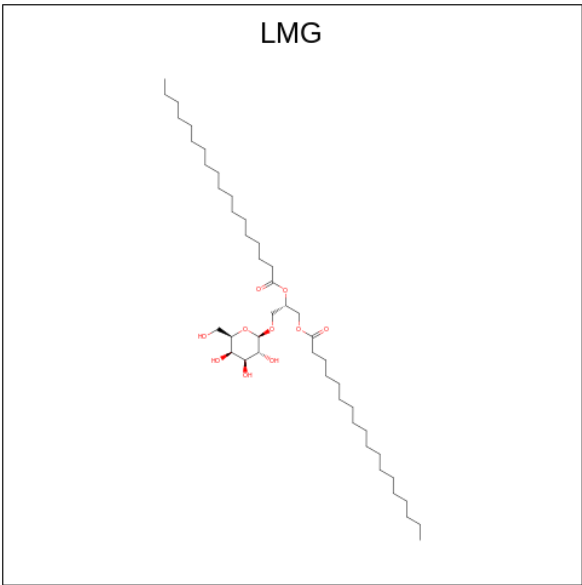
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			4	1	3	
31	a	1	Total	C	O	0
			4	1	3	

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



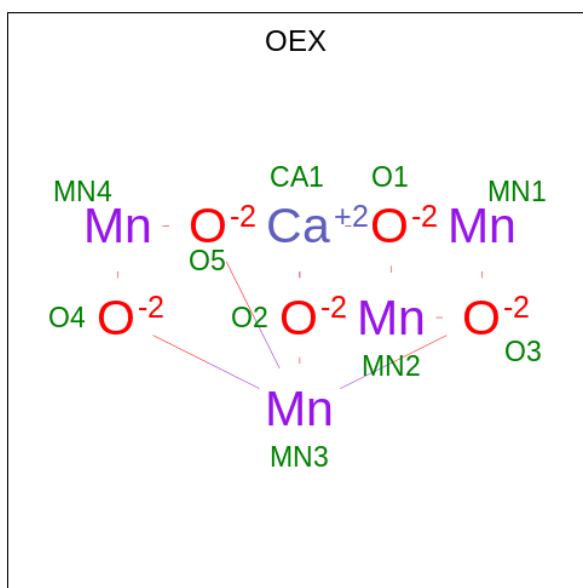
Mol	Chain	Residues	Atoms				AltConf
32	A	1	Total	C	O	P	0
			46	35	10	1	
32	B	1	Total	C	O	P	0
			49	38	10	1	
32	L	1	Total	C	O	P	0
			49	38	10	1	
32	L	1	Total	C	O	P	0
			49	38	10	1	
32	a	1	Total	C	O	P	0
			46	35	10	1	
32	b	1	Total	C	O	P	0
			49	38	10	1	
32	l	1	Total	C	O	P	0
			49	38	10	1	
32	l	1	Total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

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



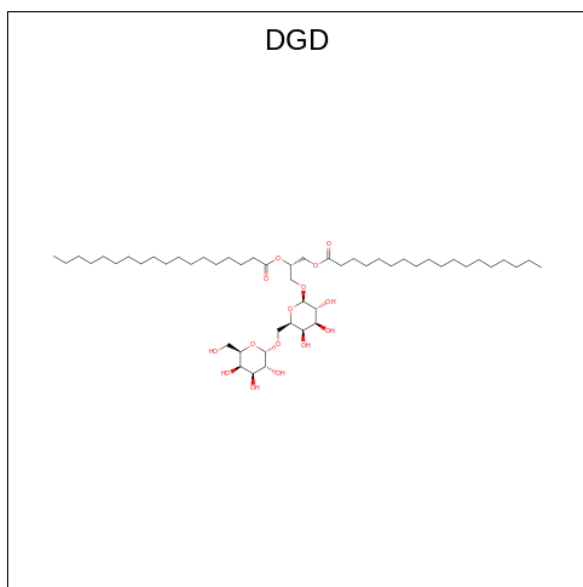
Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			51	41	10	
33	B	1	Total	C	O	0
			51	41	10	
33	C	1	Total	C	O	0
			51	41	10	
33	D	1	Total	C	O	0
			51	41	10	
33	M	1	Total	C	O	0
			40	30	10	
33	W	1	Total	C	O	0
			51	41	10	
33	b	1	Total	C	O	0
			51	41	10	
33	b	1	Total	C	O	0
			51	41	10	
33	d	1	Total	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).



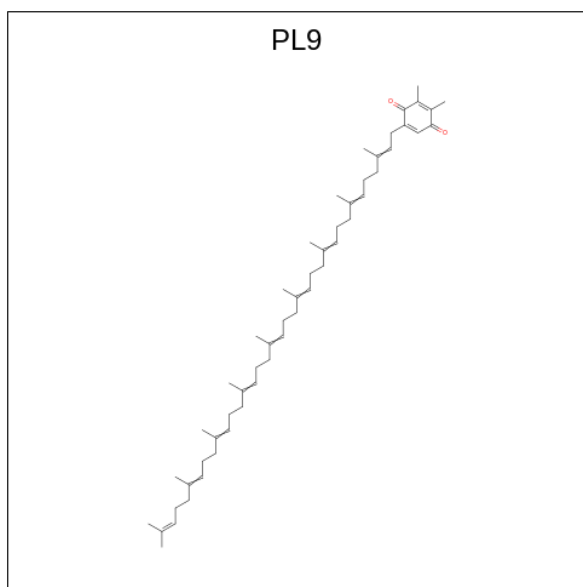
Mol	Chain	Residues	Atoms				AltConf
			Total	Ca	Mn	O	
34	C	1	10	1	4	5	0
34	c	1	10	1	4	5	0

- 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).



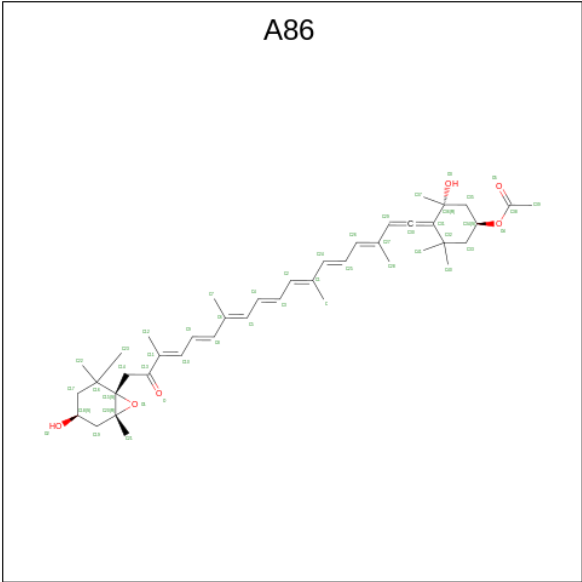
Mol	Chain	Residues	Atoms			AltConf
36	D	1	Total	C	O	0
			55	53	2	
36	D	1	Total	C	O	0
			55	53	2	
36	d	1	Total	C	O	0
			55	53	2	

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

- # HEM

- 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	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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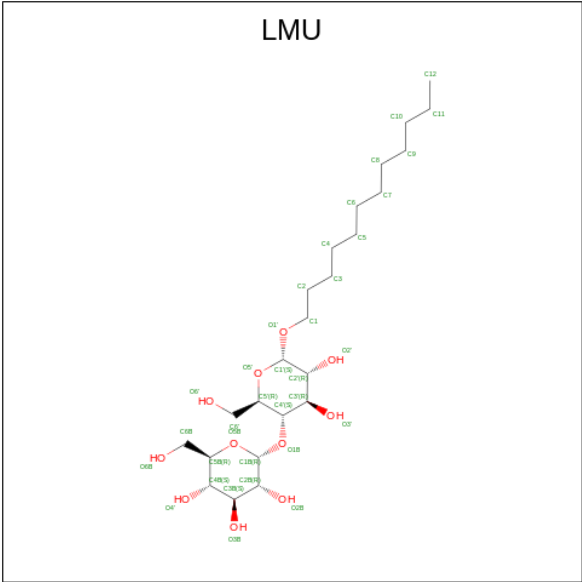
Mol	Chain	Residues	Atoms			AltConf
38	13	1	Total	C	O	0
			48	42	6	
38	13	1	Total	C	O	0
			48	42	6	
38	13	1	Total	C	O	0
			48	42	6	
38	13	1	Total	C	O	0
			48	42	6	
38	14	1	Total	C	O	0
			48	42	6	
38	14	1	Total	C	O	0
			48	42	6	
38	14	1	Total	C	O	0
			48	42	6	
38	14	1	Total	C	O	0
			48	42	6	
38	14	1	Total	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).

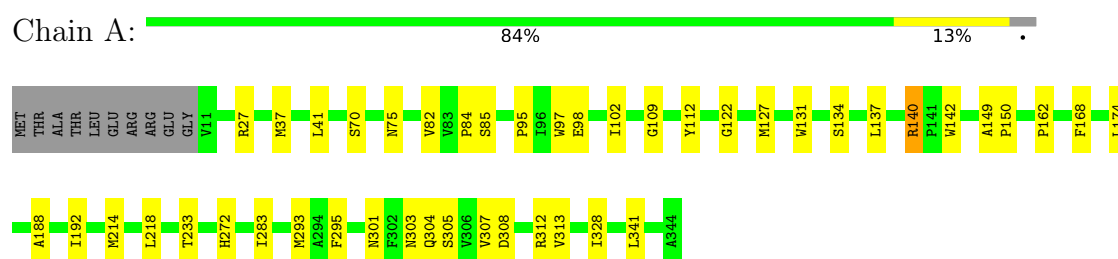


Mol	Chain	Residues	Atoms			AltConf
39	12	1	Total	C	O	0
			32	21	11	
39	32	1	Total	C	O	0
			32	21	11	

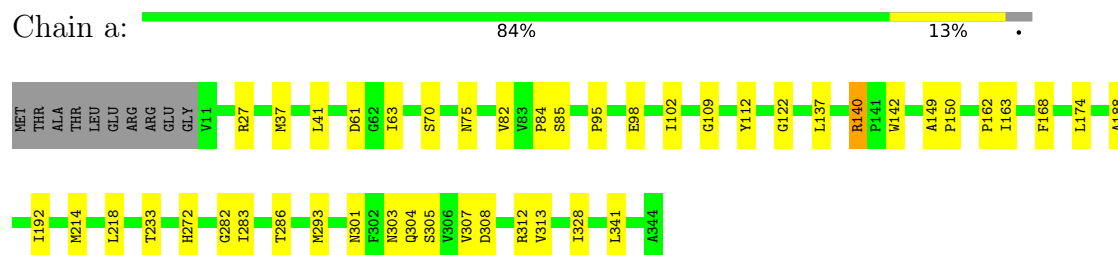
3 Residue-property plots [i](#)

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.

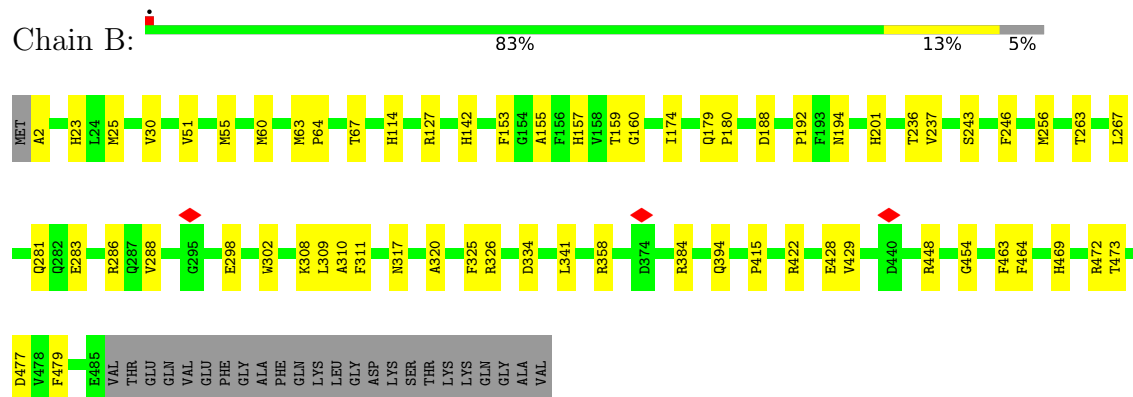
- Molecule 1: Photosystem II reaction center protein D1



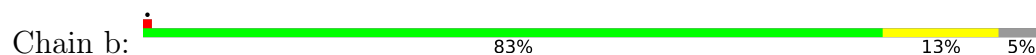
- Molecule 1: Photosystem II reaction center protein D1

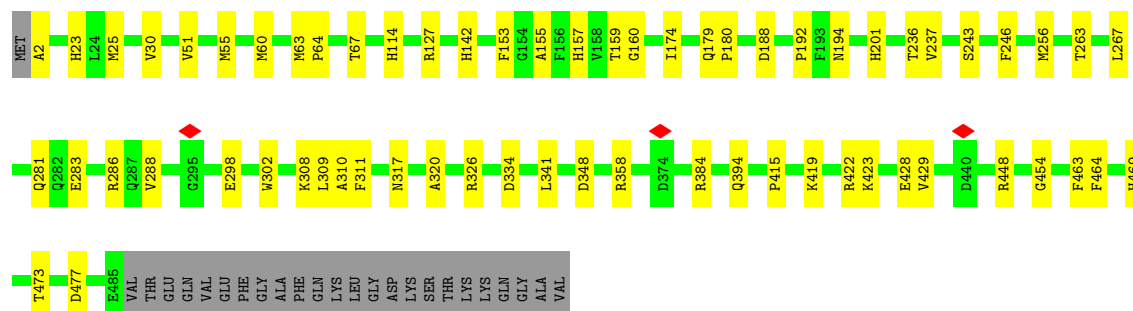


- Molecule 2: Photosystem II chlorophyll protein CP47



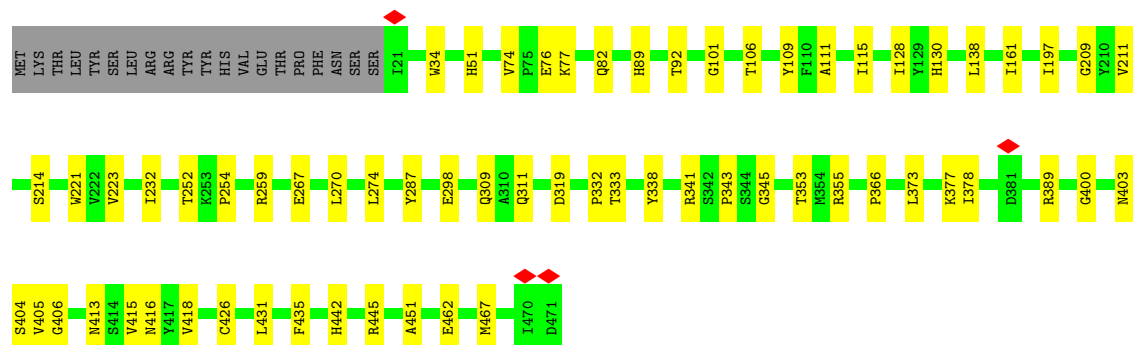
- Molecule 2: Photosystem II chlorophyll protein CP47





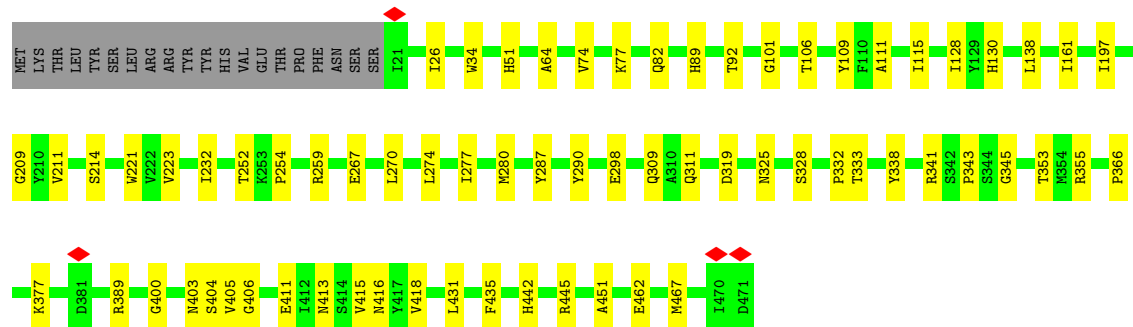
• Molecule 3: Photosystem II chlorophyll protein CP43

Chain C: 82% 14%



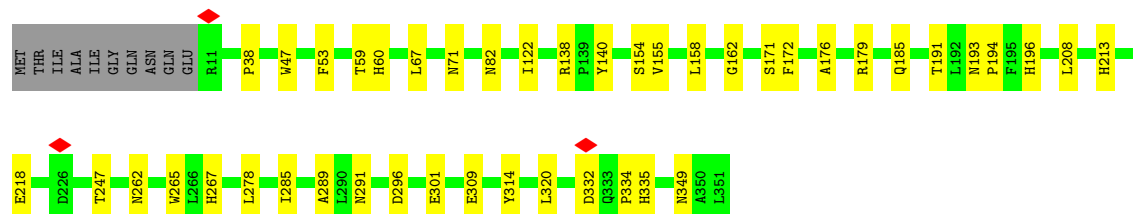
• Molecule 3: Photosystem II chlorophyll protein CP43

Chain c: 81% 15%

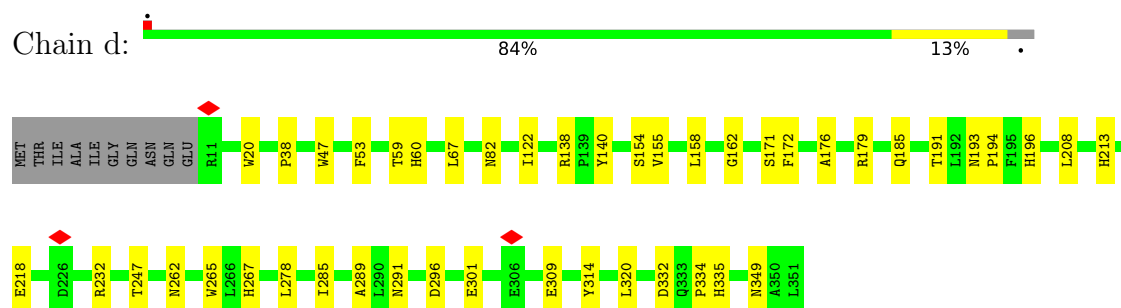


• Molecule 4: Photosystem II reaction center protein D2

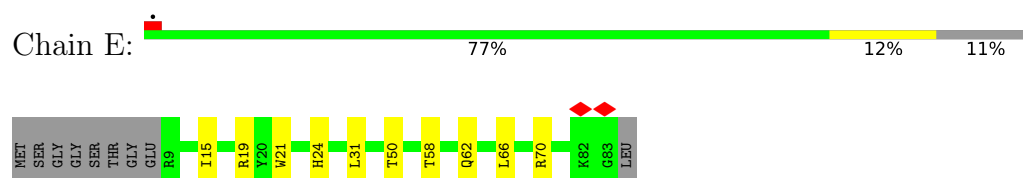
Chain D: 85% 13%



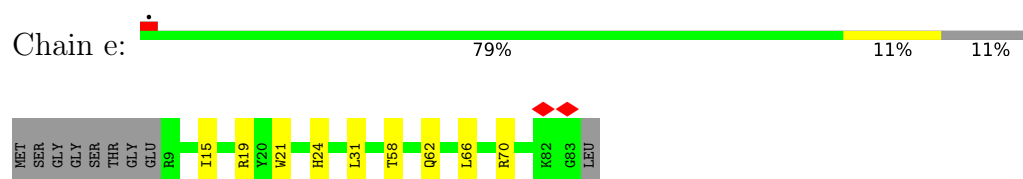
- Molecule 4: Photosystem II reaction center protein D2



- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha



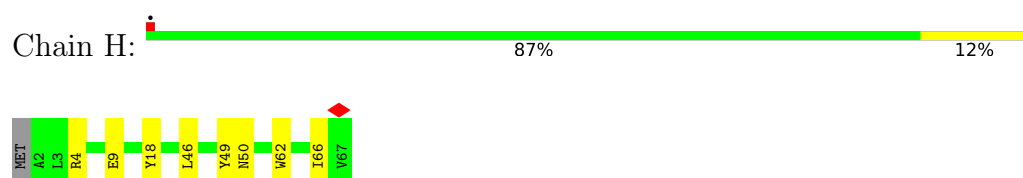
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 6: Cytochrome b559 subunit beta

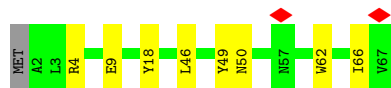


- Molecule 7: Photosystem II reaction center protein H



- 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%



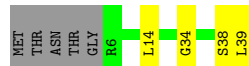
- Molecule 8: Photosystem II reaction center protein I

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%

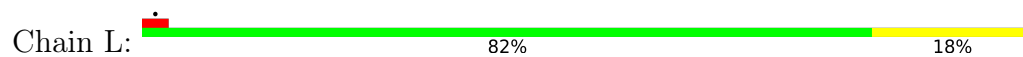


- Molecule 10: Photosystem II reaction center protein K

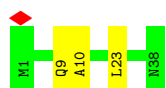
Chain k:  73% 11% 16%



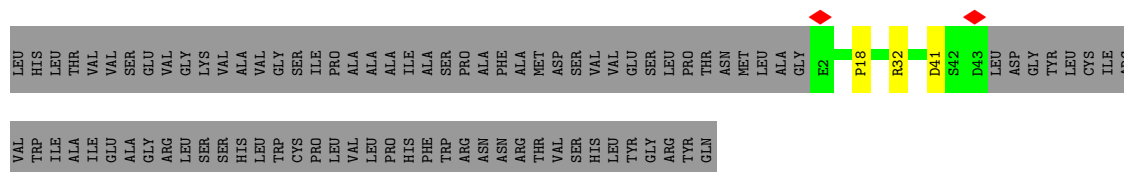
- Molecule 11: Photosystem II reaction center protein L



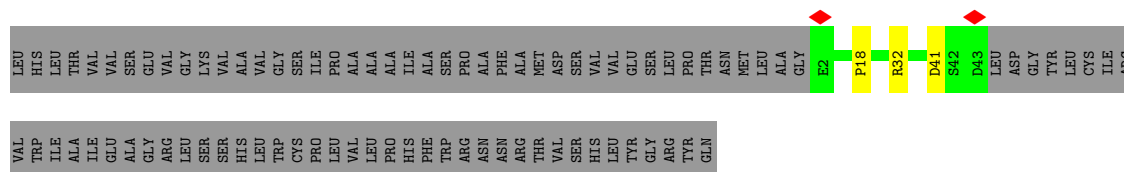
- Molecule 11: Photosystem II reaction center protein L



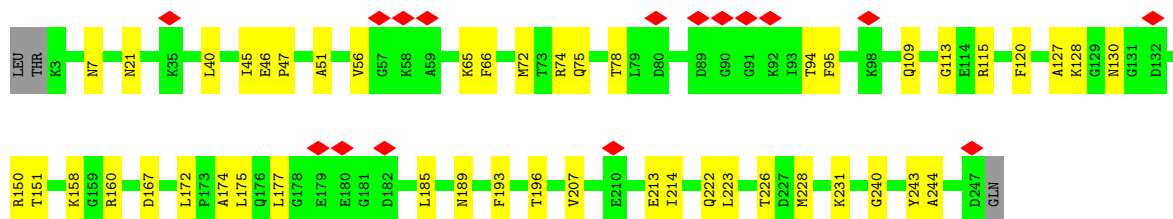
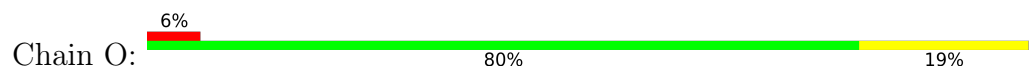
- Molecule 12: Photosystem II reaction center protein M



- Molecule 12: Photosystem II reaction center protein M

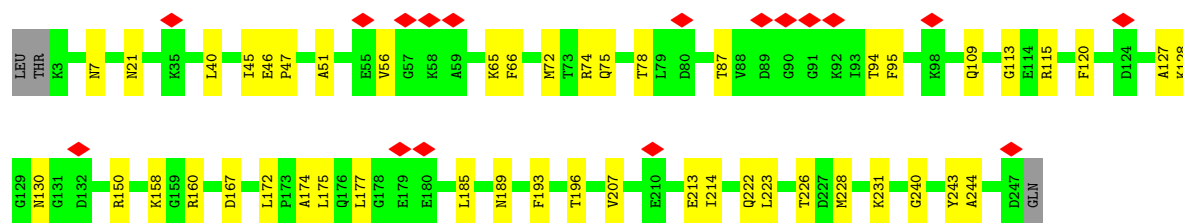


- Molecule 13: Extrinsic protein in photosystem II

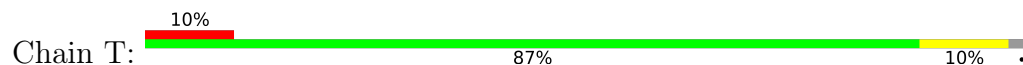


- Molecule 13: Extrinsic protein in photosystem II

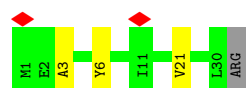
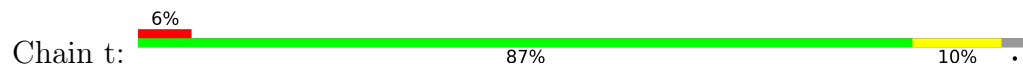




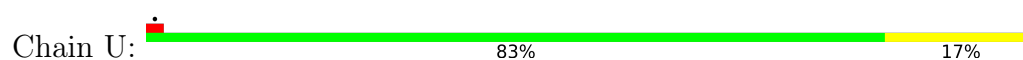
- Molecule 14: Photosystem II reaction center protein T



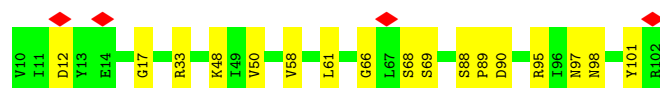
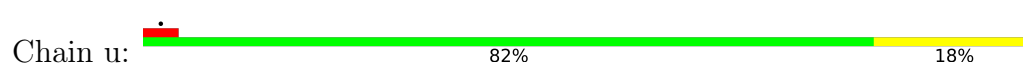
- Molecule 14: Photosystem II reaction center protein T



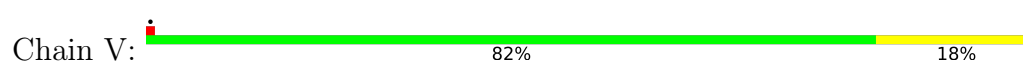
- Molecule 15: Extrinsic protein in photosystem II



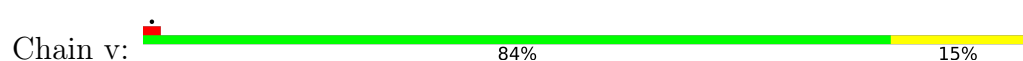
- Molecule 15: Extrinsic protein in photosystem II

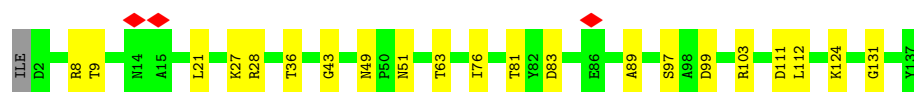


- Molecule 16: Cytochrome c-550



- Molecule 16: Cytochrome c-550

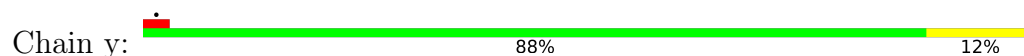




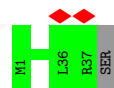
- Molecule 17: Photosystem II reaction center protein Ycf12



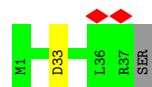
- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center X protein



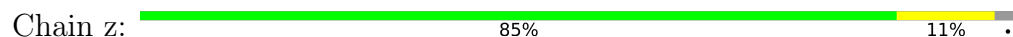
- Molecule 18: Photosystem II reaction center X protein



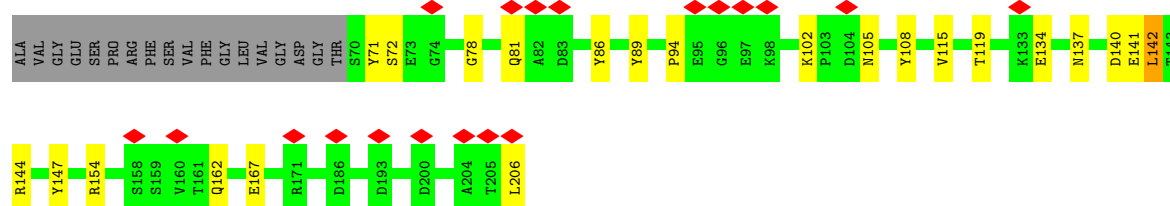
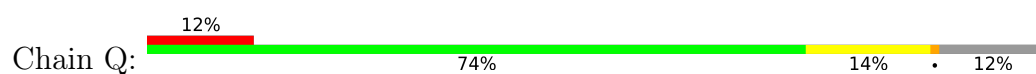
- Molecule 19: Photosystem II reaction center protein Z



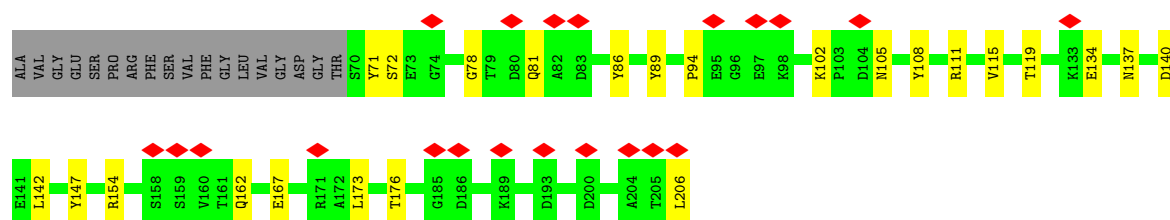
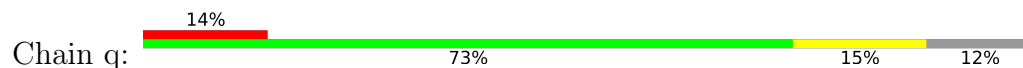
- Molecule 19: Photosystem II reaction center protein Z



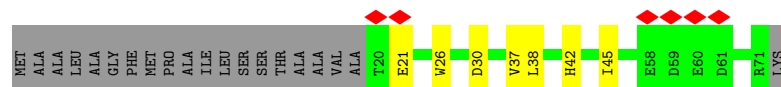
- Molecule 20: Extrinsic protein in photosystem II



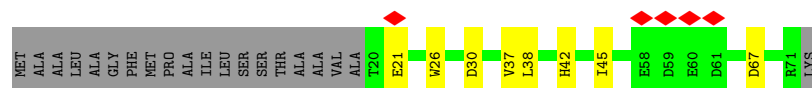
- Molecule 20: Extrinsic protein in photosystem II



- 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.

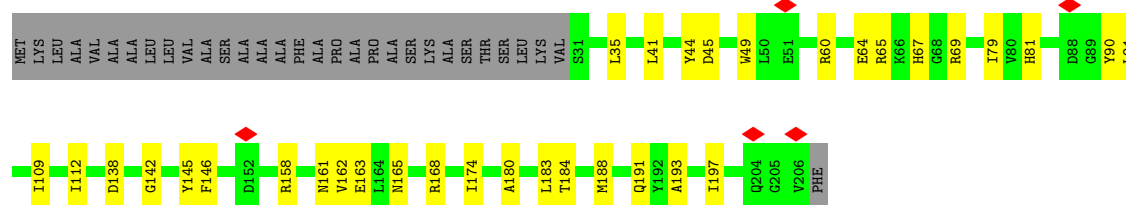
- Molecule 24: Unknown protein 2

Chain 7:  100%

There are no outlier residues recorded for this chain.

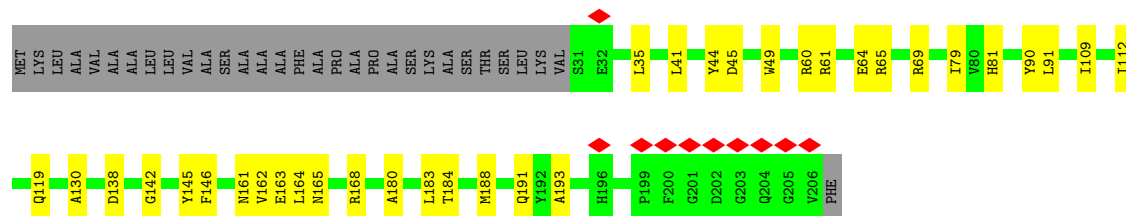
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 11:  69% 16% 15%



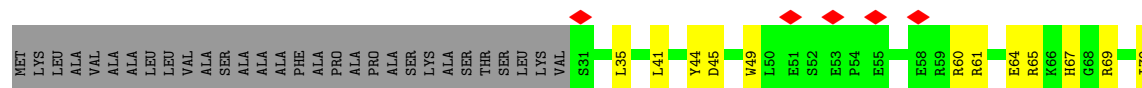
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

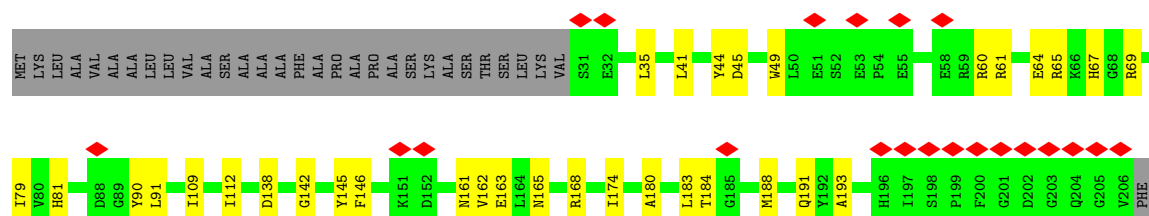
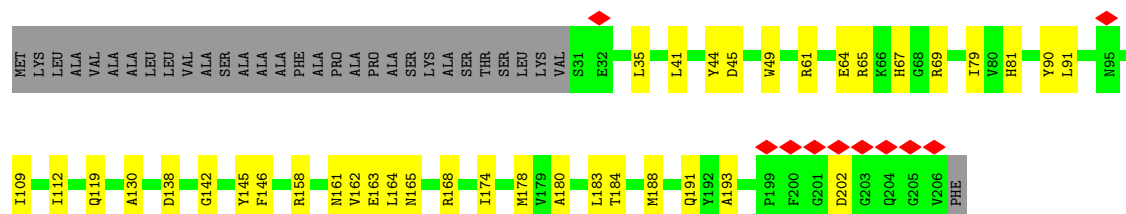
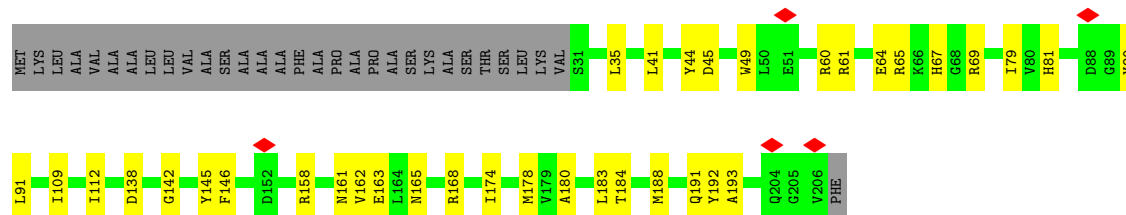
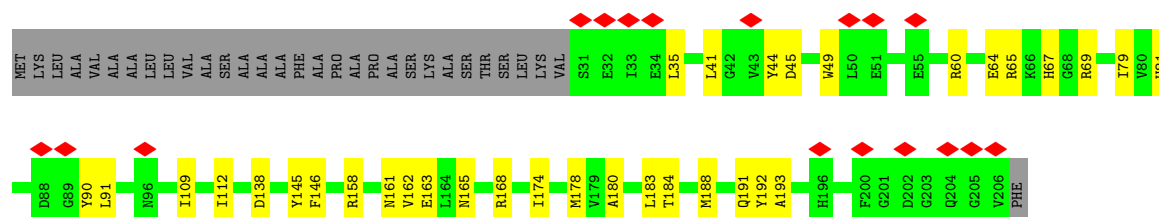
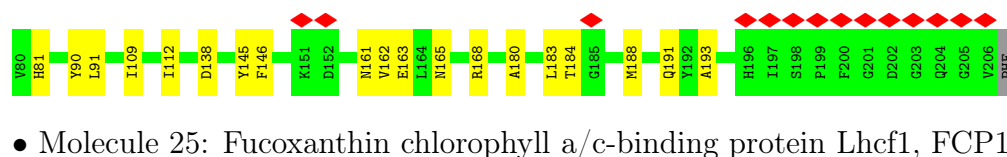
Chain 12:  5% 69% 16% 15%

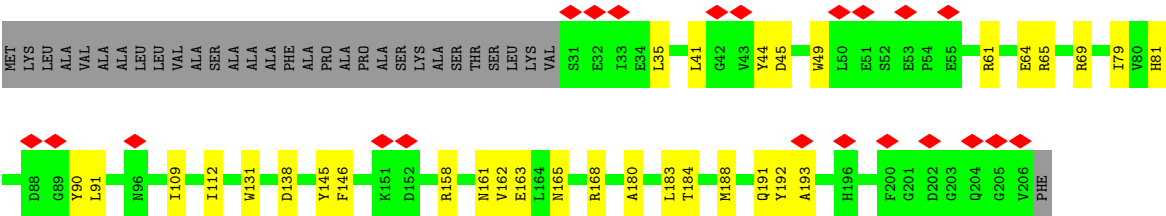


- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 13:  9% 70% 15% 15%







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 ($\text{\AA}$)	573.44, 573.44, 573.44	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.12, 1.12, 1.12	Depositor

5 Model quality

5.1 Standard geometry

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

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:HH2	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	31	306	25	49,53,73	1.46	9 (18%)	59,89,113	1.69	8 (13%)
27	CLA	14	311	-	49,53,73	1.48	10 (20%)	59,89,113	1.52	6 (10%)
27	CLA	13	303	25	69,73,73	1.27	10 (14%)	83,113,113	1.58	8 (9%)
30	SQD	L	103	-	53,54,54	0.93	5 (9%)	62,65,65	1.84	12 (19%)
27	CLA	33	309	25	69,73,73	1.31	11 (15%)	83,113,113	1.45	11 (13%)
27	CLA	C	507	3	69,73,73	1.30	10 (14%)	83,113,113	1.44	11 (13%)
33	LMG	D	408	-	51,51,55	0.90	3 (5%)	59,59,63	1.42	7 (11%)
27	CLA	C	506	3	69,73,73	1.26	9 (13%)	83,113,113	1.46	11 (13%)
27	CLA	C	504	3	69,73,73	1.28	11 (15%)	83,113,113	1.45	10 (12%)
27	CLA	12	308	25,33	49,53,73	1.50	10 (20%)	59,89,113	1.84	13 (22%)
27	CLA	34	312	-	49,53,73	1.46	10 (20%)	59,89,113	1.53	7 (11%)
27	CLA	B	609	2	69,73,73	1.24	10 (14%)	83,113,113	1.44	8 (9%)
27	CLA	13	310	25	49,53,73	1.49	11 (22%)	59,89,113	1.60	7 (11%)
27	CLA	12	307	25	69,73,73	1.24	11 (15%)	83,113,113	1.48	9 (10%)
27	CLA	c	512	3	69,73,73	1.32	11 (15%)	83,113,113	1.50	11 (13%)
27	CLA	B	614	2	69,73,73	1.24	11 (15%)	83,113,113	1.46	8 (9%)
27	CLA	12	303	25	69,73,73	1.27	10 (14%)	83,113,113	1.38	6 (7%)
33	LMG	b	619	-	51,51,55	0.98	5 (9%)	59,59,63	1.44	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	13	307	-	49,53,73	1.46	10 (20%)	59,89,113	1.54	7 (11%)
34	OEX	C	501	1,3	0,14,14	-	-	-		
35	DGD	c	518	-	63,63,67	1.25	10 (15%)	77,77,81	1.52	15 (19%)
38	A86	33	312	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
33	LMG	w	101	-	51,51,55	0.89	2 (3%)	59,59,63	1.40	7 (11%)
36	PL9	d	407	-	55,55,55	2.32	14 (25%)	68,69,69	1.48	14 (20%)
35	DGD	C	517	-	63,63,67	1.05	7 (11%)	77,77,81	1.60	15 (19%)
27	CLA	13	305	25	69,73,73	1.23	11 (15%)	83,113,113	1.48	9 (10%)
30	SQD	b	620	-	36,37,54	1.20	7 (19%)	45,48,65	1.64	9 (20%)
38	A86	33	302	-	44,50,50	4.00	23 (52%)	51,76,76	7.61	20 (39%)
27	CLA	D	401	-	69,73,73	1.33	10 (14%)	83,113,113	1.45	11 (13%)
29	BCR	c	519	-	41,41,41	1.27	2 (4%)	56,56,56	1.37	6 (10%)
33	LMG	M	103	27	40,40,55	0.96	3 (7%)	48,48,63	1.34	7 (14%)
27	CLA	34	308	-	49,53,73	1.45	9 (18%)	59,89,113	1.53	7 (11%)
33	LMG	12	301	27	39,39,55	1.01	4 (10%)	47,47,63	1.21	5 (10%)
34	OEX	c	501	1,3	0,14,14	-	-	-		
27	CLA	C	505	-	69,73,73	1.26	10 (14%)	83,113,113	1.57	10 (12%)
27	CLA	c	513	3	69,73,73	1.27	10 (14%)	83,113,113	1.38	7 (8%)
27	CLA	11	315	25	69,73,73	1.27	11 (15%)	83,113,113	1.38	6 (7%)
31	BCT	A	407	1,26	2,3,3	1.26	0	2,3,3	3.93	2 (100%)
38	A86	11	314	-	44,50,50	3.94	23 (52%)	51,76,76	7.97	19 (37%)
39	LMU	32	302	25,27	33,33,36	1.29	3 (9%)	44,44,47	1.57	8 (18%)
27	CLA	b	615	2	69,73,73	1.33	11 (15%)	83,113,113	1.38	11 (13%)
27	CLA	31	308	25	49,53,73	1.49	11 (22%)	59,89,113	1.59	7 (11%)
38	A86	12	314	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
30	SQD	l	101	-	53,54,54	0.93	5 (9%)	62,65,65	1.84	12 (19%)
35	DGD	C	518	-	63,63,67	1.25	10 (15%)	77,77,81	1.52	15 (19%)
38	A86	13	314	-	44,50,50	4.05	23 (52%)	51,76,76	7.81	19 (37%)
27	CLA	B	613	2	69,73,73	1.34	10 (14%)	83,113,113	1.46	11 (13%)
27	CLA	A	404	1	69,73,73	1.27	11 (15%)	83,113,113	1.50	9 (10%)
27	CLA	b	611	2	69,73,73	1.34	11 (15%)	83,113,113	1.50	11 (13%)
27	CLA	34	310	25	69,73,73	1.29	11 (15%)	83,113,113	1.44	12 (14%)
38	A86	13	312	-	44,50,50	3.93	23 (52%)	51,76,76	8.33	17 (33%)
27	CLA	B	601	-	69,73,73	1.25	10 (14%)	83,113,113	1.42	8 (9%)
27	CLA	32	306	39,25	49,53,73	1.46	11 (22%)	59,89,113	1.61	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	13	309	25	69,73,73	1.28	10 (14%)	83,113,113	1.44	12 (14%)
27	CLA	c	509	3	69,73,73	1.33	10 (14%)	83,113,113	1.53	11 (13%)
27	CLA	33	311	-	49,53,73	1.47	10 (20%)	59,89,113	1.52	6 (10%)
38	A86	12	315	-	44,50,50	3.97	23 (52%)	51,76,76	7.95	18 (35%)
38	A86	13	302	-	44,50,50	4.00	23 (52%)	51,76,76	7.60	20 (39%)
29	BCR	a	405	-	41,41,41	1.29	2 (4%)	56,56,56	1.39	6 (10%)
36	PL9	D	407	-	55,55,55	2.32	15 (27%)	68,69,69	1.48	14 (20%)
27	CLA	c	505	-	69,73,73	1.27	11 (15%)	83,113,113	1.57	10 (12%)
27	CLA	34	305	25	49,53,73	1.45	11 (22%)	59,89,113	1.61	7 (11%)
29	BCR	B	617	-	41,41,41	1.23	2 (4%)	56,56,56	1.42	10 (17%)
27	CLA	31	305	-	49,53,73	1.46	11 (22%)	59,89,113	1.53	7 (11%)
29	BCR	B	623	-	41,41,41	1.13	3 (7%)	56,56,56	1.31	7 (12%)
38	A86	13	315	-	44,50,50	4.01	23 (52%)	51,76,76	8.22	20 (39%)
27	CLA	c	504	3	69,73,73	1.28	11 (15%)	83,113,113	1.44	9 (10%)
38	A86	12	304	-	44,50,50	4.00	23 (52%)	51,76,76	7.60	20 (39%)
27	CLA	32	308	25,33	49,53,73	1.51	10 (20%)	59,89,113	1.84	13 (22%)
38	A86	32	314	-	44,50,50	3.93	23 (52%)	51,76,76	8.33	17 (33%)
27	CLA	14	309	25	69,73,73	1.27	10 (14%)	83,113,113	1.44	12 (14%)
38	A86	32	316	-	44,50,50	4.04	22 (50%)	51,76,76	7.81	19 (37%)
38	A86	11	316	-	44,50,50	4.00	23 (52%)	51,76,76	7.59	20 (39%)
38	A86	14	315	-	44,50,50	4.01	23 (52%)	51,76,76	8.23	20 (39%)
29	BCR	Z	101	-	41,41,41	1.27	4 (9%)	56,56,56	1.46	10 (17%)
27	CLA	31	315	25	69,73,73	1.27	11 (15%)	83,113,113	1.37	6 (7%)
27	CLA	B	622	-	69,73,73	1.29	11 (15%)	83,113,113	1.50	13 (15%)
27	CLA	32	309	-	49,53,73	1.45	10 (20%)	59,89,113	1.53	7 (11%)
29	BCR	b	617	-	41,41,41	1.23	2 (4%)	56,56,56	1.41	10 (17%)
38	A86	32	317	-	44,50,50	4.01	23 (52%)	51,76,76	8.22	20 (39%)
30	SQD	B	620	-	36,37,54	1.20	6 (16%)	45,48,65	1.64	9 (20%)
27	CLA	C	502	3	69,73,73	1.26	11 (15%)	83,113,113	1.53	12 (14%)
38	A86	34	314	-	44,50,50	3.96	23 (52%)	51,76,76	7.95	18 (35%)
29	BCR	B	616	-	41,41,41	1.21	2 (4%)	56,56,56	1.36	9 (16%)
27	CLA	b	614	2	69,73,73	1.24	11 (15%)	83,113,113	1.47	8 (9%)
27	CLA	13	308	25	49,53,73	1.46	9 (18%)	59,89,113	1.71	8 (13%)
27	CLA	B	610	-	69,73,73	1.33	11 (15%)	83,113,113	1.43	7 (8%)
27	CLA	a	404	1	69,73,73	1.27	11 (15%)	83,113,113	1.50	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	33	310	25	49,53,73	1.48	11 (22%)	59,89,113	1.60	7 (11%)
27	CLA	32	312	25	49,53,73	1.49	11 (22%)	59,89,113	1.59	7 (11%)
27	CLA	c	511	3	69,73,73	1.36	12 (17%)	83,113,113	1.46	12 (14%)
27	CLA	m	101	12,2,33	69,73,73	1.25	10 (14%)	83,113,113	1.28	6 (7%)
27	CLA	34	309	25	49,53,73	1.46	9 (18%)	59,89,113	1.70	9 (15%)
32	LHG	b	621	-	48,48,48	0.75	1 (2%)	51,54,54	1.29	6 (11%)
32	LHG	A	408	-	45,45,48	0.78	2 (4%)	48,51,54	1.35	6 (12%)
38	A86	34	315	-	44,50,50	4.03	23 (52%)	51,76,76	7.81	19 (37%)
29	BCR	z	101	-	41,41,41	1.27	3 (7%)	56,56,56	1.46	9 (16%)
27	CLA	33	305	25	69,73,73	1.24	11 (15%)	83,113,113	1.48	9 (10%)
29	BCR	a	409	-	41,41,41	1.17	2 (4%)	56,56,56	1.29	5 (8%)
27	CLA	d	405	4	69,73,73	1.33	12 (17%)	83,113,113	1.46	12 (14%)
27	CLA	13	304	25	49,53,73	1.45	11 (22%)	59,89,113	1.62	7 (11%)
27	CLA	b	609	2	69,73,73	1.24	10 (14%)	83,113,113	1.44	8 (9%)
38	A86	14	312	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
38	A86	32	318	-	44,50,50	3.94	23 (52%)	51,76,76	7.97	19 (37%)
27	CLA	B	611	2	69,73,73	1.34	11 (15%)	83,113,113	1.50	11 (13%)
27	CLA	w	102	21	69,73,73	1.25	10 (14%)	83,113,113	1.35	9 (10%)
27	CLA	32	307	25	69,73,73	1.24	11 (15%)	83,113,113	1.48	9 (10%)
27	CLA	11	307	25	69,73,73	1.27	10 (14%)	83,113,113	1.44	11 (13%)
27	CLA	12	311	25	69,73,73	1.27	10 (14%)	83,113,113	1.44	11 (13%)
27	CLA	C	510	3	69,73,73	1.35	10 (14%)	83,113,113	1.61	12 (14%)
33	LMG	B	618	-	51,51,55	0.89	4 (7%)	59,59,63	1.43	8 (13%)
29	BCR	M	101	-	41,41,41	1.31	2 (4%)	56,56,56	1.39	8 (14%)
29	BCR	A	409	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	5 (8%)
27	CLA	B	606	2	69,73,73	1.37	12 (17%)	83,113,113	1.49	13 (15%)
27	CLA	b	605	2	69,73,73	1.26	10 (14%)	83,113,113	1.41	8 (9%)
27	CLA	12	310	25	49,53,73	1.46	9 (18%)	59,89,113	1.70	8 (13%)
38	A86	33	314	-	44,50,50	4.04	22 (50%)	51,76,76	7.81	20 (39%)
27	CLA	B	604	2	69,73,73	1.34	10 (14%)	83,113,113	1.56	16 (19%)
27	CLA	31	304	25	49,53,73	1.51	10 (20%)	59,89,113	1.85	13 (22%)
27	CLA	c	510	3	69,73,73	1.36	10 (14%)	83,113,113	1.61	12 (14%)
27	CLA	b	606	2	69,73,73	1.36	12 (17%)	83,113,113	1.48	13 (15%)
27	CLA	34	311	25	49,53,73	1.49	11 (22%)	59,89,113	1.59	7 (11%)
36	PL9	D	404	4	55,55,55	1.35	6 (10%)	68,69,69	1.49	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	BCT	a	407	1,26	2,3,3	1.27	0	2,3,3	3.95	2 (100%)
33	LMG	m	102	27	40,40,55	0.96	3 (7%)	48,48,63	1.34	7 (14%)
35	DGD	h	102	-	63,63,67	0.94	3 (4%)	77,77,81	1.42	8 (10%)
29	BCR	A	405	-	41,41,41	1.29	2 (4%)	56,56,56	1.39	6 (10%)
27	CLA	C	503	3	69,73,73	1.38	11 (15%)	83,113,113	1.45	12 (14%)
27	CLA	C	508	-	69,73,73	1.30	10 (14%)	83,113,113	1.56	13 (15%)
27	CLA	32	311	25	69,73,73	1.28	10 (14%)	83,113,113	1.45	11 (13%)
27	CLA	14	308	25	49,53,73	1.45	9 (18%)	59,89,113	1.69	8 (13%)
27	CLA	34	304	25	69,73,73	1.27	11 (15%)	83,113,113	1.57	8 (9%)
27	CLA	31	303	25	69,73,73	1.24	11 (15%)	83,113,113	1.48	9 (10%)
29	BCR	C	516	-	41,41,41	1.31	5 (12%)	56,56,56	1.41	10 (17%)
33	LMG	d	408	-	51,51,55	0.90	3 (5%)	59,59,63	1.43	7 (11%)
27	CLA	31	307	25	69,73,73	1.28	10 (14%)	83,113,113	1.44	12 (14%)
27	CLA	c	508	-	69,73,73	1.30	10 (14%)	83,113,113	1.55	13 (15%)
29	BCR	c	515	-	41,41,41	1.33	3 (7%)	56,56,56	1.41	8 (14%)
38	A86	31	313	-	44,50,50	4.01	23 (52%)	51,76,76	8.23	20 (39%)
27	CLA	b	603	2	69,73,73	1.27	11 (15%)	83,113,113	1.52	12 (14%)
27	CLA	11	303	25	69,73,73	1.23	11 (15%)	83,113,113	1.48	9 (10%)
27	CLA	C	512	3	69,73,73	1.32	11 (15%)	83,113,113	1.51	12 (14%)
27	CLA	32	303	25	69,73,73	1.28	10 (14%)	83,113,113	1.38	6 (7%)
35	DGD	c	517	-	63,63,67	1.05	8 (12%)	77,77,81	1.60	15 (19%)
27	CLA	c	503	3	69,73,73	1.38	11 (15%)	83,113,113	1.45	12 (14%)
27	CLA	33	303	25	69,73,73	1.28	11 (15%)	83,113,113	1.58	8 (9%)
27	CLA	B	608	2	69,73,73	1.24	9 (13%)	83,113,113	1.39	7 (8%)
27	CLA	33	307	-	49,53,73	1.46	9 (18%)	59,89,113	1.53	7 (11%)
27	CLA	14	307	-	49,53,73	1.45	10 (20%)	59,89,113	1.53	7 (11%)
27	CLA	c	514	3	69,73,73	1.26	10 (14%)	83,113,113	1.47	7 (8%)
27	CLA	d	406	4	69,73,73	1.25	11 (15%)	83,113,113	1.52	7 (8%)
32	LHG	B	621	-	48,48,48	0.74	1 (2%)	51,54,54	1.29	6 (11%)
32	LHG	L	102	-	48,48,48	0.76	1 (2%)	51,54,54	1.31	6 (11%)
27	CLA	13	306	25	49,53,73	1.51	10 (20%)	59,89,113	1.83	13 (22%)
27	CLA	b	601	-	69,73,73	1.26	10 (14%)	83,113,113	1.42	7 (8%)
27	CLA	B	615	2	69,73,73	1.33	11 (15%)	83,113,113	1.38	11 (13%)
33	LMG	q	301	-	51,51,55	0.96	5 (9%)	59,59,63	1.46	9 (15%)
37	HEM	V	201	16	50,50,50	1.32	5 (10%)	66,82,82	1.29	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LMG	32	301	27	39,39,55	1.00	4 (10%)	47,47,63	1.18	4 (8%)
27	CLA	11	301	25	69,73,73	1.27	11 (15%)	83,113,113	1.58	8 (9%)
27	CLA	34	302	25	69,73,73	1.27	10 (14%)	83,113,113	1.37	6 (7%)
27	CLA	14	302	25	69,73,73	1.27	10 (14%)	83,113,113	1.38	6 (7%)
27	CLA	b	622	-	69,73,73	1.29	10 (14%)	83,113,113	1.52	13 (15%)
38	A86	33	316	-	44,50,50	3.94	23 (52%)	51,76,76	7.97	17 (33%)
27	CLA	32	310	25	49,53,73	1.46	9 (18%)	59,89,113	1.69	9 (15%)
27	CLA	A	402	1	69,73,73	1.29	11 (15%)	83,113,113	1.47	9 (10%)
27	CLA	M	102	2,12,33	69,73,73	1.25	10 (14%)	83,113,113	1.29	6 (7%)
27	CLA	b	604	2	69,73,73	1.33	10 (14%)	83,113,113	1.57	16 (19%)
27	CLA	11	304	25	49,53,73	1.51	10 (20%)	59,89,113	1.84	13 (22%)
29	BCR	C	515	-	41,41,41	1.32	3 (7%)	56,56,56	1.41	8 (14%)
29	BCR	H	101	-	41,41,41	1.27	4 (9%)	56,56,56	1.31	6 (10%)
38	A86	13	316	-	44,50,50	3.94	23 (52%)	51,76,76	7.98	18 (35%)
38	A86	31	314	-	44,50,50	3.94	23 (52%)	51,76,76	7.98	19 (37%)
27	CLA	B	602	2	69,73,73	1.27	9 (13%)	83,113,113	1.42	10 (12%)
27	CLA	b	613	2	69,73,73	1.34	10 (14%)	83,113,113	1.47	10 (12%)
38	A86	14	301	-	44,50,50	3.93	23 (52%)	51,76,76	7.97	19 (37%)
38	A86	13	317	-	44,50,50	4.00	23 (52%)	51,76,76	7.60	20 (39%)
27	CLA	31	301	25	69,73,73	1.27	11 (15%)	83,113,113	1.57	8 (9%)
37	HEM	E	101	6,5	50,50,50	1.35	4 (8%)	66,82,82	1.15	4 (6%)
27	CLA	13	311	-	49,53,73	1.47	10 (20%)	59,89,113	1.53	6 (10%)
27	CLA	14	305	25	69,73,73	1.23	11 (15%)	83,113,113	1.48	9 (10%)
37	HEM	f	102	6,5	50,50,50	1.35	4 (8%)	66,82,82	1.16	4 (6%)
27	CLA	b	610	-	69,73,73	1.33	11 (15%)	83,113,113	1.43	7 (8%)
29	BCR	c	516	-	41,41,41	1.31	4 (9%)	56,56,56	1.40	9 (16%)
38	A86	31	312	-	44,50,50	4.03	22 (50%)	51,76,76	7.81	20 (39%)
38	A86	14	316	-	44,50,50	3.93	23 (52%)	51,76,76	7.97	18 (35%)
38	A86	34	303	-	44,50,50	4.00	23 (52%)	51,76,76	7.60	20 (39%)
27	CLA	D	405	4	69,73,73	1.33	12 (17%)	83,113,113	1.46	11 (13%)
27	CLA	B	605	2	69,73,73	1.27	10 (14%)	83,113,113	1.41	8 (9%)
33	LMG	B	619	-	51,51,55	0.98	5 (9%)	59,59,63	1.44	8 (13%)
36	PL9	d	404	4	55,55,55	1.36	6 (10%)	68,69,69	1.49	14 (20%)
29	BCR	b	623	-	41,41,41	1.13	3 (7%)	56,56,56	1.28	7 (12%)
27	CLA	d	401	-	69,73,73	1.32	9 (13%)	83,113,113	1.45	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	B	607	-	69,73,73	1.26	11 (15%)	83,113,113	1.42	9 (10%)
27	CLA	w	103	-	69,73,73	1.26	9 (13%)	83,113,113	1.30	7 (8%)
27	CLA	34	306	25	69,73,73	1.23	10 (14%)	83,113,113	1.48	9 (10%)
35	DGD	J	101	-	63,63,67	1.10	10 (15%)	77,77,81	1.55	15 (19%)
38	A86	12	317	-	44,50,50	4.01	23 (52%)	51,76,76	8.22	20 (39%)
27	CLA	C	511	3	69,73,73	1.37	12 (17%)	83,113,113	1.46	12 (14%)
35	DGD	H	102	-	63,63,67	0.94	3 (4%)	77,77,81	1.42	8 (10%)
29	BCR	f	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.32	9 (16%)
38	A86	34	301	-	44,50,50	3.93	23 (52%)	51,76,76	7.97	18 (35%)
27	CLA	C	514	3	69,73,73	1.26	10 (14%)	83,113,113	1.46	7 (8%)
27	CLA	b	608	2	69,73,73	1.24	9 (13%)	83,113,113	1.39	7 (8%)
27	CLA	a	402	1	69,73,73	1.30	11 (15%)	83,113,113	1.46	7 (8%)
38	A86	34	316	-	44,50,50	4.02	23 (52%)	51,76,76	8.21	20 (39%)
29	BCR	b	616	-	41,41,41	1.21	2 (4%)	56,56,56	1.36	9 (16%)
33	LMG	C	519	-	51,51,55	0.96	5 (9%)	59,59,63	1.46	9 (15%)
27	CLA	c	507	3	69,73,73	1.30	10 (14%)	83,113,113	1.45	11 (13%)
27	CLA	32	305	25	69,73,73	1.27	10 (14%)	83,113,113	1.57	8 (9%)
27	CLA	11	305	-	49,53,73	1.46	11 (22%)	59,89,113	1.54	7 (11%)
38	A86	34	313	-	44,50,50	3.93	23 (52%)	51,76,76	8.33	17 (33%)
27	CLA	14	303	25	69,73,73	1.27	11 (15%)	83,113,113	1.57	8 (9%)
38	A86	31	311	-	44,50,50	3.97	23 (52%)	51,76,76	7.94	18 (35%)
38	A86	11	312	-	44,50,50	4.04	22 (50%)	51,76,76	7.82	19 (37%)
29	BCR	m	103	-	41,41,41	1.31	2 (4%)	56,56,56	1.39	8 (14%)
37	HEM	v	201	16	50,50,50	1.32	5 (10%)	66,82,82	1.29	7 (10%)
28	PHO	D	403	-	58,69,69	1.91	12 (20%)	56,99,99	1.76	8 (14%)
27	CLA	14	306	25	49,53,73	1.50	10 (20%)	59,89,113	1.84	13 (22%)
28	PHO	a	403	-	58,69,69	1.97	13 (22%)	56,99,99	1.83	10 (17%)
27	CLA	B	612	2	69,73,73	1.38	8 (11%)	83,113,113	1.67	11 (13%)
27	CLA	C	509	3	69,73,73	1.33	10 (14%)	83,113,113	1.53	10 (12%)
27	CLA	14	304	25	49,53,73	1.45	11 (22%)	59,89,113	1.62	7 (11%)
33	LMG	b	618	-	51,51,55	0.89	4 (7%)	59,59,63	1.43	9 (15%)
35	DGD	j	101	-	63,63,67	1.10	10 (15%)	77,77,81	1.55	15 (19%)
27	CLA	d	402	-	69,73,73	1.27	10 (14%)	83,113,113	1.42	7 (8%)
38	A86	14	313	-	44,50,50	3.97	23 (52%)	51,76,76	7.95	18 (35%)
27	CLA	12	306	39,25	49,53,73	1.45	11 (22%)	59,89,113	1.61	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	b	607	-	69,73,73	1.27	10 (14%)	83,113,113	1.42	9 (10%)
27	CLA	Z	102	-	69,73,73	1.28	11 (15%)	83,113,113	1.42	7 (8%)
27	CLA	32	313	-	49,53,73	1.47	10 (20%)	59,89,113	1.52	6 (10%)
27	CLA	11	309	-	49,53,73	1.47	10 (20%)	59,89,113	1.52	5 (8%)
28	PHO	A	403	-	58,69,69	1.97	13 (22%)	56,99,99	1.82	10 (17%)
39	LMU	12	302	25,27	33,33,36	1.30	3 (9%)	44,44,47	1.54	7 (15%)
38	A86	13	313	-	44,50,50	3.97	23 (52%)	51,76,76	7.95	18 (35%)
30	SQD	a	406	-	53,54,54	0.96	6 (11%)	62,65,65	1.58	11 (17%)
38	A86	14	314	-	44,50,50	4.04	22 (50%)	51,76,76	7.81	19 (37%)
29	BCR	h	101	-	41,41,41	1.28	4 (9%)	56,56,56	1.31	7 (12%)
38	A86	31	310	-	44,50,50	3.92	23 (52%)	51,76,76	8.32	17 (33%)
32	LHG	a	408	-	45,45,48	0.78	2 (4%)	48,51,54	1.35	7 (14%)
38	A86	12	316	-	44,50,50	4.04	22 (50%)	51,76,76	7.81	20 (39%)
27	CLA	13	301	25	69,73,73	1.28	10 (14%)	83,113,113	1.37	6 (7%)
27	CLA	11	308	25	49,53,73	1.49	11 (22%)	59,89,113	1.60	7 (11%)
33	LMG	W	101	-	51,51,55	0.88	2 (3%)	59,59,63	1.40	7 (11%)
38	A86	31	316	-	44,50,50	4.01	23 (52%)	51,76,76	7.60	20 (39%)
27	CLA	12	305	25	69,73,73	1.27	11 (15%)	83,113,113	1.57	8 (9%)
32	LHG	l	102	-	48,48,48	0.81	1 (2%)	51,54,54	1.27	5 (9%)
38	A86	11	311	-	44,50,50	3.97	23 (52%)	51,76,76	7.94	18 (35%)
27	CLA	D	402	-	69,73,73	1.27	10 (14%)	83,113,113	1.42	7 (8%)
27	CLA	z	102	-	69,73,73	1.28	11 (15%)	83,113,113	1.42	7 (8%)
27	CLA	C	513	3	69,73,73	1.26	11 (15%)	83,113,113	1.39	7 (8%)
27	CLA	D	406	4	69,73,73	1.25	11 (15%)	83,113,113	1.52	7 (8%)
38	A86	32	315	-	44,50,50	3.97	23 (52%)	51,76,76	7.94	18 (35%)
27	CLA	12	313	-	49,53,73	1.47	10 (20%)	59,89,113	1.52	5 (8%)
27	CLA	14	310	25	49,53,73	1.49	11 (22%)	59,89,113	1.59	6 (10%)
38	A86	11	313	-	44,50,50	4.02	23 (52%)	51,76,76	8.22	20 (39%)
27	CLA	12	312	25	49,53,73	1.49	11 (22%)	59,89,113	1.60	7 (11%)
38	A86	33	315	-	44,50,50	4.01	23 (52%)	51,76,76	8.22	20 (39%)
38	A86	33	313	-	44,50,50	3.96	23 (52%)	51,76,76	7.93	18 (35%)
27	CLA	31	302	25	49,53,73	1.45	11 (22%)	59,89,113	1.61	7 (11%)
27	CLA	34	307	25	49,53,73	1.50	10 (20%)	59,89,113	1.85	13 (22%)
38	A86	11	310	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
38	A86	32	304	-	44,50,50	4.01	23 (52%)	51,76,76	7.60	21 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	SQD	A	406	-	53,54,54	0.97	6 (11%)	62,65,65	1.58	11 (17%)
27	CLA	B	603	2	69,73,73	1.26	10 (14%)	83,113,113	1.51	12 (14%)
27	CLA	c	502	3	69,73,73	1.26	11 (15%)	83,113,113	1.53	12 (14%)
27	CLA	11	306	25	49,53,73	1.45	8 (16%)	59,89,113	1.71	8 (13%)
32	LHG	l	103	-	48,48,48	0.76	1 (2%)	51,54,54	1.31	6 (11%)
27	CLA	33	306	25	49,53,73	1.51	10 (20%)	59,89,113	1.85	13 (22%)
27	CLA	33	301	25	69,73,73	1.28	11 (15%)	83,113,113	1.38	6 (7%)
27	CLA	W	103	-	69,73,73	1.26	9 (13%)	83,113,113	1.30	7 (8%)
27	CLA	c	506	3	69,73,73	1.26	9 (13%)	83,113,113	1.46	10 (12%)
27	CLA	33	304	25	49,53,73	1.44	11 (22%)	59,89,113	1.61	7 (11%)
32	LHG	L	101	-	48,48,48	0.81	1 (2%)	51,54,54	1.27	5 (9%)
27	CLA	12	309	-	49,53,73	1.46	9 (18%)	59,89,113	1.54	7 (11%)
29	BCR	F	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.32	8 (14%)
27	CLA	b	612	2	69,73,73	1.39	9 (13%)	83,113,113	1.67	11 (13%)
27	CLA	31	309	-	49,53,73	1.48	10 (20%)	59,89,113	1.52	6 (10%)
27	CLA	33	308	25	49,53,73	1.47	9 (18%)	59,89,113	1.70	8 (13%)
29	BCR	C	520	-	41,41,41	1.28	2 (4%)	56,56,56	1.37	6 (10%)
27	CLA	11	302	25	49,53,73	1.45	11 (22%)	59,89,113	1.60	7 (11%)
28	PHO	d	403	-	58,69,69	1.90	12 (20%)	56,99,99	1.76	8 (14%)
27	CLA	b	602	2	69,73,73	1.27	10 (14%)	83,113,113	1.41	10 (12%)
27	CLA	W	102	21	69,73,73	1.26	11 (15%)	83,113,113	1.35	9 (10%)

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	31	306	25	-	10/15/91/115	-
27	CLA	14	311	-	-	8/15/91/115	-
27	CLA	13	303	25	-	14/39/115/115	-
30	SQD	L	103	-	-	21/49/69/69	0/1/1/1
27	CLA	33	309	25	-	16/39/115/115	-
27	CLA	C	507	3	-	19/39/115/115	-
33	LMG	D	408	-	-	14/46/66/70	0/1/1/1
27	CLA	C	506	3	-	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	C	504	3	-	19/39/115/115	-
27	CLA	12	308	25,33	-	9/15/91/115	-
27	CLA	34	312	-	-	8/15/91/115	-
27	CLA	B	609	2	-	10/39/115/115	-
27	CLA	13	310	25	-	8/15/91/115	-
27	CLA	12	307	25	-	15/39/115/115	-
27	CLA	c	512	3	-	10/39/115/115	-
27	CLA	B	614	2	-	8/39/115/115	-
27	CLA	12	303	25	-	13/39/115/115	-
33	LMG	b	619	-	-	20/46/66/70	0/1/1/1
27	CLA	13	307	-	-	10/15/91/115	-
35	DGD	c	518	-	-	22/51/91/95	0/2/2/2
38	A86	33	312	-	-	8/34/90/90	0/3/3/3
33	LMG	w	101	-	-	28/46/66/70	0/1/1/1
36	PL9	d	407	-	-	13/53/73/73	0/1/1/1
35	DGD	C	517	-	-	19/51/91/95	0/2/2/2
27	CLA	13	305	25	-	15/39/115/115	-
30	SQD	b	620	-	-	9/32/52/69	0/1/1/1
38	A86	33	302	-	-	16/34/90/90	0/3/3/3
27	CLA	D	401	-	-	14/39/115/115	-
29	BCR	c	519	-	-	8/29/63/63	0/2/2/2
33	LMG	M	103	27	-	10/35/55/70	0/1/1/1
27	CLA	34	308	-	-	10/15/91/115	-
33	LMG	12	301	27	-	17/34/54/70	0/1/1/1
27	CLA	C	505	-	-	19/39/115/115	-
27	CLA	c	513	3	-	18/39/115/115	-
27	CLA	11	315	25	-	13/39/115/115	-
38	A86	11	314	-	-	7/34/90/90	0/3/3/3
39	LMU	32	302	25,27	-	7/18/58/61	0/2/2/2
27	CLA	b	615	2	-	13/39/115/115	-
27	CLA	31	308	25	-	8/15/91/115	-
38	A86	12	314	-	-	8/34/90/90	0/3/3/3
30	SQD	l	101	-	-	21/49/69/69	0/1/1/1
35	DGD	C	518	-	-	22/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	A86	13	314	-	-	9/34/90/90	0/3/3/3
27	CLA	B	613	2	-	8/39/115/115	-
27	CLA	A	404	1	-	12/39/115/115	-
27	CLA	b	611	2	-	14/39/115/115	-
27	CLA	34	310	25	-	16/39/115/115	-
38	A86	13	312	-	-	8/34/90/90	0/3/3/3
27	CLA	B	601	-	-	20/39/115/115	-
27	CLA	32	306	39,25	-	5/15/91/115	-
27	CLA	13	309	25	-	16/39/115/115	-
27	CLA	c	509	3	-	12/39/115/115	-
27	CLA	33	311	-	-	8/15/91/115	-
38	A86	12	315	-	-	3/34/90/90	0/3/3/3
38	A86	13	302	-	-	15/34/90/90	0/3/3/3
29	BCR	a	405	-	-	12/29/63/63	0/2/2/2
36	PL9	D	407	-	-	13/53/73/73	0/1/1/1
27	CLA	c	505	-	-	19/39/115/115	-
27	CLA	34	305	25	-	5/15/91/115	-
29	BCR	B	617	-	-	9/29/63/63	0/2/2/2
27	CLA	31	305	-	-	10/15/91/115	-
29	BCR	B	623	-	-	18/29/63/63	0/2/2/2
38	A86	13	315	-	-	10/34/90/90	0/3/3/3
27	CLA	c	504	3	-	19/39/115/115	-
38	A86	12	304	-	-	16/34/90/90	0/3/3/3
27	CLA	32	308	25,33	-	9/15/91/115	-
38	A86	32	314	-	-	7/34/90/90	0/3/3/3
27	CLA	14	309	25	-	16/39/115/115	-
38	A86	32	316	-	-	8/34/90/90	0/3/3/3
38	A86	11	316	-	-	15/34/90/90	0/3/3/3
38	A86	14	315	-	-	10/34/90/90	0/3/3/3
29	BCR	Z	101	-	-	16/29/63/63	0/2/2/2
27	CLA	31	315	25	-	13/39/115/115	-
27	CLA	B	622	-	-	17/39/115/115	-
27	CLA	32	309	-	-	10/15/91/115	-
29	BCR	b	617	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	A86	32	317	-	-	10/34/90/90	0/3/3/3
30	SQD	B	620	-	-	9/32/52/69	0/1/1/1
27	CLA	C	502	3	-	14/39/115/115	-
38	A86	34	314	-	-	3/34/90/90	0/3/3/3
29	BCR	B	616	-	-	9/29/63/63	0/2/2/2
27	CLA	b	614	2	-	8/39/115/115	-
27	CLA	13	308	25	-	10/15/91/115	-
27	CLA	B	610	-	-	16/39/115/115	-
27	CLA	a	404	1	-	12/39/115/115	-
27	CLA	33	310	25	-	8/15/91/115	-
27	CLA	32	312	25	-	8/15/91/115	-
27	CLA	c	511	3	-	12/39/115/115	-
27	CLA	m	101	12,2,33	-	21/39/115/115	-
27	CLA	34	309	25	-	10/15/91/115	-
32	LHG	b	621	-	-	20/53/53/53	-
32	LHG	A	408	-	-	23/50/50/53	-
38	A86	34	315	-	-	9/34/90/90	0/3/3/3
29	BCR	z	101	-	-	16/29/63/63	0/2/2/2
27	CLA	33	305	25	-	15/39/115/115	-
29	BCR	a	409	-	-	9/29/63/63	0/2/2/2
27	CLA	d	405	4	-	8/39/115/115	-
27	CLA	13	304	25	-	5/15/91/115	-
27	CLA	b	609	2	-	10/39/115/115	-
38	A86	14	312	-	-	8/34/90/90	0/3/3/3
38	A86	32	318	-	-	7/34/90/90	0/3/3/3
27	CLA	B	611	2	-	14/39/115/115	-
27	CLA	w	102	21	-	16/39/115/115	-
27	CLA	32	307	25	-	15/39/115/115	-
27	CLA	11	307	25	-	16/39/115/115	-
27	CLA	12	311	25	-	16/39/115/115	-
27	CLA	C	510	3	-	12/39/115/115	-
33	LMG	B	618	-	-	18/46/66/70	0/1/1/1
29	BCR	M	101	-	-	8/29/63/63	0/2/2/2
29	BCR	A	409	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	B	606	2	-	7/39/115/115	-
27	CLA	b	605	2	-	19/39/115/115	-
27	CLA	12	310	25	-	10/15/91/115	-
38	A86	33	314	-	-	8/34/90/90	0/3/3/3
27	CLA	B	604	2	-	14/39/115/115	-
27	CLA	31	304	25	-	9/15/91/115	-
27	CLA	c	510	3	-	12/39/115/115	-
27	CLA	b	606	2	-	7/39/115/115	-
27	CLA	34	311	25	-	8/15/91/115	-
36	PL9	D	404	4	-	17/53/73/73	0/1/1/1
33	LMG	m	102	27	-	10/35/55/70	0/1/1/1
35	DGD	h	102	-	-	24/51/91/95	0/2/2/2
29	BCR	A	405	-	-	12/29/63/63	0/2/2/2
27	CLA	C	503	3	-	13/39/115/115	-
27	CLA	C	508	-	-	18/39/115/115	-
27	CLA	32	311	25	-	16/39/115/115	-
27	CLA	14	308	25	-	10/15/91/115	-
27	CLA	34	304	25	-	14/39/115/115	-
27	CLA	31	303	25	-	15/39/115/115	-
29	BCR	C	516	-	-	10/29/63/63	0/2/2/2
33	LMG	d	408	-	-	14/46/66/70	0/1/1/1
27	CLA	31	307	25	-	16/39/115/115	-
27	CLA	c	508	-	-	18/39/115/115	-
29	BCR	c	515	-	-	15/29/63/63	0/2/2/2
38	A86	31	313	-	-	10/34/90/90	0/3/3/3
27	CLA	b	603	2	-	12/39/115/115	-
27	CLA	11	303	25	-	15/39/115/115	-
27	CLA	C	512	3	-	10/39/115/115	-
27	CLA	32	303	25	-	13/39/115/115	-
35	DGD	c	517	-	-	19/51/91/95	0/2/2/2
27	CLA	c	503	3	-	13/39/115/115	-
27	CLA	33	303	25	-	14/39/115/115	-
27	CLA	B	608	2	-	9/39/115/115	-
27	CLA	33	307	-	-	10/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	14	307	-	-	10/15/91/115	-
27	CLA	c	514	3	-	13/39/115/115	-
27	CLA	d	406	4	-	6/39/115/115	-
32	LHG	B	621	-	-	20/53/53/53	-
32	LHG	L	102	-	-	22/53/53/53	-
27	CLA	13	306	25	-	9/15/91/115	-
27	CLA	b	601	-	-	20/39/115/115	-
27	CLA	B	615	2	-	13/39/115/115	-
33	LMG	q	301	-	-	22/46/66/70	0/1/1/1
37	HEM	V	201	16	-	1/14/54/54	-
33	LMG	32	301	27	-	14/34/54/70	0/1/1/1
27	CLA	11	301	25	-	13/39/115/115	-
27	CLA	34	302	25	-	13/39/115/115	-
27	CLA	14	302	25	-	13/39/115/115	-
27	CLA	b	622	-	-	17/39/115/115	-
38	A86	33	316	-	-	7/34/90/90	0/3/3/3
27	CLA	32	310	25	-	10/15/91/115	-
27	CLA	A	402	1	-	7/39/115/115	-
27	CLA	M	102	2,12,33	-	21/39/115/115	-
27	CLA	b	604	2	-	14/39/115/115	-
27	CLA	11	304	25	-	9/15/91/115	-
29	BCR	C	515	-	-	15/29/63/63	0/2/2/2
29	BCR	H	101	-	-	7/29/63/63	0/2/2/2
38	A86	13	316	-	-	7/34/90/90	0/3/3/3
38	A86	31	314	-	-	7/34/90/90	0/3/3/3
27	CLA	B	602	2	-	15/39/115/115	-
27	CLA	b	613	2	-	8/39/115/115	-
38	A86	14	301	-	-	7/34/90/90	0/3/3/3
38	A86	13	317	-	-	16/34/90/90	0/3/3/3
27	CLA	31	301	25	-	14/39/115/115	-
37	HEM	E	101	6,5	-	7/14/54/54	-
27	CLA	13	311	-	-	8/15/91/115	-
27	CLA	14	305	25	-	15/39/115/115	-
37	HEM	f	102	6,5	-	7/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	b	610	-	-	16/39/115/115	-
29	BCR	c	516	-	-	10/29/63/63	0/2/2/2
38	A86	31	312	-	-	8/34/90/90	0/3/3/3
38	A86	14	316	-	-	7/34/90/90	0/3/3/3
38	A86	34	303	-	-	15/34/90/90	0/3/3/3
27	CLA	D	405	4	-	8/39/115/115	-
27	CLA	B	605	2	-	19/39/115/115	-
33	LMG	B	619	-	-	21/46/66/70	0/1/1/1
36	PL9	d	404	4	-	17/53/73/73	0/1/1/1
29	BCR	b	623	-	-	18/29/63/63	0/2/2/2
27	CLA	d	401	-	-	14/39/115/115	-
27	CLA	B	607	-	-	12/39/115/115	-
27	CLA	w	103	-	-	21/39/115/115	-
27	CLA	34	306	25	-	15/39/115/115	-
35	DGD	J	101	-	-	15/51/91/95	0/2/2/2
38	A86	12	317	-	-	10/34/90/90	0/3/3/3
27	CLA	C	511	3	-	12/39/115/115	-
35	DGD	H	102	-	-	24/51/91/95	0/2/2/2
29	BCR	f	101	-	-	15/29/63/63	0/2/2/2
38	A86	34	301	-	-	7/34/90/90	0/3/3/3
27	CLA	C	514	3	-	13/39/115/115	-
27	CLA	b	608	2	-	9/39/115/115	-
27	CLA	a	402	1	-	7/39/115/115	-
38	A86	34	316	-	-	10/34/90/90	0/3/3/3
29	BCR	b	616	-	-	9/29/63/63	0/2/2/2
33	LMG	C	519	-	-	22/46/66/70	0/1/1/1
27	CLA	c	507	3	-	19/39/115/115	-
27	CLA	32	305	25	-	14/39/115/115	-
27	CLA	11	305	-	-	10/15/91/115	-
38	A86	34	313	-	-	8/34/90/90	0/3/3/3
27	CLA	14	303	25	-	14/39/115/115	-
38	A86	31	311	-	-	3/34/90/90	0/3/3/3
38	A86	11	312	-	-	8/34/90/90	0/3/3/3
29	BCR	m	103	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	HEM	v	201	16	-	1/14/54/54	-
28	PHO	D	403	-	-	8/37/103/103	0/5/6/6
27	CLA	14	306	25	-	9/15/91/115	-
28	PHO	a	403	-	-	12/37/103/103	0/5/6/6
27	CLA	B	612	2	-	13/39/115/115	-
27	CLA	C	509	3	-	12/39/115/115	-
27	CLA	14	304	25	-	4/15/91/115	-
33	LMG	b	618	-	-	18/46/66/70	0/1/1/1
35	DGD	j	101	-	-	15/51/91/95	0/2/2/2
27	CLA	d	402	-	-	15/39/115/115	-
38	A86	14	313	-	-	3/34/90/90	0/3/3/3
27	CLA	12	306	39,25	-	5/15/91/115	-
27	CLA	b	607	-	-	12/39/115/115	-
27	CLA	Z	102	-	-	23/39/115/115	-
27	CLA	32	313	-	-	8/15/91/115	-
27	CLA	11	309	-	-	8/15/91/115	-
28	PHO	A	403	-	-	12/37/103/103	0/5/6/6
39	LMU	12	302	25,27	-	7/18/58/61	0/2/2/2
38	A86	13	313	-	-	3/34/90/90	0/3/3/3
30	SQD	a	406	-	-	14/49/69/69	0/1/1/1
38	A86	14	314	-	-	8/34/90/90	0/3/3/3
29	BCR	h	101	-	-	7/29/63/63	0/2/2/2
38	A86	31	310	-	-	8/34/90/90	0/3/3/3
32	LHG	a	408	-	-	23/50/50/53	-
38	A86	12	316	-	-	9/34/90/90	0/3/3/3
27	CLA	13	301	25	-	13/39/115/115	-
27	CLA	11	308	25	-	8/15/91/115	-
33	LMG	W	101	-	-	28/46/66/70	0/1/1/1
38	A86	31	316	-	-	15/34/90/90	0/3/3/3
27	CLA	12	305	25	-	14/39/115/115	-
32	LHG	l	102	-	-	29/53/53/53	-
38	A86	11	311	-	-	3/34/90/90	0/3/3/3
27	CLA	D	402	-	-	15/39/115/115	-
27	CLA	z	102	-	-	23/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	C	513	3	-	18/39/115/115	-
27	CLA	D	406	4	-	6/39/115/115	-
38	A86	32	315	-	-	3/34/90/90	0/3/3/3
27	CLA	12	313	-	-	8/15/91/115	-
27	CLA	14	310	25	-	8/15/91/115	-
38	A86	11	313	-	-	10/34/90/90	0/3/3/3
27	CLA	12	312	25	-	8/15/91/115	-
38	A86	33	315	-	-	10/34/90/90	0/3/3/3
38	A86	33	313	-	-	3/34/90/90	0/3/3/3
27	CLA	31	302	25	-	4/15/91/115	-
27	CLA	34	307	25	-	9/15/91/115	-
38	A86	11	310	-	-	8/34/90/90	0/3/3/3
38	A86	32	304	-	-	15/34/90/90	0/3/3/3
30	SQD	A	406	-	-	14/49/69/69	0/1/1/1
27	CLA	B	603	2	-	12/39/115/115	-
27	CLA	c	502	3	-	14/39/115/115	-
27	CLA	11	306	25	-	10/15/91/115	-
32	LHG	l	103	-	-	22/53/53/53	-
27	CLA	33	306	25	-	9/15/91/115	-
27	CLA	33	301	25	-	13/39/115/115	-
27	CLA	W	103	-	-	21/39/115/115	-
27	CLA	c	506	3	-	18/39/115/115	-
27	CLA	33	304	25	-	5/15/91/115	-
32	LHG	L	101	-	-	29/53/53/53	-
27	CLA	12	309	-	-	10/15/91/115	-
29	BCR	F	101	-	-	15/29/63/63	0/2/2/2
27	CLA	b	612	2	-	13/39/115/115	-
27	CLA	31	309	-	-	8/15/91/115	-
27	CLA	33	308	25	-	10/15/91/115	-
29	BCR	C	520	-	-	8/29/63/63	0/2/2/2
27	CLA	11	302	25	-	5/15/91/115	-
28	PHO	d	403	-	-	8/37/103/103	0/5/6/6
27	CLA	b	602	2	-	15/39/115/115	-
27	CLA	W	102	21	-	16/39/115/115	-

All (3072) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	34	316	A86	C14-C13	14.10	1.68	1.51
38	11	313	A86	C14-C13	14.03	1.68	1.51
38	13	315	A86	C14-C13	14.01	1.68	1.51
38	12	317	A86	C14-C13	14.01	1.68	1.51
38	31	313	A86	C14-C13	14.00	1.68	1.51
38	32	317	A86	C14-C13	14.00	1.68	1.51
38	33	315	A86	C14-C13	14.00	1.68	1.51
38	14	315	A86	C14-C13	13.98	1.68	1.51
38	33	316	A86	C14-C13	13.97	1.68	1.51
38	13	314	A86	C14-C13	13.93	1.68	1.51
38	32	318	A86	C14-C13	13.92	1.68	1.51
38	11	312	A86	C14-C13	13.90	1.68	1.51
38	11	314	A86	C14-C13	13.90	1.68	1.51
38	12	316	A86	C14-C13	13.89	1.68	1.51
38	31	314	A86	C14-C13	13.89	1.68	1.51
38	32	316	A86	C14-C13	13.88	1.68	1.51
38	14	314	A86	C14-C13	13.88	1.68	1.51
38	14	316	A86	C14-C13	13.87	1.68	1.51
38	14	301	A86	C14-C13	13.86	1.68	1.51
38	13	316	A86	C14-C13	13.85	1.68	1.51
38	33	314	A86	C14-C13	13.85	1.68	1.51
38	31	312	A86	C14-C13	13.84	1.68	1.51
38	34	301	A86	C14-C13	13.83	1.67	1.51
38	12	314	A86	C14-C13	13.82	1.67	1.51
38	34	315	A86	C14-C13	13.81	1.67	1.51
38	14	312	A86	C14-C13	13.80	1.67	1.51
38	31	316	A86	C14-C13	13.80	1.67	1.51
38	32	314	A86	C14-C13	13.80	1.67	1.51
38	11	310	A86	C14-C13	13.80	1.67	1.51
38	33	312	A86	C14-C13	13.78	1.67	1.51
38	13	312	A86	C14-C13	13.77	1.67	1.51
38	34	313	A86	C14-C13	13.77	1.67	1.51
38	31	310	A86	C14-C13	13.77	1.67	1.51
38	32	304	A86	C14-C13	13.76	1.67	1.51
38	13	317	A86	C14-C13	13.74	1.67	1.51
38	12	304	A86	C14-C13	13.73	1.67	1.51
38	34	303	A86	C14-C13	13.72	1.67	1.51
38	33	302	A86	C14-C13	13.71	1.67	1.51
38	11	316	A86	C14-C13	13.69	1.67	1.51
38	13	302	A86	C14-C13	13.69	1.67	1.51
38	31	311	A86	C14-C13	13.67	1.67	1.51
38	12	315	A86	C14-C13	13.67	1.67	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	32	315	A86	C14-C13	13.66	1.67	1.51
38	14	313	A86	C14-C13	13.65	1.67	1.51
38	13	313	A86	C14-C13	13.64	1.67	1.51
38	34	314	A86	C14-C13	13.63	1.67	1.51
38	33	313	A86	C14-C13	13.63	1.67	1.51
38	11	311	A86	C14-C13	13.63	1.67	1.51
38	31	316	A86	C30-C29	8.90	1.46	1.32
38	12	304	A86	C30-C29	8.88	1.46	1.32
38	32	304	A86	C30-C29	8.88	1.46	1.32
38	33	302	A86	C30-C29	8.87	1.46	1.32
38	34	303	A86	C30-C29	8.87	1.46	1.32
38	13	317	A86	C30-C29	8.87	1.46	1.32
38	11	316	A86	C30-C29	8.86	1.46	1.32
38	13	302	A86	C30-C29	8.85	1.46	1.32
38	32	316	A86	C30-C29	8.71	1.46	1.32
38	33	314	A86	C30-C29	8.70	1.46	1.32
38	31	311	A86	C30-C29	8.70	1.46	1.32
38	11	312	A86	C30-C29	8.69	1.46	1.32
38	14	314	A86	C30-C29	8.68	1.46	1.32
38	12	316	A86	C30-C29	8.68	1.46	1.32
38	13	313	A86	C30-C29	8.68	1.46	1.32
38	34	315	A86	C30-C29	8.68	1.46	1.32
38	32	315	A86	C30-C29	8.67	1.46	1.32
38	31	312	A86	C30-C29	8.67	1.46	1.32
38	11	311	A86	C30-C29	8.66	1.46	1.32
38	13	314	A86	C30-C29	8.65	1.46	1.32
38	14	313	A86	C30-C29	8.64	1.46	1.32
38	12	315	A86	C30-C29	8.63	1.46	1.32
38	33	313	A86	C30-C29	8.62	1.46	1.32
38	34	314	A86	C30-C29	8.62	1.46	1.32
38	12	317	A86	C30-C29	8.60	1.46	1.32
38	31	313	A86	C30-C29	8.59	1.46	1.32
38	33	315	A86	C30-C29	8.58	1.46	1.32
38	11	313	A86	C30-C29	8.58	1.46	1.32
38	34	316	A86	C30-C29	8.58	1.46	1.32
38	32	317	A86	C30-C29	8.56	1.46	1.32
38	14	315	A86	C30-C29	8.55	1.46	1.32
38	13	315	A86	C30-C29	8.53	1.46	1.32
38	32	314	A86	C30-C29	8.53	1.46	1.32
38	31	310	A86	C30-C29	8.51	1.46	1.32
38	34	313	A86	C30-C29	8.51	1.46	1.32
38	12	314	A86	C30-C29	8.49	1.46	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	33	312	A86	C30-C29	8.49	1.46	1.32
38	14	312	A86	C30-C29	8.49	1.46	1.32
38	11	310	A86	C30-C29	8.47	1.46	1.32
38	13	312	A86	C30-C29	8.47	1.46	1.32
28	D	403	PHO	C1B-C2B	8.34	1.48	1.39
28	d	403	PHO	C1B-C2B	8.32	1.48	1.39
38	14	301	A86	C30-C29	8.31	1.45	1.32
28	a	403	PHO	C1B-C2B	8.31	1.48	1.39
38	14	316	A86	C30-C29	8.31	1.45	1.32
38	13	316	A86	C30-C29	8.30	1.45	1.32
38	11	314	A86	C30-C29	8.30	1.45	1.32
38	31	314	A86	C30-C29	8.30	1.45	1.32
28	A	403	PHO	C1B-C2B	8.29	1.48	1.39
38	34	301	A86	C30-C29	8.26	1.45	1.32
38	33	316	A86	C30-C29	8.25	1.45	1.32
38	32	318	A86	C30-C29	8.24	1.45	1.32
36	D	407	PL9	C7-C3	-7.76	1.43	1.51
36	d	407	PL9	C7-C3	-7.65	1.43	1.51
38	32	304	A86	C4-C5	7.51	1.66	1.43
38	33	302	A86	C4-C5	7.49	1.66	1.43
38	11	316	A86	C4-C5	7.49	1.66	1.43
38	13	317	A86	C4-C5	7.49	1.66	1.43
38	12	304	A86	C4-C5	7.48	1.66	1.43
38	34	303	A86	C4-C5	7.47	1.66	1.43
38	13	302	A86	C4-C5	7.47	1.66	1.43
38	31	316	A86	C4-C5	7.46	1.66	1.43
38	12	304	A86	C8-C6	7.45	1.61	1.45
38	32	304	A86	C8-C6	7.42	1.61	1.45
38	11	316	A86	C8-C6	7.41	1.61	1.45
38	13	317	A86	C8-C6	7.41	1.61	1.45
38	31	316	A86	C8-C6	7.40	1.61	1.45
38	13	302	A86	C8-C6	7.40	1.61	1.45
38	13	314	A86	C4-C5	7.40	1.66	1.43
38	14	314	A86	C4-C5	7.40	1.66	1.43
38	33	302	A86	C8-C6	7.40	1.61	1.45
38	12	316	A86	C4-C5	7.39	1.66	1.43
38	31	312	A86	C4-C5	7.39	1.66	1.43
38	32	316	A86	C4-C5	7.39	1.66	1.43
38	11	312	A86	C4-C5	7.38	1.66	1.43
38	33	314	A86	C4-C5	7.38	1.66	1.43
38	34	303	A86	C8-C6	7.37	1.61	1.45
38	34	315	A86	C4-C5	7.37	1.66	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	11	314	A86	C4-C5	7.32	1.66	1.43
38	31	314	A86	C4-C5	7.31	1.66	1.43
38	32	318	A86	C4-C5	7.31	1.66	1.43
38	32	315	A86	C4-C5	7.31	1.66	1.43
38	11	311	A86	C4-C5	7.30	1.66	1.43
38	33	315	A86	C4-C5	7.30	1.66	1.43
38	11	313	A86	C4-C5	7.30	1.66	1.43
38	32	317	A86	C4-C5	7.30	1.66	1.43
38	14	301	A86	C4-C5	7.30	1.66	1.43
38	12	315	A86	C4-C5	7.30	1.66	1.43
38	13	316	A86	C4-C5	7.30	1.66	1.43
38	31	311	A86	C4-C5	7.30	1.66	1.43
38	14	315	A86	C4-C5	7.29	1.66	1.43
38	33	316	A86	C4-C5	7.29	1.66	1.43
38	13	315	A86	C4-C5	7.29	1.66	1.43
38	34	314	A86	C4-C5	7.29	1.66	1.43
38	34	316	A86	C4-C5	7.29	1.66	1.43
38	13	313	A86	C4-C5	7.29	1.66	1.43
38	14	313	A86	C4-C5	7.28	1.66	1.43
38	14	316	A86	C4-C5	7.28	1.66	1.43
38	34	301	A86	C4-C5	7.28	1.66	1.43
38	12	317	A86	C4-C5	7.28	1.66	1.43
38	33	313	A86	C4-C5	7.27	1.66	1.43
38	31	313	A86	C4-C5	7.26	1.65	1.43
38	14	312	A86	C4-C5	7.26	1.65	1.43
38	11	310	A86	C4-C5	7.25	1.65	1.43
38	33	312	A86	C4-C5	7.25	1.65	1.43
38	13	314	A86	C8-C6	7.25	1.61	1.45
38	14	314	A86	C8-C6	7.25	1.61	1.45
38	33	314	A86	C8-C6	7.25	1.61	1.45
38	13	312	A86	C4-C5	7.25	1.65	1.43
38	32	314	A86	C4-C5	7.25	1.65	1.43
38	31	312	A86	C8-C6	7.24	1.61	1.45
38	12	314	A86	C4-C5	7.24	1.65	1.43
38	31	310	A86	C4-C5	7.24	1.65	1.43
38	11	312	A86	C8-C6	7.24	1.61	1.45
38	34	313	A86	C4-C5	7.24	1.65	1.43
38	34	315	A86	C8-C6	7.24	1.61	1.45
38	32	316	A86	C8-C6	7.23	1.61	1.45
38	12	316	A86	C8-C6	7.23	1.61	1.45
38	11	313	A86	C19-C20	7.14	1.62	1.52
38	34	316	A86	C19-C20	7.14	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	14	315	A86	C19-C20	7.14	1.62	1.52
38	14	315	A86	C8-C6	7.14	1.61	1.45
38	11	313	A86	C8-C6	7.12	1.61	1.45
38	31	313	A86	C19-C20	7.12	1.62	1.52
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	32	317	A86	C8-C6	7.10	1.61	1.45
38	34	316	A86	C8-C6	7.10	1.61	1.45
38	13	315	A86	C8-C6	7.10	1.61	1.45
38	31	313	A86	C8-C6	7.10	1.61	1.45
38	33	315	A86	C8-C6	7.09	1.61	1.45
38	13	315	A86	C19-C20	7.07	1.62	1.52
38	12	317	A86	C8-C6	7.06	1.61	1.45
38	12	315	A86	C8-C6	7.06	1.61	1.45
38	33	315	A86	C19-C20	7.05	1.62	1.52
38	13	313	A86	C8-C6	7.04	1.61	1.45
38	33	313	A86	C8-C6	7.03	1.61	1.45
38	11	311	A86	C8-C6	7.03	1.61	1.45
38	34	314	A86	C8-C6	7.01	1.61	1.45
38	31	311	A86	C8-C6	7.00	1.61	1.45
38	11	314	A86	C8-C6	6.99	1.61	1.45
38	14	313	A86	C8-C6	6.99	1.61	1.45
36	d	407	PL9	C3-C4	-6.99	1.38	1.49
38	32	315	A86	C8-C6	6.98	1.60	1.45
38	14	316	A86	C8-C6	6.98	1.60	1.45
38	34	301	A86	C8-C6	6.98	1.60	1.45
38	31	314	A86	C8-C6	6.97	1.60	1.45
36	D	407	PL9	C3-C4	-6.96	1.38	1.49
38	14	301	A86	C8-C6	6.96	1.60	1.45
38	13	316	A86	C8-C6	6.96	1.60	1.45
38	33	312	A86	C8-C6	6.95	1.60	1.45
38	33	316	A86	C8-C6	6.95	1.60	1.45
38	32	318	A86	C8-C6	6.94	1.60	1.45
38	31	310	A86	C8-C6	6.93	1.60	1.45
38	11	310	A86	C8-C6	6.93	1.60	1.45
38	13	312	A86	C8-C6	6.93	1.60	1.45
38	32	314	A86	C8-C6	6.91	1.60	1.45
38	34	313	A86	C8-C6	6.89	1.60	1.45
38	14	312	A86	C8-C6	6.89	1.60	1.45
38	12	314	A86	C8-C6	6.87	1.60	1.45
38	11	311	A86	C19-C20	6.84	1.61	1.52
38	12	315	A86	C19-C20	6.83	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	33	313	A86	C19-C20	6.83	1.61	1.52
38	32	315	A86	C19-C20	6.83	1.61	1.52
38	13	312	A86	C19-C20	6.83	1.61	1.52
38	14	312	A86	C19-C20	6.83	1.61	1.52
38	33	313	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	31	311	A86	C19-C20	6.80	1.61	1.52
38	13	313	A86	C25-C26	6.80	1.64	1.43
38	31	311	A86	C25-C26	6.80	1.64	1.43
38	34	314	A86	C19-C20	6.80	1.61	1.52
38	11	311	A86	C25-C26	6.79	1.64	1.43
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	14	313	A86	C25-C26	6.79	1.64	1.43
38	12	315	A86	C25-C26	6.79	1.64	1.43
38	34	314	A86	C25-C26	6.79	1.64	1.43
38	32	314	A86	C19-C20	6.77	1.61	1.52
38	32	315	A86	C25-C26	6.76	1.64	1.43
38	13	314	A86	C25-C26	6.75	1.64	1.43
38	33	314	A86	C25-C26	6.75	1.64	1.43
38	33	302	A86	C25-C26	6.75	1.64	1.43
38	31	316	A86	C25-C26	6.75	1.64	1.43
38	14	314	A86	C25-C26	6.74	1.64	1.43
38	31	312	A86	C25-C26	6.74	1.64	1.43
38	34	315	A86	C25-C26	6.74	1.64	1.43
38	12	316	A86	C25-C26	6.74	1.64	1.43
38	13	302	A86	C25-C26	6.73	1.64	1.43
38	34	303	A86	C25-C26	6.73	1.64	1.43
38	12	304	A86	C25-C26	6.73	1.64	1.43
38	13	317	A86	C25-C26	6.73	1.64	1.43
38	11	316	A86	C25-C26	6.73	1.64	1.43
38	14	313	A86	C19-C20	6.73	1.61	1.52
38	32	316	A86	C25-C26	6.73	1.64	1.43
38	11	312	A86	C25-C26	6.73	1.64	1.43
38	32	304	A86	C25-C26	6.71	1.64	1.43
38	33	316	A86	C25-C26	6.63	1.64	1.43
38	14	316	A86	C25-C26	6.61	1.63	1.43
38	34	301	A86	C25-C26	6.61	1.63	1.43
38	32	318	A86	C25-C26	6.60	1.63	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	11	314	A86	C25-C26	6.60	1.63	1.43
38	31	314	A86	C25-C26	6.60	1.63	1.43
28	A	403	PHO	C3B-C4B	6.60	1.49	1.41
38	14	301	A86	C25-C26	6.60	1.63	1.43
38	13	316	A86	C25-C26	6.59	1.63	1.43
28	a	403	PHO	C3B-C4B	6.59	1.49	1.41
38	33	315	A86	C25-C26	6.59	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	310	A86	C25-C26	6.57	1.63	1.43
38	34	313	A86	C25-C26	6.57	1.63	1.43
38	11	313	A86	C25-C26	6.56	1.63	1.43
38	31	310	A86	C25-C26	6.56	1.63	1.43
38	13	315	A86	C25-C26	6.56	1.63	1.43
38	34	316	A86	C25-C26	6.56	1.63	1.43
38	32	314	A86	C25-C26	6.55	1.63	1.43
38	12	317	A86	C25-C26	6.55	1.63	1.43
38	32	317	A86	C25-C26	6.55	1.63	1.43
38	31	313	A86	C25-C26	6.55	1.63	1.43
38	13	312	A86	C25-C26	6.55	1.63	1.43
38	33	312	A86	C25-C26	6.55	1.63	1.43
38	14	315	A86	C25-C26	6.54	1.63	1.43
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	14	312	A86	C25-C26	6.53	1.63	1.43
38	12	314	A86	C25-C26	6.53	1.63	1.43
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
36	d	407	PL9	C6-C1	-6.48	1.37	1.48
36	D	407	PL9	C6-C1	-6.44	1.37	1.48
28	D	403	PHO	C3B-C4B	6.42	1.48	1.41
28	d	403	PHO	C3B-C4B	6.42	1.48	1.41
38	13	316	A86	C19-C20	6.40	1.61	1.52
38	31	314	A86	C19-C20	6.38	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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	31	316	A86	C19-C20	6.12	1.60	1.52
38	33	302	A86	C19-C20	6.11	1.60	1.52
38	13	317	A86	C19-C20	6.10	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	404	PL9	C7-C3	-5.73	1.45	1.51
36	d	404	PL9	C7-C3	-5.72	1.45	1.51
38	12	316	A86	C9-C8	4.97	1.47	1.34
38	13	314	A86	C9-C8	4.96	1.47	1.34
38	34	315	A86	C9-C8	4.95	1.47	1.34
38	32	316	A86	C9-C8	4.94	1.47	1.34
38	11	312	A86	C9-C8	4.93	1.47	1.34
38	33	314	A86	C9-C8	4.92	1.47	1.34
38	14	314	A86	C9-C8	4.92	1.47	1.34
38	31	312	A86	C9-C8	4.92	1.47	1.34
38	13	302	A86	C9-C8	4.89	1.47	1.34
38	34	303	A86	C9-C8	4.87	1.47	1.34
38	11	316	A86	C9-C8	4.86	1.47	1.34
38	32	304	A86	C9-C8	4.86	1.47	1.34
38	33	302	A86	C9-C8	4.86	1.47	1.34
38	13	317	A86	C9-C8	4.85	1.47	1.34
38	31	316	A86	C9-C8	4.84	1.47	1.34
38	12	304	A86	C9-C8	4.84	1.47	1.34
27	c	510	CLA	C4D-ND	-4.75	1.31	1.37
38	32	315	A86	C9-C8	4.74	1.46	1.34
38	33	313	A86	C9-C8	4.73	1.46	1.34
38	31	311	A86	C9-C8	4.72	1.46	1.34
38	14	313	A86	C9-C8	4.72	1.46	1.34
38	13	313	A86	C9-C8	4.71	1.46	1.34
38	11	311	A86	C9-C8	4.71	1.46	1.34
27	C	510	CLA	C4D-ND	-4.71	1.31	1.37
38	33	316	A86	C9-C8	4.70	1.46	1.34
38	12	315	A86	C9-C8	4.70	1.46	1.34
38	14	301	A86	C9-C8	4.69	1.46	1.34
38	34	314	A86	C9-C8	4.69	1.46	1.34
38	11	310	A86	C9-C8	4.68	1.46	1.34
38	14	312	A86	C9-C8	4.68	1.46	1.34
38	12	314	A86	C9-C8	4.68	1.46	1.34
38	34	313	A86	C9-C8	4.67	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	13	312	A86	C9-C8	4.67	1.46	1.34
38	34	301	A86	C9-C8	4.66	1.46	1.34
27	b	612	CLA	C4D-ND	-4.66	1.31	1.37
38	31	314	A86	C9-C8	4.66	1.46	1.34
38	31	310	A86	C9-C8	4.66	1.46	1.34
38	33	315	A86	C9-C8	4.66	1.46	1.34
38	32	318	A86	C9-C8	4.66	1.46	1.34
38	34	316	A86	C9-C8	4.65	1.46	1.34
38	14	314	A86	C26-C27	4.65	1.42	1.35
38	13	316	A86	C9-C8	4.65	1.46	1.34
38	33	312	A86	C9-C8	4.65	1.46	1.34
38	11	314	A86	C9-C8	4.65	1.46	1.34
38	31	313	A86	C9-C8	4.65	1.46	1.34
38	12	317	A86	C9-C8	4.65	1.46	1.34
38	32	314	A86	C9-C8	4.64	1.46	1.34
38	11	313	A86	C9-C8	4.64	1.46	1.34
27	B	612	CLA	C4D-ND	-4.64	1.31	1.37
38	33	314	A86	C26-C27	4.64	1.41	1.35
38	14	316	A86	C9-C8	4.63	1.46	1.34
38	31	312	A86	C26-C27	4.63	1.41	1.35
38	13	314	A86	C26-C27	4.63	1.41	1.35
38	13	315	A86	C9-C8	4.62	1.46	1.34
38	32	317	A86	C9-C8	4.61	1.46	1.34
38	14	315	A86	C9-C8	4.61	1.46	1.34
38	12	316	A86	C26-C27	4.61	1.41	1.35
38	12	316	A86	O4-C38	4.58	1.45	1.35
38	11	312	A86	O4-C38	4.58	1.45	1.35
38	13	314	A86	O4-C38	4.58	1.45	1.35
38	14	314	A86	O4-C38	4.57	1.45	1.35
38	11	312	A86	C26-C27	4.56	1.41	1.35
38	31	312	A86	O4-C38	4.56	1.45	1.35
38	32	316	A86	C26-C27	4.56	1.41	1.35
38	32	316	A86	O4-C38	4.56	1.45	1.35
38	34	315	A86	O4-C38	4.55	1.45	1.35
38	33	314	A86	O4-C38	4.55	1.45	1.35
38	34	315	A86	C26-C27	4.54	1.41	1.35
38	31	311	A86	C17-C18	-4.49	1.45	1.52
38	11	311	A86	C17-C18	-4.47	1.45	1.52
38	12	315	A86	C17-C18	-4.47	1.45	1.52
38	34	314	A86	C17-C18	-4.46	1.45	1.52
38	32	315	A86	C26-C27	4.46	1.41	1.35
38	33	313	A86	C17-C18	-4.44	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	32	315	A86	C17-C18	-4.44	1.45	1.52
38	13	313	A86	C17-C18	-4.43	1.45	1.52
38	14	313	A86	C26-C27	4.43	1.41	1.35
38	14	313	A86	C17-C18	-4.42	1.46	1.52
38	32	304	A86	C26-C27	4.41	1.41	1.35
38	33	313	A86	C26-C27	4.40	1.41	1.35
38	31	311	A86	C26-C27	4.40	1.41	1.35
38	11	316	A86	C26-C27	4.37	1.41	1.35
38	12	304	A86	C26-C27	4.37	1.41	1.35
38	12	315	A86	C26-C27	4.37	1.41	1.35
38	33	302	A86	C26-C27	4.37	1.41	1.35
38	13	302	A86	C26-C27	4.37	1.41	1.35
38	13	314	A86	C17-C18	-4.37	1.46	1.52
38	34	303	A86	C26-C27	4.37	1.41	1.35
38	34	314	A86	C26-C27	4.36	1.41	1.35
38	31	316	A86	C26-C27	4.35	1.41	1.35
38	11	311	A86	C26-C27	4.35	1.41	1.35
38	13	317	A86	C26-C27	4.35	1.41	1.35
38	31	312	A86	C17-C18	-4.34	1.46	1.52
38	32	316	A86	C2-C1	4.33	1.41	1.35
38	11	312	A86	C17-C18	-4.33	1.46	1.52
38	11	314	A86	C26-C27	4.33	1.41	1.35
38	13	313	A86	C26-C27	4.33	1.41	1.35
27	d	401	CLA	C4D-ND	-4.32	1.31	1.37
38	13	316	A86	C26-C27	4.32	1.41	1.35
38	14	314	A86	C17-C18	-4.32	1.46	1.52
38	11	312	A86	C2-C1	4.32	1.41	1.35
38	12	316	A86	C2-C1	4.32	1.41	1.35
38	33	314	A86	C17-C18	-4.32	1.46	1.52
38	31	314	A86	C26-C27	4.31	1.41	1.35
38	34	315	A86	C2-C1	4.30	1.41	1.35
38	34	315	A86	C17-C18	-4.30	1.46	1.52
38	12	316	A86	C17-C18	-4.30	1.46	1.52
38	14	316	A86	C26-C27	4.29	1.41	1.35
38	34	301	A86	C26-C27	4.29	1.41	1.35
38	32	318	A86	C17-C18	-4.29	1.46	1.52
27	b	613	CLA	C4D-ND	-4.29	1.31	1.37
38	14	314	A86	C2-C1	4.28	1.41	1.35
27	B	613	CLA	C4D-ND	-4.28	1.31	1.37
38	33	316	A86	C26-C27	4.28	1.41	1.35
27	D	401	CLA	C4D-ND	-4.28	1.31	1.37
38	14	315	A86	C26-C27	4.28	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	14	301	A86	C26-C27	4.28	1.41	1.35
38	33	316	A86	C17-C18	-4.28	1.46	1.52
38	32	318	A86	C26-C27	4.28	1.41	1.35
38	13	302	A86	O4-C38	4.26	1.44	1.35
38	33	315	A86	C7-C6	4.26	1.59	1.50
38	31	313	A86	C7-C6	4.26	1.59	1.50
38	33	315	A86	O4-C38	4.25	1.44	1.35
38	32	316	A86	C17-C18	-4.25	1.46	1.52
38	13	314	A86	C2-C1	4.25	1.41	1.35
38	31	312	A86	C2-C1	4.25	1.41	1.35
27	B	611	CLA	C4D-ND	-4.25	1.31	1.37
38	34	301	A86	C17-C18	-4.25	1.46	1.52
38	12	317	A86	C26-C27	4.24	1.41	1.35
38	12	317	A86	O4-C38	4.24	1.44	1.35
38	34	303	A86	C7-C6	4.24	1.59	1.50
38	13	316	A86	C17-C18	-4.24	1.46	1.52
38	31	313	A86	C26-C27	4.24	1.41	1.35
27	d	405	CLA	C4D-ND	-4.24	1.31	1.37
38	11	313	A86	C26-C27	4.24	1.41	1.35
38	33	302	A86	O4-C38	4.24	1.44	1.35
38	13	317	A86	C2-C1	4.23	1.41	1.35
38	12	317	A86	C7-C6	4.23	1.59	1.50
38	13	317	A86	C17-C18	-4.23	1.46	1.52
38	33	314	A86	C2-C1	4.23	1.41	1.35
38	11	313	A86	O4-C38	4.23	1.44	1.35
27	C	509	CLA	C4D-ND	-4.23	1.31	1.37
38	32	304	A86	O4-C38	4.23	1.44	1.35
38	34	303	A86	C17-C18	-4.23	1.46	1.52
38	13	302	A86	C17-C18	-4.23	1.46	1.52
38	13	315	A86	O4-C38	4.23	1.44	1.35
38	12	304	A86	O4-C38	4.22	1.44	1.35
38	33	302	A86	C17-C18	-4.22	1.46	1.52
38	14	316	A86	C17-C18	-4.22	1.46	1.52
27	c	502	CLA	C4D-ND	-4.22	1.31	1.37
38	32	317	A86	O4-C38	4.22	1.44	1.35
27	D	405	CLA	C4D-ND	-4.22	1.31	1.37
38	31	314	A86	C17-C18	-4.22	1.46	1.52
38	32	304	A86	C17-C18	-4.22	1.46	1.52
38	14	315	A86	O4-C38	4.22	1.44	1.35
38	11	316	A86	O4-C38	4.22	1.44	1.35
38	11	314	A86	C17-C18	-4.22	1.46	1.52
38	13	317	A86	O4-C38	4.21	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	11	316	A86	C17-C18	-4.21	1.46	1.52
38	32	317	A86	C26-C27	4.21	1.41	1.35
38	31	313	A86	O4-C38	4.21	1.44	1.35
38	31	316	A86	O4-C38	4.21	1.44	1.35
38	11	313	A86	C7-C6	4.21	1.59	1.50
38	34	303	A86	O4-C38	4.21	1.44	1.35
38	12	304	A86	C7-C6	4.21	1.59	1.50
38	13	315	A86	C26-C27	4.21	1.41	1.35
38	31	316	A86	C7-C6	4.21	1.59	1.50
38	13	315	A86	C7-C6	4.21	1.59	1.50
38	34	316	A86	O4-C38	4.21	1.44	1.35
38	13	302	A86	C7-C6	4.21	1.59	1.50
38	34	316	A86	C7-C6	4.21	1.59	1.50
38	13	317	A86	C7-C6	4.20	1.59	1.50
38	31	316	A86	C17-C18	-4.20	1.46	1.52
38	11	316	A86	C7-C6	4.20	1.59	1.50
38	32	317	A86	C7-C6	4.20	1.59	1.50
38	12	304	A86	C2-C1	4.20	1.41	1.35
27	b	611	CLA	C4D-ND	-4.20	1.31	1.37
38	32	304	A86	C7-C6	4.19	1.59	1.50
38	14	301	A86	C17-C18	-4.19	1.46	1.52
38	32	304	A86	C2-C1	4.19	1.41	1.35
38	33	302	A86	C7-C6	4.19	1.59	1.50
38	33	315	A86	C26-C27	4.18	1.41	1.35
38	12	304	A86	C17-C18	-4.18	1.46	1.52
38	11	316	A86	C2-C1	4.18	1.41	1.35
38	34	316	A86	C17-C18	-4.18	1.46	1.52
38	14	315	A86	C7-C6	4.17	1.59	1.50
38	34	316	A86	C26-C27	4.17	1.41	1.35
38	34	303	A86	C2-C1	4.17	1.41	1.35
27	C	502	CLA	C4D-ND	-4.17	1.32	1.37
38	13	302	A86	C2-C1	4.16	1.41	1.35
38	34	315	A86	C7-C6	4.16	1.59	1.50
27	13	303	CLA	C4D-ND	-4.16	1.32	1.37
38	31	316	A86	C2-C1	4.16	1.41	1.35
38	13	313	A86	O4-C38	4.15	1.44	1.35
38	11	312	A86	C7-C6	4.15	1.59	1.50
27	B	604	CLA	C4D-ND	-4.15	1.32	1.37
38	11	313	A86	C17-C18	-4.15	1.46	1.52
27	12	305	CLA	C4D-ND	-4.15	1.32	1.37
38	32	315	A86	O4-C38	4.15	1.44	1.35
27	a	402	CLA	C4D-ND	-4.15	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	33	314	A86	C7-C6	4.14	1.59	1.50
38	14	301	A86	C21-C20	4.14	1.58	1.51
38	14	316	A86	C7-C6	4.14	1.59	1.50
38	14	313	A86	O4-C38	4.14	1.44	1.35
38	33	316	A86	C7-C6	4.14	1.59	1.50
38	34	314	A86	O4-C38	4.14	1.44	1.35
38	12	315	A86	O4-C38	4.14	1.44	1.35
38	31	312	A86	C7-C6	4.13	1.59	1.50
38	11	311	A86	O4-C38	4.13	1.44	1.35
38	12	317	A86	C17-C18	-4.13	1.46	1.52
38	34	301	A86	C7-C6	4.13	1.59	1.50
27	c	509	CLA	C4D-ND	-4.13	1.32	1.37
38	31	311	A86	O4-C38	4.12	1.44	1.35
27	33	303	CLA	C4D-ND	-4.12	1.32	1.37
38	13	316	A86	C7-C6	4.12	1.59	1.50
38	33	302	A86	C2-C1	4.12	1.41	1.35
38	11	314	A86	C7-C6	4.12	1.59	1.50
38	12	316	A86	C7-C6	4.11	1.59	1.50
27	31	301	CLA	C4D-ND	-4.11	1.32	1.37
38	33	313	A86	O4-C38	4.11	1.44	1.35
27	34	304	CLA	C4D-ND	-4.11	1.32	1.37
38	12	314	A86	C17-C18	-4.11	1.46	1.52
38	13	314	A86	C7-C6	4.11	1.59	1.50
27	b	622	CLA	C4D-ND	-4.11	1.32	1.37
38	13	315	A86	C17-C18	-4.11	1.46	1.52
38	14	312	A86	C17-C18	-4.11	1.46	1.52
27	a	404	CLA	C4D-ND	-4.11	1.32	1.37
38	14	314	A86	C7-C6	4.11	1.59	1.50
27	A	404	CLA	C4D-ND	-4.11	1.32	1.37
38	14	301	A86	C7-C6	4.11	1.59	1.50
27	B	610	CLA	C4D-ND	-4.10	1.32	1.37
38	32	318	A86	C2-C1	4.10	1.41	1.35
27	B	622	CLA	C4D-ND	-4.10	1.32	1.37
27	b	604	CLA	C4D-ND	-4.10	1.32	1.37
38	33	316	A86	C21-C20	4.10	1.58	1.51
38	32	316	A86	C7-C6	4.10	1.59	1.50
38	33	316	A86	C2-C1	4.10	1.41	1.35
27	b	610	CLA	C4D-ND	-4.09	1.32	1.37
27	A	402	CLA	C4D-ND	-4.09	1.32	1.37
38	31	314	A86	C21-C20	4.09	1.58	1.51
38	32	314	A86	C17-C18	-4.09	1.46	1.52
27	14	303	CLA	C4D-ND	-4.09	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	31	313	A86	C17-C18	-4.09	1.46	1.52
38	32	318	A86	C21-C20	4.09	1.58	1.51
38	14	315	A86	C17-C18	-4.09	1.46	1.52
27	32	305	CLA	C4D-ND	-4.09	1.32	1.37
27	11	301	CLA	C4D-ND	-4.08	1.32	1.37
38	32	317	A86	C17-C18	-4.08	1.46	1.52
38	11	314	A86	C21-C20	4.08	1.58	1.51
27	c	503	CLA	C4D-ND	-4.08	1.32	1.37
38	13	316	A86	C21-C20	4.08	1.58	1.51
38	14	313	A86	C7-C6	4.08	1.59	1.50
38	31	310	A86	C17-C18	-4.07	1.46	1.52
38	13	316	A86	C2-C1	4.07	1.41	1.35
38	32	318	A86	C7-C6	4.07	1.59	1.50
27	C	503	CLA	C4D-ND	-4.07	1.32	1.37
27	d	402	CLA	C4D-ND	-4.07	1.32	1.37
38	31	314	A86	C7-C6	4.07	1.59	1.50
27	c	508	CLA	C4D-ND	-4.07	1.32	1.37
38	14	316	A86	C21-C20	4.06	1.58	1.51
38	34	301	A86	O4-C38	4.06	1.44	1.35
38	34	301	A86	C21-C20	4.06	1.58	1.51
38	11	311	A86	C7-C6	4.06	1.59	1.50
38	34	314	A86	C7-C6	4.06	1.59	1.50
38	13	316	A86	O4-C38	4.06	1.44	1.35
38	14	301	A86	O4-C38	4.05	1.44	1.35
38	13	315	A86	C2-C1	4.05	1.41	1.35
38	11	314	A86	C2-C1	4.05	1.41	1.35
38	31	314	A86	C2-C1	4.05	1.41	1.35
38	33	312	A86	C17-C18	-4.05	1.46	1.52
38	34	313	A86	C17-C18	-4.05	1.46	1.52
38	14	316	A86	O4-C38	4.05	1.44	1.35
27	C	508	CLA	C4D-ND	-4.05	1.32	1.37
38	11	313	A86	C2-C1	4.05	1.41	1.35
38	33	315	A86	C2-C1	4.05	1.41	1.35
27	D	402	CLA	C4D-ND	-4.04	1.32	1.37
38	33	313	A86	C7-C6	4.04	1.59	1.50
38	32	315	A86	C7-C6	4.04	1.59	1.50
38	11	314	A86	O4-C38	4.04	1.44	1.35
38	12	315	A86	C7-C6	4.04	1.59	1.50
38	33	316	A86	O4-C38	4.04	1.44	1.35
38	13	312	A86	C17-C18	-4.04	1.46	1.52
38	33	315	A86	C17-C18	-4.04	1.46	1.52
38	11	310	A86	C17-C18	-4.03	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	31	313	A86	C21-C20	4.03	1.58	1.51
38	31	311	A86	C7-C6	4.03	1.59	1.50
38	13	313	A86	C7-C6	4.03	1.59	1.50
38	31	314	A86	O4-C38	4.03	1.44	1.35
38	12	314	A86	C7-C6	4.03	1.59	1.50
27	c	514	CLA	C4D-ND	-4.03	1.32	1.37
38	32	318	A86	O4-C38	4.02	1.44	1.35
38	11	313	A86	C21-C20	4.02	1.58	1.51
38	31	310	A86	C7-C6	4.02	1.59	1.50
38	34	313	A86	C7-C6	4.02	1.59	1.50
38	33	312	A86	C21-C20	4.01	1.58	1.51
38	14	301	A86	C2-C1	4.01	1.41	1.35
38	34	313	A86	C21-C20	4.01	1.58	1.51
27	C	514	CLA	C4D-ND	-4.01	1.32	1.37
27	c	505	CLA	C4D-ND	-4.01	1.32	1.37
38	31	311	A86	C2-C1	4.01	1.41	1.35
38	11	316	A86	C21-C20	4.00	1.58	1.51
38	12	317	A86	C21-C20	4.00	1.58	1.51
38	32	317	A86	C2-C1	4.00	1.41	1.35
38	33	315	A86	C21-C20	4.00	1.58	1.51
38	14	315	A86	C2-C1	4.00	1.41	1.35
38	14	315	A86	C21-C20	4.00	1.58	1.51
38	14	312	A86	C7-C6	4.00	1.59	1.50
38	34	301	A86	C2-C1	4.00	1.41	1.35
38	32	314	A86	C7-C6	4.00	1.59	1.50
38	33	312	A86	C7-C6	4.00	1.59	1.50
38	11	310	A86	C7-C6	4.00	1.59	1.50
38	12	304	A86	C21-C20	3.99	1.58	1.51
36	d	407	PL9	C7-C8	-3.99	1.44	1.50
27	b	607	CLA	C4D-ND	-3.99	1.32	1.37
38	32	314	A86	C21-C20	3.99	1.58	1.51
27	c	513	CLA	C4D-ND	-3.98	1.32	1.37
38	13	317	A86	C21-C20	3.98	1.58	1.51
38	31	310	A86	C21-C20	3.98	1.58	1.51
38	31	316	A86	C21-C20	3.98	1.58	1.51
38	13	302	A86	C21-C20	3.98	1.58	1.51
38	12	317	A86	C2-C1	3.98	1.41	1.35
38	33	302	A86	C21-C20	3.98	1.58	1.51
38	14	312	A86	C26-C27	3.98	1.41	1.35
38	13	312	A86	C7-C6	3.97	1.59	1.50
38	14	312	A86	C21-C20	3.97	1.58	1.51
38	13	313	A86	C2-C1	3.97	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	31	313	A86	C2-C1	3.97	1.41	1.35
38	34	316	A86	C2-C1	3.97	1.41	1.35
27	B	607	CLA	C4D-ND	-3.97	1.32	1.37
38	14	316	A86	C2-C1	3.97	1.41	1.35
38	32	304	A86	C21-C20	3.97	1.58	1.51
36	D	407	PL9	C7-C8	-3.97	1.44	1.50
38	32	315	A86	C2-C1	3.97	1.41	1.35
38	13	312	A86	O4-C38	3.97	1.44	1.35
38	32	317	A86	C21-C20	3.97	1.58	1.51
38	11	310	A86	C21-C20	3.96	1.58	1.51
38	12	314	A86	C21-C20	3.96	1.58	1.51
38	11	311	A86	C2-C1	3.96	1.41	1.35
38	14	313	A86	C2-C1	3.96	1.41	1.35
38	34	303	A86	C21-C20	3.96	1.58	1.51
38	34	313	A86	O4-C38	3.96	1.44	1.35
38	13	312	A86	C26-C27	3.95	1.41	1.35
38	34	314	A86	C2-C1	3.95	1.41	1.35
38	31	310	A86	O4-C38	3.95	1.44	1.35
38	13	315	A86	C21-C20	3.95	1.58	1.51
27	C	513	CLA	C4D-ND	-3.95	1.32	1.37
38	13	312	A86	C21-C20	3.94	1.58	1.51
38	12	314	A86	C26-C27	3.94	1.41	1.35
38	32	314	A86	O4-C38	3.94	1.44	1.35
38	11	310	A86	C2-C1	3.94	1.41	1.35
38	11	310	A86	O4-C38	3.93	1.44	1.35
38	12	315	A86	C2-C1	3.93	1.41	1.35
27	B	606	CLA	C4D-ND	-3.93	1.32	1.37
38	32	314	A86	C26-C27	3.93	1.41	1.35
38	14	312	A86	O4-C38	3.92	1.44	1.35
27	C	512	CLA	C4D-ND	-3.92	1.32	1.37
38	33	312	A86	O4-C38	3.92	1.44	1.35
38	32	314	A86	C2-C1	3.92	1.41	1.35
27	c	511	CLA	C4D-ND	-3.92	1.32	1.37
27	d	406	CLA	C4D-ND	-3.92	1.32	1.37
27	C	505	CLA	C4D-ND	-3.91	1.32	1.37
38	31	310	A86	C26-C27	3.91	1.41	1.35
38	33	312	A86	C2-C1	3.91	1.41	1.35
27	C	511	CLA	C4D-ND	-3.91	1.32	1.37
38	34	313	A86	C2-C1	3.91	1.41	1.35
38	34	316	A86	C21-C20	3.90	1.57	1.51
38	13	312	A86	C2-C1	3.90	1.41	1.35
38	33	313	A86	C2-C1	3.90	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	11	310	A86	C26-C27	3.90	1.41	1.35
38	12	314	A86	O4-C38	3.90	1.44	1.35
38	34	313	A86	C26-C27	3.90	1.41	1.35
27	D	406	CLA	C4D-ND	-3.89	1.32	1.37
27	c	512	CLA	C4D-ND	-3.89	1.32	1.37
27	b	606	CLA	C4D-ND	-3.89	1.32	1.37
38	31	310	A86	C2-C1	3.87	1.40	1.35
38	33	312	A86	C26-C27	3.87	1.40	1.35
38	14	312	A86	C2-C1	3.86	1.40	1.35
27	C	507	CLA	C4D-ND	-3.85	1.32	1.37
38	31	316	A86	C9-C10	3.85	1.55	1.43
36	D	407	PL9	C52-C5	-3.85	1.42	1.50
27	W	103	CLA	C1D-ND	3.84	1.42	1.37
38	12	315	A86	C21-C20	3.84	1.57	1.51
38	14	314	A86	C9-C10	3.84	1.55	1.43
27	b	603	CLA	C4D-ND	-3.84	1.32	1.37
27	w	103	CLA	C1D-ND	3.84	1.42	1.37
38	32	316	A86	C9-C10	3.84	1.55	1.43
38	33	314	A86	C9-C10	3.84	1.55	1.43
38	32	304	A86	C9-C10	3.83	1.55	1.43
38	31	312	A86	C9-C10	3.83	1.55	1.43
38	32	315	A86	C21-C20	3.82	1.57	1.51
38	11	316	A86	C9-C10	3.82	1.55	1.43
38	34	315	A86	C9-C10	3.82	1.55	1.43
38	11	312	A86	C9-C10	3.82	1.55	1.43
38	13	302	A86	C9-C10	3.82	1.55	1.43
38	12	304	A86	C9-C10	3.82	1.55	1.43
38	33	302	A86	C9-C10	3.81	1.55	1.43
29	M	101	BCR	C30-C25	-3.81	1.48	1.53
38	12	314	A86	C2-C1	3.81	1.40	1.35
38	13	314	A86	C9-C10	3.81	1.55	1.43
38	12	316	A86	C9-C10	3.81	1.55	1.43
27	Z	102	CLA	C4D-ND	-3.81	1.32	1.37
36	d	407	PL9	C52-C5	-3.81	1.42	1.50
32	l	102	LHG	O7-C5	-3.81	1.37	1.46
38	34	303	A86	C9-C10	3.80	1.55	1.43
38	13	317	A86	C9-C10	3.80	1.55	1.43
38	11	312	A86	C10-C11	3.80	1.45	1.34
27	B	603	CLA	C4D-ND	-3.80	1.32	1.37
38	33	314	A86	C10-C11	3.79	1.45	1.34
27	C	504	CLA	C4D-ND	-3.79	1.32	1.37
38	32	316	A86	C10-C11	3.79	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	14	314	A86	C10-C11	3.79	1.45	1.34
38	34	315	A86	C10-C11	3.79	1.45	1.34
38	13	314	A86	C10-C11	3.79	1.45	1.34
38	12	316	A86	C10-C11	3.78	1.45	1.34
32	L	101	LHG	O7-C5	-3.78	1.37	1.46
38	34	314	A86	C21-C20	3.78	1.57	1.51
27	c	504	CLA	C4D-ND	-3.77	1.32	1.37
38	31	311	A86	C21-C20	3.77	1.57	1.51
29	m	103	BCR	C30-C25	-3.77	1.48	1.53
38	31	312	A86	C10-C11	3.77	1.45	1.34
29	h	101	BCR	C1-C6	-3.77	1.48	1.53
27	c	507	CLA	C4D-ND	-3.76	1.32	1.37
38	13	313	A86	C21-C20	3.76	1.57	1.51
38	33	313	A86	C21-C20	3.76	1.57	1.51
27	B	601	CLA	C4D-ND	-3.75	1.32	1.37
38	13	316	A86	C9-C10	3.75	1.55	1.43
27	z	102	CLA	C4D-ND	-3.75	1.32	1.37
38	32	318	A86	C9-C10	3.75	1.55	1.43
38	14	313	A86	C21-C20	3.75	1.57	1.51
38	11	311	A86	C21-C20	3.74	1.57	1.51
38	14	301	A86	C9-C10	3.74	1.55	1.43
38	14	316	A86	C9-C10	3.74	1.55	1.43
38	11	314	A86	C9-C10	3.73	1.55	1.43
38	34	314	A86	C9-C10	3.73	1.55	1.43
38	14	313	A86	C9-C10	3.73	1.55	1.43
38	31	311	A86	C9-C10	3.72	1.55	1.43
38	34	301	A86	C9-C10	3.72	1.55	1.43
38	34	316	A86	C9-C10	3.72	1.55	1.43
38	31	314	A86	C9-C10	3.72	1.55	1.43
38	33	316	A86	C9-C10	3.72	1.55	1.43
38	32	316	A86	C5-C6	3.72	1.40	1.35
38	32	315	A86	C9-C10	3.72	1.55	1.43
29	H	101	BCR	C1-C6	-3.72	1.48	1.53
38	34	315	A86	C21-C20	3.71	1.57	1.51
38	11	311	A86	C9-C10	3.71	1.54	1.43
38	11	313	A86	C9-C10	3.70	1.54	1.43
38	33	313	A86	C9-C10	3.70	1.54	1.43
38	13	313	A86	C9-C10	3.70	1.54	1.43
38	13	315	A86	C9-C10	3.70	1.54	1.43
38	34	315	A86	C5-C6	3.70	1.40	1.35
27	m	101	CLA	C4D-ND	-3.70	1.32	1.37
38	12	315	A86	C9-C10	3.69	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	14	314	A86	C21-C20	3.69	1.57	1.51
27	M	102	CLA	C4D-ND	-3.69	1.32	1.37
38	11	312	A86	C21-C20	3.69	1.57	1.51
27	B	608	CLA	C4D-ND	-3.69	1.32	1.37
38	14	314	A86	C5-C6	3.69	1.40	1.35
38	13	313	A86	C10-C11	3.69	1.45	1.34
38	32	317	A86	C9-C10	3.68	1.54	1.43
38	32	315	A86	C10-C11	3.68	1.45	1.34
38	34	314	A86	C10-C11	3.68	1.45	1.34
38	12	316	A86	C5-C6	3.68	1.40	1.35
38	31	312	A86	C21-C20	3.68	1.57	1.51
27	b	601	CLA	C4D-ND	-3.68	1.32	1.37
38	33	314	A86	C5-C6	3.68	1.40	1.35
29	C	520	BCR	C30-C25	-3.68	1.48	1.53
38	14	315	A86	C9-C10	3.68	1.54	1.43
38	31	313	A86	C9-C10	3.68	1.54	1.43
27	b	608	CLA	C4D-ND	-3.68	1.32	1.37
38	33	315	A86	C9-C10	3.68	1.54	1.43
38	11	311	A86	C10-C11	3.68	1.45	1.34
38	12	317	A86	C9-C10	3.67	1.54	1.43
27	31	303	CLA	C4D-ND	-3.67	1.32	1.37
27	32	307	CLA	C4D-ND	-3.67	1.32	1.37
38	12	316	A86	C21-C20	3.67	1.57	1.51
38	13	314	A86	C5-C6	3.67	1.40	1.35
27	b	602	CLA	C4D-ND	-3.66	1.32	1.37
38	14	313	A86	C10-C11	3.66	1.45	1.34
38	32	316	A86	C21-C20	3.66	1.57	1.51
27	W	102	CLA	C4D-ND	-3.66	1.32	1.37
38	31	311	A86	C10-C11	3.66	1.45	1.34
27	B	602	CLA	C4D-ND	-3.66	1.32	1.37
38	12	315	A86	C10-C11	3.66	1.45	1.34
27	32	311	CLA	C4D-ND	-3.66	1.32	1.37
38	33	314	A86	C21-C20	3.65	1.57	1.51
38	13	314	A86	C21-C20	3.65	1.57	1.51
27	33	305	CLA	C4D-ND	-3.65	1.32	1.37
38	33	313	A86	C10-C11	3.65	1.45	1.34
38	11	312	A86	C5-C6	3.65	1.40	1.35
27	14	309	CLA	C4D-ND	-3.64	1.32	1.37
38	33	316	A86	C10-C11	3.64	1.45	1.34
29	c	515	BCR	C30-C25	-3.64	1.48	1.53
29	c	519	BCR	C30-C25	-3.64	1.48	1.53
38	32	318	A86	C10-C11	3.64	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	12	311	CLA	C4D-ND	-3.64	1.32	1.37
38	34	301	A86	C10-C11	3.64	1.45	1.34
29	C	515	BCR	C30-C25	-3.64	1.48	1.53
38	14	301	A86	C10-C11	3.64	1.45	1.34
38	11	314	A86	C10-C11	3.63	1.45	1.34
38	13	316	A86	C10-C11	3.63	1.45	1.34
27	b	615	CLA	C4D-ND	-3.63	1.32	1.37
27	w	102	CLA	C4D-ND	-3.63	1.32	1.37
27	12	307	CLA	C4D-ND	-3.63	1.32	1.37
27	b	614	CLA	C4D-ND	-3.62	1.32	1.37
38	11	316	A86	C10-C11	3.62	1.45	1.34
38	31	310	A86	C9-C10	3.62	1.54	1.43
38	14	316	A86	C10-C11	3.62	1.45	1.34
38	13	312	A86	C10-C11	3.62	1.45	1.34
38	33	302	A86	C10-C11	3.62	1.45	1.34
27	13	309	CLA	C4D-ND	-3.62	1.32	1.37
39	12	302	LMU	O5B-C1B	3.62	1.51	1.41
38	13	312	A86	C9-C10	3.62	1.54	1.43
38	34	303	A86	C10-C11	3.62	1.45	1.34
38	13	317	A86	C5-C6	3.62	1.40	1.35
38	31	314	A86	C10-C11	3.62	1.45	1.34
38	14	312	A86	C9-C10	3.62	1.54	1.43
38	33	312	A86	C9-C10	3.61	1.54	1.43
38	31	312	A86	C5-C6	3.61	1.40	1.35
38	12	304	A86	C10-C11	3.61	1.45	1.34
39	32	302	LMU	O5B-C1B	3.61	1.51	1.41
38	14	312	A86	C10-C11	3.61	1.45	1.34
38	12	317	A86	C19-C18	3.61	1.57	1.52
38	13	315	A86	C19-C18	3.61	1.57	1.52
38	14	315	A86	C19-C18	3.61	1.57	1.52
38	11	310	A86	C9-C10	3.61	1.54	1.43
27	11	307	CLA	C4D-ND	-3.61	1.32	1.37
38	12	314	A86	C9-C10	3.61	1.54	1.43
27	31	307	CLA	C4D-ND	-3.61	1.32	1.37
38	12	314	A86	C10-C11	3.61	1.45	1.34
27	34	306	CLA	C4D-ND	-3.61	1.32	1.37
38	31	310	A86	C10-C11	3.61	1.45	1.34
38	13	317	A86	C10-C11	3.61	1.45	1.34
27	34	310	CLA	C4D-ND	-3.61	1.32	1.37
27	B	605	CLA	C4D-ND	-3.60	1.32	1.37
27	33	309	CLA	C4D-ND	-3.60	1.32	1.37
38	32	314	A86	C9-C10	3.60	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	34	313	A86	C9-C10	3.60	1.54	1.43
27	B	615	CLA	C4D-ND	-3.60	1.32	1.37
38	32	314	A86	C10-C11	3.60	1.45	1.34
38	33	302	A86	C5-C6	3.60	1.40	1.35
38	11	310	A86	C10-C11	3.60	1.45	1.34
38	13	302	A86	C10-C11	3.60	1.45	1.34
38	34	316	A86	C19-C18	3.60	1.57	1.52
38	32	317	A86	C19-C18	3.59	1.57	1.52
38	34	313	A86	C10-C11	3.59	1.45	1.34
38	31	316	A86	C10-C11	3.58	1.45	1.34
27	11	303	CLA	C4D-ND	-3.58	1.32	1.37
38	33	312	A86	C10-C11	3.58	1.45	1.34
38	11	313	A86	C19-C18	3.58	1.57	1.52
28	A	403	PHO	C4D-ND	-3.58	1.33	1.38
28	a	403	PHO	C4D-ND	-3.58	1.33	1.38
29	M	101	BCR	C1-C6	-3.58	1.48	1.53
27	c	506	CLA	C4D-ND	-3.58	1.32	1.37
38	12	304	A86	C5-C6	3.58	1.40	1.35
27	14	305	CLA	C4D-ND	-3.57	1.32	1.37
38	31	313	A86	C10-C11	3.57	1.44	1.34
38	11	316	A86	C5-C6	3.57	1.40	1.35
38	31	313	A86	C19-C18	3.57	1.57	1.52
38	32	304	A86	C10-C11	3.57	1.44	1.34
38	14	315	A86	C10-C11	3.57	1.44	1.34
38	12	317	A86	C10-C11	3.56	1.44	1.34
38	33	315	A86	C10-C11	3.56	1.44	1.34
38	11	313	A86	C10-C11	3.56	1.44	1.34
38	34	303	A86	C5-C6	3.56	1.40	1.35
27	b	605	CLA	C4D-ND	-3.56	1.32	1.37
38	32	317	A86	C10-C11	3.56	1.44	1.34
27	B	614	CLA	C4D-ND	-3.56	1.32	1.37
38	31	316	A86	C5-C6	3.56	1.40	1.35
36	d	404	PL9	C3-C4	-3.55	1.43	1.49
27	13	305	CLA	C4D-ND	-3.55	1.32	1.37
38	34	316	A86	C10-C11	3.55	1.44	1.34
38	13	302	A86	C5-C6	3.54	1.40	1.35
38	13	315	A86	C10-C11	3.54	1.44	1.34
29	m	103	BCR	C1-C6	-3.53	1.48	1.53
38	33	315	A86	C19-C18	3.53	1.57	1.52
29	z	101	BCR	C1-C6	-3.53	1.48	1.53
38	32	318	A86	C5-C6	3.52	1.40	1.35
27	C	506	CLA	C4D-ND	-3.52	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	32	304	A86	C5-C6	3.51	1.40	1.35
27	b	609	CLA	C4D-ND	-3.51	1.32	1.37
29	Z	101	BCR	C1-C6	-3.51	1.49	1.53
27	11	305	CLA	C1D-ND	3.50	1.42	1.37
27	11	315	CLA	C4D-ND	-3.50	1.32	1.37
27	13	301	CLA	C4D-ND	-3.50	1.32	1.37
27	33	301	CLA	C4D-ND	-3.50	1.32	1.37
27	32	303	CLA	C4D-ND	-3.49	1.32	1.37
27	c	507	CLA	CMB-C2B	-3.49	1.43	1.50
27	b	612	CLA	CMD-C2D	-3.49	1.43	1.50
27	C	507	CLA	CMB-C2B	-3.48	1.43	1.50
27	31	315	CLA	C4D-ND	-3.47	1.32	1.37
36	D	404	PL9	C3-C4	-3.47	1.43	1.49
29	C	516	BCR	C1-C6	-3.47	1.49	1.53
27	33	307	CLA	C1D-ND	3.47	1.42	1.37
27	34	302	CLA	C4D-ND	-3.47	1.32	1.37
38	14	301	A86	C5-C6	3.46	1.40	1.35
27	B	612	CLA	CMD-C2D	-3.45	1.43	1.50
27	12	312	CLA	C4D-ND	-3.45	1.32	1.37
27	12	303	CLA	C4D-ND	-3.45	1.33	1.37
27	b	611	CLA	CMB-C2B	-3.45	1.43	1.50
27	31	305	CLA	C1D-ND	3.45	1.42	1.37
27	B	609	CLA	C4D-ND	-3.45	1.33	1.37
38	33	316	A86	C5-C6	3.45	1.40	1.35
27	14	307	CLA	C1D-ND	3.44	1.42	1.37
27	11	308	CLA	C4D-ND	-3.43	1.33	1.37
29	c	516	BCR	C1-C6	-3.43	1.49	1.53
27	B	611	CLA	CMB-C2B	-3.43	1.43	1.50
27	13	310	CLA	C4D-ND	-3.43	1.33	1.37
38	31	314	A86	C5-C6	3.43	1.40	1.35
38	14	316	A86	C5-C6	3.43	1.40	1.35
38	34	301	A86	C5-C6	3.42	1.40	1.35
29	a	405	BCR	C1-C6	-3.42	1.49	1.53
27	14	302	CLA	C4D-ND	-3.42	1.33	1.37
27	c	509	CLA	CMB-C2B	-3.42	1.43	1.50
27	31	308	CLA	C4D-ND	-3.42	1.33	1.37
38	13	316	A86	C5-C6	3.41	1.40	1.35
27	b	602	CLA	C1D-ND	3.41	1.42	1.37
29	A	405	BCR	C1-C6	-3.41	1.49	1.53
38	14	315	A86	C5-C6	3.40	1.40	1.35
27	34	308	CLA	C1D-ND	3.40	1.42	1.37
38	11	314	A86	C5-C6	3.40	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	33	310	CLA	C4D-ND	-3.40	1.33	1.37
27	32	309	CLA	C1D-ND	3.39	1.42	1.37
27	14	310	CLA	C4D-ND	-3.39	1.33	1.37
27	C	509	CLA	CMB-C2B	-3.39	1.43	1.50
27	12	309	CLA	C1D-ND	3.39	1.41	1.37
27	32	312	CLA	C4D-ND	-3.39	1.33	1.37
38	12	314	A86	C19-C18	3.39	1.57	1.52
38	13	312	A86	C19-C18	3.38	1.57	1.52
27	z	102	CLA	C1D-ND	3.38	1.41	1.37
27	33	309	CLA	C1D-ND	3.38	1.41	1.37
27	13	307	CLA	C1D-ND	3.38	1.41	1.37
27	B	602	CLA	C1D-ND	3.37	1.41	1.37
38	32	317	A86	C5-C6	3.37	1.40	1.35
27	12	309	CLA	C4D-ND	-3.37	1.33	1.37
27	13	307	CLA	C4D-ND	-3.37	1.33	1.37
27	32	306	CLA	C4D-ND	-3.37	1.33	1.37
38	12	317	A86	C5-C6	3.37	1.40	1.35
27	Z	102	CLA	C1D-ND	3.37	1.41	1.37
27	31	305	CLA	C4D-ND	-3.37	1.33	1.37
29	c	515	BCR	C1-C6	-3.36	1.49	1.53
38	32	314	A86	C19-C18	3.36	1.57	1.52
27	c	511	CLA	MG-NB	-3.36	1.99	2.05
27	11	302	CLA	C4D-ND	-3.36	1.33	1.37
27	13	309	CLA	C1D-ND	3.36	1.41	1.37
38	13	315	A86	C5-C6	3.36	1.40	1.35
38	31	310	A86	C19-C18	3.35	1.57	1.52
27	C	511	CLA	MG-NB	-3.35	1.99	2.05
38	31	313	A86	C5-C6	3.35	1.40	1.35
27	13	311	CLA	C1D-ND	3.35	1.41	1.37
27	33	311	CLA	C4D-ND	-3.35	1.33	1.37
38	11	313	A86	C5-C6	3.35	1.40	1.35
29	C	515	BCR	C1-C6	-3.34	1.49	1.53
38	14	312	A86	C19-C18	3.34	1.57	1.52
27	12	306	CLA	C4D-ND	-3.34	1.33	1.37
27	31	307	CLA	C1D-ND	3.34	1.41	1.37
38	34	313	A86	C19-C18	3.34	1.57	1.52
27	34	311	CLA	C4D-ND	-3.34	1.33	1.37
38	34	316	A86	C5-C6	3.33	1.40	1.35
38	33	315	A86	C5-C6	3.33	1.40	1.35
27	11	305	CLA	C4D-ND	-3.33	1.33	1.37
36	D	407	PL9	C53-C6	-3.33	1.43	1.50
27	33	303	CLA	C1D-ND	3.33	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	34	305	CLA	C4D-ND	-3.33	1.33	1.37
27	34	308	CLA	C4D-ND	-3.32	1.33	1.37
27	B	615	CLA	C1D-ND	3.32	1.41	1.37
29	b	623	BCR	C1-C6	-3.32	1.49	1.53
27	14	307	CLA	C4D-ND	-3.32	1.33	1.37
27	11	309	CLA	C1D-ND	3.32	1.41	1.37
27	13	304	CLA	C4D-ND	-3.32	1.33	1.37
27	13	301	CLA	C1D-ND	3.32	1.41	1.37
27	32	311	CLA	C1D-ND	3.32	1.41	1.37
38	11	310	A86	C19-C18	3.32	1.57	1.52
28	D	403	PHO	C4D-ND	-3.31	1.33	1.38
27	32	309	CLA	C4D-ND	-3.31	1.33	1.37
27	31	301	CLA	C1D-ND	3.31	1.41	1.37
27	B	612	CLA	MG-ND	-3.31	1.99	2.05
27	b	615	CLA	C1D-ND	3.31	1.41	1.37
27	31	302	CLA	C4D-ND	-3.31	1.33	1.37
27	14	311	CLA	C4D-ND	-3.31	1.33	1.37
27	b	612	CLA	MG-ND	-3.31	1.99	2.05
27	14	311	CLA	C1D-ND	3.31	1.41	1.37
27	31	309	CLA	C1D-ND	3.31	1.41	1.37
38	33	312	A86	C19-C18	3.31	1.57	1.52
27	14	304	CLA	C4D-ND	-3.31	1.33	1.37
27	14	302	CLA	C1D-ND	3.31	1.41	1.37
27	14	309	CLA	C1D-ND	3.30	1.41	1.37
27	33	301	CLA	C1D-ND	3.30	1.41	1.37
27	32	313	CLA	C1D-ND	3.30	1.41	1.37
27	33	307	CLA	C4D-ND	-3.29	1.33	1.37
27	12	305	CLA	C1D-ND	3.29	1.41	1.37
38	14	313	A86	C5-C6	3.29	1.40	1.35
36	d	407	PL9	C53-C6	-3.29	1.43	1.50
27	34	312	CLA	C1D-ND	3.29	1.41	1.37
27	11	309	CLA	C4D-ND	-3.29	1.33	1.37
27	33	308	CLA	C4B-NB	3.29	1.41	1.37
27	34	310	CLA	C1D-ND	3.29	1.41	1.37
27	33	306	CLA	C1D-ND	3.29	1.41	1.37
27	33	311	CLA	C1D-ND	3.28	1.41	1.37
27	31	304	CLA	C4D-ND	-3.28	1.33	1.37
27	31	309	CLA	C4D-ND	-3.28	1.33	1.37
27	12	311	CLA	C1D-ND	3.28	1.41	1.37
27	11	307	CLA	C1D-ND	3.28	1.41	1.37
27	32	305	CLA	C1D-ND	3.28	1.41	1.37
27	14	303	CLA	C1D-ND	3.28	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	13	303	CLA	C1D-ND	3.28	1.41	1.37
27	33	304	CLA	C4D-ND	-3.28	1.33	1.37
27	c	511	CLA	CMD-C2D	-3.27	1.43	1.50
27	12	313	CLA	C1D-ND	3.27	1.41	1.37
27	32	313	CLA	C4D-ND	-3.27	1.33	1.37
27	12	303	CLA	C1D-ND	3.27	1.41	1.37
27	b	604	CLA	C1D-ND	3.27	1.41	1.37
28	d	403	PHO	C4D-ND	-3.27	1.34	1.38
27	32	303	CLA	C1D-ND	3.27	1.41	1.37
29	B	623	BCR	C1-C6	-3.26	1.49	1.53
27	c	503	CLA	C1D-ND	3.26	1.41	1.37
27	31	315	CLA	C1D-ND	3.25	1.41	1.37
38	33	313	A86	C5-C6	3.25	1.40	1.35
27	12	313	CLA	C4D-ND	-3.25	1.33	1.37
27	13	311	CLA	C4D-ND	-3.25	1.33	1.37
27	34	304	CLA	C1D-ND	3.25	1.41	1.37
27	11	315	CLA	C1D-ND	3.24	1.41	1.37
27	13	306	CLA	C4D-ND	-3.24	1.33	1.37
27	11	304	CLA	C1D-ND	3.24	1.41	1.37
38	13	313	A86	C5-C6	3.24	1.40	1.35
27	B	604	CLA	C1D-ND	3.24	1.41	1.37
27	C	503	CLA	C1D-ND	3.24	1.41	1.37
27	32	308	CLA	C4D-ND	-3.24	1.33	1.37
27	14	310	CLA	C1D-ND	3.24	1.41	1.37
27	31	308	CLA	C1D-ND	3.24	1.41	1.37
27	11	301	CLA	C1D-ND	3.24	1.41	1.37
27	12	308	CLA	C4D-ND	-3.23	1.33	1.37
38	14	313	A86	C19-C18	3.23	1.57	1.52
27	31	306	CLA	C4B-NB	3.23	1.41	1.37
27	13	306	CLA	C1D-ND	3.23	1.41	1.37
38	11	311	A86	C19-C18	3.23	1.57	1.52
27	C	511	CLA	CMD-C2D	-3.23	1.44	1.50
27	14	306	CLA	C4D-ND	-3.23	1.33	1.37
27	32	308	CLA	C1D-ND	3.23	1.41	1.37
27	W	103	CLA	C4B-NB	3.22	1.41	1.37
27	11	304	CLA	C4D-ND	-3.22	1.33	1.37
29	f	101	BCR	C1-C6	-3.22	1.49	1.53
27	34	302	CLA	C1D-ND	3.22	1.41	1.37
27	12	310	CLA	C4B-NB	3.22	1.41	1.37
27	b	612	CLA	MG-NB	-3.22	1.99	2.05
27	33	306	CLA	C4D-ND	-3.21	1.33	1.37
27	13	308	CLA	C4B-NB	3.21	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	512	CLA	C1D-ND	3.21	1.41	1.37
29	F	101	BCR	C1-C6	-3.21	1.49	1.53
38	32	315	A86	C19-C18	3.21	1.56	1.52
27	33	308	CLA	C4D-ND	-3.20	1.33	1.37
38	32	315	A86	C5-C6	3.20	1.40	1.35
38	31	311	A86	C5-C6	3.20	1.40	1.35
38	34	314	A86	C19-C18	3.20	1.56	1.52
27	c	509	CLA	MG-NB	-3.19	1.99	2.05
27	11	308	CLA	C1D-ND	3.19	1.41	1.37
38	31	311	A86	C19-C18	3.19	1.56	1.52
27	w	103	CLA	C4B-NB	3.19	1.41	1.37
27	c	512	CLA	C1D-ND	3.19	1.41	1.37
27	32	310	CLA	C4B-NB	3.19	1.41	1.37
27	11	306	CLA	C4B-NB	3.19	1.41	1.37
27	C	511	CLA	C1B-NB	-3.19	1.33	1.37
27	31	304	CLA	C1D-ND	3.19	1.41	1.37
27	13	310	CLA	C1D-ND	3.19	1.41	1.37
38	12	315	A86	C5-C6	3.19	1.40	1.35
27	34	307	CLA	C4D-ND	-3.18	1.33	1.37
27	14	308	CLA	C4B-NB	3.18	1.41	1.37
29	b	616	BCR	C1-C6	-3.18	1.49	1.53
38	34	314	A86	C5-C6	3.18	1.40	1.35
38	11	311	A86	C25-C24	3.18	1.42	1.34
27	34	309	CLA	C4D-ND	-3.18	1.33	1.37
27	34	312	CLA	C4D-ND	-3.18	1.33	1.37
38	12	315	A86	C19-C18	3.18	1.56	1.52
38	11	311	A86	C5-C6	3.17	1.40	1.35
27	B	612	CLA	MG-NB	-3.17	1.99	2.05
27	32	312	CLA	C1D-ND	3.17	1.41	1.37
27	33	310	CLA	C1D-ND	3.17	1.41	1.37
27	34	309	CLA	C4B-NB	3.17	1.41	1.37
27	12	308	CLA	C1D-ND	3.17	1.41	1.37
27	14	306	CLA	C1D-ND	3.17	1.41	1.37
27	31	306	CLA	C1D-ND	3.17	1.41	1.37
27	34	305	CLA	C1D-ND	3.17	1.41	1.37
38	33	313	A86	C25-C24	3.17	1.42	1.34
27	34	311	CLA	C1D-ND	3.16	1.41	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
38	31	311	A86	C25-C24	3.16	1.42	1.34
38	32	315	A86	C25-C24	3.16	1.42	1.34
38	13	313	A86	C19-C18	3.16	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	W	103	CLA	C4D-ND	-3.16	1.33	1.37
27	33	308	CLA	C1D-ND	3.16	1.41	1.37
38	13	313	A86	C25-C24	3.16	1.42	1.34
27	w	103	CLA	C4D-ND	-3.16	1.33	1.37
38	12	315	A86	C25-C24	3.16	1.42	1.34
38	33	313	A86	C19-C18	3.16	1.56	1.52
27	D	401	CLA	MG-NB	-3.15	1.99	2.05
27	34	309	CLA	C1D-ND	3.15	1.41	1.37
27	13	308	CLA	C4D-ND	-3.15	1.33	1.37
35	c	518	DGD	O2G-C2G	-3.15	1.38	1.46
38	34	314	A86	C25-C24	3.15	1.42	1.34
38	13	312	A86	C5-C6	3.15	1.40	1.35
38	34	313	A86	C5-C6	3.14	1.40	1.35
38	14	313	A86	C25-C24	3.14	1.42	1.34
29	B	616	BCR	C1-C6	-3.14	1.49	1.53
39	32	302	LMU	O5'-C1'	3.14	1.49	1.41
27	12	310	CLA	C1D-ND	3.14	1.41	1.37
27	31	306	CLA	C4D-ND	-3.13	1.33	1.37
27	12	310	CLA	C4D-ND	-3.13	1.33	1.37
27	12	312	CLA	C1D-ND	3.13	1.41	1.37
27	32	310	CLA	C1D-ND	3.13	1.41	1.37
29	C	520	BCR	C1-C6	-3.13	1.49	1.53
27	d	401	CLA	MG-NB	-3.13	1.99	2.05
29	c	519	BCR	C1-C6	-3.13	1.49	1.53
27	11	306	CLA	C4D-ND	-3.12	1.33	1.37
27	14	308	CLA	C1D-ND	3.12	1.41	1.37
27	13	308	CLA	C1D-ND	3.12	1.41	1.37
39	12	302	LMU	O5'-C1'	3.12	1.49	1.41
27	C	503	CLA	MG-NB	-3.12	1.99	2.05
27	c	511	CLA	C1B-NB	-3.12	1.34	1.37
27	11	302	CLA	C1D-ND	3.11	1.41	1.37
27	14	308	CLA	C4D-ND	-3.11	1.33	1.37
35	C	518	DGD	O2G-C2G	-3.11	1.38	1.46
27	32	306	CLA	C1D-ND	3.11	1.41	1.37
27	b	605	CLA	C1D-ND	3.11	1.41	1.37
27	12	307	CLA	C1D-ND	3.10	1.41	1.37
27	31	302	CLA	C1D-ND	3.10	1.41	1.37
29	A	405	BCR	C30-C25	-3.10	1.49	1.53
27	B	605	CLA	C1D-ND	3.10	1.41	1.37
38	31	312	A86	C25-C24	3.09	1.42	1.34
27	34	307	CLA	C1D-ND	3.09	1.41	1.37
29	a	405	BCR	C30-C25	-3.09	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	32	310	CLA	C4D-ND	-3.09	1.33	1.37
36	D	407	PL9	C36-C34	-3.09	1.44	1.51
27	12	306	CLA	C1D-ND	3.09	1.41	1.37
27	B	606	CLA	C4B-NB	3.09	1.41	1.37
27	B	604	CLA	MG-NB	-3.08	1.99	2.05
29	B	617	BCR	C1-C6	-3.08	1.49	1.53
38	31	310	A86	C5-C6	3.08	1.39	1.35
38	11	312	A86	C25-C24	3.08	1.42	1.34
27	c	508	CLA	MG-NB	-3.08	1.99	2.05
29	b	617	BCR	C1-C6	-3.08	1.49	1.53
36	d	407	PL9	C36-C34	-3.08	1.44	1.51
27	b	601	CLA	C1D-ND	3.07	1.41	1.37
32	L	102	LHG	O7-C5	-3.07	1.38	1.46
38	32	316	A86	C25-C24	3.07	1.42	1.34
38	14	312	A86	C5-C6	3.07	1.39	1.35
28	A	403	PHO	CMC-C2C	-3.07	1.45	1.50
28	a	403	PHO	CMC-C2C	-3.07	1.45	1.50
27	C	510	CLA	MG-NB	-3.07	1.99	2.05
38	14	314	A86	C25-C24	3.07	1.42	1.34
27	13	304	CLA	C1D-ND	3.07	1.41	1.37
38	12	314	A86	C5-C6	3.06	1.39	1.35
27	11	306	CLA	C1D-ND	3.06	1.41	1.37
38	11	310	A86	C5-C6	3.06	1.39	1.35
27	c	510	CLA	MG-NB	-3.06	1.99	2.05
38	34	315	A86	C25-C24	3.06	1.42	1.34
32	l	103	LHG	O7-C5	-3.06	1.38	1.46
38	13	314	A86	C25-C24	3.06	1.42	1.34
38	33	312	A86	C5-C6	3.05	1.39	1.35
33	C	519	LMG	O7-C8	-3.05	1.39	1.46
28	A	403	PHO	CAC-C3C	-3.05	1.46	1.51
38	12	316	A86	C25-C24	3.05	1.42	1.34
27	14	305	CLA	C1D-ND	3.05	1.41	1.37
27	C	508	CLA	MG-NB	-3.05	1.99	2.05
33	b	619	LMG	O8-C9	-3.05	1.38	1.45
38	32	314	A86	C5-C6	3.04	1.39	1.35
27	b	604	CLA	MG-NB	-3.04	1.99	2.05
27	32	307	CLA	C1D-ND	3.04	1.41	1.37
27	b	613	CLA	C1B-NB	-3.04	1.34	1.37
38	33	314	A86	C25-C24	3.04	1.42	1.34
27	14	304	CLA	C1D-ND	3.04	1.41	1.37
28	a	403	PHO	CAC-C3C	-3.04	1.46	1.51
28	A	403	PHO	CMD-C2D	-3.04	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	606	CLA	C4B-NB	3.03	1.41	1.37
38	31	312	A86	C19-C18	3.03	1.56	1.52
38	32	304	A86	C19-C18	3.03	1.56	1.52
33	q	301	LMG	O7-C8	-3.03	1.39	1.46
30	L	103	SQD	O47-C7	3.03	1.42	1.34
29	B	617	BCR	C30-C25	-3.03	1.49	1.53
35	j	101	DGD	O2G-C2G	-3.03	1.39	1.46
38	11	312	A86	C19-C18	3.02	1.56	1.52
27	b	610	CLA	MG-NB	-3.02	1.99	2.05
33	B	619	LMG	O8-C9	-3.02	1.38	1.45
27	B	601	CLA	C1D-ND	3.02	1.41	1.37
27	31	303	CLA	C1D-ND	3.02	1.41	1.37
35	J	101	DGD	O2G-C2G	-3.02	1.39	1.46
30	l	101	SQD	O47-C7	3.02	1.42	1.34
27	d	406	CLA	MG-NB	-3.02	1.99	2.05
38	12	316	A86	C19-C18	3.01	1.56	1.52
38	33	314	A86	C19-C18	3.01	1.56	1.52
27	B	613	CLA	MG-NB	-3.01	1.99	2.05
27	b	613	CLA	MG-NB	-3.01	1.99	2.05
28	A	403	PHO	C1D-C2D	3.01	1.42	1.39
27	13	305	CLA	C1D-ND	3.01	1.41	1.37
38	32	317	A86	C25-C24	3.00	1.42	1.34
27	B	613	CLA	C1B-NB	-2.99	1.34	1.37
28	a	403	PHO	CMD-C2D	-2.99	1.45	1.51
35	c	517	DGD	O1G-C1G	-2.99	1.38	1.45
27	B	610	CLA	MG-NB	-2.99	1.99	2.05
38	31	316	A86	C25-C24	2.99	1.42	1.34
27	B	606	CLA	C1D-ND	2.99	1.41	1.37
38	13	314	A86	C19-C18	2.99	1.56	1.52
27	D	406	CLA	MG-NB	-2.99	1.99	2.05
38	12	304	A86	C19-C18	2.98	1.56	1.52
38	32	316	A86	C19-C18	2.98	1.56	1.52
27	b	611	CLA	MG-NB	-2.98	1.99	2.05
27	b	606	CLA	C1D-ND	2.98	1.41	1.37
38	14	315	A86	C25-C24	2.98	1.42	1.34
33	D	408	LMG	O7-C8	-2.98	1.39	1.46
38	32	304	A86	C25-C24	2.98	1.42	1.34
27	33	304	CLA	C1D-ND	2.98	1.41	1.37
33	d	408	LMG	O7-C8	-2.98	1.39	1.46
27	34	306	CLA	C1D-ND	2.98	1.41	1.37
35	C	517	DGD	O1G-C1G	-2.98	1.38	1.45
38	13	315	A86	C25-C24	2.98	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	611	CLA	MG-NB	-2.98	1.99	2.05
38	34	303	A86	C19-C18	2.98	1.56	1.52
38	12	317	A86	C25-C24	2.97	1.42	1.34
38	31	313	A86	C25-C24	2.97	1.42	1.34
27	c	510	CLA	CMB-C2B	-2.97	1.44	1.50
28	D	403	PHO	CMC-C2C	-2.97	1.45	1.50
38	34	303	A86	C25-C24	2.97	1.42	1.34
38	33	302	A86	C19-C18	2.97	1.56	1.52
38	11	313	A86	C25-C24	2.97	1.42	1.34
38	34	316	A86	C25-C24	2.97	1.42	1.34
38	13	302	A86	C25-C24	2.97	1.42	1.34
28	D	403	PHO	C4D-CHA	2.97	1.44	1.39
27	11	303	CLA	C1D-ND	2.97	1.41	1.37
29	b	617	BCR	C30-C25	-2.97	1.49	1.53
33	C	519	LMG	O1-C7	-2.96	1.38	1.43
38	13	317	A86	C25-C24	2.96	1.42	1.34
27	b	622	CLA	MG-NB	-2.96	1.99	2.05
38	12	304	A86	C25-C24	2.96	1.42	1.34
38	14	314	A86	C19-C18	2.96	1.56	1.52
27	c	507	CLA	MG-NB	-2.96	1.99	2.05
27	w	102	CLA	C1D-ND	2.96	1.41	1.37
28	d	403	PHO	C4D-CHA	2.96	1.44	1.39
38	33	315	A86	C25-C24	2.96	1.42	1.34
38	33	302	A86	C25-C24	2.96	1.42	1.34
27	B	622	CLA	CMD-C2D	-2.96	1.44	1.50
27	b	622	CLA	CMD-C2D	-2.95	1.44	1.50
27	C	506	CLA	C1D-ND	2.95	1.41	1.37
38	13	302	A86	C19-C18	2.95	1.56	1.52
27	B	608	CLA	C4B-NB	2.95	1.41	1.37
33	q	301	LMG	O1-C7	-2.95	1.38	1.43
27	d	402	CLA	C1D-ND	2.94	1.41	1.37
38	13	317	A86	C19-C18	2.94	1.56	1.52
27	C	510	CLA	CMB-C2B	-2.94	1.44	1.50
27	b	608	CLA	C4B-NB	2.94	1.41	1.37
27	13	311	CLA	C4B-NB	2.94	1.41	1.37
38	11	316	A86	C19-C18	2.94	1.56	1.52
32	b	621	LHG	O7-C5	-2.94	1.39	1.46
38	31	316	A86	C19-C18	2.94	1.56	1.52
38	11	316	A86	C25-C24	2.93	1.42	1.34
38	34	315	A86	C19-C18	2.93	1.56	1.52
29	a	409	BCR	C1-C6	-2.93	1.49	1.53
27	B	622	CLA	MG-NB	-2.93	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	D	402	CLA	C1D-ND	2.93	1.41	1.37
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	C	507	CLA	MG-NB	-2.93	2.00	2.05
27	33	305	CLA	C1D-ND	2.93	1.41	1.37
27	14	306	CLA	MG-NB	-2.92	2.00	2.05
27	a	404	CLA	MG-NB	-2.92	2.00	2.05
27	W	102	CLA	C1D-ND	2.92	1.41	1.37
27	c	506	CLA	C1D-ND	2.92	1.41	1.37
30	b	620	SQD	O48-C23	2.92	1.41	1.33
29	b	616	BCR	C30-C25	-2.92	1.49	1.53
27	13	306	CLA	MG-NB	-2.92	2.00	2.05
27	12	313	CLA	C4B-NB	2.92	1.41	1.37
27	34	312	CLA	C4B-NB	2.92	1.41	1.37
28	d	403	PHO	CMC-C2C	-2.91	1.45	1.50
27	31	309	CLA	C4B-NB	2.91	1.41	1.37
30	B	620	SQD	O48-C23	2.91	1.41	1.33
27	11	304	CLA	MG-NB	-2.91	2.00	2.05
29	z	101	BCR	C30-C25	-2.91	1.49	1.53
27	C	511	CLA	MG-ND	-2.91	2.00	2.05
27	b	609	CLA	C1D-ND	2.91	1.41	1.37
28	a	403	PHO	C1D-C2D	2.91	1.42	1.39
29	A	409	BCR	C1-C6	-2.91	1.49	1.53
27	12	308	CLA	MG-NB	-2.90	2.00	2.05
27	33	311	CLA	C4B-NB	2.90	1.41	1.37
27	C	509	CLA	C1B-NB	-2.90	1.34	1.37
27	11	309	CLA	C4B-NB	2.90	1.41	1.37
27	C	504	CLA	C1D-ND	2.89	1.41	1.37
27	32	313	CLA	C4B-NB	2.89	1.41	1.37
32	B	621	LHG	O7-C5	-2.89	1.39	1.46
27	C	503	CLA	MG-ND	-2.89	2.00	2.05
27	D	405	CLA	CMD-C2D	-2.88	1.44	1.50
27	14	311	CLA	C4B-NB	2.88	1.41	1.37
27	32	308	CLA	MG-NB	-2.88	2.00	2.05
29	B	616	BCR	C30-C25	-2.88	1.49	1.53
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	c	509	CLA	C1B-NB	-2.87	1.34	1.37
27	C	508	CLA	C1D-ND	2.87	1.41	1.37
27	c	504	CLA	C1D-ND	2.87	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	d	407	PL9	C26-C24	-2.87	1.45	1.51
27	z	102	CLA	MG-NB	-2.87	2.00	2.05
27	c	503	CLA	CMC-C2C	-2.87	1.44	1.50
29	Z	101	BCR	C30-C25	-2.87	1.49	1.53
27	B	608	CLA	C3B-C4B	2.86	1.49	1.42
36	d	407	PL9	C11-C9	-2.86	1.45	1.51
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	b	607	CLA	MG-NB	-2.86	2.00	2.05
27	c	503	CLA	MG-ND	-2.85	2.00	2.05
27	B	611	CLA	CMC-C2C	-2.85	1.44	1.50
27	b	611	CLA	CMC-C2C	-2.85	1.44	1.50
27	c	506	CLA	CMD-C2D	-2.85	1.44	1.50
27	b	608	CLA	C3B-C4B	2.85	1.49	1.42
27	b	603	CLA	MG-NB	-2.84	2.00	2.05
27	b	606	CLA	CMD-C2D	-2.84	1.44	1.50
38	13	312	A86	C25-C24	2.84	1.41	1.34
27	11	307	CLA	MG-NB	-2.84	2.00	2.05
27	c	513	CLA	C1D-ND	2.84	1.41	1.37
27	d	405	CLA	CMD-C2D	-2.84	1.44	1.50
36	D	407	PL9	C11-C9	-2.84	1.45	1.51
27	b	614	CLA	C1D-ND	2.84	1.41	1.37
27	13	309	CLA	MG-NB	-2.84	2.00	2.05
29	a	409	BCR	C30-C25	-2.84	1.49	1.53
38	34	301	A86	C25-C24	2.83	1.41	1.34
27	C	506	CLA	CMD-C2D	-2.83	1.44	1.50
27	B	609	CLA	C1D-ND	2.83	1.41	1.37
27	B	603	CLA	MG-NB	-2.83	2.00	2.05
27	a	402	CLA	C1D-ND	2.83	1.41	1.37
27	b	615	CLA	C1B-NB	-2.83	1.34	1.37
38	14	312	A86	C25-C24	2.83	1.41	1.34
38	31	314	A86	C25-C24	2.83	1.41	1.34
27	B	606	CLA	CMD-C2D	-2.83	1.44	1.50
27	31	307	CLA	MG-NB	-2.83	2.00	2.05
30	A	406	SQD	O48-C23	2.83	1.41	1.33
38	32	318	A86	C25-C24	2.83	1.41	1.34
36	D	407	PL9	C26-C24	-2.83	1.45	1.51
27	C	503	CLA	CMC-C2C	-2.82	1.44	1.50
29	c	516	BCR	C30-C25	-2.82	1.49	1.53
38	11	314	A86	C25-C24	2.82	1.41	1.34
29	A	409	BCR	C30-C25	-2.82	1.49	1.53
27	34	310	CLA	MG-NB	-2.82	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	504	CLA	CMD-C2D	-2.82	1.44	1.50
27	D	401	CLA	CMB-C2B	-2.82	1.44	1.50
27	d	401	CLA	CMB-C2B	-2.82	1.44	1.50
27	c	508	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
27	C	514	CLA	C1D-ND	2.81	1.41	1.37
27	c	508	CLA	MG-ND	-2.81	2.00	2.05
38	31	310	A86	C25-C24	2.81	1.41	1.34
38	34	313	A86	C25-C24	2.81	1.41	1.34
29	H	101	BCR	C30-C25	-2.81	1.49	1.53
27	b	604	CLA	MG-ND	-2.81	2.00	2.05
27	14	309	CLA	MG-NB	-2.81	2.00	2.05
38	13	316	A86	C25-C24	2.81	1.41	1.34
28	a	403	PHO	CBD-CGD	-2.81	1.48	1.52
38	33	312	A86	C25-C24	2.81	1.41	1.34
38	32	314	A86	C25-C24	2.81	1.41	1.34
27	B	601	CLA	MG-NB	-2.81	2.00	2.05
27	B	604	CLA	MG-ND	-2.81	2.00	2.05
28	A	403	PHO	CMB-C2B	-2.81	1.45	1.51
27	32	303	CLA	C4B-NB	2.81	1.41	1.37
27	13	301	CLA	C4B-NB	2.81	1.41	1.37
27	33	309	CLA	MG-NB	-2.81	2.00	2.05
27	B	615	CLA	C3B-C4B	2.81	1.49	1.42
30	a	406	SQD	O48-C23	2.81	1.41	1.33
27	b	615	CLA	C3B-C4B	2.81	1.49	1.42
38	14	301	A86	C25-C24	2.81	1.41	1.34
27	d	405	CLA	MG-NB	-2.81	2.00	2.05
27	w	102	CLA	C3B-C4B	2.80	1.49	1.42
27	32	311	CLA	MG-NB	-2.80	2.00	2.05
38	14	316	A86	C25-C24	2.80	1.41	1.34
28	a	403	PHO	CMB-C2B	-2.80	1.45	1.51
27	C	513	CLA	C1D-ND	2.80	1.41	1.37
38	33	316	A86	C25-C24	2.80	1.41	1.34
28	A	403	PHO	CBD-CGD	-2.80	1.48	1.52
38	11	310	A86	C25-C24	2.80	1.41	1.34
27	c	514	CLA	C1D-ND	2.80	1.41	1.37
27	b	606	CLA	C3B-C4B	2.80	1.49	1.42
27	13	307	CLA	C4B-NB	2.80	1.41	1.37
29	h	101	BCR	C30-C25	-2.80	1.49	1.53
27	12	303	CLA	C3B-C4B	2.79	1.49	1.42
27	b	607	CLA	C1D-ND	2.79	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	v	201	HEM	CAB-C3B	2.79	1.55	1.47
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	11	315	CLA	C3B-C4B	2.78	1.49	1.42
27	32	303	CLA	C3B-C4B	2.78	1.49	1.42
36	D	407	PL9	C41-C39	-2.78	1.45	1.51
27	w	103	CLA	C3B-C4B	2.78	1.49	1.42
27	b	601	CLA	MG-NB	-2.78	2.00	2.05
27	31	315	CLA	C3B-C4B	2.78	1.49	1.42
38	12	314	A86	C25-C24	2.78	1.41	1.34
27	B	614	CLA	C1D-ND	2.78	1.41	1.37
27	D	401	CLA	CMD-C2D	-2.78	1.44	1.50
27	13	301	CLA	C3B-C4B	2.78	1.49	1.42
27	14	302	CLA	C3B-C4B	2.78	1.49	1.42
38	13	316	A86	C19-C18	2.77	1.56	1.52
27	C	502	CLA	MG-NB	-2.77	2.00	2.05
36	D	404	PL9	C6-C1	-2.77	1.43	1.48
27	33	301	CLA	C4B-NB	2.77	1.41	1.37
27	B	607	CLA	C1D-ND	2.77	1.41	1.37
27	B	615	CLA	C1B-NB	-2.77	1.34	1.37
27	34	302	CLA	C4B-NB	2.77	1.41	1.37
37	E	101	HEM	CAB-C3B	2.77	1.55	1.47
27	33	301	CLA	C3B-C4B	2.77	1.49	1.42
28	D	403	PHO	CMD-C2D	-2.77	1.45	1.51
27	c	505	CLA	MG-NB	-2.77	2.00	2.05
36	d	404	PL9	C6-C1	-2.77	1.43	1.48
27	31	315	CLA	C4B-NB	2.77	1.41	1.37
37	f	102	HEM	CAB-C3B	2.77	1.55	1.47
27	W	102	CLA	C3B-C4B	2.77	1.49	1.42
27	C	504	CLA	CMD-C2D	-2.77	1.44	1.50
27	c	510	CLA	C1B-NB	-2.77	1.34	1.37
29	C	516	BCR	C30-C25	-2.77	1.50	1.53
27	B	606	CLA	C1B-NB	-2.77	1.34	1.37
27	A	402	CLA	C1D-ND	2.76	1.41	1.37
27	b	610	CLA	C1B-NB	-2.76	1.34	1.37
27	B	606	CLA	C3B-C4B	2.76	1.49	1.42
27	a	404	CLA	CMD-C2D	-2.76	1.44	1.50
27	c	507	CLA	MG-ND	-2.76	2.00	2.05
37	V	201	HEM	CAB-C3B	2.76	1.54	1.47
27	11	304	CLA	C3B-C4B	2.76	1.49	1.42
27	31	304	CLA	C3B-C4B	2.76	1.49	1.42
27	B	612	CLA	CMC-C2C	-2.75	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d	401	CLA	CMD-C2D	-2.75	1.45	1.50
27	33	307	CLA	C4B-NB	2.75	1.41	1.37
27	c	514	CLA	C1B-NB	-2.75	1.34	1.37
36	D	407	PL9	C46-C44	-2.75	1.45	1.51
36	d	407	PL9	C46-C44	-2.75	1.45	1.51
27	C	503	CLA	CMB-C2B	-2.75	1.45	1.50
27	34	302	CLA	C3B-C4B	2.75	1.49	1.42
27	b	612	CLA	CMC-C2C	-2.75	1.45	1.50
27	11	315	CLA	C4B-NB	2.75	1.41	1.37
27	12	309	CLA	C4B-NB	2.75	1.41	1.37
38	34	316	A86	O-C13	-2.75	1.17	1.23
27	C	510	CLA	C1B-NB	-2.75	1.34	1.37
27	12	308	CLA	C3B-C4B	2.75	1.49	1.42
27	m	101	CLA	MG-NB	-2.75	2.00	2.05
36	d	407	PL9	C41-C39	-2.75	1.45	1.51
27	11	305	CLA	C4B-NB	2.75	1.41	1.37
27	31	305	CLA	C4B-NB	2.75	1.41	1.37
27	W	103	CLA	C3B-C4B	2.75	1.49	1.42
36	d	404	PL9	C53-C6	-2.74	1.45	1.50
27	A	404	CLA	CMD-C2D	-2.74	1.45	1.50
38	14	316	A86	C19-C18	2.74	1.56	1.52
38	34	301	A86	C19-C18	2.74	1.56	1.52
27	33	306	CLA	C3B-C4B	2.74	1.49	1.42
27	B	604	CLA	CMD-C2D	-2.74	1.45	1.50
27	b	615	CLA	CMC-C2C	-2.74	1.45	1.50
38	32	318	A86	C19-C18	2.74	1.56	1.52
27	14	306	CLA	C3B-C4B	2.74	1.49	1.42
27	M	102	CLA	MG-NB	-2.74	2.00	2.05
38	11	314	A86	C19-C18	2.74	1.56	1.52
35	c	518	DGD	O6D-C5D	-2.74	1.37	1.44
27	C	507	CLA	MG-ND	-2.74	2.00	2.05
27	c	507	CLA	C4B-NB	2.73	1.41	1.37
38	32	317	A86	O-C13	-2.73	1.17	1.23
28	d	403	PHO	CMD-C2D	-2.73	1.46	1.51
27	c	502	CLA	MG-NB	-2.73	2.00	2.05
38	33	312	A86	O-C13	-2.73	1.17	1.23
36	D	404	PL9	C53-C6	-2.73	1.45	1.50
27	34	307	CLA	C3B-C4B	2.73	1.49	1.42
27	c	509	CLA	MG-ND	-2.73	2.00	2.05
27	b	604	CLA	CMD-C2D	-2.73	1.45	1.50
27	C	509	CLA	CMC-C2C	-2.73	1.45	1.50
27	C	509	CLA	MG-ND	-2.73	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	13	312	A86	O-C13	-2.73	1.17	1.23
27	32	309	CLA	C4B-NB	2.73	1.41	1.37
37	E	101	HEM	CAC-C3C	2.73	1.54	1.47
27	32	308	CLA	C3B-C4B	2.73	1.49	1.42
27	32	305	CLA	MG-NB	-2.72	2.00	2.05
27	14	302	CLA	C4B-NB	2.72	1.41	1.37
35	J	101	DGD	O5D-C6D	-2.72	1.38	1.43
27	b	603	CLA	C1D-ND	2.72	1.41	1.37
27	B	609	CLA	MG-NB	-2.72	2.00	2.05
27	13	303	CLA	MG-NB	-2.72	2.00	2.05
27	b	612	CLA	C1B-NB	-2.72	1.34	1.37
27	c	509	CLA	CMC-C2C	-2.72	1.45	1.50
27	12	305	CLA	MG-NB	-2.72	2.00	2.05
38	12	317	A86	O-C13	-2.72	1.17	1.23
33	12	301	LMG	O1-C1	2.72	1.44	1.40
38	12	314	A86	O-C13	-2.72	1.17	1.23
27	b	615	CLA	CMD-C2D	-2.71	1.45	1.50
38	33	315	A86	O-C13	-2.71	1.17	1.23
27	B	610	CLA	C1B-NB	-2.71	1.34	1.37
27	14	307	CLA	C4B-NB	2.71	1.41	1.37
38	31	314	A86	C19-C18	2.71	1.56	1.52
27	b	609	CLA	MG-NB	-2.71	2.00	2.05
30	l	101	SQD	O48-C23	2.71	1.41	1.33
27	B	602	CLA	CMC-C2C	-2.71	1.45	1.50
38	32	314	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
27	c	503	CLA	CMB-C2B	-2.71	1.45	1.50
38	11	310	A86	O-C13	-2.71	1.17	1.23
38	13	315	A86	O-C13	-2.71	1.17	1.23
27	C	514	CLA	C1B-NB	-2.71	1.34	1.37
27	b	611	CLA	C1D-ND	2.71	1.41	1.37
27	34	308	CLA	C4B-NB	2.71	1.41	1.37
27	C	505	CLA	C1B-NB	-2.71	1.34	1.37
27	m	101	CLA	C1D-ND	2.71	1.41	1.37
38	14	312	A86	O-C13	-2.70	1.17	1.23
27	C	505	CLA	MG-NB	-2.70	2.00	2.05
38	34	313	A86	O-C13	-2.70	1.17	1.23
27	B	612	CLA	C1B-NB	-2.70	1.34	1.37
38	11	313	A86	O-C13	-2.70	1.17	1.23
30	L	103	SQD	O48-C23	2.70	1.41	1.33
37	f	102	HEM	CAC-C3C	2.70	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	32	313	CLA	C3B-C4B	2.70	1.49	1.42
27	B	615	CLA	CMC-C2C	-2.70	1.45	1.50
27	B	615	CLA	CMD-C2D	-2.70	1.45	1.50
27	13	306	CLA	C3B-C4B	2.70	1.49	1.42
27	b	606	CLA	C1B-NB	-2.70	1.34	1.37
27	33	303	CLA	MG-NB	-2.70	2.00	2.05
38	34	316	A86	C-C1	2.70	1.56	1.50
35	C	518	DGD	O5D-C6D	-2.69	1.38	1.43
38	33	315	A86	C-C1	2.69	1.56	1.50
27	B	613	CLA	C1D-ND	2.69	1.41	1.37
27	b	602	CLA	CMC-C2C	-2.69	1.45	1.50
38	14	315	A86	O-C13	-2.69	1.17	1.23
38	11	312	A86	C-C1	2.69	1.56	1.50
35	c	518	DGD	O5D-C6D	-2.69	1.38	1.43
35	C	518	DGD	O6D-C5D	-2.69	1.37	1.44
38	34	315	A86	C14-C15	2.69	1.58	1.52
27	B	609	CLA	C4B-NB	2.69	1.41	1.37
27	31	309	CLA	C3B-C4B	2.69	1.49	1.42
27	34	312	CLA	C3B-C4B	2.69	1.49	1.42
27	33	309	CLA	O2A-C1	-2.69	1.38	1.46
27	B	603	CLA	CMB-C2B	-2.69	1.45	1.50
27	c	505	CLA	C1B-NB	-2.69	1.34	1.37
27	13	311	CLA	C3B-C4B	2.69	1.49	1.42
27	C	512	CLA	MG-NB	-2.69	2.00	2.05
27	C	505	CLA	C1D-ND	2.69	1.41	1.37
38	31	310	A86	O-C13	-2.68	1.17	1.23
27	b	604	CLA	CMB-C2B	-2.68	1.45	1.50
38	31	312	A86	C-C1	2.68	1.56	1.50
27	m	101	CLA	CMD-C2D	-2.68	1.45	1.50
27	14	311	CLA	C3B-C4B	2.68	1.49	1.42
28	D	403	PHO	CBD-CGD	-2.68	1.48	1.52
27	11	301	CLA	MG-NB	-2.68	2.00	2.05
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	12	313	CLA	C3B-C4B	2.68	1.49	1.42
27	M	102	CLA	CMD-C2D	-2.68	1.45	1.50
38	31	313	A86	O-C13	-2.68	1.17	1.23
27	b	613	CLA	C1D-ND	2.68	1.41	1.37
27	33	311	CLA	C3B-C4B	2.68	1.49	1.42
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	502	CLA	CMD-C2D	-2.68	1.45	1.50
35	j	101	DGD	O5D-C6D	-2.67	1.38	1.43
27	34	304	CLA	MG-NB	-2.67	2.00	2.05
27	C	508	CLA	C1B-NB	-2.67	1.34	1.37
28	d	403	PHO	CMB-C2B	-2.67	1.46	1.51
36	D	407	PL9	C5-C4	-2.67	1.37	1.47
27	B	604	CLA	CMB-C2B	-2.67	1.45	1.50
27	w	103	CLA	CMD-C2D	-2.67	1.45	1.50
27	C	505	CLA	CMB-C2B	-2.67	1.45	1.50
27	b	608	CLA	CMB-C2B	-2.67	1.45	1.50
27	12	303	CLA	C4B-NB	2.67	1.41	1.37
27	b	622	CLA	MG-ND	-2.67	2.00	2.05
28	D	403	PHO	CMB-C2B	-2.67	1.46	1.51
27	c	512	CLA	MG-NB	-2.67	2.00	2.05
38	32	318	A86	C-C1	2.67	1.56	1.50
38	14	301	A86	C19-C18	2.67	1.56	1.52
38	12	316	A86	C-C1	2.67	1.56	1.50
27	b	603	CLA	CMB-C2B	-2.67	1.45	1.50
38	33	315	A86	C14-C15	2.67	1.57	1.52
27	b	608	CLA	C1D-ND	2.67	1.41	1.37
35	C	518	DGD	O4D-C4D	-2.67	1.36	1.43
38	31	314	A86	C-C1	2.67	1.56	1.50
38	13	316	A86	C-C1	2.67	1.56	1.50
37	V	201	HEM	C3C-C2C	-2.66	1.31	1.37
27	C	507	CLA	C4B-NB	2.66	1.41	1.37
38	32	316	A86	C14-C15	2.66	1.57	1.52
27	W	103	CLA	CMD-C2D	-2.66	1.45	1.50
38	11	313	A86	C-C1	2.66	1.56	1.50
38	31	313	A86	C-C1	2.66	1.56	1.50
37	v	201	HEM	C3C-C2C	-2.66	1.31	1.37
36	d	407	PL9	C5-C4	-2.66	1.37	1.47
38	14	314	A86	C-C1	2.66	1.56	1.50
27	B	608	CLA	CMB-C2B	-2.66	1.45	1.50
27	c	510	CLA	MG-ND	-2.66	2.00	2.05
38	13	314	A86	C14-C15	2.66	1.57	1.52
38	32	317	A86	C14-C15	2.66	1.57	1.52
28	d	403	PHO	CBD-CGD	-2.66	1.48	1.52
27	C	510	CLA	MG-ND	-2.66	2.00	2.05
27	11	309	CLA	C3B-C4B	2.66	1.49	1.42
38	34	315	A86	C-C1	2.65	1.56	1.50
38	33	316	A86	C19-C18	2.65	1.56	1.52
27	12	307	CLA	MG-NB	-2.65	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	610	CLA	C1D-ND	2.65	1.41	1.37
28	D	403	PHO	CAC-C3C	-2.65	1.46	1.51
27	C	502	CLA	C1D-ND	2.65	1.41	1.37
27	c	502	CLA	C1D-ND	2.65	1.41	1.37
38	14	316	A86	C-C1	2.65	1.56	1.50
38	13	314	A86	C-C1	2.65	1.56	1.50
27	33	305	CLA	MG-NB	-2.65	2.00	2.05
35	c	518	DGD	O4D-C4D	-2.65	1.36	1.43
38	34	316	A86	C14-C15	2.65	1.57	1.52
38	12	317	A86	C-C1	2.65	1.56	1.50
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	603	CLA	C1D-ND	2.65	1.41	1.37
38	14	301	A86	C-C1	2.65	1.56	1.50
27	B	610	CLA	CMC-C2C	-2.65	1.45	1.50
27	b	604	CLA	C1B-NB	-2.64	1.34	1.37
27	B	611	CLA	C1B-NB	-2.64	1.34	1.37
38	11	314	A86	C-C1	2.64	1.56	1.50
33	B	619	LMG	O4-C4	-2.64	1.36	1.43
27	B	611	CLA	C1D-ND	2.64	1.41	1.37
38	32	317	A86	C-C1	2.64	1.56	1.50
27	d	401	CLA	C1D-ND	2.64	1.41	1.37
27	b	610	CLA	CMC-C2C	-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
27	B	615	CLA	MG-NB	-2.64	2.00	2.05
38	14	315	A86	C-C1	2.64	1.56	1.50
27	A	402	CLA	MG-NB	-2.64	2.00	2.05
27	11	304	CLA	CMD-C2D	-2.64	1.45	1.50
27	c	502	CLA	CMD-C2D	-2.63	1.45	1.50
37	V	201	HEM	CAC-C3C	2.63	1.54	1.47
33	b	619	LMG	O4-C4	-2.63	1.36	1.43
38	33	314	A86	C-C1	2.63	1.56	1.50
30	A	406	SQD	O47-C7	2.63	1.41	1.34
27	32	308	CLA	CMD-C2D	-2.63	1.45	1.50
38	31	313	A86	C14-C15	2.63	1.57	1.52
27	14	307	CLA	C3B-C4B	2.63	1.48	1.42
35	C	518	DGD	O4E-C4E	-2.63	1.36	1.43
27	31	305	CLA	C3B-C4B	2.63	1.48	1.42
27	32	309	CLA	C3B-C4B	2.63	1.48	1.42
38	32	316	A86	C-C1	2.63	1.56	1.50
35	c	518	DGD	O4E-C4E	-2.63	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
27	B	608	CLA	C1D-ND	2.63	1.41	1.37
27	b	603	CLA	C1B-NB	-2.63	1.34	1.37
27	C	506	CLA	MG-NB	-2.63	2.00	2.05
30	a	406	SQD	O47-C7	2.63	1.41	1.34
38	12	317	A86	C14-C15	2.63	1.57	1.52
33	W	101	LMG	O7-C8	-2.63	1.40	1.46
33	w	101	LMG	O7-C8	-2.62	1.40	1.46
27	b	603	CLA	CMD-C2D	-2.62	1.45	1.50
37	v	201	HEM	CAC-C3C	2.62	1.54	1.47
27	33	307	CLA	C3B-C4B	2.62	1.48	1.42
27	c	505	CLA	CMB-C2B	-2.62	1.45	1.50
27	B	603	CLA	CMD-C2D	-2.62	1.45	1.50
27	c	514	CLA	C3B-C4B	2.62	1.48	1.42
27	12	308	CLA	CMD-C2D	-2.62	1.45	1.50
38	33	316	A86	C-C1	2.62	1.56	1.50
35	C	518	DGD	O3G-C1D	-2.62	1.35	1.40
35	c	518	DGD	O3G-C1D	-2.62	1.35	1.40
28	d	403	PHO	CAC-C3C	-2.62	1.46	1.51
27	34	308	CLA	C3B-C4B	2.62	1.48	1.42
27	32	307	CLA	MG-NB	-2.62	2.00	2.05
27	14	305	CLA	MG-NB	-2.62	2.00	2.05
27	c	508	CLA	C1B-NB	-2.61	1.34	1.37
27	b	610	CLA	C1D-ND	2.61	1.41	1.37
27	b	615	CLA	MG-NB	-2.61	2.00	2.05
27	b	613	CLA	CAA-C2A	-2.61	1.49	1.54
33	B	618	LMG	O7-C8	-2.61	1.40	1.46
38	34	301	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	C14-C15	2.61	1.57	1.52
33	b	618	LMG	O7-C8	-2.61	1.40	1.46
27	B	612	CLA	CMA-C3A	-2.61	1.47	1.53
27	b	612	CLA	CMA-C3A	-2.61	1.47	1.53
27	13	307	CLA	C3B-C4B	2.61	1.48	1.42
38	11	311	A86	O-C13	-2.61	1.17	1.23
27	12	309	CLA	C3B-C4B	2.61	1.48	1.42
38	13	314	A86	O-C13	-2.61	1.17	1.23
27	b	614	CLA	MG-NB	-2.61	2.00	2.05
27	13	306	CLA	CMD-C2D	-2.61	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	13	315	A86	C-C1	2.60	1.56	1.50
27	M	102	CLA	C1D-ND	2.60	1.41	1.37
38	31	311	A86	O-C13	-2.60	1.17	1.23
38	33	313	A86	O-C13	-2.60	1.17	1.23
28	a	403	PHO	C3B-C2B	-2.60	1.36	1.40
27	B	610	CLA	MG-ND	-2.60	2.00	2.05
27	B	604	CLA	C1B-NB	-2.60	1.34	1.37
27	B	613	CLA	CAA-C2A	-2.60	1.49	1.54
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	11	305	CLA	C3B-C4B	2.60	1.48	1.42
27	D	401	CLA	CMC-C2C	-2.60	1.45	1.50
27	d	401	CLA	CMC-C2C	-2.60	1.45	1.50
27	B	622	CLA	MG-ND	-2.60	2.00	2.05
27	b	611	CLA	C1B-NB	-2.60	1.34	1.37
27	C	514	CLA	C3B-C4B	2.60	1.48	1.42
38	12	315	A86	O-C13	-2.60	1.17	1.23
27	C	513	CLA	MG-NB	-2.60	2.00	2.05
38	14	313	A86	O-C13	-2.59	1.17	1.23
27	Z	102	CLA	C4B-NB	2.59	1.41	1.37
38	33	302	A86	C24-C1	2.59	1.51	1.45
38	11	316	A86	C24-C1	2.59	1.51	1.45
38	34	314	A86	O-C13	-2.59	1.17	1.23
27	b	615	CLA	CMB-C2B	-2.59	1.45	1.50
27	31	304	CLA	CMD-C2D	-2.59	1.45	1.50
38	13	315	A86	C14-C15	2.59	1.57	1.52
27	B	610	CLA	CMD-C2D	-2.59	1.45	1.50
38	13	302	A86	C24-C1	2.59	1.51	1.45
27	B	603	CLA	MG-ND	-2.59	2.00	2.05
27	b	603	CLA	MG-ND	-2.59	2.00	2.05
27	b	609	CLA	C4B-NB	2.59	1.41	1.37
27	31	303	CLA	MG-NB	-2.59	2.00	2.05
38	12	304	A86	C24-C1	2.59	1.51	1.45
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	c	503	CLA	C1B-NB	-2.58	1.34	1.37
35	C	518	DGD	O3G-C3G	-2.58	1.39	1.43
27	C	513	CLA	C3B-C4B	2.58	1.48	1.42
27	b	609	CLA	CMD-C2D	-2.58	1.45	1.50
27	33	306	CLA	CMD-C2D	-2.58	1.45	1.50
33	32	301	LMG	O1-C1	2.58	1.44	1.40
38	14	314	A86	O-C13	-2.58	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	605	CLA	CMD-C2D	-2.58	1.45	1.50
27	34	307	CLA	CMD-C2D	-2.58	1.45	1.50
38	31	312	A86	O-C13	-2.58	1.17	1.23
27	B	604	CLA	CAC-C3C	-2.58	1.44	1.51
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	B	614	CLA	MG-NB	-2.58	2.00	2.05
28	A	403	PHO	C3B-C2B	-2.58	1.36	1.40
27	c	505	CLA	C1D-ND	2.58	1.41	1.37
38	12	316	A86	C24-C1	2.57	1.51	1.45
27	33	306	CLA	C4B-NB	2.57	1.40	1.37
27	33	308	CLA	MG-NB	-2.57	2.00	2.05
33	q	301	LMG	O8-C9	-2.57	1.39	1.45
27	c	503	CLA	CMD-C2D	-2.57	1.45	1.50
38	33	314	A86	O-C13	-2.57	1.17	1.23
27	b	605	CLA	CMD-C2D	-2.57	1.45	1.50
27	11	303	CLA	MG-NB	-2.57	2.00	2.05
27	C	503	CLA	C1B-NB	-2.57	1.34	1.37
38	11	316	A86	C-C1	2.57	1.56	1.50
27	B	615	CLA	CMB-C2B	-2.57	1.45	1.50
27	c	506	CLA	MG-NB	-2.57	2.00	2.05
27	W	102	CLA	C4B-NB	2.57	1.40	1.37
38	32	316	A86	O-C13	-2.57	1.17	1.23
27	z	102	CLA	C4B-NB	2.57	1.40	1.37
38	33	316	A86	O-C13	-2.57	1.17	1.23
27	D	401	CLA	C1D-ND	2.57	1.40	1.37
38	34	303	A86	C-C1	2.57	1.56	1.50
27	34	311	CLA	CMD-C2D	-2.57	1.45	1.50
27	c	513	CLA	CMD-C2D	-2.57	1.45	1.50
27	B	609	CLA	CMD-C2D	-2.57	1.45	1.50
38	11	312	A86	O-C13	-2.57	1.17	1.23
38	33	314	A86	C24-C1	2.57	1.51	1.45
27	C	508	CLA	CMD-C2D	-2.56	1.45	1.50
27	C	514	CLA	MG-NB	-2.56	2.00	2.05
27	b	610	CLA	MG-ND	-2.56	2.00	2.05
27	c	505	CLA	CAC-C3C	-2.56	1.44	1.51
27	b	610	CLA	CMD-C2D	-2.56	1.45	1.50
27	c	513	CLA	C3B-C4B	2.56	1.48	1.42
27	31	304	CLA	C4B-NB	2.56	1.40	1.37
33	C	519	LMG	O8-C9	-2.56	1.39	1.45
27	C	510	CLA	CMC-C2C	-2.56	1.45	1.50
33	w	101	LMG	O8-C9	-2.56	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	14	314	A86	C24-C1	2.56	1.51	1.45
27	b	606	CLA	CMB-C2B	-2.56	1.45	1.50
38	31	316	A86	C24-C1	2.56	1.51	1.45
37	v	201	HEM	C2A-C3A	-2.56	1.32	1.38
38	13	314	A86	C24-C1	2.56	1.51	1.45
27	C	505	CLA	CAC-C3C	-2.56	1.44	1.51
27	b	602	CLA	MG-NB	-2.56	2.00	2.05
38	13	317	A86	C-C1	2.56	1.56	1.50
27	32	312	CLA	C4B-NB	2.56	1.40	1.37
38	33	302	A86	C-C1	2.56	1.56	1.50
38	32	304	A86	C24-C1	2.56	1.51	1.45
38	13	317	A86	C24-C1	2.55	1.51	1.45
27	b	622	CLA	C4B-NB	2.55	1.40	1.37
38	12	304	A86	C-C1	2.55	1.56	1.50
27	B	622	CLA	C4B-NB	2.55	1.40	1.37
27	14	302	CLA	CMD-C2D	-2.55	1.45	1.50
27	B	610	CLA	CMB-C2B	-2.55	1.45	1.50
27	C	504	CLA	MG-NB	-2.55	2.00	2.05
27	c	508	CLA	CMD-C2D	-2.55	1.45	1.50
27	B	605	CLA	MG-NB	-2.55	2.00	2.05
27	31	315	CLA	CMD-C2D	-2.55	1.45	1.50
27	C	503	CLA	CMD-C2D	-2.55	1.45	1.50
38	34	303	A86	C24-C1	2.55	1.51	1.45
38	31	316	A86	C-C1	2.55	1.56	1.50
27	31	301	CLA	CMC-C2C	-2.55	1.45	1.50
38	32	316	A86	C24-C1	2.55	1.51	1.45
27	13	306	CLA	C4B-NB	2.55	1.40	1.37
27	14	306	CLA	CMD-C2D	-2.55	1.45	1.50
27	c	510	CLA	C1D-ND	2.55	1.40	1.37
27	12	303	CLA	CMD-C2D	-2.55	1.45	1.50
27	32	308	CLA	C4B-NB	2.55	1.40	1.37
27	c	514	CLA	MG-NB	-2.54	2.00	2.05
27	12	308	CLA	MG-ND	-2.54	2.00	2.05
35	c	518	DGD	O3G-C3G	-2.54	1.39	1.43
27	D	405	CLA	CMC-C2C	-2.54	1.45	1.50
37	V	201	HEM	C2A-C3A	-2.54	1.32	1.38
27	34	304	CLA	CMC-C2C	-2.54	1.45	1.50
38	13	302	A86	C-C1	2.54	1.56	1.50
30	A	406	SQD	O2-C2	-2.54	1.37	1.43
27	13	310	CLA	C4B-NB	2.54	1.40	1.37
39	12	302	LMU	O3'-C3'	2.54	1.49	1.43
38	34	315	A86	C24-C1	2.54	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	512	CLA	MG-ND	-2.54	2.00	2.05
27	B	608	CLA	CMD-C2D	-2.54	1.45	1.50
27	b	605	CLA	MG-NB	-2.54	2.00	2.05
38	32	304	A86	C-C1	2.54	1.56	1.50
27	C	513	CLA	CMD-C2D	-2.54	1.45	1.50
27	33	303	CLA	CMC-C2C	-2.54	1.45	1.50
33	D	408	LMG	O1-C7	-2.54	1.39	1.43
33	W	101	LMG	O8-C9	-2.54	1.39	1.45
27	b	604	CLA	CAC-C3C	-2.54	1.44	1.51
27	B	606	CLA	CMB-C2B	-2.53	1.45	1.50
38	11	312	A86	C24-C1	2.53	1.51	1.45
27	13	301	CLA	CMD-C2D	-2.53	1.45	1.50
32	A	408	LHG	O7-C5	-2.53	1.40	1.46
38	32	318	A86	O-C13	-2.53	1.18	1.23
27	C	510	CLA	C1D-ND	2.53	1.40	1.37
27	B	602	CLA	MG-NB	-2.53	2.00	2.05
27	d	406	CLA	C1D-ND	2.53	1.40	1.37
27	14	310	CLA	CMD-C2D	-2.53	1.45	1.50
38	31	312	A86	C24-C1	2.53	1.51	1.45
27	33	306	CLA	MG-ND	-2.53	2.00	2.05
30	b	620	SQD	O47-C7	2.53	1.41	1.34
27	B	606	CLA	CMC-C2C	-2.53	1.45	1.50
27	c	503	CLA	CHC-C4B	-2.53	1.33	1.39
27	d	405	CLA	CMC-C2C	-2.53	1.45	1.50
27	B	603	CLA	C1B-NB	-2.53	1.34	1.37
27	b	608	CLA	CMD-C2D	-2.53	1.45	1.50
27	b	606	CLA	CMC-C2C	-2.53	1.45	1.50
27	A	404	CLA	CMB-C2B	-2.53	1.45	1.50
27	C	512	CLA	C3B-C4B	2.53	1.48	1.42
27	B	605	CLA	CMB-C2B	-2.52	1.45	1.50
27	z	102	CLA	MG-ND	-2.52	2.00	2.05
27	D	406	CLA	C1D-ND	2.52	1.40	1.37
27	c	510	CLA	CMC-C2C	-2.52	1.45	1.50
32	a	408	LHG	O7-C5	-2.52	1.40	1.46
27	b	605	CLA	C4B-NB	2.52	1.40	1.37
27	11	308	CLA	C4B-NB	2.52	1.40	1.37
27	14	303	CLA	CMC-C2C	-2.52	1.45	1.50
33	12	301	LMG	O4-C4	-2.52	1.37	1.43
30	B	620	SQD	O47-C7	2.52	1.41	1.34
27	12	305	CLA	CMC-C2C	-2.52	1.45	1.50
27	b	614	CLA	CMD-C2D	-2.52	1.45	1.50
27	33	301	CLA	CMD-C2D	-2.52	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	504	CLA	MG-NB	-2.52	2.00	2.05
38	12	314	A86	C-C1	2.52	1.56	1.50
27	d	405	CLA	MG-ND	-2.52	2.00	2.05
38	14	301	A86	O-C13	-2.52	1.18	1.23
27	a	404	CLA	CMB-C2B	-2.52	1.45	1.50
27	32	308	CLA	MG-ND	-2.52	2.00	2.05
27	11	301	CLA	CMC-C2C	-2.52	1.45	1.50
27	34	302	CLA	CMD-C2D	-2.52	1.45	1.50
38	31	314	A86	O-C13	-2.51	1.18	1.23
27	11	308	CLA	CMD-C2D	-2.51	1.45	1.50
27	31	306	CLA	MG-NB	-2.51	2.00	2.05
27	12	307	CLA	C4B-NB	2.51	1.40	1.37
27	12	308	CLA	C4B-NB	2.51	1.40	1.37
27	b	605	CLA	CMB-C2B	-2.51	1.45	1.50
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	b	610	CLA	CMB-C2B	-2.51	1.45	1.50
27	12	305	CLA	C4B-NB	2.51	1.40	1.37
30	a	406	SQD	O2-C2	-2.51	1.37	1.43
27	34	305	CLA	C4B-NB	2.51	1.40	1.37
27	32	303	CLA	CMD-C2D	-2.51	1.45	1.50
27	13	306	CLA	MG-ND	-2.51	2.00	2.05
27	33	305	CLA	C4B-NB	2.51	1.40	1.37
27	14	304	CLA	C4B-NB	2.51	1.40	1.37
27	31	304	CLA	MG-ND	-2.51	2.00	2.05
33	d	408	LMG	O1-C7	-2.51	1.39	1.43
27	d	406	CLA	CMD-C2D	-2.51	1.45	1.50
27	13	303	CLA	CMC-C2C	-2.51	1.45	1.50
27	32	312	CLA	CMD-C2D	-2.51	1.45	1.50
27	11	304	CLA	MG-ND	-2.51	2.00	2.05
27	w	102	CLA	C4B-NB	2.50	1.40	1.37
27	31	308	CLA	C4B-NB	2.50	1.40	1.37
27	a	404	CLA	CMC-C2C	-2.50	1.45	1.50
35	J	101	DGD	O1G-C1G	-2.50	1.39	1.45
27	B	614	CLA	CMD-C2D	-2.50	1.45	1.50
27	31	307	CLA	C4B-NB	2.50	1.40	1.37
27	12	310	CLA	MG-NB	-2.50	2.00	2.05
27	C	503	CLA	CHC-C4B	-2.50	1.33	1.39
27	32	305	CLA	CMC-C2C	-2.50	1.45	1.50
38	13	316	A86	O-C13	-2.50	1.18	1.23
27	33	303	CLA	C4B-NB	2.50	1.40	1.37
27	b	609	CLA	CMB-C2B	-2.50	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	32	310	CLA	MG-NB	-2.50	2.00	2.05
27	b	607	CLA	CMD-C2D	-2.50	1.45	1.50
27	34	305	CLA	MG-NB	-2.50	2.00	2.05
27	c	508	CLA	CMC-C2C	-2.50	1.45	1.50
27	34	309	CLA	MG-NB	-2.50	2.00	2.05
27	13	308	CLA	MG-NB	-2.50	2.00	2.05
27	c	512	CLA	C3B-C4B	2.50	1.48	1.42
27	32	306	CLA	C4B-NB	2.50	1.40	1.37
27	m	101	CLA	C3B-C4B	2.49	1.48	1.42
27	33	307	CLA	MG-NB	-2.49	2.00	2.05
27	11	306	CLA	MG-NB	-2.49	2.00	2.05
27	32	311	CLA	C4B-NB	2.49	1.40	1.37
27	C	508	CLA	CMC-C2C	-2.49	1.45	1.50
38	14	316	A86	O-C13	-2.49	1.18	1.23
38	11	310	A86	C-C1	2.49	1.56	1.50
38	34	313	A86	C-C1	2.49	1.56	1.50
27	12	312	CLA	C4B-NB	2.49	1.40	1.37
27	34	311	CLA	MG-ND	-2.49	2.00	2.05
27	31	302	CLA	MG-NB	-2.49	2.00	2.05
27	33	301	CLA	MG-NB	-2.49	2.00	2.05
27	11	307	CLA	C4B-NB	2.49	1.40	1.37
38	31	310	A86	C-C1	2.49	1.56	1.50
27	34	307	CLA	C4B-NB	2.49	1.40	1.37
27	B	622	CLA	C3B-C4B	2.49	1.48	1.42
27	33	310	CLA	CMD-C2D	-2.49	1.45	1.50
27	D	406	CLA	CMD-C2D	-2.49	1.45	1.50
27	32	306	CLA	MG-NB	-2.49	2.00	2.05
27	11	315	CLA	CMD-C2D	-2.49	1.45	1.50
27	33	310	CLA	C4B-NB	2.49	1.40	1.37
27	14	310	CLA	MG-ND	-2.49	2.00	2.05
38	34	303	A86	O-C13	-2.49	1.18	1.23
38	33	312	A86	C-C1	2.48	1.56	1.50
27	31	302	CLA	C4B-NB	2.48	1.40	1.37
27	B	613	CLA	CMD-C2D	-2.48	1.45	1.50
27	31	308	CLA	CMD-C2D	-2.48	1.45	1.50
38	32	314	A86	C-C1	2.48	1.56	1.50
27	13	304	CLA	MG-NB	-2.48	2.00	2.05
27	11	304	CLA	C4B-NB	2.48	1.40	1.37
27	A	402	CLA	CMC-C2C	-2.48	1.45	1.50
27	a	402	CLA	CMC-C2C	-2.48	1.45	1.50
27	b	613	CLA	CMD-C2D	-2.48	1.45	1.50
27	12	311	CLA	C4B-NB	2.48	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	M	102	CLA	CMB-C2B	-2.48	1.45	1.50
33	32	301	LMG	O7-C8	-2.48	1.40	1.46
38	11	314	A86	O-C13	-2.48	1.18	1.23
27	w	102	CLA	MG-NB	-2.48	2.00	2.05
38	14	312	A86	C-C1	2.48	1.56	1.50
27	b	613	CLA	CMC-C2C	-2.48	1.45	1.50
38	34	301	A86	O-C13	-2.48	1.18	1.23
27	B	615	CLA	MG-ND	-2.48	2.00	2.05
27	B	602	CLA	C4B-NB	2.48	1.40	1.37
27	12	306	CLA	C4B-NB	2.48	1.40	1.37
27	W	102	CLA	MG-NB	-2.48	2.00	2.05
27	c	507	CLA	C1B-NB	-2.48	1.34	1.37
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	13	310	CLA	CMD-C2D	-2.47	1.45	1.50
27	B	607	CLA	CMD-C2D	-2.47	1.45	1.50
27	12	312	CLA	CMD-C2D	-2.47	1.45	1.50
27	c	513	CLA	C4B-NB	2.47	1.40	1.37
38	32	304	A86	O-C13	-2.47	1.18	1.23
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	b	601	CLA	CMB-C2B	-2.47	1.45	1.50
27	b	602	CLA	C4B-NB	2.47	1.40	1.37
27	31	301	CLA	C4B-NB	2.47	1.40	1.37
27	C	509	CLA	CMD-C2D	-2.47	1.45	1.50
27	b	622	CLA	C3B-C4B	2.47	1.48	1.42
33	m	102	LMG	O4-C4	-2.47	1.37	1.43
27	C	514	CLA	CMC-C2C	-2.47	1.45	1.50
27	14	309	CLA	C4B-NB	2.47	1.40	1.37
27	13	305	CLA	C4B-NB	2.47	1.40	1.37
27	31	315	CLA	MG-NB	-2.47	2.00	2.05
27	a	402	CLA	CMD-C2D	-2.47	1.45	1.50
27	C	507	CLA	CMD-C2D	-2.47	1.45	1.50
27	b	615	CLA	MG-ND	-2.47	2.00	2.05
38	12	304	A86	O-C13	-2.47	1.18	1.23
27	13	304	CLA	C4B-NB	2.47	1.40	1.37
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	406	CLA	CMB-C2B	-2.47	1.45	1.50
35	j	101	DGD	O1G-C1G	-2.47	1.39	1.45
27	32	305	CLA	C4B-NB	2.47	1.40	1.37
27	33	306	CLA	C1B-NB	-2.47	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	33	309	CLA	C4B-NB	2.47	1.40	1.37
27	14	305	CLA	C4B-NB	2.47	1.40	1.37
27	14	306	CLA	C4B-NB	2.47	1.40	1.37
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	11	303	CLA	C4B-NB	2.47	1.40	1.37
27	31	303	CLA	C4B-NB	2.47	1.40	1.37
27	A	404	CLA	CMC-C2C	-2.46	1.45	1.50
27	B	609	CLA	CMB-C2B	-2.46	1.45	1.50
27	11	302	CLA	MG-NB	-2.46	2.00	2.05
27	14	310	CLA	C4B-NB	2.46	1.40	1.37
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	605	CLA	C4B-NB	2.46	1.40	1.37
27	A	402	CLA	CMD-C2D	-2.46	1.45	1.50
27	11	302	CLA	C4B-NB	2.46	1.40	1.37
27	a	404	CLA	MG-ND	-2.46	2.00	2.05
27	32	309	CLA	MG-NB	-2.46	2.00	2.05
27	32	307	CLA	C4B-NB	2.46	1.40	1.37
27	B	607	CLA	CMB-C2B	-2.46	1.45	1.50
27	32	308	CLA	C1B-NB	-2.46	1.34	1.37
27	c	514	CLA	CMC-C2C	-2.46	1.45	1.50
27	34	302	CLA	MG-NB	-2.46	2.00	2.05
38	13	312	A86	C-C1	2.46	1.56	1.50
27	b	607	CLA	C1B-NB	-2.46	1.34	1.37
27	13	310	CLA	MG-ND	-2.46	2.00	2.05
27	c	508	CLA	CMB-C2B	-2.46	1.45	1.50
38	13	317	A86	O-C13	-2.46	1.18	1.23
27	c	509	CLA	CMD-C2D	-2.46	1.45	1.50
27	M	102	CLA	C3B-C4B	2.46	1.48	1.42
27	11	315	CLA	MG-NB	-2.46	2.00	2.05
27	C	507	CLA	C1D-ND	2.45	1.40	1.37
27	c	507	CLA	C1D-ND	2.45	1.40	1.37
38	14	315	A86	C24-C1	2.45	1.51	1.45
27	B	601	CLA	CMB-C2B	-2.45	1.45	1.50
27	C	508	CLA	CMB-C2B	-2.45	1.45	1.50
27	12	306	CLA	MG-NB	-2.45	2.00	2.05
27	12	308	CLA	C1B-NB	-2.45	1.34	1.37
27	14	308	CLA	MG-NB	-2.45	2.00	2.05
27	c	507	CLA	CMD-C2D	-2.45	1.45	1.50
27	33	303	CLA	C1B-C2B	2.45	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	13	309	CLA	C4B-NB	2.45	1.40	1.37
27	C	504	CLA	MG-ND	-2.45	2.00	2.05
38	13	302	A86	O-C13	-2.45	1.18	1.23
35	C	517	DGD	O5D-C6D	-2.45	1.39	1.43
27	B	613	CLA	CMC-C2C	-2.45	1.45	1.50
27	11	304	CLA	C1B-NB	-2.45	1.34	1.37
27	b	622	CLA	CMB-C2B	-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	14	302	CLA	MG-NB	-2.45	2.00	2.05
27	14	304	CLA	MG-NB	-2.45	2.00	2.05
27	C	503	CLA	CAC-C3C	-2.45	1.44	1.51
27	D	406	CLA	CMB-C2B	-2.45	1.45	1.50
27	d	401	CLA	C1B-NB	-2.44	1.34	1.37
27	12	312	CLA	MG-ND	-2.44	2.00	2.05
27	m	101	CLA	CMB-C2B	-2.44	1.45	1.50
27	34	304	CLA	C1B-C2B	2.44	1.49	1.43
27	D	406	CLA	C1B-NB	-2.44	1.34	1.37
27	34	306	CLA	C4B-NB	2.44	1.40	1.37
27	c	504	CLA	MG-ND	-2.44	2.00	2.05
27	c	510	CLA	CMD-C2D	-2.44	1.45	1.50
27	14	307	CLA	MG-NB	-2.44	2.01	2.05
38	31	316	A86	O-C13	-2.44	1.18	1.23
27	32	305	CLA	C1B-C2B	2.44	1.49	1.43
27	B	607	CLA	C1B-NB	-2.44	1.34	1.37
27	14	303	CLA	C4B-NB	2.44	1.40	1.37
36	D	407	PL9	C31-C29	-2.44	1.46	1.51
36	d	407	PL9	C31-C29	-2.44	1.46	1.51
27	D	401	CLA	C1B-NB	-2.44	1.34	1.37
27	b	610	CLA	C3B-C4B	2.44	1.48	1.42
28	D	403	PHO	C1D-C2D	2.44	1.42	1.39
27	31	307	CLA	C3B-C4B	2.44	1.48	1.42
27	13	307	CLA	MG-NB	-2.43	2.01	2.05
27	B	611	CLA	CMD-C2D	-2.43	1.45	1.50
38	33	313	A86	C14-C15	2.43	1.57	1.52
27	13	309	CLA	C3B-C4B	2.43	1.48	1.42
27	12	313	CLA	MG-NB	-2.43	2.01	2.05
27	d	406	CLA	C1B-NB	-2.43	1.34	1.37
27	31	309	CLA	MG-NB	-2.43	2.01	2.05
33	M	103	LMG	O4-C4	-2.43	1.37	1.43
27	14	311	CLA	MG-NB	-2.43	2.01	2.05
27	11	301	CLA	C4B-NB	2.43	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	13	315	A86	C24-C1	2.43	1.51	1.45
38	11	311	A86	C14-C15	2.43	1.57	1.52
38	34	316	A86	C24-C1	2.43	1.51	1.45
27	13	303	CLA	C1B-C2B	2.43	1.49	1.43
27	c	512	CLA	C4B-NB	2.43	1.40	1.37
27	31	304	CLA	C1B-NB	-2.43	1.34	1.37
27	C	506	CLA	CMC-C2C	-2.43	1.45	1.50
27	c	506	CLA	CMC-C2C	-2.43	1.45	1.50
27	11	301	CLA	C1B-C2B	2.43	1.49	1.43
27	13	311	CLA	C1B-C2B	2.43	1.49	1.43
27	C	504	CLA	C4B-NB	2.43	1.40	1.37
38	31	311	A86	C14-C15	2.43	1.57	1.52
27	11	309	CLA	MG-NB	-2.43	2.01	2.05
27	14	309	CLA	C3B-C4B	2.43	1.48	1.42
27	11	308	CLA	MG-ND	-2.43	2.01	2.05
27	B	614	CLA	C1B-NB	-2.43	1.34	1.37
27	C	509	CLA	C1D-ND	2.43	1.40	1.37
27	14	303	CLA	C1B-C2B	2.43	1.49	1.43
27	12	305	CLA	C1B-C2B	2.43	1.49	1.43
27	B	610	CLA	C3B-C4B	2.43	1.48	1.42
37	E	101	HEM	FE-ND	2.43	2.02	1.94
38	11	313	A86	C24-C1	2.43	1.51	1.45
27	31	308	CLA	CMC-C2C	-2.42	1.45	1.50
27	C	505	CLA	MG-ND	-2.42	2.01	2.05
27	b	611	CLA	CMD-C2D	-2.42	1.45	1.50
27	B	622	CLA	CMB-C2B	-2.42	1.45	1.50
27	13	304	CLA	CMD-C2D	-2.42	1.45	1.50
27	31	305	CLA	MG-NB	-2.42	2.01	2.05
37	V	201	HEM	C3D-C2D	-2.42	1.31	1.36
38	13	313	A86	C14-C15	2.42	1.57	1.52
38	33	315	A86	C24-C1	2.42	1.51	1.45
38	12	317	A86	C24-C1	2.42	1.51	1.45
27	13	308	CLA	C1B-C2B	2.42	1.49	1.43
27	B	622	CLA	C1B-NB	-2.42	1.34	1.37
27	33	304	CLA	MG-NB	-2.42	2.01	2.05
27	34	304	CLA	C4B-NB	2.42	1.40	1.37
27	34	311	CLA	C4B-NB	2.42	1.40	1.37
37	f	102	HEM	FE-ND	2.42	2.02	1.94
27	34	309	CLA	CMB-C2B	-2.42	1.45	1.50
27	C	511	CLA	CMC-C2C	-2.42	1.45	1.50
27	B	605	CLA	C3B-C4B	2.42	1.48	1.42
38	34	314	A86	C14-C15	2.42	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	34	312	CLA	C1B-C2B	2.42	1.48	1.43
27	W	102	CLA	CMC-C2C	-2.42	1.45	1.50
27	31	309	CLA	C1B-C2B	2.42	1.48	1.43
27	c	506	CLA	C3B-C4B	2.42	1.48	1.42
27	B	607	CLA	MG-ND	-2.42	2.01	2.05
27	C	510	CLA	CMD-C2D	-2.41	1.45	1.50
27	33	311	CLA	MG-NB	-2.41	2.01	2.05
27	c	507	CLA	CMC-C2C	-2.41	1.45	1.50
27	b	607	CLA	MG-ND	-2.41	2.01	2.05
27	34	310	CLA	C3B-C4B	2.41	1.48	1.42
27	b	605	CLA	C3B-C4B	2.41	1.48	1.42
27	11	305	CLA	MG-NB	-2.41	2.01	2.05
27	13	303	CLA	C4B-NB	2.41	1.40	1.37
27	C	506	CLA	C3B-C4B	2.41	1.48	1.42
27	13	309	CLA	CMD-C2D	-2.41	1.45	1.50
27	C	507	CLA	C1B-NB	-2.41	1.34	1.37
27	c	512	CLA	C1B-NB	-2.41	1.34	1.37
27	34	310	CLA	C4B-NB	2.41	1.40	1.37
37	v	201	HEM	C3D-C2D	-2.41	1.31	1.36
27	c	503	CLA	CAC-C3C	-2.41	1.44	1.51
27	c	505	CLA	CMD-C2D	-2.41	1.45	1.50
27	11	308	CLA	MG-NB	-2.41	2.01	2.05
27	13	311	CLA	MG-NB	-2.41	2.01	2.05
27	c	504	CLA	C4B-NB	2.41	1.40	1.37
27	C	505	CLA	CMD-C2D	-2.41	1.45	1.50
35	c	517	DGD	O5D-C6D	-2.41	1.39	1.43
27	12	313	CLA	C1B-C2B	2.41	1.48	1.43
27	B	602	CLA	C3B-C4B	2.41	1.48	1.42
38	12	315	A86	C14-C15	2.41	1.57	1.52
27	w	102	CLA	CMC-C2C	-2.41	1.45	1.50
27	33	310	CLA	CMC-C2C	-2.41	1.45	1.50
27	13	306	CLA	C1B-NB	-2.41	1.34	1.37
27	b	602	CLA	C3B-C4B	2.41	1.48	1.42
27	12	310	CLA	CMB-C2B	-2.40	1.45	1.50
27	c	505	CLA	CMC-C2C	-2.40	1.45	1.50
27	d	402	CLA	CMB-C2B	-2.40	1.45	1.50
27	32	312	CLA	C3B-C4B	2.40	1.48	1.42
27	32	311	CLA	CMD-C2D	-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
38	31	313	A86	C24-C1	2.40	1.51	1.45
27	14	311	CLA	C1B-C2B	2.40	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	12	311	CLA	C3B-C4B	2.40	1.48	1.42
27	32	311	CLA	C3B-C4B	2.40	1.48	1.42
27	34	310	CLA	CMD-C2D	-2.40	1.45	1.50
27	d	402	CLA	MG-ND	-2.40	2.01	2.05
27	w	102	CLA	CMB-C2B	-2.40	1.45	1.50
27	13	310	CLA	CMC-C2C	-2.40	1.45	1.50
27	14	310	CLA	MG-NB	-2.40	2.01	2.05
27	b	614	CLA	C1B-NB	-2.40	1.34	1.37
27	c	514	CLA	MG-ND	-2.40	2.01	2.05
27	D	402	CLA	CMB-C2B	-2.40	1.45	1.50
27	33	308	CLA	CMB-C2B	-2.40	1.45	1.50
27	31	301	CLA	C1B-C2B	2.40	1.48	1.43
27	34	311	CLA	CMC-C2C	-2.40	1.45	1.50
27	34	312	CLA	MG-NB	-2.40	2.01	2.05
27	14	309	CLA	CMD-C2D	-2.40	1.45	1.50
27	D	402	CLA	MG-ND	-2.40	2.01	2.05
27	C	512	CLA	C1B-NB	-2.40	1.34	1.37
27	13	308	CLA	CMB-C2B	-2.40	1.45	1.50
27	31	307	CLA	CMD-C2D	-2.40	1.45	1.50
27	32	306	CLA	CMD-C2D	-2.40	1.45	1.50
27	C	512	CLA	C4B-NB	2.40	1.40	1.37
27	14	306	CLA	C1B-NB	-2.40	1.34	1.37
27	b	614	CLA	CMC-C2C	-2.40	1.45	1.50
27	b	622	CLA	C1B-NB	-2.39	1.34	1.37
27	34	307	CLA	C1B-NB	-2.39	1.34	1.37
38	13	312	A86	O4-C34	-2.39	1.40	1.46
28	d	403	PHO	C1D-C2D	2.39	1.42	1.39
38	32	317	A86	C24-C1	2.39	1.51	1.45
27	C	514	CLA	MG-ND	-2.39	2.01	2.05
27	34	305	CLA	CMD-C2D	-2.39	1.45	1.50
27	11	307	CLA	C3B-C4B	2.39	1.48	1.42
27	31	306	CLA	C1B-C2B	2.39	1.48	1.43
27	B	614	CLA	CMC-C2C	-2.39	1.45	1.50
27	34	309	CLA	C1B-C2B	2.39	1.48	1.43
27	33	308	CLA	C1B-C2B	2.39	1.48	1.43
27	33	310	CLA	MG-NB	-2.39	2.01	2.05
27	C	502	CLA	C1B-NB	-2.39	1.34	1.37
27	32	312	CLA	CMC-C2C	-2.39	1.45	1.50
27	c	509	CLA	C1D-ND	2.39	1.40	1.37
27	31	306	CLA	CMB-C2B	-2.39	1.45	1.50
38	32	314	A86	C14-C15	2.39	1.57	1.52
27	W	102	CLA	CMB-C2B	-2.39	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	607	CLA	CMB-C2B	-2.39	1.45	1.50
27	C	513	CLA	C4B-NB	2.39	1.40	1.37
27	11	309	CLA	C1B-C2B	2.39	1.48	1.43
27	C	514	CLA	CMD-C2D	-2.39	1.45	1.50
27	C	505	CLA	CMC-C2C	-2.39	1.45	1.50
38	31	310	A86	O4-C34	-2.39	1.40	1.46
38	31	310	A86	C14-C15	2.39	1.57	1.52
27	32	312	CLA	MG-NB	-2.39	2.01	2.05
33	d	408	LMG	O4-C4	-2.39	1.37	1.43
29	B	623	BCR	C30-C25	-2.38	1.50	1.53
27	14	308	CLA	CMB-C2B	-2.38	1.45	1.50
27	c	511	CLA	CMC-C2C	-2.38	1.45	1.50
27	33	309	CLA	CMD-C2D	-2.38	1.45	1.50
27	14	310	CLA	CMC-C2C	-2.38	1.45	1.50
38	33	316	A86	C14-C15	2.38	1.57	1.52
27	B	603	CLA	CMC-C2C	-2.38	1.45	1.50
27	32	310	CLA	C1B-C2B	2.38	1.48	1.43
27	32	313	CLA	C1B-C2B	2.38	1.48	1.43
27	33	309	CLA	C3B-C4B	2.38	1.48	1.42
27	D	406	CLA	MG-ND	-2.38	2.01	2.05
27	12	312	CLA	CMC-C2C	-2.38	1.45	1.50
27	b	604	CLA	CHC-C4B	-2.38	1.34	1.39
29	b	623	BCR	C30-C25	-2.38	1.50	1.53
27	31	302	CLA	CMD-C2D	-2.38	1.45	1.50
27	b	611	CLA	MG-ND	-2.38	2.01	2.05
27	11	308	CLA	CMC-C2C	-2.38	1.45	1.50
27	11	306	CLA	CMB-C2B	-2.38	1.45	1.50
27	12	311	CLA	CMD-C2D	-2.38	1.45	1.50
27	C	507	CLA	CMC-C2C	-2.38	1.45	1.50
27	31	302	CLA	C3B-C4B	2.38	1.48	1.42
27	B	604	CLA	CHC-C4B	-2.38	1.34	1.39
27	14	303	CLA	C3B-C4B	2.38	1.48	1.42
27	b	603	CLA	CMC-C2C	-2.37	1.45	1.50
27	12	306	CLA	CMD-C2D	-2.37	1.45	1.50
27	32	310	CLA	CMB-C2B	-2.37	1.45	1.50
27	34	311	CLA	C3B-C4B	2.37	1.48	1.42
33	12	301	LMG	O7-C8	-2.37	1.40	1.46
27	12	312	CLA	MG-NB	-2.37	2.01	2.05
27	c	502	CLA	C1B-NB	-2.37	1.34	1.37
30	B	620	SQD	O3-C3	-2.37	1.37	1.43
27	33	304	CLA	C1B-C2B	2.37	1.48	1.43
27	11	302	CLA	CMD-C2D	-2.37	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	33	312	A86	C14-C15	2.37	1.57	1.52
27	14	308	CLA	C1B-C2B	2.37	1.48	1.43
27	12	310	CLA	C1B-C2B	2.37	1.48	1.43
27	13	310	CLA	C3B-C4B	2.37	1.48	1.42
27	c	511	CLA	C3B-C4B	2.37	1.48	1.42
27	33	303	CLA	C3B-C4B	2.37	1.48	1.42
27	33	304	CLA	C4B-NB	2.37	1.40	1.37
27	B	608	CLA	MG-NB	-2.37	2.01	2.05
27	33	311	CLA	C1B-C2B	2.37	1.48	1.43
38	11	311	A86	C-C1	2.36	1.55	1.50
27	D	405	CLA	C1B-NB	-2.36	1.34	1.37
27	B	601	CLA	CMD-C2D	-2.36	1.45	1.50
27	D	402	CLA	CMD-C2D	-2.36	1.45	1.50
27	33	310	CLA	C3B-C4B	2.36	1.48	1.42
38	33	316	A86	O4-C34	-2.36	1.40	1.46
27	14	304	CLA	CMD-C2D	-2.36	1.45	1.50
38	14	316	A86	C24-C1	2.36	1.51	1.45
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	13	316	A86	C14-C15	2.36	1.57	1.52
27	11	308	CLA	C3B-C4B	2.36	1.48	1.42
27	32	305	CLA	C3B-C4B	2.36	1.48	1.42
38	32	314	A86	O4-C34	-2.36	1.40	1.46
38	34	313	A86	O4-C34	-2.36	1.40	1.46
27	B	611	CLA	MG-ND	-2.36	2.01	2.05
27	C	511	CLA	C3B-C4B	2.36	1.48	1.42
27	33	304	CLA	C3B-C4B	2.36	1.48	1.42
38	34	313	A86	C14-C15	2.36	1.57	1.52
27	B	604	CLA	CMC-C2C	-2.36	1.45	1.50
38	13	313	A86	C-C1	2.36	1.55	1.50
38	32	315	A86	C-C1	2.36	1.55	1.50
27	34	310	CLA	MG-ND	-2.36	2.01	2.05
27	11	306	CLA	C1B-C2B	2.36	1.48	1.43
38	33	312	A86	O4-C34	-2.36	1.40	1.46
27	11	307	CLA	CMD-C2D	-2.36	1.45	1.50
38	11	314	A86	O4-C34	-2.36	1.40	1.46
38	31	311	A86	C-C1	2.36	1.55	1.50
38	34	314	A86	C-C1	2.36	1.55	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	b	612	CLA	CMB-C2B	-2.35	1.45	1.50
27	31	302	CLA	C1B-C2B	2.35	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	14	312	A86	O4-C34	-2.35	1.40	1.46
27	31	308	CLA	MG-NB	-2.35	2.01	2.05
27	11	303	CLA	C1B-C2B	2.35	1.48	1.43
27	32	306	CLA	C1B-C2B	2.35	1.48	1.43
27	32	306	CLA	C3B-C4B	2.35	1.48	1.42
29	f	101	BCR	C30-C25	-2.35	1.50	1.53
27	d	406	CLA	MG-ND	-2.35	2.01	2.05
38	14	312	A86	C14-C15	2.35	1.57	1.52
27	32	307	CLA	C1B-C2B	2.35	1.48	1.43
27	C	506	CLA	CMB-C2B	-2.35	1.45	1.50
30	B	620	SQD	O2-C2	-2.35	1.37	1.43
27	12	306	CLA	C1B-C2B	2.35	1.48	1.43
27	33	304	CLA	CMD-C2D	-2.35	1.45	1.50
27	D	405	CLA	C3B-C4B	2.35	1.48	1.42
38	12	314	A86	C14-C15	2.35	1.57	1.52
27	11	303	CLA	CMD-C2D	-2.35	1.45	1.50
27	13	304	CLA	C3B-C4B	2.35	1.48	1.42
38	32	318	A86	C14-C15	2.35	1.57	1.52
27	c	512	CLA	CMB-C2B	-2.35	1.45	1.50
27	12	312	CLA	C3B-C4B	2.35	1.48	1.42
38	34	301	A86	C24-C1	2.35	1.51	1.45
27	31	303	CLA	C1B-C2B	2.35	1.48	1.43
38	12	315	A86	C-C1	2.34	1.55	1.50
27	31	309	CLA	CMD-C2D	-2.34	1.45	1.50
33	32	301	LMG	O4-C4	-2.34	1.37	1.43
38	14	301	A86	O4-C34	-2.34	1.40	1.46
38	14	313	A86	C-C1	2.34	1.55	1.50
35	c	518	DGD	O1G-C1G	-2.34	1.39	1.45
27	11	302	CLA	C1B-C2B	2.34	1.48	1.43
38	33	313	A86	C-C1	2.34	1.55	1.50
27	14	310	CLA	C3B-C4B	2.34	1.48	1.42
30	b	620	SQD	O3-C3	-2.34	1.37	1.43
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	B	612	CLA	CMB-C2B	-2.34	1.45	1.50
27	C	502	CLA	CMC-C2C	-2.34	1.45	1.50
27	34	304	CLA	C3B-C4B	2.34	1.48	1.42
27	c	506	CLA	CMB-C2B	-2.34	1.45	1.50
33	D	408	LMG	O4-C4	-2.34	1.37	1.43
27	W	102	CLA	CMD-C2D	-2.34	1.45	1.50
27	b	608	CLA	MG-NB	-2.34	2.01	2.05
38	14	301	A86	C24-C1	2.34	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	11	310	A86	O4-C34	-2.34	1.40	1.46
27	B	607	CLA	CMC-C2C	-2.34	1.45	1.50
27	34	306	CLA	CMD-C2D	-2.34	1.45	1.50
27	14	304	CLA	C1B-C2B	2.34	1.48	1.43
27	c	505	CLA	MG-ND	-2.34	2.01	2.05
27	d	405	CLA	C1B-NB	-2.34	1.34	1.37
27	C	512	CLA	CMB-C2B	-2.34	1.45	1.50
27	b	607	CLA	CMC-C2C	-2.34	1.45	1.50
27	c	502	CLA	CMC-C2C	-2.34	1.45	1.50
27	c	504	CLA	CMC-C2C	-2.34	1.45	1.50
35	C	518	DGD	O1G-C1G	-2.34	1.39	1.45
38	11	310	A86	C14-C15	2.34	1.57	1.52
27	14	311	CLA	CMD-C2D	-2.34	1.45	1.50
27	33	305	CLA	CMD-C2D	-2.34	1.45	1.50
27	31	308	CLA	C3B-C4B	2.34	1.48	1.42
38	11	314	A86	C14-C15	2.34	1.57	1.52
27	A	402	CLA	C3B-C4B	2.33	1.48	1.42
27	11	301	CLA	C3B-C4B	2.33	1.48	1.42
27	11	302	CLA	C3B-C4B	2.33	1.48	1.42
27	11	309	CLA	CMD-C2D	-2.33	1.45	1.50
27	12	307	CLA	CMD-C2D	-2.33	1.45	1.50
27	14	305	CLA	C1B-C2B	2.33	1.48	1.43
27	C	512	CLA	CMC-C2C	-2.33	1.45	1.50
27	z	102	CLA	C1B-C2B	2.33	1.48	1.43
27	32	313	CLA	CMD-C2D	-2.33	1.45	1.50
38	34	301	A86	C14-C15	2.33	1.57	1.52
35	C	517	DGD	O2E-C2E	-2.33	1.37	1.43
27	w	102	CLA	CMD-C2D	-2.33	1.45	1.50
33	12	301	LMG	O6-C5	-2.33	1.38	1.44
27	13	309	CLA	MG-ND	-2.33	2.01	2.05
27	D	405	CLA	C4B-NB	2.33	1.40	1.37
27	d	405	CLA	C4B-NB	2.33	1.40	1.37
38	12	314	A86	O4-C34	-2.33	1.40	1.46
38	14	301	A86	C14-C15	2.33	1.57	1.52
27	C	504	CLA	C1B-C2B	2.33	1.48	1.43
27	34	306	CLA	C1B-C2B	2.33	1.48	1.43
38	31	314	A86	O4-C34	-2.33	1.40	1.46
27	12	311	CLA	MG-ND	-2.33	2.01	2.05
38	32	318	A86	O4-C34	-2.33	1.40	1.46
38	33	316	A86	C24-C1	2.33	1.50	1.45
30	b	620	SQD	O4-C4	-2.33	1.37	1.43
27	B	614	CLA	C1B-C2B	2.33	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	12	313	CLA	CMD-C2D	-2.33	1.45	1.50
27	13	303	CLA	C3B-C4B	2.33	1.48	1.42
27	34	305	CLA	C3B-C4B	2.33	1.48	1.42
27	12	307	CLA	C1B-C2B	2.33	1.48	1.43
30	b	620	SQD	O2-C2	-2.33	1.37	1.43
27	Z	102	CLA	C1B-C2B	2.33	1.48	1.43
27	32	311	CLA	MG-ND	-2.33	2.01	2.05
27	d	405	CLA	C3B-C4B	2.33	1.48	1.42
27	w	103	CLA	MG-NB	-2.33	2.01	2.05
27	c	514	CLA	CMD-C2D	-2.33	1.45	1.50
27	d	402	CLA	CMD-C2D	-2.32	1.45	1.50
27	M	102	CLA	CMC-C2C	-2.32	1.45	1.50
28	d	403	PHO	C3B-CAB	-2.32	1.43	1.47
27	A	402	CLA	MG-ND	-2.32	2.01	2.05
27	a	402	CLA	MG-ND	-2.32	2.01	2.05
38	31	314	A86	C24-C1	2.32	1.50	1.45
35	c	517	DGD	O2E-C2E	-2.32	1.37	1.43
27	33	309	CLA	MG-ND	-2.32	2.01	2.05
27	b	604	CLA	CMC-C2C	-2.32	1.45	1.50
27	31	303	CLA	CMD-C2D	-2.32	1.45	1.50
27	c	506	CLA	MG-ND	-2.32	2.01	2.05
27	33	305	CLA	C1B-C2B	2.32	1.48	1.43
27	b	606	CLA	CAC-C3C	-2.32	1.45	1.51
27	33	311	CLA	CMD-C2D	-2.32	1.45	1.50
27	b	607	CLA	C3B-C4B	2.32	1.48	1.42
27	B	602	CLA	CMB-C2B	-2.32	1.45	1.50
27	B	606	CLA	CAC-C3C	-2.32	1.45	1.51
27	31	301	CLA	C3B-C4B	2.32	1.48	1.42
27	13	305	CLA	C1B-C2B	2.32	1.48	1.43
27	13	304	CLA	C1B-C2B	2.32	1.48	1.43
27	14	304	CLA	C3B-C4B	2.32	1.48	1.42
38	12	315	A86	C24-C1	2.32	1.50	1.45
27	a	402	CLA	C3B-C4B	2.32	1.48	1.42
38	32	318	A86	C24-C1	2.32	1.50	1.45
35	J	101	DGD	O3D-C3D	-2.31	1.37	1.43
27	A	402	CLA	CMB-C2B	-2.31	1.45	1.50
27	12	305	CLA	C3B-C4B	2.31	1.48	1.42
27	c	512	CLA	CMC-C2C	-2.31	1.45	1.50
27	13	305	CLA	C3B-C4B	2.31	1.48	1.42
27	12	306	CLA	C3B-C4B	2.31	1.48	1.42
38	34	301	A86	O4-C34	-2.31	1.40	1.46
30	B	620	SQD	O4-C4	-2.31	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	504	CLA	CMC-C2C	-2.31	1.45	1.50
27	D	406	CLA	CMC-C2C	-2.31	1.45	1.50
27	12	310	CLA	CMD-C2D	-2.31	1.45	1.50
27	b	602	CLA	CMB-C2B	-2.31	1.45	1.50
27	W	103	CLA	MG-NB	-2.31	2.01	2.05
27	32	307	CLA	C3B-C4B	2.31	1.48	1.42
27	b	601	CLA	MG-ND	-2.31	2.01	2.05
38	14	316	A86	C14-C15	2.31	1.57	1.52
27	13	309	CLA	CMC-C2C	-2.31	1.45	1.50
27	14	305	CLA	CMD-C2D	-2.31	1.45	1.50
27	c	504	CLA	C1B-C2B	2.31	1.48	1.43
27	D	406	CLA	C3B-C4B	2.31	1.48	1.42
30	a	406	SQD	O3-C3	-2.31	1.37	1.43
27	m	101	CLA	CMC-C2C	-2.30	1.45	1.50
27	11	306	CLA	CMD-C2D	-2.30	1.45	1.50
38	13	316	A86	O4-C34	-2.30	1.40	1.46
27	b	601	CLA	CMD-C2D	-2.30	1.45	1.50
27	32	307	CLA	CMD-C2D	-2.30	1.45	1.50
38	11	311	A86	C24-C1	2.30	1.50	1.45
27	B	614	CLA	CMB-C2B	-2.30	1.45	1.50
27	b	602	CLA	CMD-C2D	-2.30	1.45	1.50
27	13	310	CLA	C1B-C2B	2.30	1.48	1.43
27	B	615	CLA	C4B-NB	2.30	1.40	1.37
30	A	406	SQD	O3-C3	-2.30	1.37	1.43
27	C	511	CLA	CAA-C2A	-2.30	1.49	1.54
38	14	313	A86	C24-C1	2.30	1.50	1.45
38	13	302	A86	C14-C15	2.30	1.57	1.52
27	34	306	CLA	C3B-C4B	2.30	1.48	1.42
38	32	304	A86	C14-C15	2.30	1.57	1.52
38	13	316	A86	C24-C1	2.30	1.50	1.45
27	W	103	CLA	C1B-C2B	2.30	1.48	1.43
27	c	502	CLA	C1B-C2B	2.30	1.48	1.43
27	C	511	CLA	C1D-ND	2.30	1.40	1.37
27	12	312	CLA	C1B-C2B	2.30	1.48	1.43
27	b	601	CLA	C4B-NB	2.30	1.40	1.37
27	33	309	CLA	CMC-C2C	-2.30	1.45	1.50
27	B	602	CLA	CMD-C2D	-2.30	1.45	1.50
35	j	101	DGD	O2E-C2E	-2.30	1.37	1.43
27	34	311	CLA	C1B-C2B	2.30	1.48	1.43
38	34	314	A86	C24-C1	2.30	1.50	1.45
27	13	311	CLA	CMD-C2D	-2.30	1.45	1.50
27	34	310	CLA	CMC-C2C	-2.30	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	J	101	DGD	O2E-C2E	-2.30	1.37	1.43
38	11	314	A86	C24-C1	2.30	1.50	1.45
27	C	506	CLA	MG-ND	-2.30	2.01	2.05
27	31	306	CLA	CMD-C2D	-2.30	1.45	1.50
27	C	508	CLA	CHC-C4B	-2.30	1.34	1.39
29	F	101	BCR	C30-C25	-2.29	1.50	1.53
27	14	310	CLA	C1B-C2B	2.29	1.48	1.43
27	B	607	CLA	C3B-C4B	2.29	1.48	1.42
27	a	402	CLA	CMB-C2B	-2.29	1.45	1.50
27	31	307	CLA	CMB-C2B	-2.29	1.45	1.50
38	33	313	A86	C24-C1	2.29	1.50	1.45
38	11	316	A86	C14-C15	2.29	1.57	1.52
27	M	102	CLA	C1B-NB	-2.29	1.35	1.37
27	33	308	CLA	CMD-C2D	-2.29	1.45	1.50
35	H	102	DGD	O4D-C4D	-2.29	1.37	1.43
27	b	601	CLA	CMC-C2C	-2.29	1.45	1.50
27	34	305	CLA	C1B-C2B	2.29	1.48	1.43
33	B	618	LMG	O1-C7	-2.29	1.39	1.43
38	14	316	A86	O4-C34	-2.29	1.40	1.46
27	34	312	CLA	CMD-C2D	-2.29	1.45	1.50
27	A	404	CLA	C3B-C4B	2.29	1.48	1.42
27	d	402	CLA	C3B-C4B	2.29	1.48	1.42
27	12	311	CLA	CMC-C2C	-2.29	1.45	1.50
27	d	406	CLA	CMC-C2C	-2.29	1.45	1.50
27	13	308	CLA	CMD-C2D	-2.29	1.45	1.50
28	A	403	PHO	C4D-CHA	2.29	1.43	1.39
30	A	406	SQD	O4-C4	-2.29	1.37	1.43
39	32	302	LMU	O3'-C3'	2.29	1.48	1.43
27	11	303	CLA	C3B-C4B	2.29	1.48	1.42
28	D	403	PHO	C3B-CAB	-2.29	1.43	1.47
27	31	308	CLA	C1B-C2B	2.29	1.48	1.43
38	31	314	A86	C14-C15	2.29	1.57	1.52
35	j	101	DGD	O3D-C3D	-2.29	1.37	1.43
27	c	508	CLA	CHC-C4B	-2.29	1.34	1.39
27	C	506	CLA	C4B-NB	2.29	1.40	1.37
28	a	403	PHO	C4D-CHA	2.29	1.43	1.39
27	31	305	CLA	C1B-C2B	2.29	1.48	1.43
27	B	608	CLA	CMC-C2C	-2.28	1.46	1.50
27	32	312	CLA	C1B-C2B	2.28	1.48	1.43
27	33	307	CLA	C1B-C2B	2.28	1.48	1.43
27	b	614	CLA	CMB-C2B	-2.28	1.46	1.50
27	14	305	CLA	C3B-C4B	2.28	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	517	DGD	O4D-C4D	-2.28	1.37	1.43
27	B	601	CLA	CMC-C2C	-2.28	1.46	1.50
27	14	309	CLA	CMC-C2C	-2.28	1.46	1.50
27	33	305	CLA	C3B-C4B	2.28	1.48	1.42
27	13	305	CLA	CMD-C2D	-2.28	1.46	1.50
27	B	605	CLA	CMC-C2C	-2.28	1.46	1.50
27	C	504	CLA	CMB-C2B	-2.28	1.46	1.50
27	C	513	CLA	CMB-C2B	-2.28	1.46	1.50
27	32	311	CLA	CMC-C2C	-2.28	1.46	1.50
27	14	308	CLA	CMD-C2D	-2.28	1.46	1.50
30	l	101	SQD	O2-C2	-2.28	1.37	1.43
27	14	309	CLA	MG-ND	-2.28	2.01	2.05
35	c	517	DGD	O4D-C4D	-2.28	1.37	1.43
27	11	307	CLA	CMC-C2C	-2.28	1.46	1.50
27	14	309	CLA	CMB-C2B	-2.28	1.46	1.50
27	W	102	CLA	MG-ND	-2.28	2.01	2.05
27	c	513	CLA	CMB-C2B	-2.28	1.46	1.50
27	11	315	CLA	C1B-C2B	2.28	1.48	1.43
27	c	508	CLA	CAC-C3C	-2.28	1.45	1.51
37	f	102	HEM	C2A-C3A	-2.28	1.32	1.38
27	w	102	CLA	MG-ND	-2.28	2.01	2.05
33	b	618	LMG	O8-C9	-2.28	1.40	1.45
27	B	601	CLA	C3B-C4B	2.28	1.48	1.42
27	b	601	CLA	C3B-C4B	2.28	1.48	1.42
33	C	519	LMG	O4-C4	-2.28	1.37	1.43
38	33	302	A86	C14-C15	2.28	1.57	1.52
38	13	317	A86	C14-C15	2.28	1.57	1.52
27	34	308	CLA	C1B-C2B	2.28	1.48	1.43
27	c	511	CLA	CAA-C2A	-2.27	1.49	1.54
27	34	306	CLA	CMC-C2C	-2.27	1.46	1.50
27	34	309	CLA	CMD-C2D	-2.27	1.46	1.50
27	34	310	CLA	CMB-C2B	-2.27	1.46	1.50
27	w	103	CLA	C1B-C2B	2.27	1.48	1.43
27	32	309	CLA	C1B-C2B	2.27	1.48	1.43
27	D	402	CLA	C3B-C4B	2.27	1.48	1.42
27	14	302	CLA	C1B-C2B	2.27	1.48	1.43
27	11	307	CLA	MG-ND	-2.27	2.01	2.05
27	D	405	CLA	CMB-C2B	-2.27	1.46	1.50
27	31	303	CLA	C3B-C4B	2.27	1.48	1.42
38	32	315	A86	C24-C1	2.27	1.50	1.45
27	c	513	CLA	MG-ND	-2.27	2.01	2.05
27	c	513	CLA	CMC-C2C	-2.27	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	33	309	CLA	CMB-C2B	-2.27	1.46	1.50
30	a	406	SQD	O4-C4	-2.27	1.37	1.43
27	13	309	CLA	CMB-C2B	-2.27	1.46	1.50
27	11	305	CLA	C1B-C2B	2.27	1.48	1.43
27	32	303	CLA	C1B-C2B	2.27	1.48	1.43
27	32	311	CLA	CMB-C2B	-2.27	1.46	1.50
27	a	404	CLA	C3B-C4B	2.27	1.48	1.42
27	c	505	CLA	CHC-C4B	-2.27	1.34	1.39
38	12	304	A86	C14-C15	2.27	1.57	1.52
36	d	404	PL9	C36-C34	-2.27	1.46	1.51
27	11	307	CLA	CMB-C2B	-2.27	1.46	1.50
38	31	316	A86	C14-C15	2.27	1.57	1.52
27	32	310	CLA	CMD-C2D	-2.27	1.46	1.50
27	12	309	CLA	C1B-C2B	2.27	1.48	1.43
27	B	601	CLA	MG-ND	-2.27	2.01	2.05
35	J	101	DGD	O2D-C2D	-2.27	1.37	1.43
37	E	101	HEM	C2A-C3A	-2.26	1.32	1.38
27	c	506	CLA	C4B-NB	2.26	1.40	1.37
27	13	307	CLA	C1B-C2B	2.26	1.48	1.43
27	12	307	CLA	C3B-C4B	2.26	1.48	1.42
27	b	614	CLA	C1B-C2B	2.26	1.48	1.43
38	31	311	A86	C24-C1	2.26	1.50	1.45
27	11	308	CLA	C1B-C2B	2.26	1.48	1.43
27	b	608	CLA	CMC-C2C	-2.26	1.46	1.50
27	C	508	CLA	CAC-C3C	-2.26	1.45	1.51
27	C	502	CLA	C1B-C2B	2.26	1.48	1.43
27	c	512	CLA	CMD-C2D	-2.26	1.46	1.50
27	12	311	CLA	CMB-C2B	-2.26	1.46	1.50
27	31	307	CLA	CMC-C2C	-2.26	1.46	1.50
27	14	307	CLA	C1B-C2B	2.26	1.48	1.43
27	c	502	CLA	CMB-C2B	-2.26	1.46	1.50
38	13	313	A86	C24-C1	2.26	1.50	1.45
27	C	513	CLA	MG-ND	-2.26	2.01	2.05
27	b	601	CLA	C1B-NB	-2.26	1.35	1.37
27	b	605	CLA	CMC-C2C	-2.26	1.46	1.50
27	B	611	CLA	C3B-C4B	2.26	1.48	1.42
27	33	301	CLA	C1B-C2B	2.25	1.48	1.43
27	c	507	CLA	C3B-C4B	2.25	1.48	1.42
33	B	619	LMG	O3-C3	-2.25	1.37	1.43
27	m	101	CLA	MG-ND	-2.25	2.01	2.05
27	33	310	CLA	C1B-C2B	2.25	1.48	1.43
27	c	504	CLA	CMB-C2B	-2.25	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	609	CLA	CMC-C2C	-2.25	1.46	1.50
35	h	102	DGD	O4D-C4D	-2.25	1.37	1.43
33	b	618	LMG	O4-C4	-2.25	1.37	1.43
27	C	512	CLA	CMD-C2D	-2.25	1.46	1.50
33	b	618	LMG	O1-C7	-2.25	1.39	1.43
27	b	615	CLA	C4B-NB	2.25	1.40	1.37
33	q	301	LMG	O4-C4	-2.25	1.37	1.43
38	12	314	A86	C24-C1	2.25	1.50	1.45
35	j	101	DGD	O2D-C2D	-2.25	1.37	1.43
27	C	513	CLA	CMC-C2C	-2.25	1.46	1.50
33	B	619	LMG	O2-C2	-2.25	1.37	1.43
38	33	312	A86	C24-C1	2.25	1.50	1.45
27	34	302	CLA	C1B-C2B	2.25	1.48	1.43
38	14	313	A86	O4-C34	-2.24	1.41	1.46
33	b	619	LMG	O2-C2	-2.24	1.37	1.43
27	12	303	CLA	C1B-C2B	2.24	1.48	1.43
38	34	303	A86	C14-C15	2.24	1.57	1.52
27	11	303	CLA	MG-ND	-2.24	2.01	2.05
27	b	609	CLA	CMC-C2C	-2.24	1.46	1.50
27	12	303	CLA	CMB-C2B	-2.24	1.46	1.50
38	34	313	A86	C24-C1	2.24	1.50	1.45
27	33	304	CLA	C1B-NB	-2.24	1.35	1.37
38	32	314	A86	C24-C1	2.24	1.50	1.45
27	M	102	CLA	MG-ND	-2.24	2.01	2.05
27	14	303	CLA	CMD-C2D	-2.24	1.46	1.50
33	B	618	LMG	O8-C9	-2.24	1.40	1.45
38	12	315	A86	O4-C34	-2.24	1.41	1.46
27	B	601	CLA	C4B-NB	2.23	1.40	1.37
27	11	303	CLA	CMC-C2C	-2.23	1.46	1.50
27	m	101	CLA	C1B-NB	-2.23	1.35	1.37
27	31	315	CLA	C1B-C2B	2.23	1.48	1.43
38	13	313	A86	O4-C34	-2.23	1.41	1.46
27	b	611	CLA	C3B-C4B	2.23	1.48	1.42
38	11	310	A86	C24-C1	2.23	1.50	1.45
38	32	315	A86	O4-C34	-2.23	1.41	1.46
27	C	505	CLA	CHC-C4B	-2.23	1.34	1.39
35	c	518	DGD	O2E-C2E	-2.23	1.37	1.43
27	B	614	CLA	C3B-C4B	2.23	1.48	1.42
30	L	103	SQD	O2-C2	-2.23	1.37	1.43
27	B	622	CLA	CMC-C2C	-2.23	1.46	1.50
27	d	405	CLA	CAA-C2A	-2.23	1.50	1.54
27	a	404	CLA	CAB-C3B	-2.23	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	b	619	LMG	O3-C3	-2.23	1.37	1.43
27	c	511	CLA	C1D-ND	2.23	1.40	1.37
27	C	502	CLA	CMB-C2B	-2.23	1.46	1.50
27	11	301	CLA	CMD-C2D	-2.23	1.46	1.50
27	13	305	CLA	CMC-C2C	-2.23	1.46	1.50
27	b	614	CLA	C3B-C4B	2.22	1.48	1.42
27	11	306	CLA	C3B-C4B	2.22	1.48	1.42
27	b	614	CLA	MG-ND	-2.22	2.01	2.05
27	13	303	CLA	CMD-C2D	-2.22	1.46	1.50
27	c	504	CLA	C3B-C4B	2.22	1.48	1.42
27	B	609	CLA	MG-ND	-2.22	2.01	2.05
27	14	305	CLA	MG-ND	-2.22	2.01	2.05
27	D	405	CLA	CAA-C2A	-2.22	1.50	1.54
27	d	405	CLA	CMB-C2B	-2.22	1.46	1.50
27	31	303	CLA	CMC-C2C	-2.22	1.46	1.50
27	b	606	CLA	MG-ND	-2.22	2.01	2.05
27	d	406	CLA	C3B-C4B	2.22	1.48	1.42
27	13	305	CLA	MG-ND	-2.22	2.01	2.05
27	13	301	CLA	C1B-C2B	2.22	1.48	1.43
27	12	307	CLA	CMC-C2C	-2.22	1.46	1.50
27	12	305	CLA	CMD-C2D	-2.22	1.46	1.50
38	33	313	A86	O4-C34	-2.22	1.41	1.46
27	C	504	CLA	C3B-C4B	2.22	1.48	1.42
27	A	404	CLA	CAB-C3B	-2.22	1.41	1.47
27	11	315	CLA	CMB-C2B	-2.22	1.46	1.50
27	C	507	CLA	C3B-C4B	2.22	1.48	1.42
27	B	606	CLA	MG-ND	-2.22	2.01	2.05
27	12	307	CLA	MG-ND	-2.21	2.01	2.05
27	b	609	CLA	MG-ND	-2.21	2.01	2.05
27	B	611	CLA	CAC-C3C	-2.21	1.45	1.51
27	M	102	CLA	C4B-NB	2.21	1.40	1.37
27	A	402	CLA	C1B-C2B	2.21	1.48	1.43
27	b	611	CLA	CAC-C3C	-2.21	1.45	1.51
38	34	314	A86	O4-C34	-2.21	1.41	1.46
35	C	518	DGD	O2E-C2E	-2.21	1.37	1.43
33	B	618	LMG	O4-C4	-2.21	1.37	1.43
27	33	303	CLA	CMD-C2D	-2.21	1.46	1.50
27	34	311	CLA	CMB-C2B	-2.21	1.46	1.50
27	14	302	CLA	MG-ND	-2.21	2.01	2.05
27	13	308	CLA	C3B-C4B	2.21	1.47	1.42
27	14	305	CLA	CMC-C2C	-2.21	1.46	1.50
27	14	310	CLA	CMB-C2B	-2.21	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	32	312	CLA	CMB-C2B	-2.21	1.46	1.50
38	13	312	A86	C24-C1	2.21	1.50	1.45
36	D	404	PL9	C36-C34	-2.21	1.46	1.51
27	33	305	CLA	CMC-C2C	-2.21	1.46	1.50
38	11	311	A86	O4-C34	-2.21	1.41	1.46
27	32	307	CLA	MG-ND	-2.21	2.01	2.05
27	33	301	CLA	CMB-C2B	-2.21	1.46	1.50
27	32	305	CLA	CMD-C2D	-2.21	1.46	1.50
38	31	310	A86	C24-C1	2.21	1.50	1.45
27	11	302	CLA	MG-ND	-2.21	2.01	2.05
38	31	311	A86	O4-C34	-2.20	1.41	1.46
27	13	301	CLA	CMB-C2B	-2.20	1.46	1.50
27	31	303	CLA	MG-ND	-2.20	2.01	2.05
27	32	306	CLA	CMC-C2C	-2.20	1.46	1.50
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	b	605	CLA	C1B-NB	-2.20	1.35	1.37
27	A	402	CLA	C1B-NB	-2.20	1.35	1.37
27	32	303	CLA	CMB-C2B	-2.20	1.46	1.50
27	14	308	CLA	C3B-C4B	2.20	1.47	1.42
27	32	310	CLA	C3B-C4B	2.20	1.47	1.42
27	a	402	CLA	C1B-C2B	2.20	1.48	1.43
27	b	622	CLA	CMC-C2C	-2.20	1.46	1.50
27	34	309	CLA	C3B-C4B	2.20	1.47	1.42
27	34	304	CLA	CMD-C2D	-2.20	1.46	1.50
27	b	609	CLA	C3B-C4B	2.19	1.47	1.42
27	31	301	CLA	CMD-C2D	-2.19	1.46	1.50
35	C	517	DGD	O3D-C3D	-2.19	1.37	1.43
27	32	303	CLA	MG-ND	-2.19	2.01	2.05
27	14	302	CLA	CMB-C2B	-2.19	1.46	1.50
27	14	304	CLA	MG-ND	-2.19	2.01	2.05
27	12	310	CLA	C3B-C4B	2.19	1.47	1.42
27	d	406	CLA	C4B-NB	2.19	1.40	1.37
35	j	101	DGD	O6D-C5D	-2.19	1.39	1.44
27	32	307	CLA	CMC-C2C	-2.19	1.46	1.50
27	11	302	CLA	C1B-NB	-2.19	1.35	1.37
27	D	402	CLA	CMC-C2C	-2.19	1.46	1.50
27	34	302	CLA	CMB-C2B	-2.19	1.46	1.50
27	13	304	CLA	MG-ND	-2.19	2.01	2.05
27	d	402	CLA	CMC-C2C	-2.19	1.46	1.50
27	32	303	CLA	CMC-C2C	-2.19	1.46	1.50
29	F	101	BCR	C33-C5	-2.19	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	c	517	DGD	O3D-C3D	-2.19	1.37	1.43
27	33	301	CLA	CMC-C2C	-2.19	1.46	1.50
27	B	609	CLA	C3B-C4B	2.19	1.47	1.42
28	d	403	PHO	C3B-C2B	-2.19	1.37	1.40
27	14	302	CLA	CMC-C2C	-2.19	1.46	1.50
27	32	306	CLA	MG-ND	-2.18	2.01	2.05
38	14	312	A86	C24-C1	2.18	1.50	1.45
27	31	306	CLA	C3B-C4B	2.18	1.47	1.42
27	11	315	CLA	CMC-C2C	-2.18	1.46	1.50
27	31	302	CLA	MG-ND	-2.18	2.01	2.05
27	31	315	CLA	MG-ND	-2.18	2.01	2.05
27	B	601	CLA	C1B-NB	-2.18	1.35	1.37
27	B	605	CLA	C1B-NB	-2.18	1.35	1.37
27	31	315	CLA	CMB-C2B	-2.18	1.46	1.50
27	A	402	CLA	C4B-NB	2.18	1.40	1.37
27	12	312	CLA	CMB-C2B	-2.18	1.46	1.50
27	34	305	CLA	CMC-C2C	-2.18	1.46	1.50
28	A	403	PHO	CAA-C2A	-2.18	1.49	1.54
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	b	609	CLA	C1B-C2B	2.18	1.48	1.43
27	31	315	CLA	CMC-C2C	-2.18	1.46	1.50
27	13	301	CLA	CMC-C2C	-2.17	1.46	1.50
27	13	301	CLA	MG-ND	-2.17	2.01	2.05
27	11	308	CLA	CMB-C2B	-2.17	1.46	1.50
27	31	308	CLA	CMB-C2B	-2.17	1.46	1.50
27	12	303	CLA	CMC-C2C	-2.17	1.46	1.50
27	Z	102	CLA	C3B-C4B	2.17	1.47	1.42
35	J	101	DGD	O6D-C5D	-2.17	1.39	1.44
27	14	304	CLA	CMC-C2C	-2.17	1.46	1.50
35	c	517	DGD	O2G-C2G	-2.17	1.41	1.46
27	34	305	CLA	MG-ND	-2.17	2.01	2.05
27	12	305	CLA	CMB-C2B	-2.17	1.46	1.50
27	13	310	CLA	CMB-C2B	-2.17	1.46	1.50
29	f	101	BCR	C33-C5	-2.17	1.47	1.50
27	a	402	CLA	C4B-NB	2.17	1.40	1.37
27	31	302	CLA	CMC-C2C	-2.17	1.46	1.50
27	34	308	CLA	CMB-C2B	-2.17	1.46	1.50
27	c	514	CLA	CMB-C2B	-2.17	1.46	1.50
27	12	307	CLA	CMB-C2B	-2.17	1.46	1.50
27	12	306	CLA	C1B-NB	-2.17	1.35	1.37
27	31	301	CLA	CMB-C2B	-2.17	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	403	PHO	C3B-C2B	-2.17	1.37	1.40
27	B	609	CLA	C1B-C2B	2.16	1.48	1.43
27	31	303	CLA	CMB-C2B	-2.16	1.46	1.50
27	33	305	CLA	MG-ND	-2.16	2.01	2.05
27	33	308	CLA	C3B-C4B	2.16	1.47	1.42
35	C	517	DGD	O2G-C2G	-2.16	1.41	1.46
38	13	315	A86	O4-C34	-2.16	1.41	1.46
27	m	101	CLA	C4B-NB	2.16	1.40	1.37
28	a	403	PHO	CAA-C2A	-2.16	1.49	1.54
27	d	402	CLA	C1B-NB	-2.16	1.35	1.37
27	13	305	CLA	CMB-C2B	-2.16	1.46	1.50
27	31	305	CLA	CMD-C2D	-2.16	1.46	1.50
27	32	305	CLA	CMB-C2B	-2.16	1.46	1.50
27	C	502	CLA	CAC-C3C	-2.16	1.45	1.51
27	b	613	CLA	CMB-C2B	-2.16	1.46	1.50
27	z	102	CLA	CMB-C2B	-2.16	1.46	1.50
27	12	306	CLA	CMC-C2C	-2.16	1.46	1.50
27	14	303	CLA	CMB-C2B	-2.16	1.46	1.50
27	33	307	CLA	CMD-C2D	-2.16	1.46	1.50
27	b	610	CLA	C4B-NB	2.16	1.40	1.37
27	B	606	CLA	MG-NB	-2.16	2.01	2.05
27	13	307	CLA	CMD-C2D	-2.16	1.46	1.50
27	31	302	CLA	C1B-NB	-2.16	1.35	1.37
27	11	303	CLA	CMB-C2B	-2.16	1.46	1.50
29	z	101	BCR	C33-C5	-2.16	1.47	1.50
27	B	613	CLA	CMB-C2B	-2.16	1.46	1.50
27	11	301	CLA	CMB-C2B	-2.16	1.46	1.50
27	12	303	CLA	MG-ND	-2.16	2.01	2.05
27	z	102	CLA	C3B-C4B	2.16	1.47	1.42
27	13	304	CLA	CMC-C2C	-2.16	1.46	1.50
27	32	306	CLA	C1B-NB	-2.16	1.35	1.37
27	11	302	CLA	CMC-C2C	-2.16	1.46	1.50
27	Z	102	CLA	CMB-C2B	-2.15	1.46	1.50
38	33	315	A86	O4-C34	-2.15	1.41	1.46
27	B	613	CLA	C3B-C4B	2.15	1.47	1.42
38	32	317	A86	O4-C34	-2.15	1.41	1.46
27	11	315	CLA	MG-ND	-2.15	2.01	2.05
27	32	307	CLA	CMB-C2B	-2.15	1.46	1.50
27	D	405	CLA	C1B-C2B	2.15	1.48	1.43
27	C	504	CLA	C1B-NB	-2.15	1.35	1.37
27	c	504	CLA	C1B-NB	-2.15	1.35	1.37
27	33	301	CLA	MG-ND	-2.15	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	13	317	A86	O4-C34	-2.15	1.41	1.46
27	b	606	CLA	MG-NB	-2.15	2.01	2.05
27	13	306	CLA	CMB-C2B	-2.15	1.46	1.50
27	33	303	CLA	CMB-C2B	-2.15	1.46	1.50
38	31	313	A86	O4-C34	-2.15	1.41	1.46
27	z	102	CLA	C1B-NB	-2.15	1.35	1.37
27	13	304	CLA	C1B-NB	-2.15	1.35	1.37
27	33	307	CLA	CMB-C2B	-2.15	1.46	1.50
33	32	301	LMG	O6-C5	-2.15	1.39	1.44
27	11	307	CLA	C1B-NB	-2.14	1.35	1.37
27	z	102	CLA	CMC-C2C	-2.14	1.46	1.50
27	34	302	CLA	CMC-C2C	-2.14	1.46	1.50
27	Z	102	CLA	C1B-NB	-2.14	1.35	1.37
27	14	305	CLA	CMB-C2B	-2.14	1.46	1.50
27	c	514	CLA	C1B-C2B	2.14	1.48	1.43
27	32	309	CLA	CMD-C2D	-2.14	1.46	1.50
27	c	513	CLA	C1B-NB	-2.14	1.35	1.37
27	c	502	CLA	CAC-C3C	-2.14	1.45	1.51
27	C	510	CLA	CMA-C3A	-2.14	1.48	1.53
35	J	101	DGD	O3G-C3G	-2.14	1.39	1.43
27	14	304	CLA	C1B-NB	-2.14	1.35	1.37
27	34	306	CLA	CMB-C2B	-2.14	1.46	1.50
27	13	310	CLA	C1B-NB	-2.14	1.35	1.37
27	11	303	CLA	C1B-NB	-2.14	1.35	1.37
27	b	613	CLA	C3B-C4B	2.14	1.47	1.42
27	12	313	CLA	CMB-C2B	-2.14	1.46	1.50
27	a	402	CLA	C1B-NB	-2.14	1.35	1.37
30	b	620	SQD	O47-C45	-2.14	1.41	1.46
27	13	303	CLA	CMB-C2B	-2.14	1.46	1.50
27	34	307	CLA	CMB-C2B	-2.14	1.46	1.50
38	31	316	A86	O4-C34	-2.14	1.41	1.46
33	B	619	LMG	O7-C8	-2.13	1.41	1.46
27	32	309	CLA	CMC-C2C	-2.13	1.46	1.50
35	j	101	DGD	O3G-C3G	-2.13	1.39	1.43
29	Z	101	BCR	C33-C5	-2.13	1.47	1.50
27	D	406	CLA	C4B-NB	2.13	1.40	1.37
35	c	517	DGD	O4E-C4E	-2.13	1.38	1.43
27	C	513	CLA	C1B-NB	-2.13	1.35	1.37
38	34	303	A86	O4-C34	-2.13	1.41	1.46
27	a	404	CLA	C1D-ND	2.13	1.40	1.37
27	13	305	CLA	C1B-NB	-2.13	1.35	1.37
38	11	313	A86	O4-C34	-2.13	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	623	BCR	C33-C5	-2.13	1.47	1.50
27	14	309	CLA	C1B-NB	-2.13	1.35	1.37
27	34	302	CLA	MG-ND	-2.13	2.01	2.05
27	c	509	CLA	C3B-C4B	2.13	1.47	1.42
27	31	304	CLA	CMB-C2B	-2.13	1.46	1.50
27	34	304	CLA	CMB-C2B	-2.13	1.46	1.50
27	31	307	CLA	C1B-NB	-2.13	1.35	1.37
27	33	307	CLA	CMC-C2C	-2.13	1.46	1.50
27	34	312	CLA	CMB-C2B	-2.13	1.46	1.50
27	12	308	CLA	CMB-C2B	-2.13	1.46	1.50
38	12	317	A86	O4-C34	-2.13	1.41	1.46
27	11	305	CLA	CMB-C2B	-2.13	1.46	1.50
27	13	307	CLA	CMC-C2C	-2.13	1.46	1.50
27	12	311	CLA	C1B-NB	-2.13	1.35	1.37
38	32	304	A86	O4-C34	-2.13	1.41	1.46
27	c	511	CLA	CMB-C2B	-2.12	1.46	1.50
35	j	101	DGD	O4D-C4D	-2.12	1.38	1.43
27	13	311	CLA	MG-ND	-2.12	2.01	2.05
27	11	305	CLA	CMC-C2C	-2.12	1.46	1.50
27	14	306	CLA	CMB-C2B	-2.12	1.46	1.50
38	14	315	A86	O4-C34	-2.12	1.41	1.46
27	33	305	CLA	C1B-NB	-2.12	1.35	1.37
27	c	510	CLA	CMA-C3A	-2.12	1.48	1.53
29	c	516	BCR	C38-C26	-2.12	1.47	1.50
27	14	307	CLA	CMD-C2D	-2.12	1.46	1.50
27	32	306	CLA	CMB-C2B	-2.12	1.46	1.50
27	32	313	CLA	MG-ND	-2.12	2.01	2.05
33	b	619	LMG	O7-C8	-2.12	1.41	1.46
27	C	511	CLA	CMB-C2B	-2.12	1.46	1.50
27	32	313	CLA	CMB-C2B	-2.12	1.46	1.50
27	34	308	CLA	CMD-C2D	-2.12	1.46	1.50
27	B	603	CLA	CHC-C4B	-2.12	1.34	1.39
27	D	402	CLA	C1B-NB	-2.12	1.35	1.37
27	13	309	CLA	C1B-NB	-2.12	1.35	1.37
27	33	309	CLA	C1B-NB	-2.12	1.35	1.37
27	34	311	CLA	C1B-NB	-2.12	1.35	1.37
27	B	606	CLA	C5-C3	-2.12	1.46	1.51
27	C	514	CLA	CMB-C2B	-2.12	1.46	1.50
27	31	309	CLA	CMB-C2B	-2.12	1.46	1.50
27	11	304	CLA	CMB-C2B	-2.12	1.46	1.50
35	j	101	DGD	O4E-C4E	-2.12	1.38	1.43
27	Z	102	CLA	CMD-C2D	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	405	CLA	C1D-ND	2.12	1.40	1.37
27	33	310	CLA	CMB-C2B	-2.12	1.46	1.50
27	C	503	CLA	C1B-C2B	2.12	1.48	1.43
27	33	304	CLA	CMC-C2C	-2.12	1.46	1.50
27	Z	102	CLA	CMC-C2C	-2.12	1.46	1.50
27	13	311	CLA	CMB-C2B	-2.12	1.46	1.50
27	12	309	CLA	CMD-C2D	-2.11	1.46	1.50
27	33	305	CLA	CMB-C2B	-2.11	1.46	1.50
27	C	511	CLA	CAC-C3C	-2.11	1.45	1.51
30	L	103	SQD	O3-C3	-2.11	1.38	1.43
27	32	311	CLA	C1B-NB	-2.11	1.35	1.37
27	32	309	CLA	CMB-C2B	-2.11	1.46	1.50
27	b	605	CLA	CAC-C3C	-2.11	1.45	1.51
27	33	311	CLA	CMB-C2B	-2.11	1.46	1.50
27	33	304	CLA	CMB-C2B	-2.11	1.46	1.50
35	C	518	DGD	O2D-C2D	-2.11	1.38	1.43
27	B	603	CLA	C3B-C4B	2.11	1.47	1.42
27	d	405	CLA	C1D-ND	2.11	1.40	1.37
27	d	401	CLA	CAC-C3C	-2.11	1.45	1.51
35	h	102	DGD	O3D-C3D	-2.11	1.38	1.43
38	34	316	A86	O4-C34	-2.11	1.41	1.46
27	12	309	CLA	CMB-C2B	-2.11	1.46	1.50
27	32	307	CLA	C1B-NB	-2.11	1.35	1.37
27	D	401	CLA	CAC-C3C	-2.11	1.45	1.51
27	11	305	CLA	CMD-C2D	-2.11	1.46	1.50
27	31	305	CLA	CMB-C2B	-2.11	1.46	1.50
27	11	309	CLA	CMB-C2B	-2.11	1.46	1.50
27	12	306	CLA	CMB-C2B	-2.11	1.46	1.50
27	14	307	CLA	CMB-C2B	-2.11	1.46	1.50
27	32	308	CLA	CMB-C2B	-2.11	1.46	1.50
35	c	518	DGD	O2D-C2D	-2.10	1.38	1.43
27	34	312	CLA	MG-ND	-2.10	2.01	2.05
27	d	405	CLA	C1B-C2B	2.10	1.48	1.43
36	D	407	PL9	C15-C14	-2.10	1.45	1.50
27	A	404	CLA	C1D-ND	2.10	1.40	1.37
30	B	620	SQD	O47-C45	-2.10	1.41	1.46
27	c	511	CLA	CAC-C3C	-2.10	1.45	1.51
27	34	308	CLA	CMC-C2C	-2.10	1.46	1.50
33	m	102	LMG	O8-C9	-2.10	1.40	1.45
27	b	603	CLA	CHC-C4B	-2.10	1.34	1.39
38	13	302	A86	O4-C34	-2.10	1.41	1.46
27	C	514	CLA	C1B-C2B	2.10	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	602	CLA	CAC-C3C	-2.10	1.45	1.51
27	31	305	CLA	CMC-C2C	-2.10	1.46	1.50
27	B	605	CLA	CAC-C3C	-2.10	1.45	1.51
27	33	306	CLA	CMB-C2B	-2.10	1.46	1.50
27	14	311	CLA	CMB-C2B	-2.10	1.46	1.50
27	13	307	CLA	CMB-C2B	-2.10	1.46	1.50
27	32	312	CLA	C1B-NB	-2.10	1.35	1.37
29	C	516	BCR	C33-C5	-2.10	1.47	1.50
38	12	304	A86	O4-C34	-2.09	1.41	1.46
27	z	102	CLA	CMD-C2D	-2.09	1.46	1.50
27	31	309	CLA	MG-ND	-2.09	2.01	2.05
27	12	312	CLA	C1B-NB	-2.09	1.35	1.37
33	M	103	LMG	O2-C2	-2.09	1.38	1.43
27	11	309	CLA	MG-ND	-2.09	2.01	2.05
27	31	303	CLA	C1B-NB	-2.09	1.35	1.37
27	34	310	CLA	C1B-NB	-2.09	1.35	1.37
27	34	305	CLA	CMB-C2B	-2.09	1.46	1.50
38	11	316	A86	O4-C34	-2.09	1.41	1.46
29	C	516	BCR	C38-C26	-2.09	1.47	1.50
27	34	307	CLA	CMC-C2C	-2.09	1.46	1.50
36	d	407	PL9	C15-C14	-2.09	1.45	1.50
27	33	311	CLA	MG-ND	-2.09	2.01	2.05
27	b	610	CLA	CAC-C3C	-2.09	1.45	1.51
27	14	306	CLA	CMC-C2C	-2.09	1.46	1.50
27	31	302	CLA	CMB-C2B	-2.09	1.46	1.50
30	l	101	SQD	O3-C3	-2.09	1.38	1.43
27	14	305	CLA	C1B-NB	-2.09	1.35	1.37
35	J	101	DGD	O4D-C4D	-2.09	1.38	1.43
30	l	101	SQD	O4-C4	-2.09	1.38	1.43
27	C	509	CLA	C3B-C4B	2.08	1.47	1.42
27	b	606	CLA	C5-C3	-2.08	1.47	1.51
27	B	610	CLA	CAC-C3C	-2.08	1.45	1.51
27	32	310	CLA	C1B-NB	-2.08	1.35	1.37
38	33	302	A86	O4-C34	-2.08	1.41	1.46
35	J	101	DGD	O4E-C4E	-2.08	1.38	1.43
27	12	309	CLA	CMC-C2C	-2.08	1.46	1.50
35	H	102	DGD	O3D-C3D	-2.08	1.38	1.43
27	12	313	CLA	MG-ND	-2.08	2.01	2.05
29	c	515	BCR	C33-C5	-2.08	1.47	1.50
27	11	308	CLA	C1B-NB	-2.08	1.35	1.37
27	31	308	CLA	C1B-NB	-2.08	1.35	1.37
27	B	610	CLA	C4B-NB	2.08	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	12	307	CLA	C1B-NB	-2.08	1.35	1.37
30	L	103	SQD	O4-C4	-2.08	1.38	1.43
35	C	517	DGD	O4E-C4E	-2.07	1.38	1.43
27	14	307	CLA	CMC-C2C	-2.07	1.46	1.50
27	14	304	CLA	CMB-C2B	-2.07	1.46	1.50
28	a	403	PHO	C3B-CAB	-2.07	1.43	1.47
33	M	103	LMG	O8-C9	-2.07	1.40	1.45
27	b	603	CLA	C3B-C4B	2.07	1.47	1.42
27	C	511	CLA	CHC-C1C	2.07	1.42	1.38
27	c	509	CLA	CHC-C4B	-2.07	1.34	1.39
28	A	403	PHO	C3B-CAB	-2.07	1.43	1.47
27	11	302	CLA	CMB-C2B	-2.07	1.46	1.50
27	B	622	CLA	C1B-C2B	2.07	1.48	1.43
33	m	102	LMG	O2-C2	-2.07	1.38	1.43
27	b	608	CLA	MG-ND	-2.07	2.01	2.05
27	w	102	CLA	C1B-C2B	2.07	1.48	1.43
27	13	304	CLA	CMB-C2B	-2.07	1.46	1.50
27	c	502	CLA	CHC-C4B	-2.06	1.34	1.39
29	c	516	BCR	C33-C5	-2.06	1.47	1.50
27	c	512	CLA	CHC-C1C	2.06	1.42	1.38
29	b	623	BCR	C33-C5	-2.06	1.47	1.50
27	c	511	CLA	CHC-C1C	2.06	1.42	1.38
27	a	404	CLA	C4B-NB	2.06	1.40	1.37
27	13	308	CLA	C1B-NB	-2.06	1.35	1.37
27	11	305	CLA	MG-ND	-2.06	2.01	2.05
27	12	308	CLA	CMC-C2C	-2.06	1.46	1.50
27	b	611	CLA	C4B-NB	2.05	1.40	1.37
27	34	305	CLA	C1B-NB	-2.05	1.35	1.37
27	b	615	CLA	CAC-C3C	-2.05	1.45	1.51
27	A	404	CLA	C1B-NB	-2.05	1.35	1.37
35	c	517	DGD	O3G-C1D	-2.05	1.36	1.40
36	d	404	PL9	C41-C39	-2.05	1.47	1.51
27	A	404	CLA	C4B-NB	2.05	1.40	1.37
27	C	509	CLA	CHC-C4B	-2.05	1.34	1.39
27	c	503	CLA	C1B-C2B	2.05	1.48	1.43
27	32	305	CLA	MG-ND	-2.05	2.01	2.05
27	31	304	CLA	CMC-C2C	-2.05	1.46	1.50
27	33	311	CLA	CMC-C2C	-2.05	1.46	1.50
29	C	515	BCR	C33-C5	-2.05	1.47	1.50
30	A	406	SQD	O47-C45	-2.05	1.41	1.46
27	13	306	CLA	CMC-C2C	-2.05	1.46	1.50
35	h	102	DGD	O2D-C2D	-2.05	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	14	311	CLA	MG-ND	-2.05	2.01	2.05
27	B	602	CLA	CAC-C3C	-2.05	1.45	1.51
27	b	612	CLA	C1B-C2B	2.05	1.48	1.43
27	W	102	CLA	C1B-C2B	2.05	1.48	1.43
27	14	311	CLA	CMC-C2C	-2.05	1.46	1.50
27	D	402	CLA	C4B-NB	2.05	1.40	1.37
35	H	102	DGD	O2D-C2D	-2.05	1.38	1.43
29	H	101	BCR	C38-C26	-2.04	1.47	1.50
27	13	311	CLA	CMC-C2C	-2.04	1.46	1.50
27	B	608	CLA	MG-ND	-2.04	2.01	2.05
27	b	622	CLA	C1B-C2B	2.04	1.48	1.43
27	33	303	CLA	CHC-C1C	2.04	1.42	1.38
27	d	402	CLA	C4B-NB	2.04	1.40	1.37
27	B	615	CLA	CAC-C3C	-2.04	1.45	1.51
27	34	304	CLA	MG-ND	-2.04	2.01	2.05
27	31	309	CLA	CMC-C2C	-2.04	1.46	1.50
27	31	301	CLA	MG-ND	-2.04	2.01	2.05
36	D	404	PL9	C41-C39	-2.04	1.47	1.51
29	H	101	BCR	C33-C5	-2.03	1.47	1.50
29	h	101	BCR	C33-C5	-2.03	1.47	1.50
27	11	309	CLA	CMC-C2C	-2.03	1.46	1.50
27	11	304	CLA	CMC-C2C	-2.03	1.46	1.50
27	34	312	CLA	CMC-C2C	-2.03	1.46	1.50
27	b	602	CLA	C1B-NB	-2.03	1.35	1.37
27	b	614	CLA	CHC-C4B	-2.03	1.34	1.39
27	14	303	CLA	MG-ND	-2.03	2.01	2.05
32	A	408	LHG	C8-C7	-2.03	1.44	1.50
27	D	406	CLA	C1B-C2B	2.03	1.48	1.43
33	C	519	LMG	O2-C2	-2.03	1.38	1.43
27	32	308	CLA	CMC-C2C	-2.03	1.46	1.50
27	14	303	CLA	CHC-C1C	2.03	1.42	1.38
27	B	611	CLA	C4B-NB	2.03	1.40	1.37
27	33	310	CLA	C1B-NB	-2.03	1.35	1.37
27	W	103	CLA	CMB-C2B	-2.03	1.46	1.50
27	14	308	CLA	C1B-NB	-2.03	1.35	1.37
36	D	407	PL9	C16-C14	-2.02	1.47	1.51
27	12	305	CLA	CHC-C1C	2.02	1.42	1.38
27	W	103	CLA	CHC-C1C	2.02	1.42	1.38
29	h	101	BCR	C38-C26	-2.02	1.47	1.50
27	31	301	CLA	CHC-C1C	2.02	1.42	1.38
27	w	103	CLA	CMB-C2B	-2.02	1.46	1.50
27	C	513	CLA	C1B-C2B	2.02	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	33	303	CLA	MG-ND	-2.02	2.01	2.05
33	q	301	LMG	O2-C2	-2.02	1.38	1.43
27	B	614	CLA	CHC-C4B	-2.02	1.34	1.39
27	14	307	CLA	MG-ND	-2.02	2.01	2.05
27	33	306	CLA	CMC-C2C	-2.02	1.46	1.50
27	C	510	CLA	C3B-C4B	2.02	1.47	1.42
27	11	301	CLA	CHC-C1C	2.02	1.42	1.38
27	W	102	CLA	C1B-NB	-2.02	1.35	1.37
27	b	603	CLA	C4B-NB	2.02	1.40	1.37
27	12	313	CLA	CMC-C2C	-2.02	1.46	1.50
27	c	510	CLA	C3B-C4B	2.02	1.47	1.42
27	d	406	CLA	C1B-C2B	2.02	1.48	1.43
27	11	301	CLA	MG-ND	-2.02	2.01	2.05
27	b	607	CLA	C4B-NB	2.02	1.40	1.37
27	31	305	CLA	C1B-NB	-2.02	1.35	1.37
27	12	305	CLA	MG-ND	-2.02	2.01	2.05
27	w	103	CLA	CHC-C1C	2.01	1.42	1.38
30	a	406	SQD	O47-C45	-2.01	1.41	1.46
27	32	313	CLA	CMC-C2C	-2.01	1.46	1.50
27	C	502	CLA	CHC-C4B	-2.01	1.34	1.39
27	D	401	CLA	C3B-C4B	2.01	1.47	1.42
27	a	404	CLA	C1B-NB	-2.01	1.35	1.37
27	11	315	CLA	C1B-NB	-2.01	1.35	1.37
27	12	310	CLA	C1B-NB	-2.01	1.35	1.37
27	31	305	CLA	MG-ND	-2.01	2.01	2.05
27	B	607	CLA	C1B-C2B	2.01	1.48	1.43
27	13	307	CLA	MG-ND	-2.01	2.01	2.05
27	C	512	CLA	CHC-C1C	2.01	1.42	1.38
27	13	303	CLA	CHC-C1C	2.01	1.42	1.38
27	34	309	CLA	C1B-NB	-2.01	1.35	1.37
38	13	314	A86	C33-C34	2.01	1.55	1.51
38	34	315	A86	C33-C34	2.01	1.55	1.51
29	Z	101	BCR	C34-C9	-2.01	1.46	1.50
27	14	310	CLA	C1B-NB	-2.01	1.35	1.37
27	33	308	CLA	C1B-NB	-2.01	1.35	1.37
27	34	310	CLA	C1B-C2B	2.01	1.48	1.43
30	b	620	SQD	C4-C5	-2.01	1.48	1.53
27	B	622	CLA	C1D-ND	2.01	1.40	1.37
27	11	305	CLA	C1B-NB	-2.01	1.35	1.37
32	a	408	LHG	C8-C7	-2.00	1.44	1.50
27	31	315	CLA	C1B-NB	-2.00	1.35	1.37
27	32	309	CLA	C1B-NB	-2.00	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	505	CLA	C3B-C4B	2.00	1.47	1.42
27	31	306	CLA	C1B-NB	-2.00	1.35	1.37
29	C	516	BCR	C27-C26	-2.00	1.47	1.51
27	33	301	CLA	C1B-NB	-2.00	1.35	1.37
27	B	607	CLA	C4B-NB	2.00	1.40	1.37
27	34	304	CLA	CHC-C1C	2.00	1.42	1.38

All (2966) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	33	312	A86	O1-C20-C19	55.03	154.72	113.38
38	34	313	A86	O1-C20-C19	55.03	154.72	113.38
38	12	314	A86	O1-C20-C19	55.02	154.72	113.38
38	14	312	A86	O1-C20-C19	55.01	154.71	113.38
38	13	312	A86	O1-C20-C19	55.01	154.71	113.38
38	11	310	A86	O1-C20-C19	55.00	154.70	113.38
38	32	314	A86	O1-C20-C19	54.99	154.69	113.38
38	31	310	A86	O1-C20-C19	54.97	154.67	113.38
38	31	313	A86	O1-C20-C19	54.26	154.14	113.38
38	14	315	A86	O1-C20-C19	54.24	154.12	113.38
38	11	313	A86	O1-C20-C19	54.23	154.12	113.38
38	13	315	A86	O1-C20-C19	54.22	154.11	113.38
38	32	317	A86	O1-C20-C19	54.22	154.11	113.38
38	12	317	A86	O1-C20-C19	54.20	154.09	113.38
38	33	315	A86	O1-C20-C19	54.19	154.09	113.38
38	34	316	A86	O1-C20-C19	54.13	154.04	113.38
38	13	316	A86	O1-C20-C19	52.57	152.87	113.38
38	31	314	A86	O1-C20-C19	52.56	152.87	113.38
38	11	314	A86	O1-C20-C19	52.54	152.85	113.38
38	14	301	A86	O1-C20-C19	52.54	152.85	113.38
38	33	316	A86	O1-C20-C19	52.54	152.85	113.38
38	14	316	A86	O1-C20-C19	52.54	152.85	113.38
38	32	318	A86	O1-C20-C19	52.53	152.84	113.38
38	34	301	A86	O1-C20-C19	52.50	152.82	113.38
38	14	313	A86	O1-C20-C19	51.96	152.41	113.38
38	12	315	A86	O1-C20-C19	51.95	152.40	113.38
38	34	314	A86	O1-C20-C19	51.94	152.40	113.38
38	13	313	A86	O1-C20-C19	51.94	152.40	113.38
38	31	311	A86	O1-C20-C19	51.90	152.37	113.38
38	32	315	A86	O1-C20-C19	51.90	152.37	113.38
38	11	311	A86	O1-C20-C19	51.88	152.35	113.38
38	33	313	A86	O1-C20-C19	51.86	152.34	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	11	312	A86	O1-C20-C19	50.65	151.43	113.38
38	34	315	A86	O1-C20-C19	50.60	151.40	113.38
38	31	312	A86	O1-C20-C19	50.59	151.39	113.38
38	12	316	A86	O1-C20-C19	50.58	151.38	113.38
38	13	314	A86	O1-C20-C19	50.57	151.37	113.38
38	32	316	A86	O1-C20-C19	50.57	151.37	113.38
38	33	314	A86	O1-C20-C19	50.56	151.37	113.38
38	14	314	A86	O1-C20-C19	50.55	151.35	113.38
38	33	302	A86	O1-C20-C19	48.00	149.44	113.38
38	13	302	A86	O1-C20-C19	47.99	149.43	113.38
38	13	317	A86	O1-C20-C19	47.97	149.42	113.38
38	32	304	A86	O1-C20-C19	47.96	149.41	113.38
38	31	316	A86	O1-C20-C19	47.95	149.40	113.38
38	12	304	A86	O1-C20-C19	47.94	149.40	113.38
38	34	303	A86	O1-C20-C19	47.93	149.39	113.38
38	11	316	A86	O1-C20-C19	47.93	149.39	113.38
38	34	303	A86	C17-C16-C15	11.89	121.30	109.16
38	31	316	A86	C17-C16-C15	11.86	121.26	109.16
38	12	304	A86	C17-C16-C15	11.86	121.26	109.16
38	13	302	A86	C17-C16-C15	11.85	121.26	109.16
38	33	302	A86	C17-C16-C15	11.85	121.25	109.16
38	32	304	A86	C17-C16-C15	11.85	121.25	109.16
38	13	317	A86	C17-C16-C15	11.84	121.25	109.16
38	11	316	A86	C17-C16-C15	11.82	121.22	109.16
38	31	313	A86	O1-C20-C21	-11.26	101.56	115.06
38	33	315	A86	O1-C20-C21	-11.25	101.57	115.06
38	11	313	A86	O1-C20-C21	-11.25	101.58	115.06
38	32	317	A86	O1-C20-C21	-11.24	101.58	115.06
38	14	315	A86	O1-C20-C21	-11.23	101.59	115.06
38	13	315	A86	O1-C20-C21	-11.22	101.61	115.06
38	12	317	A86	O1-C20-C21	-11.21	101.62	115.06
38	34	316	A86	O1-C20-C21	-11.20	101.64	115.06
38	12	314	A86	O1-C20-C21	-10.92	101.97	115.06
38	33	312	A86	O1-C20-C21	-10.91	101.98	115.06
38	11	310	A86	O1-C20-C21	-10.90	102.00	115.06
38	14	312	A86	O1-C20-C21	-10.89	102.00	115.06
38	32	314	A86	O1-C20-C21	-10.89	102.00	115.06
38	34	313	A86	O1-C20-C21	-10.89	102.01	115.06
38	13	312	A86	O1-C20-C21	-10.88	102.02	115.06
38	11	314	A86	C21-C20-C19	-10.88	102.04	114.28
38	31	310	A86	O1-C20-C21	-10.88	102.02	115.06
38	13	316	A86	C21-C20-C19	-10.88	102.04	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	31	314	A86	C21-C20-C19	-10.86	102.06	114.28
38	14	316	A86	C21-C20-C19	-10.85	102.07	114.28
38	32	318	A86	C21-C20-C19	-10.85	102.08	114.28
38	14	301	A86	C21-C20-C19	-10.84	102.08	114.28
38	34	301	A86	C21-C20-C19	-10.84	102.08	114.28
38	33	316	A86	C21-C20-C19	-10.82	102.11	114.28
38	34	313	A86	C21-C20-C19	-10.62	102.33	114.28
38	13	312	A86	C21-C20-C19	-10.60	102.36	114.28
38	33	312	A86	C21-C20-C19	-10.59	102.36	114.28
38	11	310	A86	C21-C20-C19	-10.59	102.37	114.28
38	14	312	A86	C21-C20-C19	-10.58	102.37	114.28
38	32	314	A86	C21-C20-C19	-10.58	102.38	114.28
38	12	314	A86	C21-C20-C19	-10.57	102.38	114.28
38	31	310	A86	C21-C20-C19	-10.57	102.39	114.28
38	11	312	A86	C21-C20-C19	-10.54	102.43	114.28
38	13	314	A86	C21-C20-C19	-10.53	102.44	114.28
38	33	314	A86	C21-C20-C19	-10.53	102.44	114.28
38	12	316	A86	C21-C20-C19	-10.51	102.46	114.28
38	31	312	A86	C21-C20-C19	-10.51	102.46	114.28
38	34	315	A86	C21-C20-C19	-10.51	102.46	114.28
38	14	314	A86	C21-C20-C19	-10.48	102.49	114.28
38	32	316	A86	C21-C20-C19	-10.46	102.51	114.28
38	33	302	A86	C21-C20-C19	-10.17	102.84	114.28
38	31	316	A86	C21-C20-C19	-10.16	102.85	114.28
38	32	304	A86	C21-C20-C19	-10.14	102.87	114.28
38	12	304	A86	C21-C20-C19	-10.14	102.87	114.28
38	13	317	A86	C21-C20-C19	-10.13	102.89	114.28
38	13	302	A86	C21-C20-C19	-10.12	102.89	114.28
38	14	313	A86	O1-C20-C21	-10.12	102.93	115.06
38	13	313	A86	O1-C20-C21	-10.11	102.94	115.06
38	34	303	A86	C21-C20-C19	-10.11	102.91	114.28
38	11	316	A86	C21-C20-C19	-10.11	102.91	114.28
38	12	315	A86	O1-C20-C21	-10.10	102.95	115.06
38	34	314	A86	O1-C20-C21	-10.09	102.97	115.06
38	31	311	A86	O1-C20-C21	-10.08	102.98	115.06
38	33	313	A86	O1-C20-C21	-10.08	102.98	115.06
38	11	311	A86	O1-C20-C21	-10.06	103.00	115.06
38	32	315	A86	O1-C20-C21	-10.06	103.00	115.06
27	B	612	CLA	C4A-NA-C1A	10.00	111.20	106.71
27	b	612	CLA	C4A-NA-C1A	9.93	111.17	106.71
38	12	317	A86	C21-C20-C19	-9.87	103.18	114.28
38	32	315	A86	C21-C20-C19	-9.86	103.19	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	13	315	A86	C21-C20-C19	-9.86	103.19	114.28
38	14	315	A86	C21-C20-C19	-9.85	103.19	114.28
38	34	314	A86	C21-C20-C19	-9.85	103.19	114.28
38	11	313	A86	C21-C20-C19	-9.85	103.20	114.28
38	31	313	A86	C21-C20-C19	-9.85	103.20	114.28
38	12	315	A86	C21-C20-C19	-9.84	103.21	114.28
38	11	311	A86	C21-C20-C19	-9.84	103.21	114.28
38	32	317	A86	C21-C20-C19	-9.84	103.21	114.28
38	34	316	A86	C21-C20-C19	-9.83	103.22	114.28
38	14	313	A86	C21-C20-C19	-9.83	103.22	114.28
38	13	313	A86	C21-C20-C19	-9.83	103.23	114.28
38	31	311	A86	C21-C20-C19	-9.82	103.23	114.28
38	33	313	A86	C21-C20-C19	-9.80	103.25	114.28
38	33	315	A86	C21-C20-C19	-9.79	103.26	114.28
38	14	301	A86	O1-C20-C21	-9.39	103.80	115.06
38	33	316	A86	O1-C20-C21	-9.39	103.80	115.06
38	31	314	A86	O1-C20-C21	-9.38	103.82	115.06
38	14	316	A86	O1-C20-C21	-9.37	103.83	115.06
38	32	318	A86	O1-C20-C21	-9.37	103.83	115.06
38	34	301	A86	O1-C20-C21	-9.36	103.84	115.06
38	11	314	A86	O1-C20-C21	-9.36	103.84	115.06
38	13	316	A86	O1-C20-C21	-9.35	103.85	115.06
27	11	301	CLA	C4A-NA-C1A	9.09	110.79	106.71
27	13	303	CLA	C4A-NA-C1A	9.05	110.77	106.71
27	c	510	CLA	C4A-NA-C1A	9.02	110.76	106.71
38	12	304	A86	C33-C32-C31	9.02	117.98	109.21
27	33	303	CLA	C4A-NA-C1A	9.02	110.76	106.71
38	31	316	A86	C33-C32-C31	9.01	117.97	109.21
27	32	305	CLA	C4A-NA-C1A	9.01	110.76	106.71
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
27	12	305	CLA	C4A-NA-C1A	9.00	110.75	106.71
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	31	301	CLA	C4A-NA-C1A	8.96	110.74	106.71
27	34	304	CLA	C4A-NA-C1A	8.94	110.73	106.71
27	14	303	CLA	C4A-NA-C1A	8.94	110.72	106.71
27	C	510	CLA	C4A-NA-C1A	8.92	110.72	106.71
38	32	316	A86	O1-C20-C21	-8.87	104.43	115.06
38	11	312	A86	O1-C20-C21	-8.86	104.44	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	34	315	A86	O1-C20-C21	-8.85	104.45	115.06
38	12	316	A86	O1-C20-C21	-8.85	104.45	115.06
38	31	312	A86	O1-C20-C21	-8.85	104.45	115.06
38	14	314	A86	O1-C20-C21	-8.84	104.46	115.06
38	13	314	A86	O1-C20-C21	-8.82	104.49	115.06
38	33	314	A86	O1-C20-C21	-8.81	104.50	115.06
28	a	403	PHO	C4D-CHA-CBD	-8.81	104.53	108.52
28	A	403	PHO	C4D-CHA-CBD	-8.69	104.59	108.52
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	12	316	A86	C33-C32-C31	8.49	117.46	109.21
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	31	312	A86	C33-C32-C31	8.44	117.41	109.21
38	13	317	A86	C4-C5-C6	-8.37	115.36	127.31
38	33	302	A86	C4-C5-C6	-8.37	115.37	127.31
38	12	304	A86	C4-C5-C6	-8.36	115.38	127.31
38	34	315	A86	C17-C16-C15	8.36	117.69	109.16
38	11	316	A86	C4-C5-C6	-8.35	115.39	127.31
38	32	304	A86	C4-C5-C6	-8.35	115.39	127.31
38	34	303	A86	C4-C5-C6	-8.33	115.42	127.31
38	31	316	A86	C4-C5-C6	-8.33	115.42	127.31
38	13	302	A86	C4-C5-C6	-8.33	115.43	127.31
27	c	505	CLA	C4A-NA-C1A	8.32	110.45	106.71
38	33	314	A86	C17-C16-C15	8.31	117.64	109.16
38	32	316	A86	C17-C16-C15	8.30	117.63	109.16
38	11	312	A86	C17-C16-C15	8.29	117.62	109.16
38	14	314	A86	C17-C16-C15	8.28	117.61	109.16
38	12	316	A86	C17-C16-C15	8.27	117.59	109.16
27	C	505	CLA	C4A-NA-C1A	8.26	110.42	106.71
38	31	312	A86	C17-C16-C15	8.26	117.59	109.16
38	13	314	A86	C17-C16-C15	8.25	117.58	109.16
28	d	403	PHO	C4D-CHA-CBD	-8.21	104.80	108.52
28	D	403	PHO	C4D-CHA-CBD	-8.19	104.81	108.52
27	d	406	CLA	C4A-NA-C1A	8.17	110.38	106.71
27	11	306	CLA	C4A-NA-C1A	8.16	110.37	106.71
27	33	308	CLA	C4A-NA-C1A	8.15	110.37	106.71
27	13	308	CLA	C4A-NA-C1A	8.15	110.37	106.71
27	b	609	CLA	C4A-NA-C1A	8.14	110.36	106.71
27	A	402	CLA	C4A-NA-C1A	8.12	110.36	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	609	CLA	C4A-NA-C1A	8.11	110.35	106.71
27	D	406	CLA	C4A-NA-C1A	8.10	110.35	106.71
27	12	310	CLA	C4A-NA-C1A	8.08	110.34	106.71
27	C	502	CLA	C4A-NA-C1A	8.07	110.33	106.71
27	a	402	CLA	C4A-NA-C1A	8.05	110.32	106.71
27	31	306	CLA	C4A-NA-C1A	8.03	110.32	106.71
27	14	308	CLA	C4A-NA-C1A	8.02	110.31	106.71
27	c	502	CLA	C4A-NA-C1A	8.01	110.31	106.71
27	34	309	CLA	C4A-NA-C1A	8.01	110.31	106.71
27	32	310	CLA	C4A-NA-C1A	8.00	110.30	106.71
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
38	12	314	A86	C33-C32-C31	7.83	116.83	109.21
27	C	514	CLA	C4A-NA-C1A	7.83	110.23	106.71
27	c	514	CLA	C4A-NA-C1A	7.83	110.22	106.71
38	14	312	A86	C33-C32-C31	7.82	116.81	109.21
38	33	312	A86	C33-C32-C31	7.82	116.81	109.21
27	B	601	CLA	C4A-NA-C1A	7.71	110.17	106.71
27	34	306	CLA	C4A-NA-C1A	7.70	110.17	106.71
27	C	504	CLA	C4A-NA-C1A	7.68	110.16	106.71
27	32	307	CLA	C4A-NA-C1A	7.66	110.15	106.71
27	12	307	CLA	C4A-NA-C1A	7.65	110.14	106.71
27	14	305	CLA	C4A-NA-C1A	7.64	110.14	106.71
27	11	303	CLA	C4A-NA-C1A	7.64	110.14	106.71
27	13	305	CLA	C4A-NA-C1A	7.62	110.13	106.71
27	b	601	CLA	C4A-NA-C1A	7.62	110.13	106.71
27	b	608	CLA	C4A-NA-C1A	7.59	110.12	106.71
27	31	303	CLA	C4A-NA-C1A	7.58	110.11	106.71
27	33	305	CLA	C4A-NA-C1A	7.58	110.11	106.71
27	c	504	CLA	C4A-NA-C1A	7.57	110.11	106.71
27	B	608	CLA	C4A-NA-C1A	7.53	110.09	106.71
27	13	304	CLA	C4A-NA-C1A	7.51	110.08	106.71
27	32	306	CLA	C4A-NA-C1A	7.48	110.07	106.71
27	14	304	CLA	C4A-NA-C1A	7.45	110.06	106.71
27	b	603	CLA	C4A-NA-C1A	7.45	110.05	106.71
27	b	613	CLA	C4A-NA-C1A	7.45	110.05	106.71
27	34	307	CLA	C4A-NA-C1A	7.42	110.04	106.71
27	33	304	CLA	C4A-NA-C1A	7.42	110.04	106.71
27	34	305	CLA	C4A-NA-C1A	7.41	110.04	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	603	CLA	C4A-NA-C1A	7.41	110.04	106.71
27	11	302	CLA	C4A-NA-C1A	7.37	110.02	106.71
38	31	314	A86	C17-C16-C15	7.37	116.68	109.16
38	13	316	A86	C17-C16-C15	7.36	116.67	109.16
38	34	301	A86	C17-C16-C15	7.36	116.67	109.16
38	11	314	A86	C17-C16-C15	7.36	116.67	109.16
27	12	306	CLA	C4A-NA-C1A	7.36	110.01	106.71
38	14	301	A86	C17-C16-C15	7.36	116.67	109.16
27	c	509	CLA	C4A-NA-C1A	7.35	110.01	106.71
27	33	306	CLA	C4A-NA-C1A	7.34	110.01	106.71
38	14	316	A86	C17-C16-C15	7.34	116.65	109.16
27	b	611	CLA	C4A-NA-C1A	7.33	110.00	106.71
27	14	306	CLA	C4A-NA-C1A	7.33	110.00	106.71
27	31	302	CLA	C4A-NA-C1A	7.33	110.00	106.71
38	33	316	A86	C17-C16-C15	7.33	116.64	109.16
38	13	302	A86	O1-C20-C21	-7.32	106.28	115.06
27	B	611	CLA	C4A-NA-C1A	7.32	110.00	106.71
27	31	304	CLA	C4A-NA-C1A	7.32	110.00	106.71
38	32	318	A86	C17-C16-C15	7.31	116.62	109.16
38	32	304	A86	O1-C20-C21	-7.31	106.29	115.06
38	13	317	A86	O1-C20-C21	-7.31	106.30	115.06
27	C	509	CLA	C4A-NA-C1A	7.31	109.99	106.71
38	11	316	A86	O1-C20-C21	-7.31	106.30	115.06
38	34	303	A86	O1-C20-C21	-7.30	106.31	115.06
27	C	512	CLA	C4A-NA-C1A	7.30	109.99	106.71
38	12	304	A86	O1-C20-C21	-7.30	106.31	115.06
38	33	302	A86	O1-C20-C21	-7.28	106.33	115.06
27	32	308	CLA	C4A-NA-C1A	7.28	109.98	106.71
27	C	513	CLA	C4A-NA-C1A	7.27	109.98	106.71
38	31	316	A86	O1-C20-C21	-7.27	106.35	115.06
27	C	508	CLA	C4A-NA-C1A	7.26	109.97	106.71
27	B	613	CLA	C4A-NA-C1A	7.26	109.97	106.71
27	Z	102	CLA	C4A-NA-C1A	7.25	109.97	106.71
27	13	307	CLA	C4A-NA-C1A	7.25	109.96	106.71
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	z	102	CLA	C4A-NA-C1A	7.23	109.96	106.71
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
27	12	308	CLA	C4A-NA-C1A	7.22	109.95	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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	11	305	CLA	C4A-NA-C1A	7.21	109.95	106.71
27	D	402	CLA	C4A-NA-C1A	7.20	109.94	106.71
27	12	309	CLA	C4A-NA-C1A	7.20	109.94	106.71
27	c	513	CLA	C4A-NA-C1A	7.20	109.94	106.71
38	12	317	A86	C33-C32-C31	7.19	116.20	109.21
27	B	607	CLA	C4A-NA-C1A	7.19	109.94	106.71
27	b	614	CLA	C4A-NA-C1A	7.18	109.93	106.71
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	304	CLA	C4A-NA-C1A	7.17	109.93	106.71
38	33	315	A86	C33-C32-C31	7.15	116.16	109.21
27	D	405	CLA	C4A-NA-C1A	7.15	109.92	106.71
27	b	607	CLA	C4A-NA-C1A	7.15	109.92	106.71
27	A	404	CLA	C4A-NA-C1A	7.14	109.92	106.71
27	d	405	CLA	C4A-NA-C1A	7.14	109.91	106.71
27	13	306	CLA	C4A-NA-C1A	7.13	109.91	106.71
38	34	316	A86	C33-C32-C31	7.13	116.14	109.21
27	d	402	CLA	C4A-NA-C1A	7.13	109.91	106.71
27	a	404	CLA	C4A-NA-C1A	7.12	109.91	106.71
27	c	512	CLA	C4A-NA-C1A	7.12	109.91	106.71
27	B	606	CLA	C4A-NA-C1A	7.11	109.90	106.71
27	B	614	CLA	C4A-NA-C1A	7.10	109.90	106.71
27	14	307	CLA	C4A-NA-C1A	7.10	109.90	106.71
27	33	307	CLA	C4A-NA-C1A	7.08	109.89	106.71
38	31	311	A86	C17-C16-C15	7.08	116.38	109.16
27	31	305	CLA	C4A-NA-C1A	7.07	109.89	106.71
27	32	309	CLA	C4A-NA-C1A	7.07	109.89	106.71
27	34	308	CLA	C4A-NA-C1A	7.06	109.88	106.71
38	12	315	A86	C17-C16-C15	7.06	116.37	109.16
38	13	313	A86	C17-C16-C15	7.06	116.36	109.16
27	11	315	CLA	C4A-NA-C1A	7.05	109.88	106.71
27	B	622	CLA	C4A-NA-C1A	7.05	109.87	106.71
38	11	311	A86	C17-C16-C15	7.04	116.34	109.16
38	14	313	A86	C17-C16-C15	7.04	116.34	109.16
27	c	508	CLA	C4A-NA-C1A	7.04	109.87	106.71
27	33	301	CLA	C4A-NA-C1A	7.03	109.87	106.71
27	14	302	CLA	C4A-NA-C1A	7.03	109.87	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	33	313	A86	C17-C16-C15	7.02	116.33	109.16
27	32	303	CLA	C4A-NA-C1A	7.02	109.86	106.71
38	34	314	A86	C17-C16-C15	7.01	116.31	109.16
38	32	315	A86	C17-C16-C15	7.01	116.31	109.16
27	12	303	CLA	C4A-NA-C1A	7.00	109.85	106.71
27	31	315	CLA	C4A-NA-C1A	6.99	109.85	106.71
27	13	301	CLA	C4A-NA-C1A	6.99	109.85	106.71
27	b	606	CLA	C4A-NA-C1A	6.95	109.83	106.71
27	34	302	CLA	C4A-NA-C1A	6.93	109.82	106.71
27	B	610	CLA	C4A-NA-C1A	6.92	109.82	106.71
27	C	503	CLA	C4A-NA-C1A	6.92	109.82	106.71
27	b	622	CLA	C4A-NA-C1A	6.88	109.80	106.71
27	c	503	CLA	C4A-NA-C1A	6.88	109.80	106.71
27	b	610	CLA	C4A-NA-C1A	6.86	109.79	106.71
27	B	605	CLA	C4A-NA-C1A	6.81	109.77	106.71
27	b	604	CLA	C4A-NA-C1A	6.78	109.76	106.71
27	d	401	CLA	C4A-NA-C1A	6.78	109.76	106.71
27	D	401	CLA	C4A-NA-C1A	6.78	109.75	106.71
27	b	605	CLA	C4A-NA-C1A	6.75	109.74	106.71
27	B	604	CLA	C4A-NA-C1A	6.74	109.74	106.71
27	B	602	CLA	C4A-NA-C1A	6.73	109.73	106.71
27	c	506	CLA	C4A-NA-C1A	6.73	109.73	106.71
27	b	602	CLA	C4A-NA-C1A	6.69	109.71	106.71
27	C	506	CLA	C4A-NA-C1A	6.68	109.71	106.71
27	12	312	CLA	C4A-NA-C1A	6.53	109.64	106.71
27	11	308	CLA	C4A-NA-C1A	6.51	109.63	106.71
27	32	311	CLA	C4A-NA-C1A	6.49	109.63	106.71
27	33	309	CLA	C4A-NA-C1A	6.49	109.62	106.71
27	14	310	CLA	C4A-NA-C1A	6.49	109.62	106.71
27	13	310	CLA	C4A-NA-C1A	6.48	109.62	106.71
27	33	310	CLA	C4A-NA-C1A	6.47	109.61	106.71
27	31	308	CLA	C4A-NA-C1A	6.46	109.61	106.71
27	14	309	CLA	C4A-NA-C1A	6.45	109.61	106.71
27	w	103	CLA	C4A-NA-C1A	6.43	109.60	106.71
27	32	312	CLA	C4A-NA-C1A	6.40	109.58	106.71
27	11	307	CLA	C4A-NA-C1A	6.39	109.58	106.71
27	W	103	CLA	C4A-NA-C1A	6.39	109.58	106.71
38	13	314	A86	C4-C5-C6	-6.39	118.19	127.31
27	34	311	CLA	C4A-NA-C1A	6.39	109.58	106.71
38	32	316	A86	C4-C5-C6	-6.38	118.20	127.31
38	14	314	A86	C4-C5-C6	-6.38	118.21	127.31
27	13	309	CLA	C4A-NA-C1A	6.37	109.57	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	34	315	A86	C4-C5-C6	-6.36	118.23	127.31
38	12	316	A86	C4-C5-C6	-6.36	118.24	127.31
27	31	307	CLA	C4A-NA-C1A	6.35	109.56	106.71
38	11	312	A86	C4-C5-C6	-6.35	118.25	127.31
38	33	314	A86	C4-C5-C6	-6.34	118.25	127.31
38	31	312	A86	C4-C5-C6	-6.34	118.26	127.31
27	12	311	CLA	C4A-NA-C1A	6.33	109.55	106.71
27	34	310	CLA	C4A-NA-C1A	6.25	109.52	106.71
27	11	309	CLA	C4A-NA-C1A	6.11	109.45	106.71
27	34	312	CLA	C4A-NA-C1A	6.11	109.45	106.71
27	14	311	CLA	C4A-NA-C1A	6.10	109.45	106.71
27	13	311	CLA	C4A-NA-C1A	6.08	109.44	106.71
38	12	315	A86	C3-C2-C1	-6.08	118.63	127.31
27	33	311	CLA	C4A-NA-C1A	6.07	109.44	106.71
38	11	311	A86	C3-C2-C1	-6.07	118.64	127.31
38	34	314	A86	C3-C2-C1	-6.07	118.65	127.31
27	31	309	CLA	C4A-NA-C1A	6.06	109.43	106.71
38	14	313	A86	C3-C2-C1	-6.05	118.67	127.31
38	31	311	A86	C3-C2-C1	-6.05	118.68	127.31
38	33	313	A86	C3-C2-C1	-6.05	118.68	127.31
27	32	313	CLA	C4A-NA-C1A	6.04	109.42	106.71
38	32	315	A86	C3-C2-C1	-6.04	118.69	127.31
27	w	102	CLA	C4A-NA-C1A	6.03	109.42	106.71
27	W	102	CLA	C4A-NA-C1A	6.03	109.42	106.71
38	13	313	A86	C3-C2-C1	-6.03	118.70	127.31
27	12	313	CLA	C4A-NA-C1A	6.03	109.42	106.71
38	14	315	A86	C17-C16-C15	5.80	115.08	109.16
38	11	313	A86	C17-C16-C15	5.80	115.08	109.16
38	13	315	A86	C17-C16-C15	5.79	115.07	109.16
38	31	313	A86	C17-C16-C15	5.79	115.07	109.16
38	33	316	A86	C3-C2-C1	-5.78	119.06	127.31
38	12	317	A86	C17-C16-C15	5.78	115.06	109.16
38	33	315	A86	C17-C16-C15	5.77	115.05	109.16
38	32	317	A86	C17-C16-C15	5.75	115.03	109.16
38	34	316	A86	C17-C16-C15	5.75	115.02	109.16
38	14	301	A86	C3-C2-C1	-5.74	119.12	127.31
38	32	318	A86	C3-C2-C1	-5.73	119.13	127.31
38	14	316	A86	C3-C2-C1	-5.73	119.14	127.31
38	34	301	A86	C3-C2-C1	-5.73	119.14	127.31
38	31	314	A86	C3-C2-C1	-5.70	119.17	127.31
38	13	316	A86	C3-C2-C1	-5.70	119.17	127.31
38	11	314	A86	C3-C2-C1	-5.70	119.18	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	M	102	CLA	C4A-NA-C1A	5.67	109.25	106.71
27	m	101	CLA	C4A-NA-C1A	5.61	109.23	106.71
38	12	315	A86	C4-C5-C6	-5.44	119.54	127.31
38	32	315	A86	C4-C5-C6	-5.42	119.57	127.31
38	11	311	A86	C4-C5-C6	-5.42	119.57	127.31
38	13	313	A86	C4-C5-C6	-5.42	119.57	127.31
38	33	302	A86	C25-C26-C27	-5.41	119.58	127.31
38	14	313	A86	C4-C5-C6	-5.41	119.59	127.31
38	31	311	A86	C4-C5-C6	-5.41	119.59	127.31
38	33	313	A86	C4-C5-C6	-5.41	119.59	127.31
38	34	303	A86	C25-C26-C27	-5.40	119.60	127.31
38	34	314	A86	C4-C5-C6	-5.40	119.60	127.31
38	31	316	A86	C25-C26-C27	-5.39	119.62	127.31
38	13	302	A86	C25-C26-C27	-5.39	119.62	127.31
38	32	304	A86	C25-C26-C27	-5.39	119.62	127.31
38	13	317	A86	C25-C26-C27	-5.38	119.63	127.31
38	11	316	A86	C25-C26-C27	-5.38	119.64	127.31
38	12	304	A86	C25-C26-C27	-5.37	119.64	127.31
38	11	314	A86	C33-C32-C31	5.33	114.39	109.21
38	31	314	A86	C33-C32-C31	5.32	114.38	109.21
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
30	l	101	SQD	O7-S-C6	5.25	113.18	106.94
38	34	313	A86	C3-C2-C1	-5.25	119.81	127.31
38	33	312	A86	C3-C2-C1	-5.25	119.82	127.31
38	32	314	A86	C3-C2-C1	-5.24	119.83	127.31
38	33	316	A86	C33-C32-C31	5.24	114.30	109.21
38	31	310	A86	C3-C2-C1	-5.23	119.85	127.31
38	13	315	A86	C3-C2-C1	-5.22	119.86	127.31
27	c	507	CLA	CAA-C2A-C3A	-5.22	98.49	112.78
38	11	310	A86	C3-C2-C1	-5.22	119.87	127.31
38	13	312	A86	C3-C2-C1	-5.22	119.87	127.31
27	C	507	CLA	CAA-C2A-C3A	-5.21	98.50	112.78
30	L	103	SQD	O7-S-C6	5.19	113.11	106.94
38	12	314	A86	C3-C2-C1	-5.19	119.90	127.31
38	14	315	A86	C3-C2-C1	-5.19	119.90	127.31
38	14	312	A86	C3-C2-C1	-5.18	119.92	127.31
38	12	317	A86	C3-C2-C1	-5.18	119.92	127.31
38	33	315	A86	C3-C2-C1	-5.18	119.92	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	11	313	A86	C3-C2-C1	-5.17	119.93	127.31
38	34	316	A86	C3-C2-C1	-5.16	119.94	127.31
38	32	317	A86	C3-C2-C1	-5.14	119.97	127.31
38	31	313	A86	C3-C2-C1	-5.13	119.99	127.31
38	14	313	A86	O4-C38-C39	5.09	120.46	111.09
38	34	314	A86	O4-C38-C39	5.09	120.45	111.09
38	13	313	A86	O4-C38-C39	5.08	120.44	111.09
38	12	315	A86	O4-C38-C39	5.08	120.43	111.09
38	31	311	A86	O4-C38-C39	5.08	120.43	111.09
38	33	313	A86	O4-C38-C39	5.07	120.41	111.09
38	32	315	A86	O4-C38-C39	5.07	120.41	111.09
27	B	615	CLA	C4A-NA-C1A	5.06	108.98	106.71
38	11	311	A86	O4-C38-C39	5.06	120.40	111.09
27	c	511	CLA	C4A-NA-C1A	5.04	108.97	106.71
27	C	511	CLA	C4A-NA-C1A	5.04	108.97	106.71
27	b	615	CLA	C4A-NA-C1A	5.01	108.96	106.71
30	L	103	SQD	O6-C1-C2	5.00	116.11	108.30
38	32	304	A86	O4-C38-C39	5.00	120.29	111.09
38	34	303	A86	O4-C38-C39	4.99	120.27	111.09
38	13	302	A86	O4-C38-C39	4.99	120.26	111.09
38	11	316	A86	O4-C38-C39	4.98	120.26	111.09
38	13	317	A86	O4-C38-C39	4.98	120.25	111.09
38	31	316	A86	O4-C38-C39	4.97	120.24	111.09
38	12	304	A86	O4-C38-C39	4.97	120.24	111.09
38	33	312	A86	C17-C16-C15	4.97	114.23	109.16
38	32	314	A86	C17-C16-C15	4.97	114.23	109.16
38	33	302	A86	O4-C38-C39	4.97	120.23	111.09
30	l	101	SQD	O6-C1-C2	4.96	116.05	108.30
38	34	313	A86	C17-C16-C15	4.96	114.22	109.16
38	31	310	A86	C17-C16-C15	4.94	114.20	109.16
38	13	312	A86	C17-C16-C15	4.93	114.19	109.16
38	14	312	A86	C17-C16-C15	4.92	114.19	109.16
38	12	314	A86	C17-C16-C15	4.92	114.18	109.16
38	11	310	A86	C17-C16-C15	4.91	114.17	109.16
27	c	507	CLA	C4A-NA-C1A	4.90	108.91	106.71
27	C	507	CLA	C4A-NA-C1A	4.84	108.88	106.71
38	33	314	A86	O4-C38-C39	4.83	119.98	111.09
38	12	316	A86	O4-C38-C39	4.83	119.97	111.09
38	31	312	A86	O4-C38-C39	4.82	119.96	111.09
38	32	316	A86	O4-C38-C39	4.82	119.96	111.09
38	11	312	A86	O4-C38-C39	4.82	119.95	111.09
38	14	314	A86	O4-C38-C39	4.81	119.95	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	13	314	A86	O4-C38-C39	4.81	119.94	111.09
38	32	317	A86	O4-C38-C39	4.80	119.92	111.09
38	34	315	A86	O4-C38-C39	4.79	119.91	111.09
38	34	316	A86	O4-C38-C39	4.79	119.90	111.09
38	14	315	A86	O4-C38-C39	4.79	119.90	111.09
38	31	313	A86	O4-C38-C39	4.79	119.90	111.09
38	11	313	A86	O4-C38-C39	4.79	119.89	111.09
38	33	315	A86	O4-C38-C39	4.78	119.89	111.09
38	13	315	A86	O4-C38-C39	4.78	119.89	111.09
38	12	317	A86	O4-C38-C39	4.78	119.88	111.09
38	13	316	A86	O4-C38-C39	4.76	119.84	111.09
38	32	318	A86	O4-C38-C39	4.75	119.83	111.09
38	33	316	A86	O4-C38-C39	4.75	119.83	111.09
38	11	314	A86	O4-C38-C39	4.75	119.83	111.09
38	14	316	A86	O4-C38-C39	4.74	119.82	111.09
38	31	314	A86	O4-C38-C39	4.74	119.81	111.09
35	C	517	DGD	O3G-C3G-C2G	-4.73	99.48	110.90
35	c	517	DGD	O3G-C3G-C2G	-4.73	99.48	110.90
38	14	301	A86	O4-C38-C39	4.73	119.80	111.09
38	34	301	A86	O4-C38-C39	4.72	119.77	111.09
31	a	407	BCT	O2-C-O1	4.70	131.73	119.55
31	A	407	BCT	O2-C-O1	4.67	131.67	119.55
38	32	315	A86	C25-C26-C27	-4.66	120.66	127.31
38	33	313	A86	C25-C26-C27	-4.66	120.66	127.31
38	34	314	A86	C25-C26-C27	-4.66	120.66	127.31
38	31	311	A86	C25-C26-C27	-4.65	120.67	127.31
38	14	313	A86	C25-C26-C27	-4.65	120.68	127.31
38	11	311	A86	C25-C26-C27	-4.64	120.69	127.31
38	13	313	A86	C25-C26-C27	-4.63	120.70	127.31
38	12	315	A86	C25-C26-C27	-4.63	120.70	127.31
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	12	316	A86	C41-C32-C31	-4.60	106.35	110.47
38	13	314	A86	C41-C32-C31	-4.58	106.37	110.47
38	31	312	A86	C41-C32-C31	-4.57	106.38	110.47
27	b	603	CLA	O2D-CGD-O1D	-4.57	114.91	123.84
38	32	316	A86	C41-C32-C31	-4.57	106.38	110.47
38	14	314	A86	C41-C32-C31	-4.56	106.39	110.47
38	33	314	A86	C41-C32-C31	-4.56	106.39	110.47
36	d	404	PL9	C7-C3-C4	4.54	120.57	116.88
27	B	603	CLA	O2D-CGD-O1D	-4.54	114.97	123.84
28	D	403	PHO	C2B-C1B-NB	-4.53	106.40	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	33	315	A86	C25-C26-C27	-4.53	120.85	127.31
28	d	403	PHO	C2B-C1B-NB	-4.52	106.41	109.53
38	12	317	A86	C25-C26-C27	-4.52	120.86	127.31
38	12	314	A86	O4-C38-C39	4.52	119.40	111.09
38	11	310	A86	O4-C38-C39	4.51	119.39	111.09
38	14	315	A86	C25-C26-C27	-4.51	120.88	127.31
38	13	315	A86	C25-C26-C27	-4.49	120.90	127.31
38	31	313	A86	C25-C26-C27	-4.49	120.91	127.31
38	13	312	A86	O4-C38-C39	4.49	119.34	111.09
38	32	314	A86	O4-C38-C39	4.49	119.34	111.09
38	11	313	A86	C25-C26-C27	-4.48	120.92	127.31
38	34	313	A86	O4-C38-C39	4.48	119.33	111.09
38	33	312	A86	O4-C38-C39	4.47	119.32	111.09
38	14	312	A86	O4-C38-C39	4.47	119.32	111.09
38	34	316	A86	C25-C26-C27	-4.47	120.93	127.31
28	a	403	PHO	C2B-C1B-NB	-4.47	106.44	109.53
38	32	317	A86	C25-C26-C27	-4.47	120.93	127.31
28	A	403	PHO	C2B-C1B-NB	-4.46	106.45	109.53
38	31	310	A86	O4-C38-C39	4.46	119.29	111.09
36	D	404	PL9	C7-C3-C4	4.43	120.48	116.88
38	11	310	A86	C4-C5-C6	-4.33	121.12	127.31
38	13	312	A86	C4-C5-C6	-4.33	121.13	127.31
38	34	313	A86	C4-C5-C6	-4.32	121.14	127.31
32	B	621	LHG	O4-P-O5	4.32	133.58	112.24
38	33	302	A86	C20-C19-C18	-4.31	104.21	112.75
32	b	621	LHG	O4-P-O5	4.31	133.54	112.24
38	33	312	A86	C4-C5-C6	-4.31	121.16	127.31
38	13	302	A86	C20-C19-C18	-4.31	104.23	112.75
38	31	310	A86	C4-C5-C6	-4.30	121.17	127.31
38	32	304	A86	C20-C19-C18	-4.30	104.23	112.75
38	31	316	A86	C20-C19-C18	-4.30	104.24	112.75
38	32	314	A86	C4-C5-C6	-4.30	121.18	127.31
38	13	317	A86	C20-C19-C18	-4.29	104.26	112.75
38	12	304	A86	C20-C19-C18	-4.29	104.27	112.75
32	a	408	LHG	O4-P-O5	4.29	133.44	112.24
38	34	303	A86	C20-C19-C18	-4.29	104.27	112.75
32	A	408	LHG	O4-P-O5	4.29	133.43	112.24
38	12	314	A86	C4-C5-C6	-4.28	121.20	127.31
38	14	312	A86	C4-C5-C6	-4.28	121.21	127.31
38	11	316	A86	C20-C19-C18	-4.27	104.30	112.75
27	a	404	CLA	C3B-C4B-NB	-4.21	106.61	110.52
27	A	404	CLA	C3B-C4B-NB	-4.21	106.61	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	l	102	LHG	O4-P-O5	4.17	132.88	112.24
32	L	101	LHG	O4-P-O5	4.17	132.85	112.24
38	13	315	A86	C41-C32-C31	-4.13	106.78	110.47
32	l	103	LHG	O4-P-O5	4.08	132.42	112.24
32	L	102	LHG	O4-P-O5	4.08	132.40	112.24
38	34	316	A86	C41-C32-C31	-4.08	106.82	110.47
38	13	312	A86	C25-C26-C27	-4.08	121.49	127.31
38	11	313	A86	C41-C32-C31	-4.08	106.83	110.47
30	l	101	SQD	O9-S-C6	4.07	111.78	106.94
38	33	315	A86	C41-C32-C31	-4.07	106.83	110.47
38	32	314	A86	C25-C26-C27	-4.07	121.51	127.31
38	12	317	A86	C41-C32-C31	-4.07	106.83	110.47
38	14	312	A86	C25-C26-C27	-4.06	121.51	127.31
38	31	310	A86	C25-C26-C27	-4.06	121.51	127.31
38	11	310	A86	C25-C26-C27	-4.06	121.52	127.31
38	33	312	A86	C25-C26-C27	-4.06	121.52	127.31
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	34	313	A86	C25-C26-C27	-4.05	121.53	127.31
38	12	314	A86	C25-C26-C27	-4.04	121.55	127.31
30	L	103	SQD	O9-S-C6	4.03	111.73	106.94
29	c	519	BCR	C24-C23-C22	-4.03	120.15	126.23
29	C	520	BCR	C24-C23-C22	-4.03	120.15	126.23
38	32	317	A86	C41-C32-C31	-4.02	106.87	110.47
38	32	318	A86	C25-C24-C1	-4.02	115.14	126.42
38	13	316	A86	C25-C24-C1	-4.01	115.14	126.42
38	34	301	A86	C25-C24-C1	-4.01	115.16	126.42
38	14	316	A86	C25-C24-C1	-4.01	115.17	126.42
38	33	316	A86	C25-C24-C1	-4.00	115.17	126.42
38	31	314	A86	C25-C24-C1	-4.00	115.18	126.42
38	14	301	A86	C25-C24-C1	-4.00	115.19	126.42
38	11	314	A86	C25-C24-C1	-3.99	115.20	126.42
30	B	620	SQD	O7-S-C6	3.99	111.68	106.94
27	33	310	CLA	C2A-C1A-CHA	3.98	130.82	123.86
27	b	622	CLA	CBA-CAA-C2A	3.98	125.60	113.86
29	B	617	BCR	C2-C1-C6	3.97	116.60	110.48
27	32	312	CLA	C2A-C1A-CHA	3.97	130.80	123.86
39	32	302	LMU	O1'-C1'-C2'	3.97	114.49	108.30
39	32	302	LMU	C1B-O1B-C4'	-3.96	108.16	117.96
30	b	620	SQD	O7-S-C6	3.96	111.64	106.94
27	13	310	CLA	C2A-C1A-CHA	3.95	130.77	123.86
27	31	308	CLA	C2A-C1A-CHA	3.95	130.76	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	12	312	CLA	C2A-C1A-CHA	3.94	130.76	123.86
27	14	310	CLA	C2A-C1A-CHA	3.94	130.76	123.86
27	11	308	CLA	C2A-C1A-CHA	3.94	130.75	123.86
27	34	311	CLA	C2A-C1A-CHA	3.94	130.74	123.86
27	B	622	CLA	CBA-CAA-C2A	3.93	125.46	113.86
29	b	617	BCR	C2-C1-C6	3.92	116.52	110.48
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
29	M	101	BCR	C15-C16-C17	-3.90	115.49	123.47
38	32	314	A86	C41-C32-C31	-3.89	107.00	110.47
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
29	m	103	BCR	C15-C16-C17	-3.87	115.54	123.47
35	C	518	DGD	O6D-C1D-O3G	-3.86	100.82	109.97
39	12	302	LMU	O1'-C1'-C2'	3.86	114.33	108.30
30	a	406	SQD	O47-C7-C8	3.85	119.80	111.50
30	A	406	SQD	O47-C7-C8	3.84	119.79	111.50
38	14	312	A86	C41-C32-C31	-3.84	107.03	110.47
35	c	518	DGD	O6D-C1D-O3G	-3.84	100.87	109.97
38	12	314	A86	C41-C32-C31	-3.84	107.04	110.47
30	l	101	SQD	C4-C3-C2	3.83	117.51	110.82
35	h	102	DGD	C1D-C2D-C3D	-3.83	102.03	110.00
28	D	403	PHO	CMB-C2B-C3B	3.82	131.82	124.68
38	11	310	A86	C41-C32-C31	-3.82	107.06	110.47
28	d	403	PHO	CMB-C2B-C3B	3.82	131.82	124.68
35	H	102	DGD	C1D-C2D-C3D	-3.80	102.07	110.00
30	L	103	SQD	C4-C3-C2	3.80	117.45	110.82
39	12	302	LMU	C1B-O1B-C4'	-3.77	108.62	117.96
38	13	312	A86	C12-C11-C13	3.77	122.35	116.02
30	B	620	SQD	O9-S-O7	-3.76	100.95	113.95
30	b	620	SQD	O9-S-O7	-3.75	100.96	113.95
38	12	314	A86	C12-C11-C13	3.75	122.32	116.02
38	31	310	A86	C12-C11-C13	3.74	122.31	116.02
27	C	509	CLA	CMB-C2B-C1B	-3.74	119.67	125.37
38	33	312	A86	C12-C11-C13	3.74	122.31	116.02
38	14	301	A86	C4-C5-C6	-3.74	121.97	127.31
38	14	312	A86	C12-C11-C13	3.74	122.31	116.02
27	C	511	CLA	CMB-C2B-C1B	-3.74	119.67	125.37
38	11	310	A86	C12-C11-C13	3.74	122.30	116.02
38	11	314	A86	C4-C5-C6	-3.74	121.98	127.31
27	33	306	CLA	CMB-C2B-C1B	-3.73	119.68	125.37
38	34	313	A86	C12-C11-C13	3.73	122.30	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	620	SQD	O47-C7-C8	3.73	119.54	111.50
27	c	509	CLA	CMB-C2B-C1B	-3.73	119.69	125.37
38	32	318	A86	C4-C5-C6	-3.73	121.99	127.31
27	c	511	CLA	CMB-C2B-C1B	-3.73	119.69	125.37
27	32	308	CLA	CMB-C2B-C1B	-3.73	119.69	125.37
38	32	314	A86	C12-C11-C13	3.73	122.28	116.02
27	12	308	CLA	CMB-C2B-C1B	-3.72	119.70	125.37
38	31	314	A86	C4-C5-C6	-3.72	122.00	127.31
38	31	311	A86	C41-C32-C31	-3.72	107.14	110.47
27	14	306	CLA	CMB-C2B-C1B	-3.72	119.71	125.37
27	13	306	CLA	CMB-C2B-C1B	-3.71	119.71	125.37
38	33	316	A86	C4-C5-C6	-3.71	122.01	127.31
30	B	620	SQD	O47-C7-C8	3.71	119.49	111.50
38	33	314	A86	C25-C26-C27	-3.71	122.02	127.31
38	32	315	A86	C41-C32-C31	-3.71	107.15	110.47
38	34	314	A86	C41-C32-C31	-3.71	107.16	110.47
38	34	301	A86	C4-C5-C6	-3.70	122.03	127.31
38	12	315	A86	C41-C32-C31	-3.70	107.16	110.47
30	L	103	SQD	O47-C7-C8	3.70	119.48	111.50
27	A	404	CLA	O2D-CGD-O1D	-3.70	116.61	123.84
38	14	316	A86	C4-C5-C6	-3.70	122.03	127.31
27	a	404	CLA	O2D-CGD-O1D	-3.69	116.61	123.84
38	33	313	A86	C41-C32-C31	-3.69	107.17	110.47
27	11	304	CLA	CMB-C2B-C1B	-3.69	119.75	125.37
27	31	304	CLA	CMB-C2B-C1B	-3.69	119.75	125.37
38	12	316	A86	C25-C26-C27	-3.69	122.04	127.31
38	14	313	A86	C41-C32-C31	-3.69	107.17	110.47
38	13	314	A86	C25-C26-C27	-3.69	122.05	127.31
27	34	307	CLA	CMB-C2B-C1B	-3.69	119.76	125.37
38	11	311	A86	C41-C32-C31	-3.68	107.17	110.47
38	34	315	A86	C25-C26-C27	-3.68	122.05	127.31
38	32	316	A86	C25-C26-C27	-3.68	122.06	127.31
38	13	316	A86	C4-C5-C6	-3.68	122.06	127.31
27	b	622	CLA	CAA-C2A-C3A	-3.68	102.71	112.78
38	11	312	A86	C25-C26-C27	-3.68	122.06	127.31
30	l	101	SQD	O47-C7-C8	3.67	119.42	111.50
38	14	314	A86	C25-C26-C27	-3.67	122.08	127.31
30	L	103	SQD	O5-C5-C4	3.67	116.35	109.69
38	31	312	A86	C25-C26-C27	-3.67	122.08	127.31
30	A	406	SQD	O9-S-C6	3.67	111.30	106.94
27	12	308	CLA	CHB-C1B-NB	3.66	128.13	124.26
27	31	304	CLA	CHB-C1B-NB	3.66	128.13	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	13	313	A86	C41-C32-C31	-3.66	107.20	110.47
30	a	406	SQD	O9-S-C6	3.66	111.28	106.94
27	33	306	CLA	CHB-C1B-NB	3.66	128.13	124.26
27	13	306	CLA	CHB-C1B-NB	3.64	128.12	124.26
27	11	304	CLA	CHB-C1B-NB	3.64	128.11	124.26
27	B	622	CLA	CAA-C2A-C3A	-3.63	102.83	112.78
30	A	406	SQD	O9-S-O7	-3.63	101.39	113.95
30	a	406	SQD	O9-S-O7	-3.63	101.39	113.95
30	A	406	SQD	O5-C5-C4	3.63	116.28	109.69
30	l	101	SQD	O5-C5-C4	3.63	116.28	109.69
35	J	101	DGD	O3G-C3G-C2G	-3.63	102.15	110.90
30	a	406	SQD	O6-C1-C2	3.62	113.96	108.30
30	a	406	SQD	O5-C5-C4	3.61	116.26	109.69
27	34	307	CLA	CHB-C1B-NB	3.61	128.08	124.26
35	j	101	DGD	O3G-C3G-C2G	-3.61	102.19	110.90
27	32	308	CLA	CHB-C1B-NB	3.61	128.08	124.26
38	32	318	A86	C12-C11-C13	3.60	122.08	116.02
38	11	314	A86	C12-C11-C13	3.60	122.06	116.02
38	14	301	A86	C12-C11-C13	3.59	122.06	116.02
38	31	314	A86	C12-C11-C13	3.59	122.06	116.02
27	14	306	CLA	CHB-C1B-NB	3.59	128.06	124.26
30	A	406	SQD	O6-C1-C2	3.59	113.90	108.30
38	34	301	A86	C12-C11-C13	3.58	122.04	116.02
27	12	313	CLA	CAA-C2A-C3A	-3.58	102.97	112.78
27	13	311	CLA	CAA-C2A-C3A	-3.58	102.97	112.78
38	33	316	A86	C12-C11-C13	3.58	122.03	116.02
35	J	101	DGD	O6D-C1D-O3G	-3.58	101.50	109.97
38	13	316	A86	C12-C11-C13	3.58	122.03	116.02
38	14	316	A86	C12-C11-C13	3.57	122.02	116.02
27	34	312	CLA	CAA-C2A-C3A	-3.57	103.00	112.78
27	33	303	CLA	CHB-C4A-NA	3.57	129.44	124.51
27	12	305	CLA	CHB-C4A-NA	3.57	129.44	124.51
27	32	305	CLA	CHB-C4A-NA	3.57	129.44	124.51
27	c	505	CLA	CHB-C4A-NA	3.57	129.44	124.51
38	14	301	A86	C36-C31-C32	-3.56	116.16	119.70
27	31	309	CLA	CAA-C2A-C3A	-3.56	103.02	112.78
27	33	311	CLA	CAA-C2A-C3A	-3.56	103.02	112.78
27	11	309	CLA	CAA-C2A-C3A	-3.56	103.03	112.78
27	14	311	CLA	CAA-C2A-C3A	-3.56	103.03	112.78
27	32	313	CLA	CAA-C2A-C3A	-3.56	103.04	112.78
35	j	101	DGD	O6D-C1D-O3G	-3.55	101.56	109.97
27	13	303	CLA	CHB-C4A-NA	3.55	129.42	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	511	CLA	C3B-C4B-NB	-3.55	107.22	110.52
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
27	C	505	CLA	CHB-C4A-NA	3.54	129.41	124.51
27	11	301	CLA	CHB-C4A-NA	3.54	129.41	124.51
33	d	408	LMG	C1-C2-C3	-3.54	102.63	110.00
27	c	511	CLA	C3B-C4B-NB	-3.54	107.23	110.52
38	14	316	A86	C36-C31-C32	-3.54	116.19	119.70
27	31	301	CLA	CHB-C4A-NA	3.53	129.40	124.51
38	31	314	A86	C36-C31-C32	-3.53	116.19	119.70
33	D	408	LMG	C1-C2-C3	-3.53	102.65	110.00
30	L	103	SQD	O9-S-O7	-3.52	101.75	113.95
27	14	303	CLA	CHB-C4A-NA	3.52	129.38	124.51
38	33	316	A86	C36-C31-C32	-3.52	116.20	119.70
27	34	304	CLA	CHB-C4A-NA	3.52	129.38	124.51
29	c	515	BCR	C15-C16-C17	-3.51	116.28	123.47
38	11	314	A86	C36-C31-C32	-3.51	116.21	119.70
30	l	101	SQD	O9-S-O7	-3.51	101.79	113.95
29	C	515	BCR	C15-C16-C17	-3.51	116.29	123.47
30	b	620	SQD	O8-S-C6	3.51	111.33	105.74
38	14	314	A86	C36-C31-C32	-3.50	116.22	119.70
27	d	406	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
38	13	314	A86	C36-C31-C32	-3.50	116.22	119.70
38	34	315	A86	C36-C31-C32	-3.50	116.23	119.70
38	11	316	A86	C4-C3-C2	-3.49	116.32	123.47
38	13	317	A86	C4-C3-C2	-3.49	116.32	123.47
30	B	620	SQD	O8-S-C6	3.49	111.30	105.74
38	11	312	A86	C36-C31-C32	-3.49	116.23	119.70
29	C	515	BCR	C11-C10-C9	-3.49	122.33	127.31
38	33	314	A86	C36-C31-C32	-3.49	116.24	119.70
38	12	316	A86	C3-C2-C1	-3.49	122.34	127.31
35	c	518	DGD	O3G-C3G-C2G	-3.48	102.49	110.90
27	D	406	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
38	31	312	A86	C36-C31-C32	-3.48	116.24	119.70
38	33	314	A86	C3-C2-C1	-3.48	122.34	127.31
38	31	316	A86	C4-C3-C2	-3.48	116.34	123.47
35	C	518	DGD	O3G-C3G-C2G	-3.48	102.50	110.90
38	34	303	A86	C4-C3-C2	-3.48	116.35	123.47
38	12	304	A86	C4-C3-C2	-3.48	116.35	123.47
38	32	304	A86	C4-C3-C2	-3.48	116.35	123.47
38	33	302	A86	C4-C3-C2	-3.48	116.35	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	515	BCR	C11-C10-C9	-3.48	122.35	127.31
29	C	520	BCR	C15-C16-C17	-3.47	116.36	123.47
38	13	314	A86	C3-C2-C1	-3.47	122.35	127.31
38	11	310	A86	C34-O4-C38	-3.47	111.42	117.90
29	a	405	BCR	C15-C16-C17	-3.47	116.37	123.47
38	34	313	A86	C34-O4-C38	-3.47	111.43	117.90
29	c	519	BCR	C15-C16-C17	-3.47	116.37	123.47
38	11	312	A86	C3-C2-C1	-3.47	122.36	127.31
38	13	312	A86	C34-O4-C38	-3.46	111.44	117.90
38	31	310	A86	C34-O4-C38	-3.46	111.44	117.90
29	A	405	BCR	C15-C16-C17	-3.46	116.38	123.47
38	14	314	A86	C3-C2-C1	-3.46	122.37	127.31
38	32	316	A86	C3-C2-C1	-3.46	122.37	127.31
38	32	316	A86	C36-C31-C32	-3.46	116.26	119.70
38	32	314	A86	C34-O4-C38	-3.46	111.45	117.90
35	c	517	DGD	O5D-C6D-C5D	-3.46	102.65	109.05
38	31	311	A86	C36-C31-C32	-3.45	116.27	119.70
38	12	314	A86	C34-O4-C38	-3.45	111.46	117.90
38	13	302	A86	C4-C3-C2	-3.45	116.40	123.47
38	14	312	A86	C34-O4-C38	-3.45	111.47	117.90
38	33	312	A86	C34-O4-C38	-3.45	111.47	117.90
38	34	315	A86	C3-C2-C1	-3.44	122.39	127.31
38	31	314	A86	C20-C19-C18	-3.44	105.94	112.75
38	13	316	A86	C20-C19-C18	-3.44	105.94	112.75
38	12	316	A86	C36-C31-C32	-3.44	116.28	119.70
38	11	314	A86	C20-C19-C18	-3.44	105.94	112.75
38	32	318	A86	C20-C19-C18	-3.44	105.94	112.75
38	11	316	A86	C3-C2-C1	-3.44	122.40	127.31
38	31	316	A86	C3-C2-C1	-3.44	122.40	127.31
38	34	301	A86	C20-C19-C18	-3.44	105.95	112.75
29	b	617	BCR	C24-C23-C22	-3.43	121.05	126.23
38	31	312	A86	C3-C2-C1	-3.43	122.41	127.31
38	33	316	A86	C20-C19-C18	-3.43	105.96	112.75
38	14	301	A86	C20-C19-C18	-3.43	105.96	112.75
38	12	304	A86	C3-C2-C1	-3.43	122.42	127.31
38	34	303	A86	C3-C2-C1	-3.43	122.42	127.31
38	13	317	A86	C3-C2-C1	-3.43	122.42	127.31
29	B	617	BCR	C24-C23-C22	-3.43	121.06	126.23
38	32	315	A86	C36-C31-C32	-3.42	116.30	119.70
38	33	302	A86	C3-C2-C1	-3.42	122.43	127.31
38	13	302	A86	C3-C2-C1	-3.42	122.43	127.31
38	33	313	A86	C36-C31-C32	-3.42	116.30	119.70

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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
28	D	403	PHO	O1D-CGD-CBD	3.42	130.43	124.74
38	14	316	A86	C20-C19-C18	-3.41	106.00	112.75
38	12	315	A86	C36-C31-C32	-3.41	116.31	119.70
35	C	517	DGD	O5D-C6D-C5D	-3.41	102.74	109.05
27	c	514	CLA	CHB-C4A-NA	3.41	129.22	124.51
38	11	316	A86	C40-C32-C31	-3.40	107.42	110.47
38	34	314	A86	C36-C31-C32	-3.40	116.32	119.70
38	14	314	A86	C26-C25-C24	-3.40	112.60	123.22
27	34	304	CLA	C1-C2-C3	-3.40	120.17	126.04
38	31	312	A86	C26-C25-C24	-3.40	112.62	123.22
38	12	316	A86	C26-C25-C24	-3.40	112.62	123.22
38	32	316	A86	C26-C25-C24	-3.39	112.62	123.22
38	13	314	A86	C26-C25-C24	-3.39	112.63	123.22
27	C	514	CLA	CHB-C4A-NA	3.39	129.21	124.51
38	11	311	A86	C36-C31-C32	-3.39	116.33	119.70
38	34	315	A86	C26-C25-C24	-3.39	112.64	123.22
38	13	313	A86	C36-C31-C32	-3.39	116.33	119.70
27	32	305	CLA	C1-C2-C3	-3.39	120.18	126.04
38	32	304	A86	C3-C2-C1	-3.39	122.47	127.31
27	31	301	CLA	C1-C2-C3	-3.39	120.18	126.04
27	14	303	CLA	C1-C2-C3	-3.39	120.19	126.04
27	13	303	CLA	C1-C2-C3	-3.39	120.19	126.04
38	33	314	A86	C26-C25-C24	-3.39	112.65	123.22
27	b	610	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
38	11	312	A86	C26-C25-C24	-3.38	112.65	123.22
27	B	610	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
27	d	401	CLA	C3B-C4B-NB	-3.38	107.38	110.52
28	d	403	PHO	O1D-CGD-CBD	3.38	130.37	124.74
27	33	303	CLA	C1-C2-C3	-3.38	120.20	126.04
27	12	305	CLA	C1-C2-C3	-3.38	120.20	126.04
38	32	304	A86	C40-C32-C31	-3.37	107.45	110.47
27	C	511	CLA	CMB-C2B-C3B	3.37	134.75	126.59
38	31	316	A86	C40-C32-C31	-3.36	107.46	110.47
27	D	401	CLA	C3B-C4B-NB	-3.36	107.40	110.52
27	b	614	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
27	B	614	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
27	11	301	CLA	C1-C2-C3	-3.36	120.23	126.04
27	c	511	CLA	CMB-C2B-C3B	3.36	134.72	126.59
35	H	102	DGD	O3G-C3G-C2G	-3.35	102.82	110.90
38	33	302	A86	C40-C32-C31	-3.35	107.48	110.47
38	13	315	A86	C3-C4-C5	-3.34	116.63	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	612	CLA	CHB-C4A-NA	3.34	129.13	124.51
35	h	102	DGD	O3G-C3G-C2G	-3.34	102.84	110.90
36	d	404	PL9	C7-C3-C2	-3.34	118.91	123.30
38	13	317	A86	C40-C32-C31	-3.34	107.49	110.47
27	14	304	CLA	CHB-C4A-NA	3.34	129.12	124.51
27	b	601	CLA	CHB-C4A-NA	3.33	129.12	124.51
38	13	302	A86	C40-C32-C31	-3.33	107.49	110.47
27	b	612	CLA	CHB-C4A-NA	3.33	129.12	124.51
27	13	304	CLA	CHB-C4A-NA	3.33	129.12	124.51
38	12	304	A86	C40-C32-C31	-3.33	107.49	110.47
27	b	613	CLA	CMB-C2B-C1B	-3.33	120.30	125.37
27	33	304	CLA	CHB-C4A-NA	3.33	129.12	124.51
38	12	317	A86	C3-C4-C5	-3.33	116.66	123.47
38	32	317	A86	C3-C4-C5	-3.33	116.66	123.47
27	B	601	CLA	CHB-C4A-NA	3.33	129.11	124.51
38	34	303	A86	C40-C32-C31	-3.33	107.50	110.47
38	14	315	A86	C3-C4-C5	-3.33	116.66	123.47
27	14	309	CLA	CHB-C4A-NA	3.32	129.11	124.51
38	34	316	A86	C3-C4-C5	-3.32	116.67	123.47
27	34	305	CLA	CHB-C4A-NA	3.32	129.11	124.51
29	a	405	BCR	C15-C14-C13	-3.32	122.57	127.31
27	32	311	CLA	CHB-C4A-NA	3.32	129.10	124.51
38	33	315	A86	C3-C4-C5	-3.32	116.68	123.47
27	C	512	CLA	C3B-C4B-NB	-3.31	107.44	110.52
38	11	313	A86	C3-C4-C5	-3.31	116.69	123.47
27	11	307	CLA	CHB-C4A-NA	3.31	129.09	124.51
27	B	613	CLA	CMB-C2B-C1B	-3.31	120.33	125.37
36	D	404	PL9	C7-C3-C2	-3.31	118.95	123.30
27	12	306	CLA	CHB-C4A-NA	3.31	129.08	124.51
27	13	309	CLA	CHB-C4A-NA	3.31	129.08	124.51
38	31	313	A86	C3-C4-C5	-3.30	116.71	123.47
27	31	302	CLA	CHB-C4A-NA	3.30	129.08	124.51
29	A	405	BCR	C15-C14-C13	-3.30	122.60	127.31
27	d	401	CLA	CHB-C1B-NB	3.30	127.75	124.26
27	31	307	CLA	CHB-C4A-NA	3.30	129.07	124.51
27	32	306	CLA	CHB-C4A-NA	3.30	129.07	124.51
27	34	310	CLA	CHB-C4A-NA	3.30	129.07	124.51
27	c	512	CLA	C3B-C4B-NB	-3.29	107.46	110.52
27	D	401	CLA	CHB-C1B-NB	3.29	127.74	124.26
30	l	101	SQD	C1-O5-C5	3.29	120.14	113.69
27	33	309	CLA	CHB-C4A-NA	3.29	129.06	124.51
27	11	302	CLA	CHB-C4A-NA	3.28	129.05	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	512	CLA	CHB-C4A-NA	3.28	129.05	124.51
30	L	103	SQD	C1-O5-C5	3.28	120.12	113.69
36	D	407	PL9	C7-C8-C9	-3.28	121.34	126.79
27	a	404	CLA	CHB-C4A-NA	3.27	129.04	124.51
27	12	312	CLA	CHB-C4A-NA	3.27	129.04	124.51
36	d	407	PL9	C7-C8-C9	-3.27	121.35	126.79
27	A	404	CLA	CHB-C4A-NA	3.27	129.03	124.51
27	C	508	CLA	CHB-C4A-NA	3.26	129.02	124.51
27	12	311	CLA	CHB-C4A-NA	3.26	129.02	124.51
38	11	313	A86	C12-C11-C13	3.26	121.49	116.02
38	31	313	A86	C12-C11-C13	3.26	121.49	116.02
27	C	505	CLA	C3C-C4C-NC	-3.26	106.92	110.57
27	13	310	CLA	CHB-C4A-NA	3.25	129.01	124.51
27	M	102	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
30	A	406	SQD	O8-S-C6	3.25	110.92	105.74
27	31	308	CLA	CHB-C4A-NA	3.25	129.01	124.51
38	13	315	A86	C12-C11-C13	3.25	121.48	116.02
38	14	315	A86	C12-C11-C13	3.25	121.48	116.02
38	12	317	A86	C12-C11-C13	3.25	121.47	116.02
39	32	302	LMU	O5B-C5B-C4B	3.25	115.59	109.69
38	34	316	A86	C12-C11-C13	3.24	121.47	116.02
27	c	512	CLA	CHB-C4A-NA	3.24	128.99	124.51
38	33	315	A86	C12-C11-C13	3.24	121.46	116.02
30	a	406	SQD	O8-S-C6	3.24	110.90	105.74
27	32	312	CLA	CHB-C4A-NA	3.24	128.99	124.51
27	11	308	CLA	CHB-C4A-NA	3.24	128.99	124.51
38	32	317	A86	C12-C11-C13	3.23	121.46	116.02
38	34	316	A86	C10-C9-C8	-3.23	113.13	123.22
27	B	609	CLA	CHB-C4A-NA	3.23	128.98	124.51
27	B	604	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
27	m	101	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
38	31	313	A86	C10-C9-C8	-3.23	113.14	123.22
38	34	303	A86	C36-C31-C32	-3.23	116.49	119.70
27	b	604	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
38	11	313	A86	C10-C9-C8	-3.23	113.14	123.22
38	14	315	A86	C10-C9-C8	-3.23	113.15	123.22
27	C	509	CLA	CHB-C1B-NB	3.22	127.67	124.26
27	14	310	CLA	CHB-C4A-NA	3.22	128.97	124.51
27	B	608	CLA	O2D-CGD-O1D	-3.22	117.53	123.84
27	C	506	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
27	c	508	CLA	CHB-C4A-NA	3.22	128.97	124.51
38	32	317	A86	C10-C9-C8	-3.22	113.17	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	c	506	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
38	13	313	A86	C12-C11-C13	3.22	121.43	116.02
27	33	310	CLA	CHB-C4A-NA	3.22	128.97	124.51
27	c	509	CLA	CHB-C1B-NB	3.22	127.67	124.26
38	33	315	A86	C10-C9-C8	-3.22	113.17	123.22
29	a	405	BCR	C24-C23-C22	-3.22	121.37	126.23
38	34	314	A86	C12-C11-C13	3.22	121.43	116.02
27	c	505	CLA	C3C-C4C-NC	-3.21	106.97	110.57
27	b	608	CLA	CHB-C4A-NA	3.21	128.96	124.51
27	b	609	CLA	CHB-C4A-NA	3.21	128.95	124.51
29	A	405	BCR	C24-C23-C22	-3.21	121.38	126.23
38	12	317	A86	C10-C9-C8	-3.21	113.20	123.22
27	B	608	CLA	CHB-C4A-NA	3.21	128.95	124.51
38	13	302	A86	C36-C31-C32	-3.20	116.52	119.70
27	b	608	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
27	34	311	CLA	CHB-C4A-NA	3.20	128.94	124.51
38	13	315	A86	C10-C9-C8	-3.20	113.22	123.22
38	11	311	A86	C12-C11-C13	3.20	121.40	116.02
35	C	517	DGD	O6D-C1D-O3G	-3.20	102.39	109.97
38	32	315	A86	C12-C11-C13	3.20	121.40	116.02
38	11	316	A86	C36-C31-C32	-3.20	116.52	119.70
38	31	311	A86	C12-C11-C13	3.20	121.39	116.02
27	C	507	CLA	CMB-C2B-C1B	-3.19	120.50	125.37
27	13	305	CLA	CAA-C2A-C3A	-3.19	104.03	112.78
27	B	605	CLA	CHB-C4A-NA	3.19	128.93	124.51
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
39	12	302	LMU	O5B-C5B-C4B	3.19	115.48	109.69
38	14	313	A86	C12-C11-C13	3.18	121.37	116.02
27	11	303	CLA	CAA-C2A-C3A	-3.18	104.06	112.78
38	12	315	A86	C12-C11-C13	3.18	121.37	116.02
27	12	307	CLA	CAA-C2A-C3A	-3.18	104.07	112.78
38	33	302	A86	C36-C31-C32	-3.18	116.54	119.70
38	32	304	A86	C36-C31-C32	-3.18	116.54	119.70
27	32	307	CLA	CAA-C2A-C3A	-3.18	104.08	112.78
27	14	305	CLA	CAA-C2A-C3A	-3.18	104.08	112.78
27	31	303	CLA	CAA-C2A-C3A	-3.18	104.08	112.78
38	13	317	A86	C36-C31-C32	-3.17	116.55	119.70
27	c	507	CLA	CMB-C2B-C1B	-3.17	120.54	125.37
27	b	605	CLA	CHB-C4A-NA	3.17	128.89	124.51
38	33	313	A86	C12-C11-C13	3.17	121.34	116.02
27	33	305	CLA	CAA-C2A-C3A	-3.17	104.11	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	c	517	DGD	O6D-C1D-O3G	-3.16	102.48	109.97
39	12	302	LMU	C3'-C4'-C5'	3.16	118.18	110.93
27	34	306	CLA	CAA-C2A-C3A	-3.16	104.12	112.78
27	c	514	CLA	CMB-C2B-C1B	-3.16	120.55	125.37
27	w	103	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
27	C	514	CLA	CMB-C2B-C1B	-3.15	120.57	125.37
38	33	316	A86	C10-C9-C8	-3.15	113.39	123.22
27	b	607	CLA	CMB-C2B-C1B	-3.15	120.57	125.37
38	34	301	A86	C10-C9-C8	-3.15	113.39	123.22
38	13	316	A86	C10-C9-C8	-3.15	113.40	123.22
27	W	103	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
38	14	301	A86	C10-C9-C8	-3.14	113.41	123.22
38	32	318	A86	C10-C9-C8	-3.14	113.41	123.22
38	14	316	A86	C10-C9-C8	-3.14	113.42	123.22
38	11	314	A86	C10-C9-C8	-3.14	113.43	123.22
39	32	302	LMU	C3'-C4'-C5'	3.13	118.11	110.93
27	33	306	CLA	CHB-C4A-NA	3.13	128.84	124.51
38	31	314	A86	C10-C9-C8	-3.13	113.46	123.22
27	33	303	CLA	C3B-C4B-NB	-3.12	107.62	110.52
27	D	405	CLA	CAA-C2A-C3A	-3.12	104.22	112.78
27	d	405	CLA	CAA-C2A-C3A	-3.12	104.24	112.78
29	B	623	BCR	C7-C8-C9	-3.12	121.52	126.23
29	A	409	BCR	C11-C10-C9	-3.12	122.86	127.31
29	a	409	BCR	C11-C10-C9	-3.11	122.87	127.31
27	d	402	CLA	C3B-C4B-NB	-3.11	107.63	110.52
27	31	304	CLA	CHB-C4A-NA	3.11	128.81	124.51
27	14	310	CLA	CAA-C2A-C1A	3.11	122.15	111.97
27	13	310	CLA	CAA-C2A-C1A	3.10	122.14	111.97
27	B	607	CLA	CMB-C2B-C1B	-3.10	120.64	125.37
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
27	14	303	CLA	C3B-C4B-NB	-3.10	107.64	110.52
27	32	312	CLA	CAA-C2A-C1A	3.10	122.12	111.97
27	12	308	CLA	CHB-C4A-NA	3.10	128.79	124.51
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
27	b	622	CLA	CAA-C2A-C1A	3.09	122.11	111.97
27	31	308	CLA	CAA-C2A-C1A	3.09	122.10	111.97
27	B	611	CLA	CHB-C1B-NB	3.09	127.53	124.26
27	14	306	CLA	CHB-C4A-NA	3.09	128.78	124.51
37	v	201	HEM	CAC-C3C-C4C	3.09	132.35	124.90
27	b	609	CLA	CHC-C4B-NB	3.08	127.52	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	611	CLA	CHB-C1B-NB	3.07	127.51	124.26
27	32	308	CLA	CHB-C4A-NA	3.07	128.76	124.51
27	12	305	CLA	C3B-C4B-NB	-3.07	107.67	110.52
30	l	101	SQD	C3-C4-C5	3.07	115.72	110.24
27	33	305	CLA	CBA-CAA-C2A	3.07	122.93	113.86
37	V	201	HEM	CAC-C3C-C4C	3.07	132.31	124.90
27	11	304	CLA	CHB-C4A-NA	3.07	128.76	124.51
39	32	302	LMU	O5'-C5'-C4'	3.07	116.22	109.75
27	c	505	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
27	c	508	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
27	11	301	CLA	C3B-C4B-NB	-3.07	107.67	110.52
27	34	304	CLA	C3B-C4B-NB	-3.07	107.67	110.52
27	b	610	CLA	C3B-C4B-NB	-3.07	107.67	110.52
27	34	307	CLA	CHB-C4A-NA	3.07	128.75	124.51
27	B	612	CLA	CHC-C4B-NB	3.07	127.50	124.26
27	32	305	CLA	C3B-C4B-NB	-3.06	107.67	110.52
30	L	103	SQD	C3-C4-C5	3.06	115.70	110.24
27	D	402	CLA	C3B-C4B-NB	-3.06	107.68	110.52
27	C	510	CLA	CMB-C2B-C1B	-3.06	120.71	125.37
29	b	616	BCR	C15-C14-C13	-3.05	122.95	127.31
27	31	307	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
27	12	307	CLA	CBA-CAA-C2A	3.05	122.88	113.86
27	34	306	CLA	CBA-CAA-C2A	3.05	122.88	113.86
27	14	305	CLA	CBA-CAA-C2A	3.05	122.87	113.86
27	c	507	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
27	13	306	CLA	CHB-C4A-NA	3.05	128.73	124.51
27	32	307	CLA	CBA-CAA-C2A	3.05	122.86	113.86
27	13	305	CLA	CBA-CAA-C2A	3.05	122.86	113.86
35	C	517	DGD	C1D-C2D-C3D	-3.05	103.65	110.00
32	A	408	LHG	O8-C23-C24	3.05	121.47	111.91
27	11	303	CLA	CBA-CAA-C2A	3.04	122.85	113.86
32	a	408	LHG	O8-C23-C24	3.04	121.46	111.91
27	14	309	CLA	C3B-C4B-NB	-3.04	107.69	110.52
27	C	505	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
27	31	303	CLA	CBA-CAA-C2A	3.04	122.83	113.86
27	31	301	CLA	C3B-C4B-NB	-3.04	107.70	110.52
29	B	616	BCR	C15-C14-C13	-3.04	122.97	127.31
27	C	508	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
27	B	622	CLA	CAA-C2A-C1A	3.04	121.93	111.97
27	11	307	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
27	c	510	CLA	CMB-C2B-C1B	-3.03	120.75	125.37
29	c	515	BCR	C24-C23-C22	-3.03	121.65	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	33	309	CLA	C3B-C4B-NB	-3.03	107.70	110.52
27	C	507	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
27	13	303	CLA	C3B-C4B-NB	-3.03	107.70	110.52
27	11	304	CLA	C2A-C1A-CHA	3.03	129.16	123.86
27	W	102	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
27	33	309	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
30	B	620	SQD	O9-S-C6	3.03	110.54	106.94
35	c	517	DGD	C1D-C2D-C3D	-3.03	103.69	110.00
27	B	609	CLA	CHC-C4B-NB	3.02	127.46	124.26
27	12	311	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
27	B	608	CLA	C3B-C4B-NB	-3.02	107.71	110.52
38	12	317	A86	C36-C31-C32	-3.02	116.70	119.70
27	32	311	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
31	a	407	BCT	O3-C-O1	-3.02	111.72	119.55
27	w	102	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
27	13	309	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
29	c	516	BCR	C11-C10-C9	-3.01	123.01	127.31
27	31	307	CLA	C3B-C4B-NB	-3.01	107.72	110.52
27	d	402	CLA	CHB-C4A-NA	3.01	128.68	124.51
38	33	314	A86	C35-C34-C33	3.01	115.13	109.88
35	C	518	DGD	CDB-CCB-CBB	-3.01	99.13	114.42
27	b	612	CLA	CHC-C4B-NB	3.01	127.45	124.26
29	C	516	BCR	C11-C10-C9	-3.01	123.01	127.31
38	13	315	A86	C36-C31-C32	-3.01	116.71	119.70
35	c	518	DGD	CDB-CCB-CBB	-3.01	99.14	114.42
27	34	310	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
27	32	311	CLA	CHB-C1B-NB	3.01	127.44	124.26
31	A	407	BCT	O3-C-O1	-3.01	111.74	119.55
27	11	307	CLA	C3B-C4B-NB	-3.01	107.72	110.52
27	C	512	CLA	CAA-CBA-CGA	-3.01	104.47	113.25
27	32	311	CLA	C3B-C4B-NB	-3.01	107.73	110.52
27	11	306	CLA	CHC-C4B-NB	3.01	127.44	124.26
27	c	512	CLA	CAA-CBA-CGA	-3.01	104.47	113.25
27	13	308	CLA	CHC-C4B-NB	3.00	127.44	124.26
27	d	406	CLA	CHB-C4A-NA	3.00	128.67	124.51
27	32	308	CLA	C2A-C1A-CHA	3.00	129.11	123.86
27	12	308	CLA	C2A-C1A-CHA	3.00	129.11	123.86
27	b	614	CLA	CHB-C4A-NA	3.00	128.66	124.51
38	32	317	A86	C36-C31-C32	-3.00	116.72	119.70
38	12	316	A86	C35-C34-C33	3.00	115.11	109.88
38	13	314	A86	C35-C34-C33	3.00	115.11	109.88
27	14	309	CLA	O2D-CGD-O1D	-3.00	117.97	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	33	306	CLA	C2A-C1A-CHA	3.00	129.10	123.86
38	11	313	A86	C36-C31-C32	-3.00	116.72	119.70
29	C	515	BCR	C24-C23-C22	-3.00	121.70	126.23
39	12	302	LMU	O5'-C5'-C4'	3.00	116.07	109.75
27	14	306	CLA	C2A-C1A-CHA	3.00	129.10	123.86
27	13	306	CLA	C2A-C1A-CHA	2.99	129.09	123.86
38	32	316	A86	C35-C34-C33	2.99	115.10	109.88
27	34	309	CLA	CHC-C4B-NB	2.99	127.43	124.26
27	B	610	CLA	C3B-C4B-NB	-2.99	107.74	110.52
27	b	601	CLA	C3B-C4B-NB	-2.99	107.74	110.52
27	13	309	CLA	C3B-C4B-NB	-2.99	107.74	110.52
27	34	307	CLA	C2A-C1A-CHA	2.99	129.09	123.86
30	b	620	SQD	O9-S-C6	2.99	110.50	106.94
27	c	508	CLA	C2A-C1A-CHA	2.99	129.09	123.86
27	C	502	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
27	31	304	CLA	C2A-C1A-CHA	2.99	129.09	123.86
27	D	402	CLA	CHB-C4A-NA	2.99	128.64	124.51
27	b	608	CLA	C3B-C4B-NB	-2.99	107.75	110.52
38	14	314	A86	C35-C34-C33	2.99	115.08	109.88
27	Z	102	CLA	C3B-C4B-NB	-2.98	107.75	110.52
29	B	623	BCR	C11-C10-C9	-2.98	123.05	127.31
30	A	406	SQD	O48-C23-C24	2.98	121.27	111.91
27	D	406	CLA	CHB-C4A-NA	2.98	128.63	124.51
38	11	313	A86	C25-C24-C1	-2.98	118.04	126.42
27	B	612	CLA	C3B-C4B-NB	-2.98	107.75	110.52
30	a	406	SQD	O48-C23-C24	2.98	121.26	111.91
29	C	516	BCR	C15-C16-C17	-2.98	117.37	123.47
38	14	315	A86	C36-C31-C32	-2.98	116.74	119.70
38	12	317	A86	C25-C24-C1	-2.98	118.05	126.42
36	D	404	PL9	C41-C39-C38	-2.98	115.09	121.12
38	31	312	A86	C35-C34-C33	2.98	115.07	109.88
27	32	310	CLA	CHC-C4B-NB	2.98	127.41	124.26
38	13	302	A86	C7-C6-C5	-2.98	118.75	122.92
38	33	315	A86	C25-C24-C1	-2.98	118.06	126.42
27	12	311	CLA	C3B-C4B-NB	-2.98	107.75	110.52
27	b	604	CLA	CHB-C4A-NA	2.98	128.63	124.51
27	34	310	CLA	CHB-C1B-NB	2.97	127.41	124.26
36	d	404	PL9	C41-C39-C38	-2.97	115.10	121.12
38	34	316	A86	C36-C31-C32	-2.97	116.75	119.70
38	13	315	A86	C25-C24-C1	-2.97	118.06	126.42
38	34	303	A86	C7-C6-C5	-2.97	118.76	122.92
32	B	621	LHG	O8-C23-C24	2.97	121.24	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	34	310	CLA	C3B-C4B-NB	-2.97	107.76	110.52
29	A	405	BCR	C11-C10-C9	-2.97	123.07	127.31
27	D	406	CLA	C3B-C4B-NB	-2.97	107.76	110.52
32	b	621	LHG	O8-C23-C24	2.97	121.23	111.91
27	b	614	CLA	O2D-CGD-CBD	2.97	116.55	111.27
38	14	315	A86	C25-C24-C1	-2.97	118.07	126.42
27	B	614	CLA	O2D-CGD-CBD	2.97	116.55	111.27
38	31	313	A86	C25-C24-C1	-2.97	118.08	126.42
38	32	317	A86	C25-C24-C1	-2.97	118.08	126.42
38	14	313	A86	C3-C4-C5	-2.97	117.40	123.47
38	34	316	A86	C25-C24-C1	-2.97	118.08	126.42
38	13	313	A86	C3-C4-C5	-2.96	117.40	123.47
38	11	311	A86	C3-C4-C5	-2.96	117.40	123.47
29	b	623	BCR	C7-C8-C9	-2.96	121.76	126.23
38	34	315	A86	C35-C34-C33	2.96	115.05	109.88
38	11	312	A86	C35-C34-C33	2.96	115.04	109.88
29	c	516	BCR	C15-C16-C17	-2.96	117.41	123.47
38	32	315	A86	C3-C4-C5	-2.96	117.41	123.47
38	11	316	A86	C7-C6-C5	-2.96	118.78	122.92
27	C	508	CLA	C2A-C1A-CHA	2.96	129.03	123.86
38	12	304	A86	C7-C6-C5	-2.96	118.78	122.92
38	33	313	A86	C3-C4-C5	-2.96	117.42	123.47
38	33	314	A86	C12-C11-C13	2.96	120.99	116.02
27	13	309	CLA	CHB-C1B-NB	2.95	127.39	124.26
38	31	316	A86	C7-C6-C5	-2.95	118.78	122.92
38	31	311	A86	C3-C4-C5	-2.95	117.42	123.47
38	31	313	A86	C36-C31-C32	-2.95	116.77	119.70
38	34	314	A86	C3-C4-C5	-2.95	117.42	123.47
27	c	502	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
38	12	315	A86	C3-C4-C5	-2.95	117.43	123.47
27	z	102	CLA	C3B-C4B-NB	-2.95	107.78	110.52
33	b	619	LMG	O6-C1-O1	-2.95	102.99	109.97
33	B	619	LMG	O6-C1-O1	-2.95	102.99	109.97
27	B	615	CLA	CHB-C1B-NB	2.95	127.38	124.26
27	14	308	CLA	CHC-C4B-NB	2.95	127.38	124.26
27	B	604	CLA	CHB-C4A-NA	2.94	128.58	124.51
27	B	614	CLA	CHB-C4A-NA	2.94	128.58	124.51
27	C	513	CLA	CHB-C4A-NA	2.94	128.58	124.51
27	33	308	CLA	CHB-C4A-NA	2.94	128.58	124.51
27	12	310	CLA	CHC-C4B-NB	2.94	127.37	124.26
38	12	316	A86	C12-C11-C13	2.94	120.96	116.02
27	12	311	CLA	CHB-C1B-NB	2.94	127.37	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	613	CLA	CMB-C2B-C3B	2.94	133.71	126.59
28	a	403	PHO	O1D-CGD-CBD	2.94	129.63	124.74
27	b	615	CLA	CHB-C1B-NB	2.94	127.37	124.26
38	13	317	A86	C7-C6-C5	-2.94	118.81	122.92
27	12	308	CLA	CMB-C2B-C3B	2.94	133.70	126.59
27	12	311	CLA	C1-C2-C3	-2.94	120.97	126.04
38	31	314	A86	C41-C32-C31	-2.94	107.84	110.47
27	31	306	CLA	CHC-C4B-NB	2.93	127.36	124.26
27	12	309	CLA	CHB-C4A-NA	2.93	128.57	124.51
27	C	506	CLA	C2D-C1D-ND	-2.93	107.94	110.10
38	33	302	A86	C7-C6-C5	-2.93	118.81	122.92
27	33	301	CLA	CHB-C4A-NA	2.93	128.57	124.51
27	d	406	CLA	C3B-C4B-NB	-2.93	107.80	110.52
27	33	309	CLA	C1-C2-C3	-2.93	120.97	126.04
38	33	316	A86	C41-C32-C31	-2.93	107.85	110.47
38	33	315	A86	C7-C6-C8	2.93	122.69	118.08
27	31	307	CLA	C1-C2-C3	-2.93	120.98	126.04
38	34	315	A86	C12-C11-C13	2.93	120.94	116.02
27	11	307	CLA	CHB-C1B-NB	2.93	127.36	124.26
38	32	316	A86	C12-C11-C13	2.93	120.94	116.02
38	11	312	A86	C12-C11-C13	2.93	120.94	116.02
27	11	305	CLA	CHB-C4A-NA	2.93	128.56	124.51
27	14	306	CLA	CMB-C2B-C3B	2.93	133.67	126.59
38	14	315	A86	C7-C6-C8	2.92	122.69	118.08
38	13	314	A86	C12-C11-C13	2.92	120.93	116.02
27	32	308	CLA	CMB-C2B-C3B	2.92	133.67	126.59
38	14	301	A86	C41-C32-C31	-2.92	107.86	110.47
27	34	308	CLA	CHB-C4A-NA	2.92	128.55	124.51
27	14	309	CLA	CHB-C1B-NB	2.92	127.35	124.26
27	13	306	CLA	CMB-C2B-C3B	2.92	133.66	126.59
38	14	314	A86	C12-C11-C13	2.92	120.93	116.02
38	33	315	A86	C36-C31-C32	-2.92	116.80	119.70
27	13	307	CLA	CHB-C4A-NA	2.92	128.55	124.51
27	33	306	CLA	CMB-C2B-C3B	2.92	133.66	126.59
38	31	313	A86	C7-C6-C8	2.92	122.67	118.08
27	33	309	CLA	CHB-C1B-NB	2.92	127.34	124.26
27	b	612	CLA	C3B-C4B-NB	-2.92	107.81	110.52
27	c	506	CLA	C2D-C1D-ND	-2.91	107.96	110.10
27	11	304	CLA	CMB-C2B-C3B	2.91	133.65	126.59
38	32	304	A86	C7-C6-C5	-2.91	118.84	122.92
38	31	312	A86	C12-C11-C13	2.91	120.92	116.02
27	34	307	CLA	CMB-C2B-C3B	2.91	133.64	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	405	BCR	C11-C10-C9	-2.91	123.15	127.31
28	A	403	PHO	O1D-CGD-CBD	2.91	129.59	124.74
27	B	613	CLA	CMB-C2B-C3B	2.91	133.64	126.59
27	12	307	CLA	CHB-C4A-NA	2.91	128.53	124.51
27	31	303	CLA	CHB-C4A-NA	2.91	128.53	124.51
27	B	601	CLA	C3B-C4B-NB	-2.91	107.82	110.52
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
38	32	318	A86	C41-C32-C31	-2.91	107.87	110.47
27	11	315	CLA	CHB-C4A-NA	2.90	128.53	124.51
27	c	513	CLA	CHB-C4A-NA	2.90	128.53	124.51
27	13	311	CLA	C3B-C4B-NB	-2.90	107.82	110.52
27	12	303	CLA	CHB-C4A-NA	2.90	128.53	124.51
35	J	101	DGD	O5D-C6D-C5D	-2.90	103.68	109.05
27	31	304	CLA	CMB-C2B-C3B	2.90	133.62	126.59
27	34	310	CLA	C1-C2-C3	-2.90	121.03	126.04
27	c	510	CLA	CHB-C4A-NA	2.90	128.52	124.51
27	11	307	CLA	C1-C2-C3	-2.90	121.03	126.04
38	32	317	A86	C7-C6-C8	2.90	122.65	118.08
38	14	313	A86	C34-O4-C38	-2.90	112.49	117.90
38	12	317	A86	C7-C6-C8	2.90	122.64	118.08
27	32	303	CLA	CHB-C4A-NA	2.90	128.52	124.51
27	34	309	CLA	CHB-C4A-NA	2.90	128.52	124.51
27	b	610	CLA	CHB-C1B-NB	2.90	127.32	124.26
38	33	313	A86	C34-O4-C38	-2.90	112.50	117.90
38	34	314	A86	C34-O4-C38	-2.90	112.50	117.90
38	13	315	A86	C7-C6-C8	2.90	122.64	118.08
38	13	315	A86	C4-C5-C6	-2.90	123.18	127.31
33	b	619	LMG	O3-C3-C2	-2.89	103.66	110.35
27	32	307	CLA	CHB-C4A-NA	2.89	128.51	124.51
27	33	305	CLA	CHB-C4A-NA	2.89	128.51	124.51
38	11	311	A86	C34-O4-C38	-2.89	112.50	117.90
27	32	311	CLA	C1-C2-C3	-2.89	121.04	126.04
38	11	313	A86	C7-C6-C8	2.89	122.64	118.08
38	31	311	A86	C34-O4-C38	-2.89	112.51	117.90
27	14	307	CLA	CHB-C4A-NA	2.89	128.51	124.51
27	B	602	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
27	b	613	CLA	CHB-C4A-NA	2.89	128.51	124.51
27	11	306	CLA	CHB-C4A-NA	2.89	128.51	124.51
27	33	307	CLA	CHB-C4A-NA	2.89	128.51	124.51
35	J	101	DGD	O2D-C2D-C1D	-2.89	103.03	110.05
28	A	403	PHO	C2D-C1D-ND	-2.89	107.53	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	14	309	CLA	C1-C2-C3	-2.89	121.05	126.04
27	13	309	CLA	C1-C2-C3	-2.89	121.05	126.04
27	14	305	CLA	CHB-C4A-NA	2.89	128.51	124.51
27	31	315	CLA	CHB-C4A-NA	2.89	128.51	124.51
27	B	612	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
27	34	309	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
33	B	619	LMG	O3-C3-C2	-2.89	103.67	110.35
27	A	402	CLA	C7-C6-C5	-2.89	105.52	113.36
38	13	313	A86	C34-O4-C38	-2.89	112.52	117.90
27	A	404	CLA	CHB-C1B-NB	2.89	127.31	124.26
27	C	502	CLA	CHC-C4B-NB	2.89	127.31	124.26
27	B	610	CLA	CHB-C1B-NB	2.89	127.31	124.26
27	a	404	CLA	CHB-C1B-NB	2.89	127.31	124.26
38	34	301	A86	C41-C32-C31	-2.89	107.89	110.47
27	31	307	CLA	CHB-C1B-NB	2.88	127.31	124.26
38	12	315	A86	C34-O4-C38	-2.88	112.52	117.90
38	32	315	A86	C34-O4-C38	-2.88	112.52	117.90
27	c	502	CLA	CHC-C4B-NB	2.88	127.31	124.26
27	C	510	CLA	CHB-C4A-NA	2.88	128.50	124.51
27	13	305	CLA	CHB-C4A-NA	2.88	128.50	124.51
29	z	101	BCR	C24-C23-C22	-2.88	121.88	126.23
27	11	303	CLA	CHB-C4A-NA	2.88	128.49	124.51
27	31	305	CLA	CHB-C4A-NA	2.88	128.49	124.51
38	11	313	A86	C4-C5-C6	-2.88	123.20	127.31
27	34	306	CLA	CHB-C4A-NA	2.88	128.49	124.51
29	z	101	BCR	C16-C15-C14	-2.88	117.58	123.47
29	b	623	BCR	C11-C10-C9	-2.88	123.20	127.31
35	j	101	DGD	O5D-C6D-C5D	-2.88	103.72	109.05
29	Z	101	BCR	C16-C15-C14	-2.88	117.58	123.47
27	32	309	CLA	CHB-C4A-NA	2.87	128.49	124.51
38	32	317	A86	C4-C5-C6	-2.87	123.21	127.31
38	14	316	A86	C41-C32-C31	-2.87	107.90	110.47
27	a	402	CLA	C7-C6-C5	-2.87	105.55	113.36
27	33	304	CLA	C2A-C1A-CHA	2.87	128.88	123.86
35	j	101	DGD	O2D-C2D-C1D	-2.87	103.07	110.05
27	b	602	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
27	B	607	CLA	CHB-C4A-NA	2.87	128.48	124.51
27	33	308	CLA	CHC-C4B-NB	2.87	127.30	124.26
27	c	512	CLA	C2A-C1A-CHA	2.87	128.88	123.86
27	33	308	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
27	14	308	CLA	CHB-C4A-NA	2.87	128.48	124.51
27	C	512	CLA	C2A-C1A-CHA	2.87	128.88	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	403	PHO	C2D-C1D-ND	-2.87	107.54	109.53
27	b	612	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
27	32	310	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
27	b	607	CLA	CHB-C4A-NA	2.87	128.48	124.51
38	34	316	A86	C7-C6-C8	2.87	122.60	118.08
27	B	613	CLA	CHB-C4A-NA	2.87	128.48	124.51
27	13	301	CLA	CHB-C4A-NA	2.87	128.48	124.51
27	C	511	CLA	C2D-C1D-ND	-2.87	107.99	110.10
27	C	507	CLA	CHB-C1B-NB	2.87	127.29	124.26
27	12	310	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
27	14	304	CLA	C2A-C1A-CHA	2.87	128.87	123.86
27	c	510	CLA	O2D-CGD-CBD	2.86	116.36	111.27
27	c	507	CLA	CHB-C1B-NB	2.86	127.29	124.26
27	32	310	CLA	CHB-C4A-NA	2.86	128.47	124.51
27	31	302	CLA	C2A-C1A-CHA	2.86	128.86	123.86
27	14	302	CLA	CHB-C4A-NA	2.86	128.47	124.51
27	c	511	CLA	C2D-C1D-ND	-2.86	108.00	110.10
27	13	308	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
27	13	308	CLA	CHB-C4A-NA	2.86	128.47	124.51
29	Z	101	BCR	C24-C23-C22	-2.86	121.92	126.23
27	B	622	CLA	C3B-C4B-NB	-2.86	107.86	110.52
38	34	316	A86	C4-C5-C6	-2.86	123.23	127.31
27	34	302	CLA	CHB-C4A-NA	2.86	128.46	124.51
27	32	306	CLA	C2A-C1A-CHA	2.86	128.85	123.86
29	Z	101	BCR	C11-C10-C9	-2.86	123.23	127.31
27	31	306	CLA	O2D-CGD-O1D	-2.86	118.26	123.84
27	31	306	CLA	CHB-C4A-NA	2.85	128.46	124.51
27	C	510	CLA	O2D-CGD-CBD	2.85	116.34	111.27
29	c	516	BCR	C15-C14-C13	-2.85	123.24	127.31
38	14	315	A86	C4-C5-C6	-2.85	123.24	127.31
27	34	312	CLA	C3B-C4B-NB	-2.85	107.87	110.52
27	34	305	CLA	C2A-C1A-CHA	2.85	128.84	123.86
38	31	310	A86	C3-C4-C5	-2.85	117.64	123.47
27	C	511	CLA	CHB-C1B-NB	2.85	127.27	124.26
29	C	516	BCR	C15-C14-C13	-2.85	123.25	127.31
27	14	308	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
27	32	313	CLA	C3B-C4B-NB	-2.85	107.87	110.52
38	34	313	A86	C3-C4-C5	-2.85	117.64	123.47
27	33	311	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
38	13	312	A86	C3-C4-C5	-2.84	117.65	123.47
27	34	312	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
27	13	304	CLA	C2A-C1A-CHA	2.84	128.82	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	11	306	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
27	12	310	CLA	CHB-C4A-NA	2.84	128.44	124.51
38	11	310	A86	C3-C4-C5	-2.84	117.67	123.47
38	33	315	A86	C4-C5-C6	-2.83	123.26	127.31
27	12	313	CLA	C3B-C4B-NB	-2.83	107.89	110.52
27	11	302	CLA	C2A-C1A-CHA	2.83	128.81	123.86
27	b	611	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
27	B	611	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
27	b	601	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
27	12	306	CLA	C2A-C1A-CHA	2.83	128.81	123.86
27	33	311	CLA	C3B-C4B-NB	-2.83	107.89	110.52
27	D	405	CLA	CMB-C2B-C1B	-2.83	121.06	125.37
35	h	102	DGD	CDB-CCB-CBB	-2.83	100.08	114.42
29	z	101	BCR	C11-C10-C9	-2.83	123.28	127.31
38	32	314	A86	C3-C4-C5	-2.83	117.69	123.47
35	H	102	DGD	CDB-CCB-CBB	-2.82	100.09	114.42
27	14	311	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
38	12	317	A86	C4-C5-C6	-2.82	123.28	127.31
27	13	311	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
38	33	312	A86	C3-C4-C5	-2.82	117.69	123.47
27	14	311	CLA	C3B-C4B-NB	-2.82	107.90	110.52
38	14	312	A86	C3-C4-C5	-2.82	117.70	123.47
27	12	313	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
27	11	309	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
27	31	309	CLA	C3B-C4B-NB	-2.81	107.91	110.52
27	31	309	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
27	d	405	CLA	CMB-C2B-C1B	-2.81	121.09	125.37
38	12	314	A86	C3-C4-C5	-2.81	117.72	123.47
27	32	303	CLA	CAA-C2A-C3A	-2.81	105.08	112.78
38	31	313	A86	C4-C5-C6	-2.81	123.30	127.31
28	A	403	PHO	CMB-C2B-C3B	2.81	129.93	124.68
27	B	601	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
27	b	607	CLA	O2D-CGD-O1D	-2.80	118.35	123.84
27	B	607	CLA	CHB-C1B-NB	2.80	127.22	124.26
29	A	409	BCR	C15-C16-C17	-2.80	117.73	123.47
27	b	622	CLA	C3B-C4B-NB	-2.80	107.92	110.52
27	b	602	CLA	CHB-C4A-NA	2.80	128.39	124.51
27	B	607	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
35	j	101	DGD	C3G-C2G-C1G	-2.80	105.16	111.79
27	11	309	CLA	C3B-C4B-NB	-2.80	107.92	110.52
27	12	303	CLA	CAA-C2A-C3A	-2.80	105.11	112.78
27	32	313	CLA	O2D-CGD-O1D	-2.80	118.37	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	J	101	DGD	C3G-C2G-C1G	-2.80	105.17	111.79
36	D	404	PL9	C40-C39-C41	2.80	119.98	115.27
36	D	407	PL9	C40-C39-C41	2.80	119.98	115.27
27	31	315	CLA	CAA-C2A-C3A	-2.80	105.12	112.78
27	B	610	CLA	CHB-C4A-NA	2.80	128.38	124.51
29	M	101	BCR	C7-C8-C9	-2.80	122.01	126.23
27	13	301	CLA	CAA-C2A-C3A	-2.80	105.12	112.78
27	11	315	CLA	CAA-C2A-C3A	-2.79	105.13	112.78
27	c	511	CLA	CHB-C1B-NB	2.79	127.21	124.26
29	a	409	BCR	C15-C16-C17	-2.79	117.76	123.47
36	d	407	PL9	C40-C39-C41	2.79	119.97	115.27
28	a	403	PHO	CMB-C2B-C3B	2.79	129.90	124.68
33	q	301	LMG	O6-C1-O1	-2.79	103.37	109.97
27	B	602	CLA	CHB-C4A-NA	2.79	128.37	124.51
27	33	301	CLA	CAA-C2A-C3A	-2.79	105.15	112.78
33	C	519	LMG	O6-C1-O1	-2.79	103.38	109.97
27	34	302	CLA	CAA-C2A-C3A	-2.79	105.15	112.78
27	14	302	CLA	CAA-C2A-C3A	-2.78	105.15	112.78
29	m	103	BCR	C7-C8-C9	-2.78	122.03	126.23
27	b	606	CLA	C1-C2-C3	-2.78	121.23	126.04
27	c	509	CLA	CHB-C4A-NA	2.78	128.36	124.51
27	b	603	CLA	O2D-CGD-CBD	2.78	116.21	111.27
36	d	404	PL9	C40-C39-C41	2.78	119.95	115.27
27	B	603	CLA	O2D-CGD-CBD	2.78	116.21	111.27
27	c	502	CLA	CHB-C4A-NA	2.78	128.36	124.51
27	b	622	CLA	CMD-C2D-C1D	-2.78	119.82	124.71
27	C	509	CLA	CHB-C4A-NA	2.78	128.35	124.51
27	C	502	CLA	CHB-C4A-NA	2.78	128.35	124.51
30	a	406	SQD	C1-O5-C5	2.78	119.14	113.69
35	J	101	DGD	CDB-CCB-CBB	-2.77	100.34	114.42
27	34	306	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
27	b	610	CLA	CHB-C4A-NA	2.77	128.35	124.51
27	b	607	CLA	CHB-C1B-NB	2.77	127.19	124.26
35	j	101	DGD	CDB-CCB-CBB	-2.77	100.36	114.42
27	b	615	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
30	A	406	SQD	C1-O5-C5	2.77	119.12	113.69
27	d	402	CLA	O2D-CGD-CBD	2.76	116.18	111.27
27	C	509	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
27	12	307	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
27	13	305	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
27	c	506	CLA	CHB-C1B-NB	2.76	127.18	124.26
27	B	605	CLA	O2D-CGD-O1D	-2.76	118.45	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	603	CLA	CHB-C4A-NA	2.76	128.32	124.51
27	c	509	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
27	11	303	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
27	B	615	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
27	w	102	CLA	CHB-C4A-NA	2.75	128.31	124.51
27	c	514	CLA	CMB-C2B-C3B	2.75	133.24	126.59
35	C	517	DGD	C3G-C2G-C1G	-2.75	105.29	111.79
29	b	616	BCR	C11-C10-C9	-2.75	123.39	127.31
27	b	615	CLA	C3B-C4B-NB	-2.74	107.97	110.52
35	c	517	DGD	C3G-C2G-C1G	-2.74	105.31	111.79
27	D	402	CLA	O2D-CGD-CBD	2.74	116.14	111.27
27	32	307	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
27	33	305	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
27	a	402	CLA	CMB-C2B-C1B	-2.74	121.20	125.37
27	14	305	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
27	B	606	CLA	C1-C2-C3	-2.74	121.31	126.04
27	c	502	CLA	CMB-C2B-C1B	-2.73	121.20	125.37
29	C	516	BCR	C28-C27-C26	-2.73	109.20	114.08
27	31	303	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
27	C	502	CLA	CMB-C2B-C1B	-2.73	121.21	125.37
27	b	605	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
29	B	616	BCR	C11-C10-C9	-2.73	123.41	127.31
27	C	514	CLA	CMB-C2B-C3B	2.73	133.20	126.59
27	31	305	CLA	C3B-C4B-NB	-2.73	107.98	110.52
27	C	506	CLA	CHB-C1B-NB	2.73	127.14	124.26
27	b	609	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
27	W	102	CLA	CHB-C4A-NA	2.72	128.28	124.51
27	b	603	CLA	CHB-C4A-NA	2.72	128.28	124.51
27	B	606	CLA	CHB-C4A-NA	2.72	128.28	124.51
27	B	609	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
27	c	506	CLA	CHB-C4A-NA	2.72	128.27	124.51
33	b	618	LMG	C1-C2-C3	-2.72	104.34	110.00
27	b	606	CLA	CHB-C4A-NA	2.72	128.27	124.51
33	12	301	LMG	O3-C3-C2	-2.72	104.07	110.35
27	C	503	CLA	CHB-C4A-NA	2.72	128.27	124.51
27	C	506	CLA	CHB-C4A-NA	2.71	128.27	124.51
27	c	503	CLA	CHB-C4A-NA	2.71	128.26	124.51
33	B	618	LMG	C1-C2-C3	-2.71	104.34	110.00
27	d	402	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
27	A	402	CLA	CMB-C2B-C1B	-2.71	121.24	125.37
27	c	507	CLA	C2A-C1A-CHA	2.71	128.59	123.86
35	j	101	DGD	O3G-C1D-C2D	-2.70	104.09	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	11	305	CLA	C3B-C4B-NB	-2.70	108.01	110.52
27	m	101	CLA	C3B-C4B-NB	-2.70	108.01	110.52
27	34	307	CLA	C3A-C2A-C1A	2.70	105.38	101.34
27	c	508	CLA	O1D-CGD-CBD	2.70	130.00	124.48
27	11	304	CLA	C3A-C2A-C1A	2.70	105.38	101.34
29	c	516	BCR	C28-C27-C26	-2.70	109.26	114.08
27	B	615	CLA	C3B-C4B-NB	-2.70	108.01	110.52
27	12	309	CLA	C3B-C4B-NB	-2.70	108.01	110.52
27	12	308	CLA	C3A-C2A-C1A	2.69	105.37	101.34
27	C	508	CLA	O1D-CGD-CBD	2.69	129.99	124.48
27	c	502	CLA	CAA-C2A-C3A	-2.69	105.41	112.78
27	C	507	CLA	C2A-C1A-CHA	2.69	128.56	123.86
27	Z	102	CLA	CHB-C4A-NA	2.69	128.23	124.51
27	D	402	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
27	C	504	CLA	CAA-CBA-CGA	-2.69	105.40	113.25
27	b	604	CLA	C1-C2-C3	-2.69	121.40	126.04
38	14	314	A86	C3-C4-C5	-2.68	117.97	123.47
27	b	622	CLA	CHB-C4A-NA	2.68	128.22	124.51
29	c	519	BCR	C11-C10-C9	-2.68	123.48	127.31
33	32	301	LMG	O3-C3-C2	-2.68	104.15	110.35
27	M	102	CLA	C3B-C4B-NB	-2.68	108.03	110.52
27	14	307	CLA	C3B-C4B-NB	-2.68	108.03	110.52
38	32	316	A86	C3-C4-C5	-2.68	117.98	123.47
27	12	303	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
37	f	102	HEM	CMB-C2B-C1B	-2.68	120.96	125.04
27	C	502	CLA	CAA-C2A-C3A	-2.68	105.44	112.78
33	D	408	LMG	O1-C7-C8	-2.68	104.44	110.90
35	J	101	DGD	O3G-C1D-C2D	-2.68	104.12	108.30
33	d	408	LMG	O1-C7-C8	-2.68	104.44	110.90
27	B	606	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
27	32	309	CLA	C3B-C4B-NB	-2.67	108.03	110.52
27	14	302	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
36	d	407	PL9	C22-C23-C24	-2.67	121.22	127.66
27	34	308	CLA	C3B-C4B-NB	-2.67	108.03	110.52
27	c	504	CLA	CAA-CBA-CGA	-2.67	105.44	113.25
36	D	407	PL9	C22-C23-C24	-2.67	121.22	127.66
27	B	622	CLA	CHB-C4A-NA	2.67	128.21	124.51
38	34	315	A86	C3-C4-C5	-2.67	118.00	123.47
38	11	312	A86	C3-C4-C5	-2.67	118.00	123.47
27	B	604	CLA	C1-C2-C3	-2.67	121.43	126.04
38	12	316	A86	C3-C4-C5	-2.67	118.01	123.47
27	33	301	CLA	O2D-CGD-O1D	-2.66	118.63	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	33	306	CLA	C3A-C2A-C1A	2.66	105.33	101.34
29	C	520	BCR	C11-C10-C9	-2.66	123.51	127.31
27	B	604	CLA	C2D-C1D-ND	-2.66	108.14	110.10
27	11	315	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
27	14	306	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
38	11	312	A86	C20-C19-C18	-2.66	107.48	112.75
29	m	103	BCR	C11-C10-C9	-2.66	123.51	127.31
27	13	306	CLA	C3A-C2A-C1A	2.66	105.33	101.34
38	13	314	A86	C3-C4-C5	-2.66	118.02	123.47
38	33	314	A86	C3-C4-C5	-2.66	118.02	123.47
27	13	307	CLA	C3B-C4B-NB	-2.66	108.05	110.52
27	Z	102	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
27	C	510	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
27	b	606	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
27	c	510	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
38	31	312	A86	C3-C4-C5	-2.66	118.03	123.47
37	E	101	HEM	CMB-C2B-C1B	-2.66	120.99	125.04
27	z	102	CLA	CHB-C4A-NA	2.66	128.19	124.51
27	31	304	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
27	32	303	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
27	Z	102	CLA	CHC-C4B-NB	2.66	127.07	124.26
27	b	604	CLA	C2D-C1D-ND	-2.66	108.15	110.10
27	z	102	CLA	O2D-CGD-O1D	-2.66	118.65	123.84
27	b	604	CLA	CAA-C2A-C3A	-2.65	105.51	112.78
27	d	401	CLA	CHB-C4A-NA	2.65	128.18	124.51
27	31	304	CLA	C3A-C2A-C1A	2.65	105.31	101.34
38	33	314	A86	C20-C19-C18	-2.65	107.51	112.75
27	13	301	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
27	32	308	CLA	C3A-C2A-C1A	2.65	105.30	101.34
27	c	514	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
29	M	101	BCR	C11-C10-C9	-2.65	123.53	127.31
38	13	314	A86	C20-C19-C18	-2.65	107.52	112.75
27	34	302	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
27	b	614	CLA	O2A-CGA-O1A	-2.64	116.92	123.59
27	c	504	CLA	C3B-C4B-NB	-2.64	108.06	110.52
28	a	403	PHO	O2D-CGD-O1D	-2.64	118.67	123.84
27	b	606	CLA	CAA-CBA-CGA	-2.64	105.53	113.25
27	B	622	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
27	31	315	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
38	14	315	A86	C8-C6-C5	-2.64	114.89	118.94
38	12	316	A86	C20-C19-C18	-2.64	107.53	112.75
38	31	312	A86	C20-C19-C18	-2.64	107.53	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	14	306	CLA	C3A-C2A-C1A	2.64	105.29	101.34
27	b	610	CLA	O2D-CGD-CBD	2.64	115.95	111.27
27	C	504	CLA	CHB-C4A-NA	2.64	128.16	124.51
38	14	314	A86	C20-C19-C18	-2.64	107.53	112.75
27	34	307	CLA	O2D-CGD-O1D	-2.64	118.69	123.84
35	H	102	DGD	O6D-C1D-O3G	-2.63	103.73	109.97
27	B	610	CLA	O2D-CGD-CBD	2.63	115.95	111.27
32	L	102	LHG	C20-C19-C18	-2.63	101.05	114.42
38	34	315	A86	C20-C19-C18	-2.63	107.54	112.75
27	B	604	CLA	CAA-C2A-C3A	-2.63	105.56	112.78
38	13	315	A86	C8-C6-C5	-2.63	114.90	118.94
35	C	518	DGD	CBB-CAB-C9B	-2.63	101.06	114.42
27	b	612	CLA	CMB-C2B-C1B	-2.63	121.36	125.37
27	B	614	CLA	O2A-CGA-O1A	-2.63	116.95	123.59
27	D	401	CLA	CHB-C4A-NA	2.63	128.15	124.51
35	H	102	DGD	C3G-C2G-C1G	-2.63	105.57	111.79
38	11	313	A86	C8-C6-C5	-2.63	114.91	118.94
27	C	514	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
35	c	518	DGD	CBB-CAB-C9B	-2.63	101.08	114.42
38	32	316	A86	C20-C19-C18	-2.63	107.55	112.75
35	c	517	DGD	C1E-O6E-C5E	2.63	118.85	113.69
35	C	518	DGD	O2D-C2D-C1D	-2.63	103.66	110.05
38	33	315	A86	C8-C6-C5	-2.63	114.91	118.94
32	l	103	LHG	C20-C19-C18	-2.63	101.09	114.42
29	c	519	BCR	C27-C26-C25	2.63	126.54	122.73
27	C	504	CLA	C3B-C4B-NB	-2.62	108.08	110.52
27	B	606	CLA	CAA-CBA-CGA	-2.62	105.58	113.25
27	b	622	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
27	33	306	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
38	32	317	A86	C8-C6-C5	-2.62	114.91	118.94
27	d	405	CLA	CAA-CBA-CGA	-2.62	105.59	113.25
27	B	612	CLA	CMB-C2B-C1B	-2.62	121.38	125.37
29	M	101	BCR	C24-C23-C22	-2.62	122.28	126.23
27	z	102	CLA	CHC-C4B-NB	2.62	127.03	124.26
27	32	308	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
27	11	304	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
35	h	102	DGD	C3G-C2G-C1G	-2.62	105.59	111.79
35	h	102	DGD	O6D-C1D-O3G	-2.62	103.77	109.97
35	c	518	DGD	O2D-C2D-C1D	-2.62	103.69	110.05
27	12	308	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
33	C	519	LMG	O2-C2-C1	-2.62	103.69	110.05
27	C	512	CLA	O2D-CGD-O1D	-2.62	118.72	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	13	306	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
27	D	405	CLA	CAA-CBA-CGA	-2.61	105.61	113.25
36	D	407	PL9	C31-C32-C33	-2.61	103.29	111.88
33	q	301	LMG	O2-C2-C1	-2.61	103.70	110.05
27	M	102	CLA	CHB-C4A-NA	2.61	128.12	124.51
35	C	517	DGD	C1E-O6E-C5E	2.61	118.81	113.69
27	33	307	CLA	C3B-C4B-NB	-2.61	108.09	110.52
28	A	403	PHO	O2D-CGD-O1D	-2.61	118.74	123.84
36	d	407	PL9	C31-C32-C33	-2.61	103.31	111.88
38	32	318	A86	C7-C6-C8	2.61	122.19	118.08
27	32	313	CLA	CHB-C4A-NA	2.61	128.12	124.51
38	34	316	A86	C8-C6-C5	-2.60	114.94	118.94
29	z	101	BCR	C34-C9-C10	-2.60	119.28	122.92
38	31	314	A86	C7-C6-C8	2.60	122.18	118.08
29	C	520	BCR	C27-C26-C25	2.60	126.51	122.73
29	Z	101	BCR	C34-C9-C10	-2.60	119.28	122.92
27	W	102	CLA	C3B-C4B-NB	-2.60	108.10	110.52
29	B	617	BCR	C3-C4-C5	-2.60	109.44	114.08
27	b	613	CLA	C3B-C4B-NB	-2.60	108.10	110.52
29	m	103	BCR	C24-C23-C22	-2.60	122.31	126.23
27	33	311	CLA	CHB-C4A-NA	2.60	128.10	124.51
36	D	404	PL9	C7-C8-C9	-2.60	122.47	126.79
27	13	311	CLA	CHB-C4A-NA	2.60	128.10	124.51
29	z	101	BCR	C28-C27-C26	-2.60	109.44	114.08
27	w	102	CLA	C3B-C4B-NB	-2.60	108.11	110.52
38	13	316	A86	C7-C6-C8	2.59	122.16	118.08
27	C	509	CLA	O2D-CGD-CBD	2.59	115.87	111.27
27	c	512	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
36	d	404	PL9	C7-C8-C9	-2.59	122.48	126.79
38	31	313	A86	C8-C6-C5	-2.59	114.97	118.94
27	c	509	CLA	C3B-C4B-NB	-2.59	108.11	110.52
33	W	101	LMG	O3-C3-C2	-2.59	104.37	110.35
27	14	311	CLA	CHB-C4A-NA	2.59	128.09	124.51
27	c	504	CLA	CHB-C4A-NA	2.58	128.09	124.51
38	12	317	A86	C8-C6-C5	-2.58	114.98	118.94
33	M	103	LMG	O3-C3-C2	-2.58	104.38	110.35
29	b	617	BCR	C3-C4-C5	-2.58	109.47	114.08
27	c	504	CLA	C2A-C1A-CHA	2.58	128.38	123.86
27	C	509	CLA	C3B-C4B-NB	-2.58	108.12	110.52
27	11	309	CLA	CHB-C4A-NA	2.58	128.08	124.51
27	m	101	CLA	CHB-C4A-NA	2.58	128.08	124.51
38	34	301	A86	C7-C6-C8	2.58	122.14	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	11	315	CLA	C3B-C4B-NB	-2.58	108.12	110.52
38	14	301	A86	C7-C6-C8	2.58	122.14	118.08
38	11	314	A86	C7-C6-C8	2.58	122.14	118.08
33	w	101	LMG	O3-C3-C2	-2.58	104.39	110.35
29	Z	101	BCR	C28-C27-C26	-2.58	109.48	114.08
38	14	316	A86	C7-C6-C8	2.58	122.14	118.08
27	31	309	CLA	CHB-C4A-NA	2.58	128.07	124.51
33	m	102	LMG	O3-C3-C2	-2.57	104.40	110.35
27	33	307	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
27	B	604	CLA	CAA-CBA-CGA	-2.57	105.73	113.25
32	l	103	LHG	O8-C23-C24	2.57	119.97	111.91
27	c	511	CLA	CHB-C4A-NA	2.57	128.06	124.51
38	33	316	A86	C7-C6-C8	2.57	122.12	118.08
27	c	509	CLA	O2D-CGD-CBD	2.57	115.83	111.27
27	C	504	CLA	C2A-C1A-CHA	2.57	128.35	123.86
33	w	101	LMG	C1-C2-C3	-2.57	104.65	110.00
27	C	511	CLA	CHB-C4A-NA	2.57	128.06	124.51
32	L	102	LHG	O8-C23-C24	2.57	119.96	111.91
33	W	101	LMG	C1-C2-C3	-2.57	104.65	110.00
27	32	303	CLA	C3B-C4B-NB	-2.57	108.14	110.52
27	b	604	CLA	CAA-CBA-CGA	-2.57	105.76	113.25
27	D	402	CLA	CHB-C1B-NB	2.56	126.97	124.26
27	34	312	CLA	CHB-C4A-NA	2.56	128.06	124.51
27	B	613	CLA	C3B-C4B-NB	-2.56	108.14	110.52
27	b	622	CLA	CMD-C2D-C3D	2.56	133.51	127.61
27	b	610	CLA	CAA-C2A-C3A	-2.56	105.76	112.78
27	c	508	CLA	CMB-C2B-C1B	-2.56	121.47	125.37
33	W	101	LMG	C38-C37-C36	-2.56	101.44	114.42
29	B	616	BCR	C27-C26-C25	2.56	126.44	122.73
27	B	610	CLA	CAA-C2A-C3A	-2.56	105.78	112.78
27	13	301	CLA	C3B-C4B-NB	-2.56	108.14	110.52
27	12	313	CLA	CHB-C4A-NA	2.55	128.04	124.51
27	11	305	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
37	v	201	HEM	C4A-CHB-C1B	-2.55	120.28	126.34
33	w	101	LMG	C38-C37-C36	-2.55	101.46	114.42
27	W	103	CLA	CHB-C1B-NB	2.55	126.96	124.26
27	d	402	CLA	CHB-C1B-NB	2.55	126.96	124.26
29	B	623	BCR	C15-C14-C13	-2.55	123.67	127.31
29	b	616	BCR	C27-C26-C25	2.55	126.44	122.73
27	C	508	CLA	CHC-C4B-NB	2.55	126.96	124.26
27	14	306	CLA	O2D-CGD-CBD	2.55	115.80	111.27
27	32	309	CLA	O2D-CGD-O1D	-2.55	118.86	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	12	309	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
27	13	307	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
27	11	301	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
27	c	510	CLA	C3B-C4B-NB	-2.55	108.15	110.52
27	w	103	CLA	CHB-C4A-NA	2.55	128.03	124.51
27	B	611	CLA	C3B-C4B-NB	-2.54	108.15	110.52
27	b	611	CLA	C3B-C4B-NB	-2.54	108.15	110.52
27	B	606	CLA	CHD-C1D-ND	-2.54	122.12	124.45
27	34	308	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
27	W	103	CLA	C3B-C4B-NB	-2.54	108.16	110.52
27	C	506	CLA	O2D-CGD-CBD	2.54	115.79	111.27
27	33	309	CLA	CMB-C2B-C1B	-2.54	121.50	125.37
27	33	301	CLA	C3B-C4B-NB	-2.54	108.16	110.52
29	A	409	BCR	C15-C14-C13	-2.54	123.68	127.31
27	D	406	CLA	O2D-CGD-CBD	2.54	115.78	111.27
27	w	103	CLA	CHB-C1B-NB	2.54	126.95	124.26
37	V	201	HEM	C4A-CHB-C1B	-2.54	120.31	126.34
27	14	302	CLA	C3B-C4B-NB	-2.54	108.16	110.52
27	w	103	CLA	C3B-C4B-NB	-2.54	108.16	110.52
27	c	510	CLA	CHC-C4B-NB	2.54	126.94	124.26
39	32	302	LMU	O5B-C1B-C2B	2.54	115.72	110.35
38	34	313	A86	C25-C24-C1	-2.54	119.29	126.42
27	31	305	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
27	C	508	CLA	CMB-C2B-C1B	-2.54	121.51	125.37
27	14	307	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
38	32	318	A86	C3-C4-C5	-2.53	118.28	123.47
27	12	305	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
27	12	308	CLA	O2D-CGD-CBD	2.53	115.77	111.27
27	d	406	CLA	O2D-CGD-CBD	2.53	115.77	111.27
27	B	604	CLA	C2A-C1A-CHA	2.53	128.29	123.86
29	M	101	BCR	C15-C14-C13	-2.53	123.70	127.31
29	B	616	BCR	C40-C30-C25	2.53	114.41	110.30
27	31	315	CLA	C3B-C4B-NB	-2.53	108.17	110.52
27	33	303	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
38	13	312	A86	C25-C24-C1	-2.53	119.31	126.42
27	31	304	CLA	O2D-CGD-CBD	2.53	115.77	111.27
27	c	508	CLA	CHC-C4B-NB	2.53	126.94	124.26
36	D	407	PL9	C7-C3-C4	2.53	118.93	116.88
38	33	316	A86	C3-C4-C5	-2.53	118.29	123.47
27	14	303	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
27	13	306	CLA	O2D-CGD-CBD	2.53	115.76	111.27
38	31	310	A86	C25-C24-C1	-2.53	119.31	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	516	BCR	C29-C30-C25	2.53	114.37	110.48
35	c	518	DGD	O6D-C5D-C6D	-2.53	101.56	106.67
27	b	604	CLA	C2A-C1A-CHA	2.53	128.28	123.86
38	32	314	A86	C25-C24-C1	-2.53	119.31	126.42
29	F	101	BCR	C11-C10-C9	-2.53	123.70	127.31
27	13	309	CLA	C2A-C1A-CHA	2.53	128.28	123.86
27	d	401	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
38	11	310	A86	C25-C24-C1	-2.53	119.32	126.42
27	13	303	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
27	34	310	CLA	CMB-C2B-C1B	-2.53	121.52	125.37
32	B	621	LHG	C11-C10-C9	-2.53	101.60	114.42
27	34	304	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
29	b	623	BCR	C15-C14-C13	-2.53	123.71	127.31
38	13	302	A86	C41-C32-C31	-2.53	108.21	110.47
27	c	506	CLA	O2D-CGD-CBD	2.53	115.75	111.27
27	32	311	CLA	C2A-C1A-CHA	2.52	128.27	123.86
27	11	304	CLA	O2D-CGD-CBD	2.52	115.75	111.27
27	34	310	CLA	C2A-C1A-CHA	2.52	128.27	123.86
33	M	103	LMG	O2-C2-C1	-2.52	103.92	110.05
27	b	604	CLA	CHC-C4B-NB	2.52	126.93	124.26
38	14	301	A86	C3-C4-C5	-2.52	118.31	123.47
32	b	621	LHG	C11-C10-C9	-2.52	101.62	114.42
27	34	307	CLA	O2D-CGD-CBD	2.52	115.75	111.27
32	l	102	LHG	C20-C19-C18	-2.52	101.63	114.42
27	W	103	CLA	CHB-C4A-NA	2.52	128.00	124.51
29	F	101	BCR	C7-C8-C9	-2.52	122.43	126.23
32	L	101	LHG	C20-C19-C18	-2.52	101.63	114.42
27	13	305	CLA	C3B-C4B-NB	-2.52	108.18	110.52
27	B	606	CLA	CHC-C1C-NC	2.52	128.03	124.20
27	B	615	CLA	CHB-C4A-NA	2.52	128.00	124.51
35	C	518	DGD	O6D-C5D-C6D	-2.52	101.58	106.67
27	B	604	CLA	CHC-C4B-NB	2.52	126.92	124.26
27	c	507	CLA	C3B-C4B-NB	-2.52	108.18	110.52
27	C	510	CLA	CHC-C4B-NB	2.52	126.92	124.26
27	D	401	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
27	31	301	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
27	b	615	CLA	CHB-C4A-NA	2.52	127.99	124.51
27	32	308	CLA	O2D-CGD-CBD	2.52	115.74	111.27
27	33	306	CLA	O2D-CGD-CBD	2.51	115.74	111.27
38	33	312	A86	C25-C24-C1	-2.51	119.35	126.42
29	b	616	BCR	C40-C30-C25	2.51	114.38	110.30
38	11	314	A86	C3-C4-C5	-2.51	118.32	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	606	CLA	CHD-C1D-ND	-2.51	122.14	124.45
38	31	314	A86	C3-C4-C5	-2.51	118.33	123.47
32	A	408	LHG	C20-C19-C18	-2.51	101.67	114.42
29	m	103	BCR	C15-C14-C13	-2.51	123.72	127.31
27	b	608	CLA	CHB-C1B-NB	2.51	126.92	124.26
36	d	407	PL9	C7-C3-C4	2.51	118.92	116.88
27	32	305	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
27	31	307	CLA	C2A-C1A-CHA	2.51	128.25	123.86
33	W	101	LMG	O1-C1-C2	-2.51	104.39	108.30
38	33	315	A86	C40-C32-C31	-2.51	108.23	110.47
38	13	312	A86	C7-C6-C8	2.51	122.03	118.08
29	b	616	BCR	C15-C16-C17	-2.51	118.34	123.47
27	11	307	CLA	CMB-C2B-C1B	-2.51	121.55	125.37
32	a	408	LHG	C20-C19-C18	-2.51	101.70	114.42
27	C	503	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
27	34	302	CLA	C3B-C4B-NB	-2.51	108.19	110.52
27	d	405	CLA	CHB-C4A-NA	2.51	127.98	124.51
38	14	312	A86	C25-C24-C1	-2.51	119.37	126.42
38	34	301	A86	C3-C4-C5	-2.51	118.34	123.47
27	13	309	CLA	CMB-C2B-C1B	-2.51	121.55	125.37
27	12	311	CLA	C2A-C1A-CHA	2.51	128.24	123.86
27	14	309	CLA	C2A-C1A-CHA	2.51	128.24	123.86
29	B	616	BCR	C15-C16-C17	-2.51	118.34	123.47
38	34	303	A86	C41-C32-C31	-2.50	108.23	110.47
27	C	507	CLA	C3B-C4B-NB	-2.50	108.19	110.52
29	f	101	BCR	C7-C8-C9	-2.50	122.45	126.23
27	12	303	CLA	C3B-C4B-NB	-2.50	108.19	110.52
29	a	409	BCR	C15-C14-C13	-2.50	123.74	127.31
29	f	101	BCR	C11-C10-C9	-2.50	123.74	127.31
27	c	503	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
35	J	101	DGD	O3D-C3D-C4D	-2.50	104.56	110.35
27	12	311	CLA	CMB-C2B-C1B	-2.50	121.56	125.37
38	12	315	A86	C20-C19-C18	-2.50	107.80	112.75
27	B	607	CLA	CMB-C2B-C3B	2.50	132.65	126.59
33	m	102	LMG	O2-C2-C1	-2.50	103.97	110.05
38	34	313	A86	C7-C6-C8	2.50	122.02	118.08
38	14	316	A86	C3-C4-C5	-2.50	118.35	123.47
38	13	316	A86	C3-C4-C5	-2.50	118.35	123.47
27	B	605	CLA	CHB-C1B-NB	2.50	126.90	124.26
27	b	612	CLA	CMB-C2B-C3B	2.50	132.64	126.59
27	14	309	CLA	CMB-C2B-C1B	-2.50	121.56	125.37
27	31	307	CLA	CMB-C2B-C1B	-2.50	121.56	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	31	303	CLA	C3B-C4B-NB	-2.50	108.20	110.52
27	32	307	CLA	C3B-C4B-NB	-2.50	108.20	110.52
38	12	314	A86	C25-C24-C1	-2.50	119.40	126.42
27	11	302	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
27	11	303	CLA	C3B-C4B-NB	-2.50	108.20	110.52
27	33	305	CLA	C3B-C4B-NB	-2.50	108.20	110.52
27	11	307	CLA	C2A-C1A-CHA	2.50	128.23	123.86
38	13	313	A86	C20-C19-C18	-2.50	107.81	112.75
28	D	403	PHO	C2D-C1D-ND	-2.50	107.80	109.53
27	33	309	CLA	C2A-C1A-CHA	2.50	128.22	123.86
35	j	101	DGD	O3D-C3D-C4D	-2.50	104.58	110.35
38	11	316	A86	C41-C32-C31	-2.50	108.24	110.47
38	34	314	A86	C20-C19-C18	-2.50	107.81	112.75
27	14	306	CLA	CBA-CAA-C2A	-2.50	106.50	113.86
38	33	312	A86	C7-C6-C8	2.50	122.01	118.08
29	C	516	BCR	C29-C30-C25	2.49	114.32	110.48
38	31	313	A86	C40-C32-C31	-2.49	108.24	110.47
38	32	315	A86	C20-C19-C18	-2.49	107.82	112.75
38	11	313	A86	C40-C32-C31	-2.49	108.24	110.47
33	d	408	LMG	O6-C1-O1	-2.49	104.07	109.97
33	w	101	LMG	O1-C1-C2	-2.49	104.41	108.30
27	B	608	CLA	CHB-C1B-NB	2.49	126.89	124.26
38	14	312	A86	C7-C6-C8	2.49	122.00	118.08
38	11	311	A86	C20-C19-C18	-2.49	107.83	112.75
38	13	315	A86	C40-C32-C31	-2.49	108.25	110.47
27	b	607	CLA	CMB-C2B-C3B	2.49	132.62	126.59
33	D	408	LMG	O6-C1-O1	-2.49	104.08	109.97
27	c	513	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
29	H	101	BCR	C37-C22-C21	-2.49	119.44	122.92
27	32	308	CLA	CBA-CAA-C2A	-2.49	106.52	113.86
27	12	306	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
38	14	313	A86	C20-C19-C18	-2.49	107.83	112.75
27	C	513	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
27	C	510	CLA	C3B-C4B-NB	-2.49	108.21	110.52
28	d	403	PHO	C2D-C1D-ND	-2.49	107.81	109.53
27	D	406	CLA	CHC-C4B-NB	2.49	126.89	124.26
27	b	605	CLA	CHB-C1B-NB	2.49	126.89	124.26
38	14	315	A86	C40-C32-C31	-2.49	108.25	110.47
27	12	308	CLA	CBA-CAA-C2A	-2.48	106.53	113.86
38	31	311	A86	C20-C19-C18	-2.48	107.83	112.75
38	34	316	A86	C40-C32-C31	-2.48	108.25	110.47
27	13	306	CLA	CBA-CAA-C2A	-2.48	106.53	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	c	503	CLA	C2A-C1A-CHA	2.48	128.20	123.86
27	31	304	CLA	CBA-CAA-C2A	-2.48	106.53	113.86
38	12	304	A86	C41-C32-C31	-2.48	108.25	110.47
27	B	612	CLA	CMB-C2B-C3B	2.48	132.60	126.59
38	32	317	A86	C40-C32-C31	-2.48	108.25	110.47
27	14	305	CLA	C3B-C4B-NB	-2.48	108.21	110.52
30	a	406	SQD	O7-S-C6	2.48	109.89	106.94
29	c	515	BCR	C7-C8-C9	-2.48	122.49	126.23
38	11	310	A86	C7-C6-C8	2.48	121.98	118.08
33	b	618	LMG	O6-C1-O1	-2.48	104.11	109.97
27	32	311	CLA	CMB-C2B-C1B	-2.48	121.60	125.37
27	12	307	CLA	C3B-C4B-NB	-2.48	108.22	110.52
38	14	313	A86	C25-C24-C1	-2.48	119.46	126.42
27	D	406	CLA	CHB-C1B-NB	2.48	126.88	124.26
38	31	316	A86	C41-C32-C31	-2.48	108.26	110.47
27	D	405	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
38	32	304	A86	C41-C32-C31	-2.47	108.26	110.47
38	33	313	A86	C20-C19-C18	-2.47	107.85	112.75
27	c	510	CLA	CAA-C2A-C3A	-2.47	106.00	112.78
38	12	317	A86	C40-C32-C31	-2.47	108.26	110.47
35	C	517	DGD	O3D-C3D-C4D	-2.47	104.63	110.35
27	11	304	CLA	CBA-CAA-C2A	-2.47	106.56	113.86
38	11	311	A86	C25-C24-C1	-2.47	119.47	126.42
38	12	314	A86	C7-C6-C8	2.47	121.97	118.08
27	A	404	CLA	CAA-C2A-C3A	-2.47	106.01	112.78
27	a	404	CLA	CAA-C2A-C3A	-2.47	106.01	112.78
29	C	515	BCR	C7-C8-C9	-2.47	122.50	126.23
27	33	306	CLA	CBA-CAA-C2A	-2.47	106.57	113.86
38	13	317	A86	C41-C32-C31	-2.47	108.26	110.47
27	13	304	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
37	V	201	HEM	CAC-C3C-C2C	-2.47	120.46	128.60
33	B	618	LMG	O6-C1-O1	-2.47	104.12	109.97
38	32	314	A86	C7-C6-C8	2.47	121.97	118.08
35	c	517	DGD	O3D-C3D-C4D	-2.47	104.64	110.35
27	D	405	CLA	CHB-C4A-NA	2.47	127.93	124.51
28	a	403	PHO	CAA-CBA-CGA	-2.47	106.04	113.25
38	33	313	A86	C25-C24-C1	-2.47	119.48	126.42
27	14	304	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
27	b	604	CLA	C3C-C4C-NC	-2.47	107.81	110.57
27	34	307	CLA	CBA-CAA-C2A	-2.47	106.58	113.86
28	A	403	PHO	CAA-CBA-CGA	-2.47	106.05	113.25
27	b	606	CLA	CHC-C1C-NC	2.47	127.94	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	34	305	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
38	31	310	A86	C7-C6-C8	2.46	121.96	118.08
29	M	101	BCR	C27-C26-C25	2.46	126.31	122.73
27	31	302	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
27	33	304	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
27	C	503	CLA	C2A-C1A-CHA	2.46	128.17	123.86
27	D	405	CLA	CMB-C2B-C3B	2.46	132.55	126.59
27	C	510	CLA	CAA-C2A-C3A	-2.46	106.03	112.78
38	12	315	A86	C25-C24-C1	-2.46	119.50	126.42
38	33	302	A86	C41-C32-C31	-2.46	108.27	110.47
38	13	313	A86	C25-C24-C1	-2.46	119.50	126.42
38	31	311	A86	C25-C24-C1	-2.46	119.50	126.42
39	12	302	LMU	O5B-C1B-C2B	2.46	115.56	110.35
32	L	102	LHG	C11-C10-C9	-2.46	101.95	114.42
27	c	503	CLA	C1D-ND-C4D	2.46	108.08	106.33
37	v	201	HEM	CAC-C3C-C2C	-2.46	120.51	128.60
27	c	504	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
38	34	314	A86	C25-C24-C1	-2.46	119.51	126.42
29	H	101	BCR	C11-C10-C9	-2.46	123.80	127.31
29	m	103	BCR	C27-C26-C25	2.46	126.30	122.73
38	13	312	A86	C10-C9-C8	-2.46	115.56	123.22
38	31	310	A86	C10-C9-C8	-2.45	115.56	123.22
27	C	514	CLA	CAA-C2A-C3A	-2.45	106.06	112.78
38	14	312	A86	C10-C9-C8	-2.45	115.56	123.22
38	12	314	A86	C10-C9-C8	-2.45	115.56	123.22
32	l	103	LHG	C11-C10-C9	-2.45	101.97	114.42
38	32	315	A86	C25-C24-C1	-2.45	119.53	126.42
29	C	520	BCR	C15-C14-C13	-2.45	123.81	127.31
27	C	513	CLA	C3B-C4B-NB	-2.45	108.24	110.52
27	d	405	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
27	C	504	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
30	b	620	SQD	O48-C23-O10	-2.45	117.41	123.59
38	11	310	A86	C10-C9-C8	-2.45	115.57	123.22
33	q	301	LMG	C9-C8-C7	-2.45	106.00	111.79
38	34	313	A86	C10-C9-C8	-2.45	115.58	123.22
29	f	101	BCR	C35-C13-C14	-2.45	119.50	122.92
30	A	406	SQD	O7-S-C6	2.45	109.85	106.94
33	C	519	LMG	C9-C8-C7	-2.45	106.00	111.79
38	33	302	A86	C12-C11-C13	2.45	120.13	116.02
29	h	101	BCR	C11-C10-C9	-2.44	123.82	127.31
27	32	306	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
38	32	314	A86	C10-C9-C8	-2.44	115.59	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	33	312	A86	C10-C9-C8	-2.44	115.59	123.22
29	c	519	BCR	C15-C14-C13	-2.44	123.83	127.31
30	B	620	SQD	O48-C23-O10	-2.44	117.43	123.59
38	13	317	A86	C12-C11-C13	2.44	120.12	116.02
28	D	403	PHO	O2D-CGD-O1D	-2.44	119.07	123.84
38	13	302	A86	C12-C11-C13	2.44	120.12	116.02
38	34	303	A86	C12-C11-C13	2.44	120.12	116.02
36	d	404	PL9	C20-C19-C21	2.44	119.38	115.27
29	F	101	BCR	C35-C13-C14	-2.44	119.51	122.92
27	b	615	CLA	CHA-C1A-NA	-2.44	120.81	126.40
27	c	513	CLA	C3B-C4B-NB	-2.44	108.25	110.52
33	B	618	LMG	O3-C3-C2	-2.44	104.72	110.35
27	d	405	CLA	CMB-C2B-C3B	2.44	132.49	126.59
29	h	101	BCR	C37-C22-C21	-2.44	119.51	122.92
27	c	514	CLA	CAA-C2A-C3A	-2.43	106.11	112.78
38	11	316	A86	C12-C11-C13	2.43	120.11	116.02
27	B	604	CLA	C3C-C4C-NC	-2.43	107.84	110.57
27	b	612	CLA	CMD-C2D-C1D	-2.43	120.42	124.71
36	D	404	PL9	C20-C19-C21	2.43	119.36	115.27
27	b	609	CLA	C2A-C1A-CHA	2.43	128.11	123.86
35	j	101	DGD	O3E-C3E-C2E	-2.43	104.73	110.35
27	34	309	CLA	C2A-C1A-CHA	2.43	128.11	123.86
38	34	313	A86	C23-C16-C22	-2.43	103.78	107.37
27	b	611	CLA	CMB-C2B-C1B	-2.43	121.67	125.37
33	B	619	LMG	O1-C1-C2	-2.43	104.51	108.30
27	11	306	CLA	C2A-C1A-CHA	2.43	128.11	123.86
35	J	101	DGD	O3E-C3E-C2E	-2.43	104.73	110.35
38	12	304	A86	C12-C11-C13	2.43	120.10	116.02
27	B	609	CLA	C2A-C1A-CHA	2.43	128.10	123.86
27	d	406	CLA	CHB-C1B-NB	2.43	126.83	124.26
33	q	301	LMG	C40-C39-C38	-2.43	102.11	114.42
27	B	611	CLA	CMB-C2B-C1B	-2.43	121.67	125.37
27	B	605	CLA	C3C-C4C-NC	-2.43	107.85	110.57
38	32	315	A86	C40-C32-C31	-2.42	108.30	110.47
28	d	403	PHO	O2D-CGD-O1D	-2.42	119.10	123.84
33	C	519	LMG	C40-C39-C38	-2.42	102.12	114.42
27	34	310	CLA	CHA-C1A-NA	-2.42	120.85	126.40
38	11	312	A86	C9-C10-C11	-2.42	119.48	126.61
32	A	408	LHG	C11-C10-C9	-2.42	102.13	114.42
30	A	406	SQD	C1-C2-C3	-2.42	104.95	110.00
38	32	314	A86	C23-C16-C22	-2.42	103.80	107.37
27	12	310	CLA	C2A-C1A-CHA	2.42	128.09	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	32	310	CLA	C2A-C1A-CHA	2.42	128.09	123.86
38	13	314	A86	C9-C10-C11	-2.42	119.49	126.61
38	14	314	A86	C9-C10-C11	-2.42	119.49	126.61
37	f	102	HEM	CAC-C3C-C4C	-2.42	119.05	124.90
33	d	408	LMG	C6-C5-C4	-2.42	107.34	113.00
38	34	315	A86	C9-C10-C11	-2.42	119.50	126.61
33	b	618	LMG	O3-C3-C2	-2.42	104.76	110.35
38	31	316	A86	C12-C11-C13	2.42	120.08	116.02
37	E	101	HEM	CAC-C3C-C4C	-2.42	119.06	124.90
27	14	308	CLA	C2A-C1A-CHA	2.42	128.08	123.86
29	Z	101	BCR	C7-C8-C9	-2.42	122.58	126.23
38	13	313	A86	C40-C32-C31	-2.42	108.31	110.47
27	13	309	CLA	CHA-C1A-NA	-2.42	120.87	126.40
27	33	303	CLA	CHC-C4B-NB	2.42	126.81	124.26
38	31	310	A86	C23-C16-C22	-2.41	103.81	107.37
27	34	306	CLA	C3B-C4B-NB	-2.41	108.28	110.52
27	D	401	CLA	CMB-C2B-C1B	-2.41	121.69	125.37
27	B	602	CLA	CHD-C1D-ND	-2.41	122.24	124.45
33	q	301	LMG	C38-C37-C36	-2.41	102.17	114.42
27	13	308	CLA	C2A-C1A-CHA	2.41	128.08	123.86
38	32	304	A86	C12-C11-C13	2.41	120.08	116.02
38	33	312	A86	C23-C16-C22	-2.41	103.81	107.37
33	C	519	LMG	C38-C37-C36	-2.41	102.18	114.42
38	14	312	A86	C23-C16-C22	-2.41	103.81	107.37
27	31	307	CLA	CHA-C1A-NA	-2.41	120.88	126.40
27	c	502	CLA	CMB-C2B-C3B	2.41	132.43	126.59
27	14	303	CLA	CHC-C4B-NB	2.41	126.81	124.26
27	B	615	CLA	CHA-C1A-NA	-2.41	120.88	126.40
27	B	612	CLA	CMD-C2D-C1D	-2.41	120.47	124.71
38	12	316	A86	C9-C10-C11	-2.41	119.53	126.61
32	a	408	LHG	C11-C10-C9	-2.41	102.21	114.42
33	d	408	LMG	O3-C3-C2	-2.41	104.78	110.35
35	c	518	DGD	O3E-C3E-C2E	-2.41	104.78	110.35
38	32	316	A86	C9-C10-C11	-2.41	119.53	126.61
27	b	605	CLA	C3B-C4B-NB	-2.41	108.28	110.52
27	d	406	CLA	CHC-C4B-NB	2.41	126.80	124.26
35	C	518	DGD	O3E-C3E-C2E	-2.41	104.79	110.35
33	D	408	LMG	C6-C5-C4	-2.41	107.37	113.00
32	L	101	LHG	O8-C23-C24	2.40	119.45	111.91
27	c	508	CLA	CHA-C1A-NA	-2.40	120.89	126.40
30	a	406	SQD	C1-C2-C3	-2.40	104.99	110.00
33	b	619	LMG	O1-C1-C2	-2.40	104.55	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	32	308	CLA	C2D-C1D-ND	-2.40	108.33	110.10
32	l	102	LHG	O8-C23-C24	2.40	119.44	111.91
38	33	313	A86	C40-C32-C31	-2.40	108.32	110.47
33	D	408	LMG	O3-C3-C2	-2.40	104.80	110.35
27	C	505	CLA	CHD-C1D-ND	-2.40	122.25	124.45
27	W	102	CLA	CHB-C1B-NB	2.40	126.80	124.26
27	C	502	CLA	CMB-C2B-C3B	2.40	132.40	126.59
29	B	623	BCR	C33-C5-C6	-2.40	121.83	124.53
27	31	306	CLA	C2A-C1A-CHA	2.40	128.05	123.86
27	b	604	CLA	O2A-CGA-O1A	-2.40	117.55	123.59
27	12	311	CLA	CHA-C1A-NA	-2.40	120.91	126.40
38	31	312	A86	C9-C10-C11	-2.40	119.56	126.61
33	32	301	LMG	C1-C2-C3	-2.39	105.01	110.00
38	33	314	A86	C9-C10-C11	-2.39	119.57	126.61
35	c	517	DGD	O6E-C5E-C6E	-2.39	100.49	106.44
27	14	309	CLA	CHA-C1A-NA	-2.39	120.92	126.40
27	11	307	CLA	CHA-C1A-NA	-2.39	120.92	126.40
38	31	311	A86	C40-C32-C31	-2.39	108.33	110.47
27	33	308	CLA	C2A-C1A-CHA	2.39	128.04	123.86
36	d	407	PL9	C36-C34-C33	-2.39	116.28	121.12
38	12	314	A86	C23-C16-C22	-2.39	103.85	107.37
29	h	101	BCR	C15-C14-C13	-2.39	123.90	127.31
35	C	517	DGD	CDB-CCB-CBB	-2.39	102.31	114.42
27	32	311	CLA	CHA-C1A-NA	-2.39	120.93	126.40
35	c	517	DGD	CDB-CCB-CBB	-2.39	102.31	114.42
33	D	408	LMG	C40-C39-C38	-2.38	102.32	114.42
36	D	407	PL9	C36-C34-C33	-2.38	116.29	121.12
38	13	312	A86	C23-C16-C22	-2.38	103.86	107.37
27	14	306	CLA	C2D-C1D-ND	-2.38	108.35	110.10
27	31	304	CLA	C2D-C1D-ND	-2.38	108.35	110.10
27	34	307	CLA	C2D-C1D-ND	-2.38	108.35	110.10
35	c	518	DGD	C3D-C4D-C5D	-2.38	105.99	110.24
27	b	615	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
27	b	612	CLA	CMD-C2D-C3D	2.38	133.09	127.61
27	C	506	CLA	CMC-C2C-C1C	-2.38	121.42	125.04
38	11	310	A86	C23-C16-C22	-2.38	103.86	107.37
27	b	622	CLA	CHB-C1B-NB	2.38	126.77	124.26
33	d	408	LMG	C40-C39-C38	-2.38	102.36	114.42
27	C	510	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
27	34	304	CLA	CHC-C4B-NB	2.37	126.77	124.26
27	B	605	CLA	C3B-C4B-NB	-2.37	108.31	110.52
29	z	101	BCR	C7-C8-C9	-2.37	122.65	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	14	313	A86	C40-C32-C31	-2.37	108.35	110.47
30	B	620	SQD	C4-C3-C2	2.37	114.97	110.82
27	13	306	CLA	C2D-C1D-ND	-2.37	108.36	110.10
33	W	101	LMG	O2-C2-C1	-2.37	104.28	110.05
35	C	517	DGD	O6E-C5E-C6E	-2.37	100.53	106.44
32	a	408	LHG	C18-C17-C16	-2.37	102.39	114.42
27	c	506	CLA	CMC-C2C-C1C	-2.37	121.43	125.04
32	A	408	LHG	C18-C17-C16	-2.37	102.39	114.42
30	b	620	SQD	C1-O5-C5	2.37	118.34	113.69
27	b	602	CLA	CHD-C1D-ND	-2.37	122.28	124.45
27	c	509	CLA	CMB-C2B-C3B	2.37	132.33	126.59
29	c	516	BCR	C7-C8-C9	-2.37	122.66	126.23
27	D	401	CLA	CHC-C4B-NB	2.37	126.77	124.26
29	H	101	BCR	C15-C14-C13	-2.37	123.93	127.31
38	14	313	A86	C10-C9-C8	-2.37	115.83	123.22
35	C	518	DGD	C3D-C4D-C5D	-2.37	106.02	110.24
27	B	615	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
27	c	510	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
38	34	314	A86	C40-C32-C31	-2.37	108.35	110.47
27	d	401	CLA	CHC-C4B-NB	2.37	126.76	124.26
27	B	613	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
27	C	509	CLA	CMB-C2B-C3B	2.37	132.32	126.59
30	b	620	SQD	C4-C3-C2	2.37	114.95	110.82
29	C	516	BCR	C7-C8-C9	-2.37	122.66	126.23
33	W	101	LMG	C40-C39-C38	-2.37	102.41	114.42
27	w	102	CLA	CHB-C1B-NB	2.37	126.76	124.26
29	b	616	BCR	C24-C23-C22	-2.37	122.66	126.23
27	C	503	CLA	C1D-ND-C4D	2.36	108.02	106.33
38	33	313	A86	C10-C9-C8	-2.36	115.84	123.22
33	w	101	LMG	C40-C39-C38	-2.36	102.42	114.42
38	13	313	A86	C10-C9-C8	-2.36	115.84	123.22
27	B	604	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
27	33	309	CLA	CHA-C1A-NA	-2.36	120.99	126.40
27	d	401	CLA	CMB-C2B-C1B	-2.36	121.77	125.37
27	33	306	CLA	C2D-C1D-ND	-2.36	108.36	110.10
38	34	314	A86	C10-C9-C8	-2.36	115.85	123.22
33	w	101	LMG	O2-C2-C1	-2.36	104.32	110.05
38	32	315	A86	C10-C9-C8	-2.36	115.86	123.22
33	b	619	LMG	O2-C2-C1	-2.36	104.32	110.05
27	32	312	CLA	CHA-C1A-NA	-2.36	121.00	126.40
27	32	305	CLA	CHC-C4B-NB	2.36	126.75	124.26
27	A	402	CLA	CHB-C4A-NA	2.36	127.77	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	11	311	A86	C10-C9-C8	-2.36	115.86	123.22
30	B	620	SQD	C1-O5-C5	2.36	118.31	113.69
27	C	508	CLA	CHA-C1A-NA	-2.36	121.00	126.40
38	31	311	A86	C10-C9-C8	-2.36	115.87	123.22
27	b	611	CLA	CHB-C4A-NA	2.35	127.77	124.51
38	11	311	A86	C40-C32-C31	-2.35	108.36	110.47
33	B	619	LMG	O2-C2-C1	-2.35	104.33	110.05
27	b	613	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
33	w	101	LMG	C6-C5-C4	-2.35	107.49	113.00
38	12	315	A86	C40-C32-C31	-2.35	108.37	110.47
27	B	612	CLA	CMD-C2D-C3D	2.35	133.03	127.61
33	b	619	LMG	O7-C10-O9	-2.35	118.02	123.70
27	33	310	CLA	CHA-C1A-NA	-2.35	121.01	126.40
33	m	102	LMG	O6-C1-O1	-2.35	104.41	109.97
29	B	617	BCR	C15-C16-C17	-2.35	118.66	123.47
38	12	315	A86	C10-C9-C8	-2.35	115.88	123.22
35	c	517	DGD	O5E-C6E-C5E	-2.35	103.23	111.29
27	b	605	CLA	C3C-C4C-NC	-2.35	107.94	110.57
33	W	101	LMG	C6-C5-C4	-2.35	107.50	113.00
27	13	303	CLA	CHC-C4B-NB	2.35	126.74	124.26
37	V	201	HEM	CAD-CBD-CGD	-2.35	108.55	113.60
33	M	103	LMG	O6-C1-O1	-2.35	104.42	109.97
29	F	101	BCR	C16-C15-C14	-2.35	118.67	123.47
29	f	101	BCR	C16-C15-C14	-2.35	118.67	123.47
29	B	616	BCR	C24-C23-C22	-2.35	122.69	126.23
33	B	618	LMG	O1-C7-C8	-2.35	105.24	110.90
33	12	301	LMG	C1-C2-C3	-2.35	105.11	110.00
36	d	407	PL9	C42-C43-C44	-2.34	122.02	127.66
27	12	305	CLA	CHC-C4B-NB	2.34	126.74	124.26
27	31	308	CLA	CHA-C1A-NA	-2.34	121.03	126.40
27	12	308	CLA	CHB-C1B-C2B	-2.34	120.62	127.24
27	B	622	CLA	CHB-C1B-NB	2.34	126.74	124.26
27	31	301	CLA	CHC-C4B-NB	2.34	126.74	124.26
27	c	503	CLA	C2D-C1D-ND	-2.34	108.38	110.10
38	11	316	A86	C9-C10-C11	-2.34	119.72	126.61
27	b	614	CLA	C2A-C1A-CHA	2.34	127.95	123.86
27	11	304	CLA	C2D-C1D-ND	-2.34	108.38	110.10
33	b	618	LMG	O1-C7-C8	-2.34	105.25	110.90
38	31	316	A86	C9-C10-C11	-2.34	119.73	126.61
37	V	201	HEM	CHD-C4C-C3C	2.34	129.26	125.26
27	11	304	CLA	CHB-C1B-C2B	-2.34	120.63	127.24
35	j	101	DGD	CAB-C9B-C8B	-2.34	102.56	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	13	303	CLA	CHB-C1B-NB	2.34	126.73	124.26
27	31	304	CLA	CHB-C1B-C2B	-2.34	120.64	127.24
33	B	619	LMG	O7-C10-O9	-2.34	118.06	123.70
29	b	616	BCR	C30-C25-C26	-2.34	119.32	122.61
27	Z	102	CLA	CHB-C1B-NB	2.34	126.73	124.26
29	c	515	BCR	C33-C5-C6	-2.34	121.91	124.53
27	13	310	CLA	CHA-C1A-NA	-2.34	121.05	126.40
38	12	304	A86	C9-C10-C11	-2.33	119.74	126.61
27	m	101	CLA	CMB-C2B-C1B	-2.33	121.81	125.37
27	11	301	CLA	CHC-C4B-NB	2.33	126.73	124.26
38	13	302	A86	C9-C10-C11	-2.33	119.75	126.61
33	b	618	LMG	C40-C39-C38	-2.33	102.58	114.42
36	D	407	PL9	O1-C4-C3	-2.33	118.15	120.72
37	v	201	HEM	CHD-C4C-C3C	2.33	129.25	125.26
33	B	618	LMG	C40-C39-C38	-2.33	102.59	114.42
27	c	505	CLA	CHD-C1D-ND	-2.33	122.31	124.45
35	J	101	DGD	CAB-C9B-C8B	-2.33	102.59	114.42
27	B	614	CLA	C2A-C1A-CHA	2.33	127.94	123.86
27	c	511	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
27	c	507	CLA	O1D-CGD-CBD	2.33	129.25	124.48
27	B	611	CLA	CHB-C4A-NA	2.33	127.73	124.51
37	v	201	HEM	CAD-CBD-CGD	-2.33	108.59	113.60
38	34	303	A86	C9-C10-C11	-2.33	119.76	126.61
38	33	302	A86	C9-C10-C11	-2.33	119.76	126.61
27	11	301	CLA	CHB-C1B-NB	2.33	126.72	124.26
27	z	102	CLA	CHB-C1B-NB	2.33	126.72	124.26
35	C	517	DGD	O5E-C6E-C5E	-2.33	103.31	111.29
27	13	306	CLA	CHB-C1B-C2B	-2.33	120.66	127.24
36	d	407	PL9	C11-C9-C8	-2.33	116.41	121.12
29	b	617	BCR	C15-C16-C17	-2.33	118.71	123.47
27	12	312	CLA	CHA-C1A-NA	-2.33	121.07	126.40
27	C	503	CLA	C2D-C1D-ND	-2.33	108.39	110.10
27	34	307	CLA	CHB-C1B-C2B	-2.33	120.67	127.24
27	c	511	CLA	CAA-C2A-C3A	-2.33	106.41	112.78
27	a	402	CLA	CHB-C4A-NA	2.32	127.73	124.51
38	32	304	A86	C9-C10-C11	-2.32	119.77	126.61
27	W	103	CLA	CMB-C2B-C1B	-2.32	121.83	125.37
29	C	515	BCR	C33-C5-C6	-2.32	121.92	124.53
38	13	317	A86	C9-C10-C11	-2.32	119.78	126.61
33	b	618	LMG	O1-C1-C2	-2.32	104.68	108.30
27	14	303	CLA	CHB-C1B-NB	2.32	126.72	124.26
33	q	301	LMG	O3-C3-C2	-2.32	104.98	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	14	310	CLA	CHA-C1A-NA	-2.32	121.08	126.40
27	34	311	CLA	CHA-C1A-NA	-2.32	121.08	126.40
36	d	407	PL9	O1-C4-C3	-2.32	118.16	120.72
27	b	613	CLA	C4-C3-C5	2.32	119.17	115.27
27	33	306	CLA	CHB-C1B-C2B	-2.32	120.68	127.24
27	34	304	CLA	CHB-C1B-NB	2.32	126.71	124.26
27	11	308	CLA	CHA-C1A-NA	-2.32	121.09	126.40
27	c	505	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
33	B	618	LMG	O1-C1-C2	-2.32	104.68	108.30
27	b	611	CLA	C3C-C4C-NC	-2.32	107.97	110.57
27	c	504	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
27	32	308	CLA	CHB-C1B-C2B	-2.32	120.69	127.24
27	B	603	CLA	CMB-C2B-C1B	-2.32	121.84	125.37
27	c	509	CLA	CGD-CBD-CAD	-2.32	103.23	110.73
27	C	512	CLA	CHB-C1B-NB	2.32	126.71	124.26
27	c	507	CLA	CHC-C4B-NB	2.32	126.71	124.26
29	C	515	BCR	C27-C26-C25	2.31	126.09	122.73
27	C	511	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
27	M	102	CLA	CHB-C1B-NB	2.31	126.71	124.26
36	D	407	PL9	C42-C43-C44	-2.31	122.09	127.66
27	C	507	CLA	O1D-CGD-CBD	2.31	129.22	124.48
27	B	611	CLA	C7-C6-C5	-2.31	107.08	113.36
27	12	308	CLA	C2D-C1D-ND	-2.31	108.40	110.10
27	b	611	CLA	C1-C2-C3	-2.31	122.04	126.04
27	B	611	CLA	C1-C2-C3	-2.31	122.05	126.04
27	14	306	CLA	CHB-C1B-C2B	-2.31	120.71	127.24
27	33	303	CLA	CHB-C1B-NB	2.31	126.70	124.26
27	C	511	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
36	D	407	PL9	C11-C9-C8	-2.31	116.44	121.12
27	32	305	CLA	CHB-C1B-NB	2.31	126.70	124.26
27	B	613	CLA	C4-C3-C5	2.31	119.15	115.27
29	c	515	BCR	C27-C26-C25	2.31	126.08	122.73
27	12	305	CLA	CHB-C1B-NB	2.31	126.70	124.26
35	C	517	DGD	O2D-C2D-C1D	-2.31	104.44	110.05
27	C	509	CLA	CGD-CBD-CAD	-2.31	103.26	110.73
29	B	616	BCR	C30-C25-C26	-2.31	119.37	122.61
29	F	101	BCR	C15-C16-C17	-2.31	118.75	123.47
33	C	519	LMG	O3-C3-C2	-2.31	105.02	110.35
27	b	607	CLA	CAA-C2A-C3A	-2.31	106.47	112.78
27	C	505	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
27	B	606	CLA	CHB-C1B-NB	2.30	126.70	124.26
27	M	102	CLA	CMB-C2B-C1B	-2.30	121.86	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	f	101	BCR	C15-C16-C17	-2.30	118.76	123.47
32	L	101	LHG	C18-C17-C16	-2.30	102.74	114.42
27	b	611	CLA	C7-C6-C5	-2.30	107.11	113.36
35	c	517	DGD	O2D-C2D-C1D	-2.30	104.45	110.05
33	d	408	LMG	C38-C37-C36	-2.30	102.74	114.42
33	D	408	LMG	C38-C37-C36	-2.30	102.75	114.42
27	B	606	CLA	C3C-C4C-NC	-2.30	107.99	110.57
27	B	611	CLA	C3C-C4C-NC	-2.30	107.99	110.57
32	l	102	LHG	C18-C17-C16	-2.30	102.76	114.42
27	w	103	CLA	CMB-C2B-C1B	-2.30	121.87	125.37
27	B	613	CLA	C2A-C1A-CHA	2.30	127.88	123.86
30	L	103	SQD	O8-S-C6	2.30	109.40	105.74
29	h	101	BCR	C27-C26-C25	2.30	126.06	122.73
27	b	606	CLA	CHB-C1B-NB	2.30	126.69	124.26
27	C	510	CLA	CMB-C2B-C3B	2.30	132.15	126.59
27	m	101	CLA	CHB-C1B-NB	2.30	126.69	124.26
27	b	601	CLA	CHB-C1B-NB	2.29	126.68	124.26
27	Z	102	CLA	C2A-C1A-CHA	2.29	127.87	123.86
35	H	102	DGD	CBB-CAB-C9B	-2.29	102.80	114.42
27	13	305	CLA	CHC-C4B-NB	2.29	126.68	124.26
33	b	619	LMG	C6-C5-C4	-2.29	107.64	113.00
27	C	504	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
27	B	607	CLA	CAA-C2A-C3A	-2.29	106.51	112.78
27	b	603	CLA	CMB-C2B-C1B	-2.29	121.88	125.37
35	h	102	DGD	CBB-CAB-C9B	-2.29	102.80	114.42
27	B	601	CLA	CHB-C1B-NB	2.29	126.68	124.26
29	b	623	BCR	C33-C5-C6	-2.29	121.96	124.53
28	d	403	PHO	C1C-C2C-C3C	-2.29	106.71	108.61
27	c	510	CLA	CMB-C2B-C3B	2.28	132.12	126.59
27	c	507	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
29	h	101	BCR	C24-C23-C22	-2.28	122.78	126.23
27	c	512	CLA	CHB-C1B-NB	2.28	126.67	124.26
27	b	622	CLA	C1-C2-C3	-2.28	122.10	126.04
27	B	603	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
38	12	304	A86	C35-C34-C33	2.28	113.85	109.88
32	l	103	LHG	C18-C17-C16	-2.28	102.85	114.42
27	C	504	CLA	CAA-C2A-C3A	-2.28	106.54	112.78
27	b	601	CLA	C2A-C1A-CHA	2.28	127.84	123.86
27	C	513	CLA	CHB-C1B-NB	2.28	126.67	124.26
38	33	316	A86	C-C1-C24	2.28	121.67	118.08
38	11	314	A86	C-C1-C24	2.28	121.66	118.08
28	A	403	PHO	CBA-CAA-C2A	-2.28	107.16	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	601	CLA	C2A-C1A-CHA	2.28	127.84	123.86
27	z	102	CLA	C2A-C1A-CHA	2.27	127.84	123.86
27	c	504	CLA	CAA-C2A-C3A	-2.27	106.55	112.78
27	A	404	CLA	CHC-C4B-NB	2.27	126.66	124.26
27	c	503	CLA	CHA-C1A-NA	-2.27	121.19	126.40
27	b	613	CLA	C2A-C1A-CHA	2.27	127.83	123.86
38	31	314	A86	C-C1-C24	2.27	121.66	118.08
27	C	510	CLA	CHB-C1B-NB	2.27	126.66	124.26
32	L	102	LHG	C18-C17-C16	-2.27	102.90	114.42
27	b	603	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
28	a	403	PHO	CBA-CAA-C2A	-2.27	107.18	113.81
27	31	301	CLA	CHB-C1B-NB	2.27	126.66	124.26
33	B	619	LMG	C6-C5-C4	-2.27	107.69	113.00
36	d	404	PL9	C36-C34-C33	-2.27	116.53	121.12
38	12	316	A86	C7-C6-C8	2.27	121.65	118.08
27	14	307	CLA	CMB-C2B-C1B	-2.27	121.92	125.37
27	c	508	CLA	C2D-C1D-ND	-2.26	108.44	110.10
36	D	404	PL9	C36-C34-C33	-2.26	116.53	121.12
29	a	405	BCR	C35-C13-C14	-2.26	119.75	122.92
27	C	510	CLA	C16-C15-C13	-2.26	108.61	115.92
27	C	507	CLA	CHC-C4B-NB	2.26	126.65	124.26
28	D	403	PHO	C1C-C2C-C3C	-2.26	106.73	108.61
27	14	305	CLA	CHC-C4B-NB	2.26	126.65	124.26
38	13	314	A86	C7-C6-C8	2.26	121.64	118.08
27	31	305	CLA	CMB-C2B-C1B	-2.26	121.93	125.37
27	33	307	CLA	CMB-C2B-C1B	-2.26	121.93	125.37
27	B	622	CLA	CMD-C2D-C1D	-2.26	120.73	124.71
27	C	503	CLA	CHA-C1A-NA	-2.26	121.23	126.40
27	b	607	CLA	C3B-C4B-NB	-2.26	108.42	110.52
27	B	602	CLA	C3C-C4C-NC	-2.26	108.04	110.57
27	c	510	CLA	CHB-C1B-NB	2.26	126.65	124.26
38	14	301	A86	C-C1-C24	2.25	121.63	118.08
27	11	306	CLA	C3B-C4B-NB	-2.25	108.42	110.52
27	13	308	CLA	C3B-C4B-NB	-2.25	108.42	110.52
27	32	310	CLA	C3B-C4B-NB	-2.25	108.42	110.52
27	B	605	CLA	C2D-C1D-ND	-2.25	108.44	110.10
38	13	302	A86	C35-C34-C33	2.25	113.81	109.88
38	13	316	A86	C-C1-C24	2.25	121.63	118.08
29	H	101	BCR	C24-C23-C22	-2.25	122.83	126.23
33	12	301	LMG	O2-C2-C3	-2.25	105.14	110.35
33	b	618	LMG	C38-C37-C36	-2.25	103.00	114.42
27	C	507	CLA	O2A-CGA-O1A	-2.25	117.91	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	606	CLA	C3C-C4C-NC	-2.25	108.05	110.57
38	32	318	A86	C-C1-C24	2.25	121.62	118.08
38	31	316	A86	C35-C34-C33	2.25	113.80	109.88
29	A	405	BCR	C35-C13-C14	-2.25	119.77	122.92
38	32	304	A86	C35-C34-C33	2.25	113.80	109.88
38	14	316	A86	C-C1-C24	2.25	121.62	118.08
27	c	510	CLA	C16-C15-C13	-2.25	108.65	115.92
27	B	603	CLA	CHC-C4B-NB	2.25	126.64	124.26
27	34	311	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
38	34	301	A86	C-C1-C24	2.25	121.62	118.08
38	33	302	A86	C35-C34-C33	2.25	113.80	109.88
32	b	621	LHG	C18-C17-C16	-2.25	103.02	114.42
30	l	101	SQD	O8-S-C6	2.25	109.32	105.74
29	H	101	BCR	C27-C26-C25	2.24	125.99	122.73
32	B	621	LHG	C18-C17-C16	-2.24	103.04	114.42
39	32	302	LMU	C1B-O5B-C5B	2.24	118.09	113.69
27	W	102	CLA	CAA-CBA-CGA	-2.24	106.70	113.25
29	b	623	BCR	C27-C26-C25	2.24	125.99	122.73
33	B	618	LMG	C38-C37-C36	-2.24	103.05	114.42
27	13	307	CLA	CMB-C2B-C1B	-2.24	121.96	125.37
38	11	316	A86	C35-C34-C33	2.24	113.79	109.88
27	32	307	CLA	CHC-C4B-NB	2.24	126.63	124.26
27	b	615	CLA	C2A-C1A-CHA	2.24	127.77	123.86
27	b	602	CLA	C3C-C4C-NC	-2.24	108.06	110.57
38	32	316	A86	C7-C6-C8	2.24	121.60	118.08
27	C	508	CLA	CHB-C1B-NB	2.24	126.62	124.26
27	B	602	CLA	O2D-CGD-CBD	2.24	115.24	111.27
27	11	303	CLA	CHC-C4B-NB	2.23	126.62	124.26
27	31	307	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
27	B	607	CLA	C3B-C4B-NB	-2.23	108.44	110.52
27	34	308	CLA	CMB-C2B-C1B	-2.23	121.97	125.37
27	34	306	CLA	CHC-C4B-NB	2.23	126.62	124.26
27	B	615	CLA	C2A-C1A-CHA	2.23	127.76	123.86
38	13	317	A86	C35-C34-C33	2.23	113.77	109.88
36	D	404	PL9	C37-C38-C39	-2.23	122.29	127.66
27	14	309	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
27	w	102	CLA	CAA-CBA-CGA	-2.23	106.73	113.25
27	11	307	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
35	c	518	DGD	O6E-C1E-O5D	-2.23	104.69	109.97
38	34	303	A86	C35-C34-C33	2.23	113.77	109.88
27	b	602	CLA	C3B-C4B-NB	-2.23	108.45	110.52
27	a	404	CLA	CHC-C4B-NB	2.23	126.62	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	609	CLA	O1D-CGD-CBD	2.23	129.04	124.48
38	33	314	A86	C7-C6-C8	2.23	121.59	118.08
27	a	402	CLA	CMB-C2B-C3B	2.23	131.98	126.59
27	C	508	CLA	C2D-C1D-ND	-2.23	108.46	110.10
27	c	513	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
27	13	309	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
27	31	303	CLA	CHC-C4B-NB	2.22	126.61	124.26
38	14	314	A86	C7-C6-C8	2.22	121.58	118.08
38	31	312	A86	C7-C6-C8	2.22	121.58	118.08
27	c	505	CLA	CHC-C1C-NC	2.22	127.57	124.20
38	34	315	A86	C7-C6-C8	2.22	121.58	118.08
27	b	602	CLA	O2D-CGD-CBD	2.22	115.21	111.27
27	11	305	CLA	CMB-C2B-C1B	-2.22	121.99	125.37
28	D	403	PHO	C1-C2-C3	-2.22	122.20	126.04
29	z	101	BCR	C29-C30-C25	2.22	113.90	110.48
35	C	518	DGD	O6E-C1E-O5D	-2.22	104.72	109.97
27	b	604	CLA	CHA-C1A-NA	-2.22	121.32	126.40
27	12	312	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
27	33	304	CLA	CHA-C1A-NA	-2.22	121.32	126.40
27	C	505	CLA	CHC-C1C-NC	2.22	127.57	124.20
27	B	622	CLA	CMD-C2D-C3D	2.22	132.72	127.61
27	32	309	CLA	CMB-C2B-C1B	-2.22	121.99	125.37
27	c	505	CLA	C3B-C4B-NB	-2.22	108.46	110.52
29	B	617	BCR	C11-C10-C9	-2.22	124.15	127.31
27	31	308	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
28	d	403	PHO	C1-C2-C3	-2.22	122.21	126.04
27	A	402	CLA	CMB-C2B-C3B	2.22	131.95	126.59
38	11	312	A86	C7-C6-C8	2.22	121.57	118.08
35	C	518	DGD	CAB-C9B-C8B	-2.21	103.19	114.42
27	b	603	CLA	CHC-C4B-NB	2.21	126.60	124.26
27	14	304	CLA	CHA-C1A-NA	-2.21	121.33	126.40
29	b	617	BCR	C11-C10-C9	-2.21	124.15	127.31
33	B	619	LMG	C38-C37-C36	-2.21	103.20	114.42
37	E	101	HEM	C1C-CHC-C4B	-2.21	121.29	126.06
27	12	306	CLA	CHA-C1A-NA	-2.21	121.33	126.40
27	31	302	CLA	CHA-C1A-NA	-2.21	121.33	126.40
27	33	309	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
35	C	518	DGD	O5D-C6D-C5D	-2.21	104.96	109.05
27	13	310	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
27	33	308	CLA	C3B-C4B-NB	-2.21	108.47	110.52
27	12	309	CLA	CMB-C2B-C1B	-2.21	122.00	125.37
36	d	404	PL9	C37-C38-C39	-2.21	122.34	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	609	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
27	C	513	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
27	11	308	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
33	b	619	LMG	C38-C37-C36	-2.21	103.21	114.42
27	b	608	CLA	O2D-CGD-CBD	2.21	115.19	111.27
30	L	103	SQD	C44-O6-C1	2.21	118.05	113.74
35	J	101	DGD	C3D-C4D-C5D	-2.21	106.30	110.24
27	b	622	CLA	CHA-C1A-NA	-2.21	121.34	126.40
27	B	609	CLA	O1D-CGD-CBD	2.21	129.00	124.48
27	32	312	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
35	C	518	DGD	C3G-C2G-C1G	-2.21	106.57	111.79
27	31	306	CLA	C3B-C4B-NB	-2.21	108.47	110.52
27	B	608	CLA	O2D-CGD-CBD	2.21	115.19	111.27
27	B	604	CLA	CHA-C1A-NA	-2.21	121.34	126.40
27	34	310	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
27	14	308	CLA	C3B-C4B-NB	-2.21	108.47	110.52
27	33	305	CLA	CHC-C4B-NB	2.21	126.59	124.26
27	b	609	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
37	f	102	HEM	C1C-CHC-C4B	-2.20	121.30	126.06
27	32	311	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
27	B	606	CLA	CMB-C2B-C1B	-2.20	122.01	125.37
27	b	606	CLA	CMB-C2B-C1B	-2.20	122.01	125.37
27	33	310	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
27	D	405	CLA	C3B-C4B-NB	-2.20	108.47	110.52
27	C	505	CLA	C3B-C4B-NB	-2.20	108.47	110.52
27	c	506	CLA	C3B-C4B-NB	-2.20	108.47	110.52
35	c	518	DGD	O5D-C6D-C5D	-2.20	104.97	109.05
35	j	101	DGD	C3D-C4D-C5D	-2.20	106.31	110.24
37	v	201	HEM	CHC-C1C-NC	2.20	126.82	124.44
27	d	405	CLA	C3B-C4B-NB	-2.20	108.47	110.52
27	34	309	CLA	C3B-C4B-NB	-2.20	108.47	110.52
27	12	307	CLA	CHC-C4B-NB	2.20	126.59	124.26
30	a	406	SQD	O48-C23-O10	-2.20	118.04	123.59
39	12	302	LMU	C1B-O5B-C5B	2.20	118.00	113.69
27	c	502	CLA	C7-C6-C5	-2.20	107.39	113.36
29	B	623	BCR	C27-C26-C25	2.20	125.92	122.73
35	c	518	DGD	CAB-C9B-C8B	-2.20	103.27	114.42
27	d	405	CLA	CAC-C3C-C4C	2.20	127.66	124.81
27	W	102	CLA	CAA-C2A-C3A	-2.20	106.76	112.78
27	34	305	CLA	CHA-C1A-NA	-2.20	121.37	126.40
29	c	515	BCR	C15-C14-C13	-2.20	124.17	127.31
27	11	302	CLA	CHA-C1A-NA	-2.20	121.37	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	w	102	CLA	CAA-C2A-C3A	-2.20	106.77	112.78
35	j	101	DGD	CBB-CAB-C9B	-2.20	103.28	114.42
27	b	605	CLA	C2D-C1D-ND	-2.20	108.49	110.10
29	B	617	BCR	C16-C15-C14	-2.20	118.98	123.47
27	B	602	CLA	C3B-C4B-NB	-2.19	108.48	110.52
36	d	407	PL9	C36-C37-C38	-2.19	104.67	111.88
27	12	311	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
30	A	406	SQD	O48-C23-O10	-2.19	118.06	123.59
29	m	103	BCR	C33-C5-C6	-2.19	122.07	124.53
29	f	101	BCR	C27-C26-C25	2.19	125.91	122.73
36	D	407	PL9	C50-C49-C48	-2.19	116.31	122.65
27	12	310	CLA	C3B-C4B-NB	-2.19	108.48	110.52
29	B	617	BCR	C15-C14-C13	-2.19	124.18	127.31
27	B	611	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
27	C	502	CLA	C7-C6-C5	-2.19	107.41	113.36
27	d	401	CLA	O2D-CGD-CBD	2.19	115.16	111.27
35	c	518	DGD	C3G-C2G-C1G	-2.19	106.61	111.79
27	B	609	CLA	C3B-C4B-NB	-2.19	108.48	110.52
27	13	304	CLA	CHA-C1A-NA	-2.19	121.39	126.40
27	32	306	CLA	CHA-C1A-NA	-2.19	121.39	126.40
27	C	503	CLA	CHC-C1C-NC	2.19	127.52	124.20
29	F	101	BCR	C27-C26-C25	2.19	125.91	122.73
27	14	310	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
38	12	304	A86	C28-C27-C26	-2.19	119.86	122.92
27	c	508	CLA	CHB-C1B-NB	2.19	126.57	124.26
33	C	519	LMG	C3-C4-C5	-2.19	106.34	110.24
29	h	101	BCR	C40-C30-C25	2.19	113.84	110.30
27	c	513	CLA	CHB-C1B-NB	2.18	126.57	124.26
27	34	309	CLA	CHB-C1B-NB	2.18	126.57	124.26
35	J	101	DGD	CBB-CAB-C9B	-2.18	103.34	114.42
33	q	301	LMG	C3-C4-C5	-2.18	106.34	110.24
27	31	305	CLA	CHB-C1B-NB	2.18	126.57	124.26
29	M	101	BCR	C33-C5-C6	-2.18	122.08	124.53
36	D	407	PL9	C36-C37-C38	-2.18	104.71	111.88
29	Z	101	BCR	C29-C30-C25	2.18	113.84	110.48
27	D	405	CLA	CAC-C3C-C4C	2.18	127.64	124.81
27	C	506	CLA	C3B-C4B-NB	-2.18	108.49	110.52
29	b	617	BCR	C15-C14-C13	-2.18	124.20	127.31
27	c	508	CLA	CAA-C2A-C3A	-2.18	106.82	112.78
32	b	621	LHG	C20-C19-C18	-2.18	103.38	114.42
33	b	619	LMG	C40-C39-C38	-2.18	103.38	114.42
30	l	101	SQD	C44-O6-C1	2.17	117.99	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	c	514	CLA	C2A-C1A-CHA	2.17	127.66	123.86
27	B	606	CLA	C6-C7-C8	-2.17	108.89	115.92
27	B	622	CLA	C1-C2-C3	-2.17	122.29	126.04
38	33	315	A86	C-C1-C24	2.17	121.50	118.08
27	C	508	CLA	CAA-C2A-C3A	-2.17	106.83	112.78
27	32	310	CLA	CHB-C1B-NB	2.17	126.56	124.26
32	B	621	LHG	C20-C19-C18	-2.17	103.41	114.42
36	d	404	PL9	O2-C1-C6	2.17	124.35	120.59
29	b	623	BCR	C38-C26-C27	-2.17	109.45	113.62
36	d	407	PL9	C50-C49-C48	-2.17	116.38	122.65
29	b	617	BCR	C16-C15-C14	-2.17	119.03	123.47
30	b	620	SQD	O48-C23-C24	2.17	118.71	111.91
27	b	611	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
27	13	304	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
29	b	617	BCR	C27-C26-C25	2.17	125.88	122.73
27	C	512	CLA	CHA-C4D-ND	2.17	137.03	132.50
27	C	505	CLA	CHB-C1B-NB	2.17	126.55	124.26
37	V	201	HEM	CHC-C1C-NC	2.17	126.78	124.44
29	B	623	BCR	C38-C26-C27	-2.17	109.45	113.62
27	b	606	CLA	C6-C7-C8	-2.17	108.92	115.92
32	a	408	LHG	C5-O7-C7	-2.17	112.46	117.79
27	d	401	CLA	CAA-C2A-C3A	-2.17	106.85	112.78
29	C	515	BCR	C15-C14-C13	-2.17	124.22	127.31
27	c	512	CLA	CHA-C4D-ND	2.17	137.03	132.50
33	m	102	LMG	C1-C2-C3	-2.17	105.49	110.00
27	D	401	CLA	CAA-C2A-C3A	-2.16	106.85	112.78
27	11	302	CLA	CAA-C2A-C3A	-2.16	106.85	112.78
27	14	304	CLA	CAA-C2A-C3A	-2.16	106.85	112.78
27	b	609	CLA	C3B-C4B-NB	-2.16	108.51	110.52
27	33	304	CLA	CAA-C2A-C3A	-2.16	106.85	112.78
35	H	102	DGD	C5B-C4B-C3B	-2.16	103.44	114.42
33	M	103	LMG	C1-C2-C3	-2.16	105.49	110.00
27	a	402	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
33	B	619	LMG	C40-C39-C38	-2.16	103.44	114.42
35	c	518	DGD	O5E-C6E-C5E	-2.16	103.87	111.29
30	B	620	SQD	O48-C23-C24	2.16	118.69	111.91
29	f	101	BCR	C24-C23-C22	-2.16	122.97	126.23
35	h	102	DGD	C5B-C4B-C3B	-2.16	103.45	114.42
38	32	304	A86	C28-C27-C26	-2.16	119.89	122.92
29	H	101	BCR	C40-C30-C25	2.16	113.81	110.30
27	32	306	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
27	12	306	CLA	CAA-C2A-C3A	-2.16	106.86	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	519	BCR	C20-C21-C22	-2.16	124.23	127.31
27	w	102	CLA	C2D-C1D-ND	-2.16	108.51	110.10
27	34	305	CLA	CAA-C2A-C3A	-2.16	106.87	112.78
27	C	503	CLA	CHC-C4B-NB	2.16	126.54	124.26
27	31	302	CLA	CAA-C2A-C3A	-2.16	106.87	112.78
27	D	401	CLA	O2D-CGD-CBD	2.16	115.10	111.27
33	M	103	LMG	C9-C8-C7	-2.16	106.69	111.79
27	B	622	CLA	CHA-C1A-NA	-2.16	121.46	126.40
27	c	503	CLA	CHC-C4B-NB	2.16	126.54	124.26
27	13	307	CLA	CHB-C1B-NB	2.16	126.54	124.26
27	c	512	CLA	CHA-C1A-NA	-2.16	121.46	126.40
32	A	408	LHG	C5-O7-C7	-2.16	112.48	117.79
38	31	316	A86	C28-C27-C26	-2.16	119.90	122.92
27	C	514	CLA	C2A-C1A-CHA	2.15	127.63	123.86
27	13	308	CLA	CHB-C1B-NB	2.15	126.54	124.26
38	11	316	A86	C28-C27-C26	-2.15	119.91	122.92
38	32	316	A86	C-C1-C24	2.15	121.47	118.08
35	C	518	DGD	O5E-C6E-C5E	-2.15	103.91	111.29
38	14	315	A86	C-C1-C24	2.15	121.47	118.08
27	b	613	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
27	c	503	CLA	CHC-C1C-NC	2.15	127.47	124.20
27	b	603	CLA	O1D-CGD-CBD	2.15	128.88	124.48
27	14	307	CLA	CHB-C1B-NB	2.15	126.53	124.26
33	q	301	LMG	C1-C2-C3	-2.15	105.52	110.00
38	32	317	A86	C-C1-C24	2.15	121.46	118.08
29	B	617	BCR	C27-C26-C25	2.15	125.85	122.73
27	b	607	CLA	CHC-C4B-NB	2.15	126.53	124.26
27	31	306	CLA	CHB-C1B-NB	2.15	126.53	124.26
29	C	515	BCR	C16-C15-C14	-2.15	119.07	123.47
33	m	102	LMG	O1-C7-C8	-2.15	105.72	110.90
27	14	308	CLA	CHB-C1B-NB	2.15	126.53	124.26
38	13	302	A86	C28-C27-C26	-2.15	119.92	122.92
38	12	317	A86	C-C1-C24	2.15	121.46	118.08
27	B	613	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
27	c	505	CLA	CHB-C1B-NB	2.15	126.53	124.26
38	13	315	A86	C-C1-C24	2.14	121.46	118.08
29	F	101	BCR	C24-C23-C22	-2.14	123.00	126.23
36	D	404	PL9	O2-C1-C6	2.14	124.30	120.59
29	a	409	BCR	C27-C26-C25	2.14	125.84	122.73
38	13	317	A86	C28-C27-C26	-2.14	119.92	122.92
27	c	508	CLA	CMB-C2B-C3B	2.14	131.78	126.59
33	m	102	LMG	C9-C8-C7	-2.14	106.72	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	14	314	A86	C-C1-C24	2.14	121.45	118.08
27	31	302	CLA	CHC-C4B-NB	2.14	126.53	124.26
38	11	313	A86	C-C1-C24	2.14	121.45	118.08
35	C	518	DGD	C8B-C7B-C6B	-2.14	103.55	114.42
27	b	603	CLA	CAA-CBA-CGA	-2.14	107.00	113.25
35	j	101	DGD	O6E-C1E-O5D	-2.14	104.91	109.97
27	W	102	CLA	C2D-C1D-ND	-2.14	108.53	110.10
27	12	309	CLA	CHB-C1B-NB	2.14	126.52	124.26
27	A	402	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
33	M	103	LMG	O1-C7-C8	-2.14	105.74	110.90
27	34	308	CLA	CHB-C1B-NB	2.14	126.52	124.26
38	34	303	A86	C28-C27-C26	-2.14	119.93	122.92
27	B	603	CLA	CAA-CBA-CGA	-2.14	107.01	113.25
29	c	515	BCR	C16-C15-C14	-2.13	119.10	123.47
38	31	313	A86	C-C1-C24	2.13	121.44	118.08
27	C	512	CLA	CHA-C1A-NA	-2.13	121.51	126.40
27	C	511	CLA	C1-C2-C3	-2.13	122.35	126.04
29	C	520	BCR	C20-C21-C22	-2.13	124.27	127.31
35	c	518	DGD	C8B-C7B-C6B	-2.13	103.60	114.42
27	11	305	CLA	CHB-C1B-NB	2.13	126.51	124.26
27	14	307	CLA	C2A-C1A-CHA	2.13	127.59	123.86
38	33	302	A86	C28-C27-C26	-2.13	119.94	122.92
27	34	308	CLA	C2A-C1A-CHA	2.13	127.58	123.86
27	b	602	CLA	CAA-C2A-C3A	-2.13	106.95	112.78
33	M	103	LMG	C1-O6-C5	-2.13	109.51	113.69
27	c	511	CLA	C2A-C1A-CHA	2.13	127.58	123.86
38	34	316	A86	C-C1-C24	2.13	121.43	118.08
33	b	618	LMG	O2-C2-C1	-2.13	104.88	110.05
27	B	607	CLA	CHC-C4B-NB	2.13	126.51	124.26
27	C	508	CLA	CMB-C2B-C3B	2.12	131.73	126.59
29	B	617	BCR	C40-C30-C25	2.12	113.75	110.30
38	11	313	A86	C34-O4-C38	-2.12	113.94	117.90
27	C	511	CLA	C2A-C1A-CHA	2.12	127.57	123.86
27	33	304	CLA	CHC-C4B-NB	2.12	126.50	124.26
38	34	315	A86	C-C1-C24	2.12	121.42	118.08
27	A	404	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
27	32	309	CLA	CHB-C1B-NB	2.12	126.50	124.26
29	z	101	BCR	C16-C17-C18	-2.12	124.28	127.31
27	a	404	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
27	c	511	CLA	C1-C2-C3	-2.12	122.38	126.04
27	B	615	CLA	CMA-C3A-C4A	-2.12	106.08	111.77
38	12	317	A86	C34-O4-C38	-2.12	113.95	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	34	303	A86	C8-C6-C5	2.12	122.19	118.94
27	B	603	CLA	O1D-CGD-CBD	2.12	128.82	124.48
33	C	519	LMG	C1-C2-C3	-2.12	105.58	110.00
27	c	505	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
29	A	409	BCR	C27-C26-C25	2.12	125.81	122.73
33	m	102	LMG	C1-O6-C5	-2.12	109.53	113.69
27	b	615	CLA	CMA-C3A-C4A	-2.12	106.08	111.77
37	f	102	HEM	CAA-C2A-C1A	2.12	129.06	124.89
27	33	307	CLA	C2A-C1A-CHA	2.12	127.56	123.86
27	31	304	CLA	C3B-C4B-NB	-2.12	108.55	110.52
38	13	314	A86	C-C1-C24	2.12	121.41	118.08
38	31	312	A86	C-C1-C24	2.12	121.41	118.08
37	V	201	HEM	CAA-CBA-CGA	-2.12	109.05	113.60
38	34	316	A86	C34-O4-C38	-2.12	113.95	117.90
27	c	502	CLA	C11-C12-C13	-2.12	109.08	115.92
32	l	103	LHG	C27-C26-C25	-2.11	103.69	114.42
32	L	102	LHG	C27-C26-C25	-2.11	103.69	114.42
38	13	315	A86	C34-O4-C38	-2.11	113.96	117.90
38	12	316	A86	C-C1-C24	2.11	121.41	118.08
37	v	201	HEM	CAA-CBA-CGA	-2.11	109.06	113.60
27	11	306	CLA	CHB-C1B-NB	2.11	126.49	124.26
27	11	304	CLA	C3B-C4B-NB	-2.11	108.56	110.52
27	B	603	CLA	C4-C3-C5	2.11	118.83	115.27
33	B	618	LMG	O2-C2-C1	-2.11	104.92	110.05
27	13	307	CLA	C2A-C1A-CHA	2.11	127.55	123.86
27	b	601	CLA	CHC-C4B-NB	2.11	126.49	124.26
27	B	614	CLA	C3A-C2A-C1A	2.11	104.50	101.34
27	b	611	CLA	CHD-C1D-ND	-2.11	122.51	124.45
27	12	306	CLA	CHC-C4B-NB	2.11	126.49	124.26
27	13	304	CLA	CHC-C4B-NB	2.11	126.49	124.26
27	33	307	CLA	CHB-C1B-NB	2.11	126.49	124.26
38	33	314	A86	C-C1-C24	2.11	121.40	118.08
39	32	302	LMU	C2'-C3'-C4'	2.11	114.50	109.68
29	B	616	BCR	C38-C26-C27	-2.11	109.56	113.62
27	33	306	CLA	C3B-C4B-NB	-2.11	108.56	110.52
27	C	502	CLA	C11-C12-C13	-2.11	109.10	115.92
27	32	309	CLA	C2A-C1A-CHA	2.11	127.55	123.86
38	11	312	A86	C-C1-C24	2.11	121.40	118.08
37	E	101	HEM	CAA-C2A-C1A	2.11	129.04	124.89
27	b	603	CLA	C4-C3-C5	2.11	118.82	115.27
27	W	102	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
27	b	604	CLA	CMB-C2B-C1B	-2.11	122.16	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	505	CLA	CAA-C2A-C3A	-2.11	107.01	112.78
29	c	516	BCR	C30-C25-C26	-2.11	119.65	122.61
27	34	306	CLA	CAA-C2A-C1A	2.10	118.87	111.97
27	12	310	CLA	CHB-C1B-NB	2.10	126.48	124.26
27	33	308	CLA	CHB-C1B-NB	2.10	126.48	124.26
27	c	508	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
29	b	617	BCR	C40-C30-C25	2.10	113.71	110.30
27	12	309	CLA	C2A-C1A-CHA	2.10	127.54	123.86
27	C	506	CLA	CMC-C2C-C3C	2.10	131.83	126.12
36	d	404	PL9	O2-C1-C2	-2.10	116.96	121.78
35	J	101	DGD	C7B-C6B-C5B	-2.10	103.75	114.42
35	j	101	DGD	C7B-C6B-C5B	-2.10	103.75	114.42
38	32	317	A86	C34-O4-C38	-2.10	113.98	117.90
27	11	305	CLA	C2A-C1A-CHA	2.10	127.53	123.86
27	31	305	CLA	C2A-C1A-CHA	2.10	127.53	123.86
29	C	516	BCR	C30-C25-C26	-2.10	119.65	122.61
27	32	308	CLA	C3B-C4B-NB	-2.10	108.57	110.52
27	B	602	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
27	34	310	CLA	CMB-C2B-C3B	2.10	131.68	126.59
27	B	606	CLA	C2D-C1D-ND	-2.10	108.56	110.10
33	32	301	LMG	O2-C2-C3	-2.10	105.49	110.35
38	31	313	A86	C34-O4-C38	-2.10	113.98	117.90
36	d	407	PL9	C27-C28-C29	-2.10	122.61	127.66
27	b	608	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
27	33	305	CLA	CAA-C2A-C1A	2.10	118.85	111.97
38	13	302	A86	C8-C6-C5	2.10	122.16	118.94
27	B	604	CLA	C1D-ND-C4D	2.10	107.83	106.33
29	b	616	BCR	C38-C26-C27	-2.10	109.58	113.62
27	B	622	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
38	14	315	A86	C34-O4-C38	-2.10	113.99	117.90
27	14	305	CLA	CAA-C2A-C1A	2.10	118.85	111.97
36	D	407	PL9	C27-C28-C29	-2.10	122.61	127.66
27	31	303	CLA	CAA-C2A-C1A	2.10	118.85	111.97
38	12	304	A86	C8-C6-C5	2.10	122.16	118.94
35	J	101	DGD	O6E-C1E-O5D	-2.10	105.01	109.97
38	31	316	A86	C8-C6-C5	2.10	122.16	118.94
27	b	614	CLA	C3A-C2A-C1A	2.10	104.48	101.34
29	z	101	BCR	C15-C16-C17	-2.09	119.18	123.47
36	D	404	PL9	O2-C1-C2	-2.09	116.98	121.78
27	c	503	CLA	C3B-C4B-NB	-2.09	108.57	110.52
27	C	508	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
38	33	315	A86	C34-O4-C38	-2.09	113.99	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	614	CLA	CHC-C4B-NB	2.09	126.47	124.26
27	32	307	CLA	CAA-C2A-C1A	2.09	118.83	111.97
29	Z	101	BCR	C15-C16-C17	-2.09	119.19	123.47
27	C	502	CLA	C1-C2-C3	-2.09	122.42	126.04
27	B	608	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
27	13	305	CLA	CAA-C2A-C1A	2.09	118.83	111.97
27	C	507	CLA	CHA-C1A-NA	-2.09	121.61	126.40
27	11	303	CLA	CAA-C2A-C1A	2.09	118.83	111.97
27	c	506	CLA	CMC-C2C-C3C	2.09	131.79	126.12
27	33	309	CLA	CMB-C2B-C3B	2.09	131.65	126.59
27	34	304	CLA	CAA-CBA-CGA	-2.09	107.14	113.25
27	b	606	CLA	C2D-C1D-ND	-2.09	108.56	110.10
27	12	307	CLA	CAA-C2A-C1A	2.09	118.82	111.97
27	c	511	CLA	CHA-C4D-ND	2.09	136.87	132.50
27	B	601	CLA	CHC-C4B-NB	2.09	126.47	124.26
27	32	306	CLA	CHC-C4B-NB	2.09	126.47	124.26
29	Z	101	BCR	C16-C17-C18	-2.09	124.33	127.31
27	14	304	CLA	CHC-C4B-NB	2.09	126.47	124.26
27	b	615	CLA	CHB-C1B-C2B	-2.09	121.34	127.24
27	c	507	CLA	CHA-C1A-NA	-2.09	121.62	126.40
27	B	604	CLA	CMB-C2B-C1B	-2.08	122.19	125.37
27	33	303	CLA	CAA-CBA-CGA	-2.08	107.17	113.25
27	C	513	CLA	C2A-C1A-CHA	2.08	127.50	123.86
38	11	316	A86	C8-C6-C5	2.08	122.14	118.94
29	a	405	BCR	C7-C8-C9	-2.08	123.09	126.23
27	13	303	CLA	CAA-CBA-CGA	-2.08	107.17	113.25
27	w	102	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
27	11	307	CLA	CMB-C2B-C3B	2.08	131.63	126.59
27	C	503	CLA	C3C-C4C-NC	-2.08	108.24	110.57
27	c	506	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
27	c	512	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
27	12	308	CLA	C3B-C4B-NB	-2.08	108.59	110.52
27	C	506	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
27	B	612	CLA	C2A-C1A-CHA	2.08	127.49	123.86
27	32	305	CLA	CAA-CBA-CGA	-2.08	107.18	113.25
27	11	302	CLA	CHC-C4B-NB	2.08	126.46	124.26
27	c	503	CLA	C3C-C4C-NC	-2.08	108.24	110.57
27	31	301	CLA	CAA-CBA-CGA	-2.08	107.18	113.25
27	B	614	CLA	CHC-C4B-NB	2.08	126.46	124.26
27	b	622	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
27	C	512	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
27	C	503	CLA	CHB-C1B-NB	2.08	126.45	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	504	CLA	CHC-C4B-NB	2.08	126.45	124.26
27	B	615	CLA	CHB-C1B-C2B	-2.08	121.38	127.24
38	32	304	A86	C8-C6-C5	2.07	122.12	118.94
27	c	502	CLA	C1-C2-C3	-2.07	122.46	126.04
32	l	102	LHG	C5-O7-C7	-2.07	112.69	117.79
27	A	402	CLA	CAA-C2A-C3A	-2.07	107.10	112.78
38	33	302	A86	C8-C6-C5	2.07	122.12	118.94
29	B	616	BCR	C16-C15-C14	-2.07	119.23	123.47
32	b	621	LHG	C27-C26-C25	-2.07	103.91	114.42
27	13	310	CLA	C3B-C4B-NB	-2.07	108.59	110.52
27	c	504	CLA	CHC-C4B-NB	2.07	126.45	124.26
29	B	623	BCR	C15-C16-C17	-2.07	119.23	123.47
27	12	305	CLA	CAA-CBA-CGA	-2.07	107.21	113.25
36	D	404	PL9	C22-C23-C24	-2.07	122.68	127.66
27	14	306	CLA	C3B-C4B-NB	-2.07	108.60	110.52
27	13	305	CLA	C2A-C1A-CHA	2.07	127.47	123.86
32	L	101	LHG	C5-O7-C7	-2.07	112.70	117.79
27	B	605	CLA	C1-C2-C3	-2.07	122.47	126.04
27	11	301	CLA	CAA-CBA-CGA	-2.07	107.21	113.25
27	B	612	CLA	CMA-C3A-C4A	-2.07	106.22	111.77
27	c	513	CLA	C2A-C1A-CHA	2.07	127.47	123.86
27	13	301	CLA	C2A-C1A-CHA	2.07	127.47	123.86
28	a	403	PHO	CMA-C3A-C4A	-2.07	109.85	114.38
27	14	302	CLA	C2A-C1A-CHA	2.07	127.47	123.86
32	B	621	LHG	C27-C26-C25	-2.07	103.94	114.42
27	D	405	CLA	CHC-C4B-NB	2.07	126.44	124.26
36	d	404	PL9	C22-C23-C24	-2.07	122.69	127.66
27	b	612	CLA	C2A-C1A-CHA	2.07	127.47	123.86
36	D	404	PL9	C36-C37-C38	-2.07	105.09	111.88
27	34	307	CLA	C3B-C4B-NB	-2.07	108.60	110.52
27	31	307	CLA	CMB-C2B-C3B	2.07	131.59	126.59
27	D	402	CLA	CHD-C1D-ND	-2.06	122.56	124.45
27	14	303	CLA	CAA-CBA-CGA	-2.06	107.22	113.25
27	b	615	CLA	O2D-CGD-CBD	2.06	114.94	111.27
29	b	616	BCR	C16-C15-C14	-2.06	119.25	123.47
27	13	309	CLA	CMB-C2B-C3B	2.06	131.58	126.59
28	A	403	PHO	CMA-C3A-C4A	-2.06	109.86	114.38
27	c	502	CLA	C3C-C4C-NC	-2.06	108.26	110.57
27	32	311	CLA	CMB-C2B-C3B	2.06	131.58	126.59
27	b	604	CLA	CHB-C1B-NB	2.06	126.44	124.26
27	B	611	CLA	CHD-C1D-ND	-2.06	122.56	124.45
38	13	317	A86	C8-C6-C5	2.06	122.11	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	12	311	CLA	CMB-C2B-C3B	2.06	131.58	126.59
29	a	409	BCR	C24-C23-C22	-2.06	123.12	126.23
27	31	303	CLA	C2A-C1A-CHA	2.06	127.46	123.86
27	34	306	CLA	C2A-C1A-CHA	2.06	127.46	123.86
27	32	312	CLA	C3B-C4B-NB	-2.06	108.60	110.52
27	34	310	CLA	CHC-C4B-NB	2.06	126.44	124.26
36	D	407	PL9	C46-C47-C48	-2.06	105.11	111.88
27	12	303	CLA	C2A-C1A-CHA	2.06	127.46	123.86
27	32	303	CLA	C2A-C1A-CHA	2.06	127.46	123.86
33	12	301	LMG	O6-C1-O1	-2.06	105.10	109.97
27	B	603	CLA	C2D-C1D-ND	-2.06	108.59	110.10
27	C	511	CLA	CHA-C4D-ND	2.06	136.80	132.50
27	a	402	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
28	A	403	PHO	C1C-C2C-C3C	-2.06	106.90	108.61
27	34	302	CLA	C2A-C1A-CHA	2.06	127.45	123.86
35	c	517	DGD	C4E-C3E-C2E	-2.06	107.23	110.82
36	d	404	PL9	C36-C37-C38	-2.06	105.12	111.88
27	b	612	CLA	CMA-C3A-C4A	-2.06	106.25	111.77
27	W	103	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
27	14	309	CLA	CMB-C2B-C3B	2.06	131.57	126.59
27	32	307	CLA	C2A-C1A-CHA	2.05	127.45	123.86
36	d	404	PL9	O1-C4-C3	-2.05	118.46	120.72
27	13	306	CLA	C3B-C4B-NB	-2.05	108.61	110.52
30	L	103	SQD	O48-C23-O10	-2.05	118.42	123.59
27	b	604	CLA	C1D-ND-C4D	2.05	107.79	106.33
27	33	301	CLA	C2A-C1A-CHA	2.05	127.44	123.86
27	34	305	CLA	CHC-C4B-NB	2.05	126.42	124.26
27	31	308	CLA	C3B-C4B-NB	-2.05	108.62	110.52
27	B	604	CLA	CHB-C1B-NB	2.05	126.42	124.26
27	14	305	CLA	C2A-C1A-CHA	2.05	127.44	123.86
29	A	405	BCR	C7-C8-C9	-2.04	123.15	126.23
35	C	517	DGD	C4E-C3E-C2E	-2.04	107.25	110.82
27	B	606	CLA	C3B-C4B-NB	-2.04	108.62	110.52
27	11	315	CLA	C2A-C1A-CHA	2.04	127.43	123.86
27	b	602	CLA	CAA-CBA-CGA	-2.04	107.28	113.25
29	A	409	BCR	C24-C23-C22	-2.04	123.15	126.23
27	d	402	CLA	CHD-C1D-ND	-2.04	122.58	124.45
38	14	316	A86	C19-C18-C17	-2.04	106.83	110.77
30	l	101	SQD	O48-C23-O10	-2.04	118.44	123.59
27	12	307	CLA	C2A-C1A-CHA	2.04	127.43	123.86
27	C	512	CLA	C7-C6-C5	-2.04	107.82	113.36
27	31	315	CLA	C2A-C1A-CHA	2.04	127.42	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	C	517	DGD	CBB-CAB-C9B	-2.04	104.07	114.42
36	d	407	PL9	C46-C47-C48	-2.04	105.18	111.88
29	C	516	BCR	C24-C23-C22	-2.04	123.16	126.23
27	b	603	CLA	C2D-C1D-ND	-2.04	108.60	110.10
29	Z	101	BCR	C37-C22-C21	-2.04	120.07	122.92
27	c	503	CLA	CHB-C1B-NB	2.04	126.41	124.26
27	B	602	CLA	CAA-CBA-CGA	-2.04	107.30	113.25
27	34	311	CLA	C3B-C4B-NB	-2.04	108.62	110.52
35	c	517	DGD	CBB-CAB-C9B	-2.04	104.08	114.42
27	b	605	CLA	C1-C2-C3	-2.04	122.52	126.04
29	B	617	BCR	C1-C6-C5	-2.04	119.75	122.61
27	B	615	CLA	O2D-CGD-CBD	2.04	114.89	111.27
27	D	401	CLA	CMB-C2B-C3B	2.03	131.52	126.59
27	13	309	CLA	CHC-C4B-NB	2.03	126.41	124.26
27	12	312	CLA	C3B-C4B-NB	-2.03	108.63	110.52
27	D	401	CLA	C3A-C2A-C1A	2.03	104.39	101.34
27	c	512	CLA	C7-C6-C5	-2.03	107.84	113.36
35	C	517	DGD	O3E-C3E-C2E	-2.03	105.65	110.35
33	12	301	LMG	O7-C10-O9	-2.03	118.79	123.70
27	B	603	CLA	C3B-C4B-NB	-2.03	108.63	110.52
27	33	310	CLA	C3B-C4B-NB	-2.03	108.63	110.52
27	A	402	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
27	b	603	CLA	C3B-C4B-NB	-2.03	108.63	110.52
27	c	502	CLA	C3B-C4B-NB	-2.03	108.63	110.52
27	C	506	CLA	C3C-C4C-NC	-2.03	108.29	110.57
27	d	405	CLA	C1-C2-C3	-2.03	122.53	126.04
36	D	404	PL9	O1-C4-C3	-2.03	118.48	120.72
38	34	301	A86	C19-C18-C17	-2.03	106.85	110.77
27	B	613	CLA	CHB-C1B-NB	2.03	126.41	124.26
27	w	103	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
27	13	311	CLA	CHB-C1B-NB	2.03	126.40	124.26
27	C	503	CLA	C3B-C4B-NB	-2.03	108.63	110.52
27	11	303	CLA	C2A-C1A-CHA	2.03	127.40	123.86
38	14	301	A86	C8-C6-C5	-2.03	115.83	118.94
28	a	403	PHO	C1C-C2C-C3C	-2.03	106.92	108.61
38	13	316	A86	C19-C18-C17	-2.03	106.86	110.77
29	F	101	BCR	C40-C30-C25	2.03	113.58	110.30
27	d	401	CLA	CMB-C2B-C3B	2.03	131.49	126.59
36	d	404	PL9	C31-C32-C33	-2.03	105.22	111.88
27	b	602	CLA	C4-C3-C5	2.03	118.68	115.27
36	D	404	PL9	C31-C32-C33	-2.03	105.22	111.88
35	j	101	DGD	C5B-C4B-C3B	-2.02	104.15	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	31	314	A86	C8-C6-C5	-2.02	115.83	118.94
27	14	311	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
27	b	606	CLA	C3B-C4B-NB	-2.02	108.64	110.52
29	b	617	BCR	C1-C6-C5	-2.02	119.76	122.61
29	f	101	BCR	C40-C30-C25	2.02	113.58	110.30
27	C	509	CLA	C16-C15-C13	-2.02	109.38	115.92
27	c	509	CLA	C16-C15-C13	-2.02	109.38	115.92
35	c	517	DGD	C7A-C6A-C5A	-2.02	104.16	114.42
27	A	402	CLA	C3B-C4B-NB	-2.02	108.64	110.52
27	11	308	CLA	C3B-C4B-NB	-2.02	108.64	110.52
29	C	516	BCR	C16-C15-C14	-2.02	119.33	123.47
27	d	401	CLA	C3A-C2A-C1A	2.02	104.37	101.34
27	33	308	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
33	b	618	LMG	C6-C5-C4	-2.02	108.27	113.00
38	11	314	A86	C19-C18-C17	-2.02	106.87	110.77
29	h	101	BCR	C20-C21-C22	-2.02	124.43	127.31
27	14	308	CLA	CHA-C1A-NA	-2.02	121.77	126.40
29	C	516	BCR	C21-C20-C19	-2.02	116.92	123.22
27	b	613	CLA	CHB-C1B-NB	2.02	126.39	124.26
35	C	517	DGD	C7A-C6A-C5A	-2.02	104.18	114.42
36	d	407	PL9	C20-C19-C21	2.02	118.67	115.27
38	11	314	A86	C8-C6-C5	-2.02	115.84	118.94
35	H	102	DGD	O6E-C1E-O5D	-2.02	105.20	109.97
29	M	101	BCR	C16-C15-C14	-2.02	119.34	123.47
27	d	405	CLA	CHC-C4B-NB	2.02	126.39	124.26
27	A	404	CLA	O2D-CGD-CBD	2.02	114.85	111.27
27	C	502	CLA	C3C-C4C-NC	-2.02	108.31	110.57
36	D	407	PL9	C20-C19-C21	2.02	118.66	115.27
27	32	310	CLA	O2A-CGA-O1A	-2.02	118.28	123.30
38	32	318	A86	C8-C6-C5	-2.01	115.85	118.94
27	14	309	CLA	CHC-C4B-NB	2.01	126.39	124.26
27	31	309	CLA	CHB-C1B-NB	2.01	126.39	124.26
33	q	301	LMG	C22-C21-C20	-2.01	104.20	114.42
27	33	305	CLA	C2A-C1A-CHA	2.01	127.38	123.86
27	34	312	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
38	14	301	A86	C19-C18-C17	-2.01	106.88	110.77
29	c	516	BCR	C16-C15-C14	-2.01	119.35	123.47
35	J	101	DGD	C5B-C4B-C3B	-2.01	104.20	114.42
35	h	102	DGD	O6E-C1E-O5D	-2.01	105.21	109.97
38	32	318	A86	C19-C18-C17	-2.01	106.89	110.77
35	c	517	DGD	O3E-C3E-C2E	-2.01	105.70	110.35
27	B	604	CLA	CHA-C4D-ND	2.01	136.71	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	31	307	CLA	CHC-C4B-NB	2.01	126.39	124.26
33	32	301	LMG	O7-C10-O9	-2.01	118.84	123.70
29	f	101	BCR	C33-C5-C6	-2.01	122.27	124.53
35	c	518	DGD	C7B-C6B-C5B	-2.01	104.22	114.42
27	32	313	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
29	b	623	BCR	C15-C16-C17	-2.01	119.36	123.47
27	B	602	CLA	C4-C3-C5	2.01	118.65	115.27
27	34	312	CLA	CHB-C1B-NB	2.01	126.38	124.26
27	34	309	CLA	CHA-C1A-NA	-2.01	121.80	126.40
27	a	404	CLA	O2D-CGD-CBD	2.01	114.84	111.27
27	B	601	CLA	C3A-C2A-C1A	2.01	104.35	101.34
29	m	103	BCR	C16-C15-C14	-2.01	119.36	123.47
27	31	306	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
27	32	310	CLA	CHA-C1A-NA	-2.01	121.80	126.40
38	12	316	A86	C7-C6-C5	-2.01	120.11	122.92
27	12	310	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
27	33	311	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
38	31	312	A86	C7-C6-C5	-2.01	120.11	122.92
35	C	518	DGD	C7B-C6B-C5B	-2.01	104.24	114.42
27	D	405	CLA	C11-C12-C13	-2.01	109.44	115.92
27	C	502	CLA	CHD-C1D-ND	-2.01	122.61	124.45
27	c	509	CLA	CHC-C4B-NB	2.01	126.38	124.26
38	32	304	A86	C23-C16-C17	-2.00	105.50	108.98
27	11	306	CLA	O2A-CGA-O1A	-2.00	118.30	123.30
27	13	308	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
27	C	512	CLA	O2D-CGD-CBD	2.00	114.83	111.27
32	a	408	LHG	O8-C23-O10	-2.00	118.54	123.59
27	34	309	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
38	33	314	A86	C23-C16-C22	-2.00	104.42	107.37
33	C	519	LMG	C22-C21-C20	-2.00	104.26	114.42
38	31	314	A86	C19-C18-C17	-2.00	106.91	110.77
27	d	405	CLA	C11-C12-C13	-2.00	109.45	115.92
27	B	613	CLA	O1D-CGD-CBD	2.00	128.58	124.48
29	c	516	BCR	C21-C20-C19	-2.00	116.97	123.22
27	C	504	CLA	C3A-C2A-C1A	2.00	104.33	101.34
27	b	604	CLA	CHA-C4D-ND	2.00	136.68	132.50

There are no chirality outliers.

All (3462) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	A	402	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
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	CHA-CBD-CGD-O1D
27	B	601	CLA	CHA-CBD-CGD-O2D
27	B	601	CLA	CAD-CBD-CGD-O1D
27	B	602	CLA	C2-C3-C5-C6
27	B	602	CLA	C4-C3-C5-C6
27	B	603	CLA	CAD-CBD-CGD-O1D
27	B	603	CLA	CAD-CBD-CGD-O2D
27	B	603	CLA	C4-C3-C5-C6
27	B	604	CLA	CHA-CBD-CGD-O1D
27	B	604	CLA	CHA-CBD-CGD-O2D
27	B	605	CLA	C2B-C3B-CAB-CBB
27	B	605	CLA	C4B-C3B-CAB-CBB
27	B	605	CLA	C2-C3-C5-C6
27	B	605	CLA	C4-C3-C5-C6
27	B	608	CLA	CHA-CBD-CGD-O1D
27	B	608	CLA	CHA-CBD-CGD-O2D
27	B	610	CLA	CHA-CBD-CGD-O2D
27	B	611	CLA	CHA-CBD-CGD-O1D
27	B	611	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	614	CLA	CHA-CBD-CGD-O1D
27	B	614	CLA	CHA-CBD-CGD-O2D
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	CHA-CBD-CGD-O1D
27	C	505	CLA	CHA-CBD-CGD-O2D
27	C	506	CLA	CHA-CBD-CGD-O1D
27	C	506	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
27	C	510	CLA	CBD-CGD-O2D-CED
27	C	510	CLA	C6-C7-C8-C9
27	C	512	CLA	CHA-CBD-CGD-O1D
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	401	CLA	CHA-CBD-CGD-O1D
27	D	401	CLA	CHA-CBD-CGD-O2D
27	D	402	CLA	C2B-C3B-CAB-CBB
27	D	402	CLA	C4B-C3B-CAB-CBB
27	D	402	CLA	CHA-CBD-CGD-O1D
27	D	402	CLA	CHA-CBD-CGD-O2D
27	D	405	CLA	C1A-C2A-CAA-CBA
27	M	102	CLA	CHA-CBD-CGD-O1D
27	M	102	CLA	CHA-CBD-CGD-O2D
27	M	102	CLA	CAD-CBD-CGD-O1D
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	CHA-CBD-CGD-O1D
27	b	601	CLA	CHA-CBD-CGD-O2D
27	b	601	CLA	CAD-CBD-CGD-O1D
27	b	602	CLA	C2-C3-C5-C6
27	b	602	CLA	C4-C3-C5-C6
27	b	603	CLA	CAD-CBD-CGD-O1D
27	b	603	CLA	CAD-CBD-CGD-O2D
27	b	603	CLA	C4-C3-C5-C6
27	b	604	CLA	CHA-CBD-CGD-O1D
27	b	604	CLA	CHA-CBD-CGD-O2D
27	b	605	CLA	C2B-C3B-CAB-CBB
27	b	605	CLA	C4B-C3B-CAB-CBB
27	b	605	CLA	C2-C3-C5-C6
27	b	605	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	b	608	CLA	CHA-CBD-CGD-O1D
27	b	608	CLA	CHA-CBD-CGD-O2D
27	b	610	CLA	CHA-CBD-CGD-O2D
27	b	611	CLA	CHA-CBD-CGD-O1D
27	b	611	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	614	CLA	CHA-CBD-CGD-O1D
27	b	614	CLA	CHA-CBD-CGD-O2D
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	CHA-CBD-CGD-O1D
27	c	505	CLA	CHA-CBD-CGD-O2D
27	c	506	CLA	CHA-CBD-CGD-O1D
27	c	506	CLA	CHA-CBD-CGD-O2D
27	c	510	CLA	CBD-CGD-O2D-CED
27	c	510	CLA	C6-C7-C8-C9
27	c	512	CLA	CHA-CBD-CGD-O1D
27	c	513	CLA	C1A-C2A-CAA-CBA
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	401	CLA	CHA-CBD-CGD-O1D
27	d	401	CLA	CHA-CBD-CGD-O2D
27	d	402	CLA	C2B-C3B-CAB-CBB
27	d	402	CLA	C4B-C3B-CAB-CBB
27	d	402	CLA	CHA-CBD-CGD-O1D
27	d	402	CLA	CHA-CBD-CGD-O2D
27	d	405	CLA	C1A-C2A-CAA-CBA
27	m	101	CLA	CHA-CBD-CGD-O1D
27	m	101	CLA	CHA-CBD-CGD-O2D
27	m	101	CLA	CAD-CBD-CGD-O1D
27	m	101	CLA	CAD-CBD-CGD-O2D
27	m	101	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
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	305	CLA	CHA-CBD-CGD-O1D
27	11	308	CLA	C1A-C2A-CAA-CBA
27	11	309	CLA	C1A-C2A-CAA-CBA
27	11	309	CLA	C4B-C3B-CAB-CBB
27	11	315	CLA	CHA-CBD-CGD-O1D
27	11	315	CLA	CHA-CBD-CGD-O2D
27	12	303	CLA	CHA-CBD-CGD-O1D
27	12	303	CLA	CHA-CBD-CGD-O2D
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	309	CLA	CHA-CBD-CGD-O1D
27	12	312	CLA	C1A-C2A-CAA-CBA
27	12	313	CLA	C1A-C2A-CAA-CBA
27	12	313	CLA	C4B-C3B-CAB-CBB
27	13	301	CLA	CHA-CBD-CGD-O1D
27	13	301	CLA	CHA-CBD-CGD-O2D
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	307	CLA	CHA-CBD-CGD-O1D
27	13	310	CLA	C1A-C2A-CAA-CBA
27	13	311	CLA	C1A-C2A-CAA-CBA
27	13	311	CLA	C4B-C3B-CAB-CBB
27	14	302	CLA	CHA-CBD-CGD-O1D
27	14	302	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
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	307	CLA	CHA-CBD-CGD-O1D
27	14	310	CLA	C1A-C2A-CAA-CBA
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	305	CLA	CHA-CBD-CGD-O1D
27	31	308	CLA	C1A-C2A-CAA-CBA
27	31	309	CLA	C1A-C2A-CAA-CBA
27	31	309	CLA	C4B-C3B-CAB-CBB
27	31	315	CLA	CHA-CBD-CGD-O1D
27	31	315	CLA	CHA-CBD-CGD-O2D
27	32	303	CLA	CHA-CBD-CGD-O1D
27	32	303	CLA	CHA-CBD-CGD-O2D
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	309	CLA	CHA-CBD-CGD-O1D
27	32	312	CLA	C1A-C2A-CAA-CBA
27	32	313	CLA	C1A-C2A-CAA-CBA
27	32	313	CLA	C4B-C3B-CAB-CBB
27	33	301	CLA	CHA-CBD-CGD-O1D
27	33	301	CLA	CHA-CBD-CGD-O2D
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	307	CLA	CHA-CBD-CGD-O1D
27	33	310	CLA	C1A-C2A-CAA-CBA
27	33	311	CLA	C1A-C2A-CAA-CBA
27	33	311	CLA	C4B-C3B-CAB-CBB
27	34	302	CLA	CHA-CBD-CGD-O1D
27	34	302	CLA	CHA-CBD-CGD-O2D
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	308	CLA	CHA-CBD-CGD-O1D
27	34	311	CLA	C1A-C2A-CAA-CBA
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	C1-C6-C7-C8
29	B	616	BCR	C7-C8-C9-C10
29	B	616	BCR	C20-C21-C22-C37
29	B	617	BCR	C1-C6-C7-C8
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	515	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
29	C	516	BCR	C1-C6-C7-C8
29	C	516	BCR	C22-C23-C24-C25
29	C	520	BCR	C1-C6-C7-C8
29	C	520	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
29	F	101	BCR	C37-C22-C23-C24
29	F	101	BCR	C22-C23-C24-C25
29	H	101	BCR	C1-C6-C7-C8
29	H	101	BCR	C20-C21-C22-C37
29	H	101	BCR	C37-C22-C23-C24
29	M	101	BCR	C23-C24-C25-C30
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	C1-C6-C7-C8
29	b	616	BCR	C7-C8-C9-C10
29	b	616	BCR	C20-C21-C22-C37
29	b	617	BCR	C1-C6-C7-C8
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

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Mol	Chain	Res	Type	Atoms
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	515	BCR	C23-C24-C25-C30
29	c	516	BCR	C1-C6-C7-C8
29	c	516	BCR	C22-C23-C24-C25
29	c	519	BCR	C1-C6-C7-C8
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
29	f	101	BCR	C37-C22-C23-C24
29	f	101	BCR	C22-C23-C24-C25
29	h	101	BCR	C1-C6-C7-C8
29	h	101	BCR	C20-C21-C22-C37
29	h	101	BCR	C37-C22-C23-C24
29	m	103	BCR	C23-C24-C25-C30
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	C4-O6-P-O3
32	B	621	LHG	C3-O3-P-O4
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	102	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
32	a	408	LHG	C3-O3-P-O5
32	a	408	LHG	C4-O6-P-O3
32	b	621	LHG	C3-O3-P-O4
32	b	621	LHG	C4-O6-P-O4
32	l	102	LHG	O1-C1-C2-C3
32	l	102	LHG	C3-O3-P-O4
32	l	102	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	C24-C26-C27-C28
36	D	404	PL9	C37-C38-C39-C40
36	D	404	PL9	C44-C46-C47-C48
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	C24-C26-C27-C28
36	d	404	PL9	C37-C38-C39-C40
36	d	404	PL9	C44-C46-C47-C48
36	d	407	PL9	C12-C13-C14-C16
36	d	407	PL9	C42-C43-C44-C45
38	11	310	A86	C39-C38-O4-C34
38	11	310	A86	C5-C6-C8-C9
38	11	310	A86	C7-C6-C8-C9
38	11	312	A86	C26-C27-C29-C30
38	11	312	A86	C28-C27-C29-C30
38	11	312	A86	C35-C34-O4-C38
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

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Mol	Chain	Res	Type	Atoms
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	C39-C38-O4-C34
38	12	314	A86	C5-C6-C8-C9
38	12	314	A86	C7-C6-C8-C9
38	12	316	A86	C26-C27-C29-C30
38	12	316	A86	C28-C27-C29-C30
38	12	316	A86	C35-C34-O4-C38
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	C39-C38-O4-C34
38	13	312	A86	C5-C6-C8-C9
38	13	312	A86	C7-C6-C8-C9
38	13	314	A86	C26-C27-C29-C30
38	13	314	A86	C28-C27-C29-C30
38	13	314	A86	C35-C34-O4-C38
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	C39-C38-O4-C34
38	14	312	A86	C5-C6-C8-C9
38	14	312	A86	C7-C6-C8-C9
38	14	314	A86	C26-C27-C29-C30
38	14	314	A86	C28-C27-C29-C30
38	14	314	A86	C35-C34-O4-C38
38	14	315	A86	C2-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
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	C39-C38-O4-C34
38	31	310	A86	C5-C6-C8-C9
38	31	310	A86	C7-C6-C8-C9
38	31	312	A86	C26-C27-C29-C30
38	31	312	A86	C28-C27-C29-C30
38	31	312	A86	C35-C34-O4-C38
38	31	313	A86	C2-C1-C24-C25
38	31	313	A86	C12-C11-C13-O
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	C39-C38-O4-C34
38	32	314	A86	C5-C6-C8-C9
38	32	314	A86	C7-C6-C8-C9
38	32	316	A86	C26-C27-C29-C30
38	32	316	A86	C28-C27-C29-C30
38	32	316	A86	C35-C34-O4-C38
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	C39-C38-O4-C34
38	33	312	A86	C5-C6-C8-C9
38	33	312	A86	C7-C6-C8-C9
38	33	314	A86	C26-C27-C29-C30

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Mol	Chain	Res	Type	Atoms
38	33	314	A86	C28-C27-C29-C30
38	33	314	A86	C35-C34-O4-C38
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
38	34	313	A86	C39-C38-O4-C34
38	34	313	A86	C5-C6-C8-C9
38	34	313	A86	C7-C6-C8-C9
38	34	315	A86	C26-C27-C29-C30
38	34	315	A86	C28-C27-C29-C30
38	34	315	A86	C35-C34-O4-C38
38	34	316	A86	C2-C1-C24-C25
38	34	316	A86	C12-C11-C13-O
39	12	302	LMU	C2-C1-O1'-C1'
38	11	311	A86	C39-C38-O4-C34
38	11	312	A86	C39-C38-O4-C34
38	12	315	A86	C39-C38-O4-C34
38	12	316	A86	C39-C38-O4-C34
38	13	313	A86	C39-C38-O4-C34
38	13	314	A86	C39-C38-O4-C34
38	14	313	A86	C39-C38-O4-C34
38	14	314	A86	C39-C38-O4-C34
38	31	311	A86	C39-C38-O4-C34
38	31	312	A86	C39-C38-O4-C34
38	32	315	A86	C39-C38-O4-C34
38	32	316	A86	C39-C38-O4-C34
38	33	313	A86	C39-C38-O4-C34
38	33	314	A86	C39-C38-O4-C34
38	34	314	A86	C39-C38-O4-C34
38	34	315	A86	C39-C38-O4-C34
38	11	310	A86	O5-C38-O4-C34
38	12	314	A86	O5-C38-O4-C34
38	13	312	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
38	14	312	A86	O5-C38-O4-C34
38	31	310	A86	O5-C38-O4-C34
38	32	314	A86	O5-C38-O4-C34
38	33	312	A86	O5-C38-O4-C34
38	34	313	A86	O5-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
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

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Mol	Chain	Res	Type	Atoms
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
27	B	611	CLA	O1D-CGD-O2D-CED
27	C	504	CLA	O1D-CGD-O2D-CED
27	C	514	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	c	514	CLA	O1D-CGD-O2D-CED
27	w	103	CLA	O1D-CGD-O2D-CED
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	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	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

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Mol	Chain	Res	Type	Atoms
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
27	B	615	CLA	O1A-CGA-O2A-C1
27	b	615	CLA	O1A-CGA-O2A-C1
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
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
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
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

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Mol	Chain	Res	Type	Atoms
38	34	316	A86	C39-C38-O4-C34
33	M	103	LMG	C11-C10-O7-C8
33	m	102	LMG	C11-C10-O7-C8
27	C	508	CLA	O1D-CGD-O2D-CED
27	c	508	CLA	O1D-CGD-O2D-CED
27	C	502	CLA	C4-C3-C5-C6
27	c	502	CLA	C4-C3-C5-C6
27	C	512	CLA	CBD-CGD-O2D-CED
27	c	512	CLA	CBD-CGD-O2D-CED
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	307	CLA	C2A-CAA-CBA-CGA
27	12	305	CLA	C2A-CAA-CBA-CGA
27	12	311	CLA	C2A-CAA-CBA-CGA
27	13	303	CLA	C2A-CAA-CBA-CGA
27	13	309	CLA	C2A-CAA-CBA-CGA
27	14	303	CLA	C2A-CAA-CBA-CGA
27	14	309	CLA	C2A-CAA-CBA-CGA
27	31	301	CLA	C2A-CAA-CBA-CGA
27	31	307	CLA	C2A-CAA-CBA-CGA
27	32	305	CLA	C2A-CAA-CBA-CGA
27	32	311	CLA	C2A-CAA-CBA-CGA
27	33	303	CLA	C2A-CAA-CBA-CGA
27	33	309	CLA	C2A-CAA-CBA-CGA
27	34	304	CLA	C2A-CAA-CBA-CGA
27	34	310	CLA	C2A-CAA-CBA-CGA
27	C	505	CLA	C3-C5-C6-C7
27	c	505	CLA	C3-C5-C6-C7
28	A	403	PHO	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
28	a	403	PHO	C3-C5-C6-C7
27	C	508	CLA	CBA-CGA-O2A-C1
27	c	508	CLA	CBA-CGA-O2A-C1
33	W	101	LMG	O6-C5-C6-O5
33	w	101	LMG	O6-C5-C6-O5
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
35	H	102	DGD	C4D-C5D-C6D-O5D
35	h	102	DGD	C4D-C5D-C6D-O5D
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
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
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
27	34	304	CLA	O1A-CGA-O2A-C1
38	11	311	A86	C24-C25-C26-C27
38	12	315	A86	C24-C25-C26-C27
38	13	313	A86	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
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	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
27	B	603	CLA	O1D-CGD-O2D-CED
27	b	603	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
28	A	403	PHO	C10-C11-C12-C13
28	a	403	PHO	C10-C11-C12-C13
27	b	604	CLA	O1D-CGD-O2D-CED
27	C	503	CLA	CBD-CGD-O2D-CED
27	c	503	CLA	CBD-CGD-O2D-CED
27	B	604	CLA	O1D-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	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	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
39	12	302	LMU	O5B-C5B-C6B-O6B
39	32	302	LMU	O5B-C5B-C6B-O6B
27	B	603	CLA	C2-C3-C5-C6
27	b	603	CLA	C2-C3-C5-C6
33	12	301	LMG	O6-C5-C6-O5
35	C	518	DGD	O6E-C1E-O5D-C6D
35	c	518	DGD	O6E-C1E-O5D-C6D
36	D	404	PL9	C19-C21-C22-C23
36	d	404	PL9	C19-C21-C22-C23
27	A	402	CLA	CBA-CGA-O2A-C1
27	C	511	CLA	CBA-CGA-O2A-C1
27	c	511	CLA	CBA-CGA-O2A-C1
35	H	102	DGD	O6E-C5E-C6E-O5E
35	h	102	DGD	O6E-C5E-C6E-O5E
27	B	602	CLA	O1D-CGD-O2D-CED
27	C	507	CLA	O1D-CGD-O2D-CED
27	b	602	CLA	O1D-CGD-O2D-CED
27	c	507	CLA	O1D-CGD-O2D-CED
27	C	512	CLA	O1A-CGA-O2A-C1
27	c	512	CLA	O1A-CGA-O2A-C1
27	B	614	CLA	O1D-CGD-O2D-CED
27	b	614	CLA	O1D-CGD-O2D-CED
27	B	602	CLA	C3-C5-C6-C7
27	b	602	CLA	C3-C5-C6-C7
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	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
27	34	309	CLA	CBD-CGD-O2D-CED
29	B	623	BCR	C15-C16-C17-C18
29	b	623	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
38	11	310	A86	C24-C25-C26-C27
38	11	312	A86	C24-C25-C26-C27
38	12	314	A86	C24-C25-C26-C27
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	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	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
27	C	511	CLA	O1A-CGA-O2A-C1
27	c	511	CLA	O1A-CGA-O2A-C1
33	B	618	LMG	C4-C5-C6-O5
33	b	618	LMG	C4-C5-C6-O5
27	C	502	CLA	C2-C3-C5-C6
27	c	502	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
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	C	511	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
27	c	511	CLA	C11-C12-C13-C14
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	609	CLA	O1D-CGD-O2D-CED
27	b	609	CLA	O1D-CGD-O2D-CED
29	B	623	BCR	C7-C8-C9-C34
29	B	623	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	520	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	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	f	101	BCR	C7-C8-C9-C34
29	z	101	BCR	C37-C22-C23-C24
38	11	313	A86	C-C1-C24-C25
38	12	317	A86	C-C1-C24-C25
38	13	315	A86	C-C1-C24-C25
38	14	315	A86	C-C1-C24-C25
38	31	313	A86	C-C1-C24-C25
38	32	317	A86	C-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
38	33	315	A86	C-C1-C24-C25
38	34	316	A86	C-C1-C24-C25
33	32	301	LMG	O6-C5-C6-O5
32	L	101	LHG	C8-C7-O7-C5
32	l	102	LHG	C8-C7-O7-C5
33	12	301	LMG	C4-C5-C6-O5
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
27	B	608	CLA	C15-C16-C17-C18
27	B	615	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	z	102	CLA	C8-C10-C11-C12
33	C	519	LMG	O6-C5-C6-O5
33	q	301	LMG	O6-C5-C6-O5
27	11	303	CLA	O1D-CGD-O2D-CED
27	34	306	CLA	O1D-CGD-O2D-CED
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	615	CLA	C13-C15-C16-C17
27	C	514	CLA	C8-C10-C11-C12
27	b	615	CLA	C13-C15-C16-C17
27	b	622	CLA	C13-C15-C16-C17
27	c	514	CLA	C8-C10-C11-C12
28	A	403	PHO	C15-C16-C17-C18
28	a	403	PHO	C15-C16-C17-C18
33	32	301	LMG	C10-C11-C12-C13
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

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Mol	Chain	Res	Type	Atoms
27	C	513	CLA	CBD-CGD-O2D-CED
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	D	402	CLA	C15-C16-C17-C18
27	W	102	CLA	C10-C11-C12-C13
27	W	103	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	d	402	CLA	C15-C16-C17-C18
27	w	102	CLA	C10-C11-C12-C13
27	w	103	CLA	C10-C11-C12-C13
36	D	407	PL9	C7-C8-C9-C10
32	B	621	LHG	C23-C24-C25-C26
32	L	101	LHG	C7-C8-C9-C10
32	b	621	LHG	C23-C24-C25-C26
32	l	102	LHG	C7-C8-C9-C10
33	12	301	LMG	C10-C11-C12-C13
27	c	513	CLA	CBD-CGD-O2D-CED
27	A	404	CLA	C8-C10-C11-C12
27	B	601	CLA	C5-C6-C7-C8
27	C	511	CLA	C8-C10-C11-C12
27	a	404	CLA	C8-C10-C11-C12
27	b	601	CLA	C5-C6-C7-C8
27	c	511	CLA	C8-C10-C11-C12
37	E	101	HEM	C1A-C2A-CAA-CBA
37	f	102	HEM	C1A-C2A-CAA-CBA
27	C	513	CLA	C8-C10-C11-C12
33	B	618	LMG	C28-C29-C30-C31
33	b	618	LMG	C28-C29-C30-C31
27	C	504	CLA	C5-C6-C7-C8
27	C	505	CLA	C15-C16-C17-C18
27	c	504	CLA	C5-C6-C7-C8
27	c	505	CLA	C15-C16-C17-C18
27	c	513	CLA	C8-C10-C11-C12
27	C	502	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	c	502	CLA	O1D-CGD-O2D-CED
27	34	312	CLA	O1D-CGD-O2D-CED
27	B	615	CLA	C6-C7-C8-C10
27	C	504	CLA	C6-C7-C8-C10
27	C	505	CLA	C6-C7-C8-C10
27	W	103	CLA	C12-C13-C15-C16
27	b	615	CLA	C6-C7-C8-C10
27	c	504	CLA	C6-C7-C8-C10
27	c	505	CLA	C6-C7-C8-C10
27	w	103	CLA	C12-C13-C15-C16
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
27	c	505	CLA	O1A-CGA-O2A-C1
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	11	306	CLA	C2A-CAA-CBA-CGA
27	12	310	CLA	C2A-CAA-CBA-CGA
27	13	308	CLA	C2A-CAA-CBA-CGA
27	14	308	CLA	C2A-CAA-CBA-CGA
27	31	306	CLA	C2A-CAA-CBA-CGA
27	32	310	CLA	C2A-CAA-CBA-CGA
27	33	308	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
27	34	309	CLA	C2A-CAA-CBA-CGA
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	B	602	CLA	C5-C6-C7-C8
27	C	505	CLA	O1A-CGA-O2A-C1
27	W	102	CLA	CBD-CGD-O2D-CED
27	w	102	CLA	CBD-CGD-O2D-CED
30	B	620	SQD	O5-C1-O6-C44
30	b	620	SQD	O5-C1-O6-C44
27	b	602	CLA	C5-C6-C7-C8
36	D	404	PL9	C9-C11-C12-C13
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	C9-C11-C12-C13
36	d	404	PL9	C29-C31-C32-C33
36	d	404	PL9	C34-C36-C37-C38
36	d	404	PL9	C39-C41-C42-C43
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
39	32	302	LMU	C4B-C5B-C6B-O6B
27	B	612	CLA	C10-C11-C12-C13
27	C	505	CLA	C8-C10-C11-C12
27	C	508	CLA	C10-C11-C12-C13
27	D	402	CLA	C10-C11-C12-C13
27	M	102	CLA	C8-C10-C11-C12
27	b	612	CLA	C10-C11-C12-C13
27	c	505	CLA	C8-C10-C11-C12
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	A	402	CLA	O1A-CGA-O2A-C1
27	a	402	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	11	307	CLA	O1A-CGA-O2A-C1
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
39	12	302	LMU	C4B-C5B-C6B-O6B
27	C	504	CLA	C10-C11-C12-C13
27	C	505	CLA	C13-C15-C16-C17
27	C	507	CLA	C10-C11-C12-C13
27	C	507	CLA	C15-C16-C17-C18
27	C	508	CLA	C15-C16-C17-C18
27	W	102	CLA	C8-C10-C11-C12
27	c	507	CLA	C10-C11-C12-C13
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	607	CLA	O1D-CGD-O2D-CED
27	b	607	CLA	O1D-CGD-O2D-CED
27	33	309	CLA	O1A-CGA-O2A-C1
27	34	310	CLA	O1A-CGA-O2A-C1
33	W	101	LMG	C11-C10-O7-C8
33	w	101	LMG	C11-C10-O7-C8
27	B	602	CLA	C15-C16-C17-C18
27	B	608	CLA	C8-C10-C11-C12
27	B	613	CLA	C5-C6-C7-C8
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	b	608	CLA	C8-C10-C11-C12
27	b	613	CLA	C5-C6-C7-C8
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
32	B	621	LHG	C4-O6-P-O3
32	L	101	LHG	C4-O6-P-O3
32	L	102	LHG	C3-O3-P-O6
32	b	621	LHG	C4-O6-P-O3
32	l	102	LHG	C4-O6-P-O3
32	l	103	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
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
38	34	316	A86	O5-C38-O4-C34
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
36	d	407	PL9	C7-C8-C9-C10
33	32	301	LMG	C4-C5-C6-O5
32	A	408	LHG	O9-C7-O7-C5
32	a	408	LHG	O9-C7-O7-C5
27	D	406	CLA	C4-C3-C5-C6
27	d	406	CLA	C4-C3-C5-C6
27	D	401	CLA	C13-C15-C16-C17
27	D	405	CLA	C15-C16-C17-C18
27	d	401	CLA	C13-C15-C16-C17
27	d	405	CLA	C15-C16-C17-C18
38	12	304	A86	C35-C34-O4-C38
27	C	502	CLA	C2A-CAA-CBA-CGA
27	c	502	CLA	C2A-CAA-CBA-CGA
27	b	611	CLA	C16-C17-C18-C19
27	B	615	CLA	C3-C5-C6-C7
27	b	615	CLA	C3-C5-C6-C7
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
33	B	619	LMG	C10-C11-C12-C13
33	b	619	LMG	C10-C11-C12-C13
38	11	316	A86	C35-C34-O4-C38
38	13	302	A86	C35-C34-O4-C38
38	13	317	A86	C35-C34-O4-C38
38	31	316	A86	C35-C34-O4-C38
38	32	304	A86	C35-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
38	33	302	A86	C35-C34-O4-C38
38	34	303	A86	C35-C34-O4-C38
33	q	301	LMG	C32-C33-C34-C35
33	12	301	LMG	C12-C13-C14-C15
35	H	102	DGD	C7A-C8A-C9A-CAA
35	h	102	DGD	C7A-C8A-C9A-CAA
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
30	A	406	SQD	C11-C12-C13-C14
30	a	406	SQD	C11-C12-C13-C14
32	B	621	LHG	C11-C10-C9-C8
32	a	408	LHG	C29-C30-C31-C32
32	b	621	LHG	C11-C10-C9-C8
33	B	618	LMG	C31-C32-C33-C34
33	C	519	LMG	C32-C33-C34-C35
33	b	618	LMG	C31-C32-C33-C34
39	12	302	LMU	C5-C6-C7-C8
39	32	302	LMU	C5-C6-C7-C8
27	B	611	CLA	C16-C17-C18-C19
30	A	406	SQD	C10-C11-C12-C13
30	a	406	SQD	C10-C11-C12-C13
32	A	408	LHG	C29-C30-C31-C32
32	a	408	LHG	C15-C16-C17-C18
33	D	408	LMG	C35-C36-C37-C38
33	d	408	LMG	C35-C36-C37-C38
30	L	103	SQD	C46-C45-O47-C7
30	l	101	SQD	C46-C45-O47-C7
35	H	102	DGD	C1B-C2B-C3B-C4B
35	h	102	DGD	C1B-C2B-C3B-C4B
32	A	408	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
32	L	102	LHG	C16-C17-C18-C19
32	l	103	LHG	C16-C17-C18-C19
33	32	301	LMG	C12-C13-C14-C15
27	C	512	CLA	O1D-CGD-O2D-CED
27	c	512	CLA	O1D-CGD-O2D-CED
30	L	103	SQD	C15-C16-C17-C18
30	l	101	SQD	C15-C16-C17-C18
33	W	101	LMG	C20-C21-C22-C23
30	l	101	SQD	C32-C33-C34-C35
33	M	103	LMG	C15-C16-C17-C18
33	M	103	LMG	C33-C34-C35-C36
33	m	102	LMG	C15-C16-C17-C18
33	m	102	LMG	C33-C34-C35-C36
33	w	101	LMG	C20-C21-C22-C23
35	C	518	DGD	C2A-C3A-C4A-C5A
35	c	518	DGD	C2A-C3A-C4A-C5A
32	L	102	LHG	C23-C24-C25-C26
32	l	103	LHG	C23-C24-C25-C26
33	b	619	LMG	C28-C29-C30-C31
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	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	612	CLA	CBA-CGA-O2A-C1
27	b	612	CLA	CBA-CGA-O2A-C1
30	L	103	SQD	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
27	A	404	CLA	C5-C6-C7-C8
27	a	404	CLA	C5-C6-C7-C8
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
27	B	605	CLA	C16-C17-C18-C20
27	b	605	CLA	C16-C17-C18-C20
27	C	507	CLA	C4-C3-C5-C6
27	c	507	CLA	C4-C3-C5-C6
32	l	103	LHG	C32-C33-C34-C35
27	C	504	CLA	C6-C7-C8-C9
27	c	504	CLA	C6-C7-C8-C9
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
32	L	102	LHG	C32-C33-C34-C35
32	a	408	LHG	C28-C29-C30-C31
33	D	408	LMG	C36-C37-C38-C39
33	d	408	LMG	C36-C37-C38-C39
27	D	406	CLA	O1A-CGA-O2A-C1
27	d	406	CLA	O1A-CGA-O2A-C1
32	A	408	LHG	C28-C29-C30-C31
32	L	101	LHG	C24-C25-C26-C27
32	l	102	LHG	C24-C25-C26-C27
33	W	101	LMG	C19-C20-C21-C22
33	d	408	LMG	C30-C31-C32-C33
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
32	L	101	LHG	C25-C26-C27-C28
32	l	102	LHG	C25-C26-C27-C28
33	D	408	LMG	C30-C31-C32-C33
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
33	w	101	LMG	C19-C20-C21-C22
32	A	408	LHG	C7-C8-C9-C10
32	a	408	LHG	C7-C8-C9-C10
32	B	621	LHG	C30-C31-C32-C33
32	b	621	LHG	C30-C31-C32-C33
33	M	103	LMG	C31-C32-C33-C34
33	m	102	LMG	C31-C32-C33-C34
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
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	C	517	DGD	O6D-C1D-O3G-C3G
35	J	101	DGD	O6E-C1E-O5D-C6D
35	c	517	DGD	O6D-C1D-O3G-C3G
35	j	101	DGD	O6E-C1E-O5D-C6D
27	C	508	CLA	C13-C15-C16-C17
27	c	508	CLA	C13-C15-C16-C17
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
35	C	517	DGD	CCA-CDA-CEA-CFA
35	c	517	DGD	CCA-CDA-CEA-CFA
30	A	406	SQD	C32-C33-C34-C35
30	a	406	SQD	C32-C33-C34-C35
33	C	519	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
33	q	301	LMG	C18-C19-C20-C21
35	J	101	DGD	C8A-C9A-CAA-CBA
35	j	101	DGD	C8A-C9A-CAA-CBA
35	C	517	DGD	C7B-C8B-C9B-CAB
35	H	102	DGD	C3A-C4A-C5A-C6A
35	c	517	DGD	C7B-C8B-C9B-CAB
35	h	102	DGD	C3A-C4A-C5A-C6A
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	b	622	CLA	O1D-CGD-O2D-CED
27	m	101	CLA	O1D-CGD-O2D-CED
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
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

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Mol	Chain	Res	Type	Atoms
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
27	C	504	CLA	C8-C10-C11-C12
27	c	504	CLA	C8-C10-C11-C12
39	32	302	LMU	C2-C1-O1'-C1'
33	W	101	LMG	C12-C13-C14-C15
33	w	101	LMG	C12-C13-C14-C15
27	B	605	CLA	C16-C17-C18-C19
27	b	605	CLA	C16-C17-C18-C19
27	B	622	CLA	O1D-CGD-O2D-CED
27	c	505	CLA	CBD-CGD-O2D-CED
27	C	503	CLA	O1D-CGD-O2D-CED
27	B	601	CLA	C3-C5-C6-C7
27	b	601	CLA	C3-C5-C6-C7
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
27	C	511	CLA	C4-C3-C5-C6
27	c	511	CLA	C4-C3-C5-C6
27	C	507	CLA	C2-C3-C5-C6
27	C	511	CLA	C2-C3-C5-C6
27	c	507	CLA	C2-C3-C5-C6
27	c	511	CLA	C2-C3-C5-C6
27	C	505	CLA	CBD-CGD-O2D-CED
32	B	621	LHG	C9-C10-C11-C12
32	b	621	LHG	C9-C10-C11-C12
33	W	101	LMG	C37-C38-C39-C40
33	w	101	LMG	C37-C38-C39-C40
35	C	518	DGD	O6E-C5E-C6E-O5E
35	c	518	DGD	O6E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
30	L	103	SQD	C14-C15-C16-C17
30	l	101	SQD	C14-C15-C16-C17
32	A	408	LHG	C14-C15-C16-C17
32	L	101	LHG	C31-C32-C33-C34
32	a	408	LHG	C14-C15-C16-C17
32	l	102	LHG	C31-C32-C33-C34
27	c	503	CLA	O1D-CGD-O2D-CED
27	B	602	CLA	C2B-C3B-CAB-CBB
27	B	622	CLA	C2B-C3B-CAB-CBB
27	C	505	CLA	C2B-C3B-CAB-CBB
27	W	103	CLA	C2B-C3B-CAB-CBB
27	b	602	CLA	C2B-C3B-CAB-CBB
27	c	505	CLA	C2B-C3B-CAB-CBB
27	w	103	CLA	C2B-C3B-CAB-CBB
27	11	308	CLA	C2B-C3B-CAB-CBB
27	11	309	CLA	C2B-C3B-CAB-CBB
27	12	312	CLA	C2B-C3B-CAB-CBB
27	12	313	CLA	C2B-C3B-CAB-CBB
27	13	310	CLA	C2B-C3B-CAB-CBB
27	13	311	CLA	C2B-C3B-CAB-CBB
27	14	310	CLA	C2B-C3B-CAB-CBB
27	14	311	CLA	C2B-C3B-CAB-CBB
27	31	308	CLA	C2B-C3B-CAB-CBB
27	31	309	CLA	C2B-C3B-CAB-CBB
27	32	312	CLA	C2B-C3B-CAB-CBB
27	32	313	CLA	C2B-C3B-CAB-CBB
27	33	310	CLA	C2B-C3B-CAB-CBB
27	33	311	CLA	C2B-C3B-CAB-CBB
27	34	311	CLA	C2B-C3B-CAB-CBB
27	34	312	CLA	C2B-C3B-CAB-CBB
30	B	620	SQD	C11-C10-C9-C8
30	L	103	SQD	C31-C32-C33-C34
30	l	101	SQD	C31-C32-C33-C34
35	C	518	DGD	CAA-CBA-CCA-CDA
30	b	620	SQD	C11-C10-C9-C8
32	L	101	LHG	C13-C14-C15-C16
32	L	101	LHG	C29-C30-C31-C32
32	l	102	LHG	C29-C30-C31-C32
33	B	619	LMG	C18-C19-C20-C21
33	b	619	LMG	C18-C19-C20-C21
35	c	518	DGD	CAA-CBA-CCA-CDA
38	11	316	A86	C33-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
38	31	316	A86	C33-C34-O4-C38
38	33	302	A86	C33-C34-O4-C38
32	l	102	LHG	C13-C14-C15-C16
33	C	519	LMG	C19-C20-C21-C22
33	D	408	LMG	C17-C18-C19-C20
33	q	301	LMG	C19-C20-C21-C22
39	12	302	LMU	C2-C3-C4-C5
32	L	101	LHG	O9-C7-O7-C5
32	l	102	LHG	O9-C7-O7-C5
27	B	612	CLA	C2-C1-O2A-CGA
27	b	612	CLA	C2-C1-O2A-CGA
30	A	406	SQD	C12-C13-C14-C15
30	a	406	SQD	C12-C13-C14-C15
33	d	408	LMG	C17-C18-C19-C20
27	C	512	CLA	C5-C6-C7-C8
27	c	512	CLA	C5-C6-C7-C8
27	B	612	CLA	O1A-CGA-O2A-C1
27	b	612	CLA	O1A-CGA-O2A-C1
33	C	519	LMG	C4-C5-C6-O5
33	q	301	LMG	C4-C5-C6-O5
30	a	406	SQD	C17-C18-C19-C20
30	L	103	SQD	C7-C8-C9-C10
30	l	101	SQD	C7-C8-C9-C10
29	A	405	BCR	C1-C6-C7-C8
29	A	405	BCR	C5-C6-C7-C8
29	A	409	BCR	C1-C6-C7-C8
29	A	409	BCR	C5-C6-C7-C8
29	B	616	BCR	C5-C6-C7-C8
29	B	617	BCR	C5-C6-C7-C8
29	B	623	BCR	C1-C6-C7-C8
29	B	623	BCR	C5-C6-C7-C8
29	C	515	BCR	C1-C6-C7-C8
29	C	515	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	C	520	BCR	C23-C24-C25-C26
29	C	520	BCR	C23-C24-C25-C30
29	F	101	BCR	C1-C6-C7-C8
29	F	101	BCR	C5-C6-C7-C8
29	H	101	BCR	C5-C6-C7-C8
29	M	101	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	M	101	BCR	C5-C6-C7-C8
29	M	101	BCR	C23-C24-C25-C26
29	Z	101	BCR	C5-C6-C7-C8
29	a	405	BCR	C1-C6-C7-C8
29	a	405	BCR	C5-C6-C7-C8
29	a	409	BCR	C1-C6-C7-C8
29	a	409	BCR	C5-C6-C7-C8
29	b	616	BCR	C5-C6-C7-C8
29	b	617	BCR	C5-C6-C7-C8
29	b	623	BCR	C1-C6-C7-C8
29	b	623	BCR	C5-C6-C7-C8
29	c	515	BCR	C1-C6-C7-C8
29	c	515	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	c	519	BCR	C23-C24-C25-C26
29	c	519	BCR	C23-C24-C25-C30
29	f	101	BCR	C1-C6-C7-C8
29	f	101	BCR	C5-C6-C7-C8
29	h	101	BCR	C5-C6-C7-C8
29	m	103	BCR	C1-C6-C7-C8
29	m	103	BCR	C5-C6-C7-C8
29	m	103	BCR	C23-C24-C25-C26
29	z	101	BCR	C5-C6-C7-C8
30	A	406	SQD	C17-C18-C19-C20
33	b	618	LMG	C29-C30-C31-C32
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
38	12	304	A86	C33-C34-O4-C38
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
33	B	618	LMG	C29-C30-C31-C32
33	C	519	LMG	C10-C11-C12-C13
33	q	301	LMG	C10-C11-C12-C13
39	32	302	LMU	C2-C3-C4-C5
27	C	508	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
27	W	102	CLA	C12-C13-C15-C16
27	W	103	CLA	C6-C7-C8-C10
27	W	103	CLA	C11-C12-C13-C15
27	c	508	CLA	C11-C10-C8-C7
27	w	102	CLA	C12-C13-C15-C16
27	w	103	CLA	C6-C7-C8-C10
27	w	103	CLA	C11-C12-C13-C15
28	A	403	PHO	C2-C3-C5-C6
28	a	403	PHO	C2-C3-C5-C6
36	D	404	PL9	C28-C29-C31-C32
36	d	404	PL9	C28-C29-C31-C32
27	M	102	CLA	O1A-CGA-O2A-C1
27	m	101	CLA	O1A-CGA-O2A-C1
30	A	406	SQD	C14-C15-C16-C17
30	a	406	SQD	C14-C15-C16-C17
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
27	B	602	CLA	C16-C17-C18-C19
27	B	611	CLA	C16-C17-C18-C20
27	b	602	CLA	C16-C17-C18-C19
27	b	611	CLA	C16-C17-C18-C20
35	h	102	DGD	O6D-C5D-C6D-O5D
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
27	B	615	CLA	C2A-CAA-CBA-CGA
27	b	615	CLA	C2A-CAA-CBA-CGA
27	C	502	CLA	C10-C11-C12-C13
27	W	102	CLA	C5-C6-C7-C8
27	c	502	CLA	C10-C11-C12-C13
33	12	301	LMG	C32-C33-C34-C35
32	L	101	LHG	C33-C34-C35-C36
32	l	102	LHG	C33-C34-C35-C36
27	w	102	CLA	C5-C6-C7-C8
27	C	510	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
27	c	510	CLA	C3-C5-C6-C7
30	l	101	SQD	C17-C18-C19-C20
33	12	301	LMG	C14-C15-C16-C17
33	32	301	LMG	C32-C33-C34-C35
35	j	101	DGD	C6A-C7A-C8A-C9A
27	D	405	CLA	C5-C6-C7-C8
27	M	102	CLA	C5-C6-C7-C8
30	L	103	SQD	C12-C13-C14-C15
30	L	103	SQD	C17-C18-C19-C20
33	B	619	LMG	C11-C12-C13-C14
33	C	519	LMG	C17-C18-C19-C20
33	b	619	LMG	C11-C12-C13-C14
33	q	301	LMG	C17-C18-C19-C20
35	J	101	DGD	C6A-C7A-C8A-C9A
30	A	406	SQD	C7-C8-C9-C10
30	a	406	SQD	C7-C8-C9-C10
33	B	619	LMG	C11-C10-O7-C8
33	b	619	LMG	C11-C10-O7-C8
30	l	101	SQD	C12-C13-C14-C15
35	C	517	DGD	C3B-C4B-C5B-C6B
35	c	517	DGD	C3B-C4B-C5B-C6B
27	C	507	CLA	C13-C15-C16-C17
27	b	614	CLA	C15-C16-C17-C18
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	C13-C14-C15-C16
32	a	408	LHG	C13-C14-C15-C16
33	C	519	LMG	O9-C10-O7-C8
33	W	101	LMG	O9-C10-O7-C8
33	w	101	LMG	O9-C10-O7-C8
39	12	302	LMU	C4-C5-C6-C7
27	B	614	CLA	C15-C16-C17-C18
27	c	514	CLA	C15-C16-C17-C18
30	B	620	SQD	O47-C45-C46-O48
30	b	620	SQD	O47-C45-C46-O48
27	C	503	CLA	C13-C15-C16-C17
27	C	514	CLA	C15-C16-C17-C18
27	c	503	CLA	C13-C15-C16-C17
27	B	609	CLA	C2-C3-C5-C6
27	D	406	CLA	C2-C3-C5-C6
27	b	609	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	d	406	CLA	C2-C3-C5-C6
27	B	615	CLA	C6-C7-C8-C9
27	C	503	CLA	C11-C12-C13-C14
27	C	505	CLA	C6-C7-C8-C9
27	W	102	CLA	C14-C13-C15-C16
27	W	103	CLA	C6-C7-C8-C9
27	b	615	CLA	C6-C7-C8-C9
27	c	503	CLA	C11-C12-C13-C14
27	c	505	CLA	C6-C7-C8-C9
27	w	102	CLA	C14-C13-C15-C16
27	w	103	CLA	C6-C7-C8-C9
27	11	307	CLA	C6-C7-C8-C9
27	12	311	CLA	C6-C7-C8-C9
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
27	C	507	CLA	C2A-CAA-CBA-CGA
27	M	102	CLA	C2A-CAA-CBA-CGA
27	c	507	CLA	C2A-CAA-CBA-CGA
27	m	101	CLA	C2A-CAA-CBA-CGA
32	L	101	LHG	C28-C29-C30-C31
32	l	102	LHG	C28-C29-C30-C31
33	W	101	LMG	C18-C19-C20-C21
33	w	101	LMG	C18-C19-C20-C21
29	a	405	BCR	C11-C12-C13-C14
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

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Mol	Chain	Res	Type	Atoms
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
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	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	q	301	LMG	O9-C10-O7-C8
33	32	301	LMG	C15-C16-C17-C18
29	B	623	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
29	b	623	BCR	C13-C14-C15-C16
39	12	302	LMU	C1-C2-C3-C4
32	A	408	LHG	C3-O3-P-O6
32	B	621	LHG	C3-O3-P-O6
32	a	408	LHG	C3-O3-P-O6
32	b	621	LHG	C3-O3-P-O6
32	B	621	LHG	C33-C34-C35-C36
32	L	101	LHG	C32-C33-C34-C35
32	l	102	LHG	C32-C33-C34-C35
35	C	517	DGD	CBA-CCA-CDA-CEA
35	c	517	DGD	CBA-CCA-CDA-CEA
32	b	621	LHG	C33-C34-C35-C36
33	W	101	LMG	C17-C18-C19-C20
33	w	101	LMG	C17-C18-C19-C20
27	C	505	CLA	C10-C11-C12-C13
27	c	505	CLA	C10-C11-C12-C13
32	B	621	LHG	O6-C4-C5-C6
32	b	621	LHG	O6-C4-C5-C6
27	C	507	CLA	C8-C10-C11-C12
27	c	507	CLA	C8-C10-C11-C12
33	D	408	LMG	O6-C5-C6-O5
33	d	408	LMG	O6-C5-C6-O5
33	B	619	LMG	C31-C32-C33-C34
33	b	619	LMG	C31-C32-C33-C34
39	32	302	LMU	C4-C5-C6-C7
27	B	601	CLA	C10-C11-C12-C13
27	b	601	CLA	C10-C11-C12-C13
35	J	101	DGD	O1B-C1B-O2G-C2G
35	j	101	DGD	O1B-C1B-O2G-C2G
33	w	101	LMG	C30-C31-C32-C33
33	W	101	LMG	C30-C31-C32-C33
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
27	B	610	CLA	C16-C17-C18-C19
27	b	610	CLA	C16-C17-C18-C19
32	A	408	LHG	C4-C5-C6-O8
32	a	408	LHG	C4-C5-C6-O8
32	a	408	LHG	C30-C31-C32-C33
33	D	408	LMG	O1-C7-C8-C9
33	W	101	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
33	W	101	LMG	C7-C8-C9-O8
33	d	408	LMG	O1-C7-C8-C9
33	w	101	LMG	O1-C7-C8-C9
33	w	101	LMG	C7-C8-C9-O8
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	A	408	LHG	C30-C31-C32-C33
33	B	618	LMG	C30-C31-C32-C33
33	B	619	LMG	C34-C35-C36-C37
33	b	618	LMG	C30-C31-C32-C33
33	b	619	LMG	C34-C35-C36-C37
35	H	102	DGD	C1A-C2A-C3A-C4A
35	h	102	DGD	C1A-C2A-C3A-C4A
35	C	518	DGD	C5D-C6D-O5D-C1E
35	c	518	DGD	C5D-C6D-O5D-C1E
27	B	604	CLA	C13-C15-C16-C17
27	b	604	CLA	C13-C15-C16-C17
27	c	511	CLA	C5-C6-C7-C8
33	B	619	LMG	C13-C14-C15-C16
33	C	519	LMG	C37-C38-C39-C40
33	q	301	LMG	C37-C38-C39-C40
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
32	L	102	LHG	C13-C14-C15-C16
32	l	103	LHG	C13-C14-C15-C16
32	L	101	LHG	O1-C1-C2-O2
32	l	102	LHG	O1-C1-C2-O2
35	H	102	DGD	CBA-CCA-CDA-CEA
35	h	102	DGD	CBA-CCA-CDA-CEA
39	32	302	LMU	C1-C2-C3-C4
32	B	621	LHG	C27-C28-C29-C30
32	b	621	LHG	C27-C28-C29-C30
27	C	509	CLA	C5-C6-C7-C8
27	c	509	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
35	C	517	DGD	O6E-C5E-C6E-O5E
35	c	517	DGD	O6E-C5E-C6E-O5E
27	B	609	CLA	C4-C3-C5-C6
27	b	609	CLA	C4-C3-C5-C6
28	A	403	PHO	C4-C3-C5-C6
28	a	403	PHO	C4-C3-C5-C6
35	H	102	DGD	CBB-CCB-CDB-CEB
35	h	102	DGD	CBB-CCB-CDB-CEB
27	C	502	CLA	CBA-CGA-O2A-C1
27	c	502	CLA	CBA-CGA-O2A-C1
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
28	D	403	PHO	C5-C6-C7-C8
28	d	403	PHO	C5-C6-C7-C8
27	34	309	CLA	O1D-CGD-O2D-CED
35	j	101	DGD	CDA-CEA-CFA-CGA
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
33	W	101	LMG	C15-C16-C17-C18
33	w	101	LMG	C15-C16-C17-C18
35	J	101	DGD	CDA-CEA-CFA-CGA
30	L	103	SQD	C24-C23-O48-C46
30	l	101	SQD	C24-C23-O48-C46
32	l	103	LHG	O10-C23-O8-C6
27	Z	102	CLA	C16-C17-C18-C19
27	z	102	CLA	C16-C17-C18-C19
27	B	611	CLA	C15-C16-C17-C18
27	b	611	CLA	C15-C16-C17-C18
27	C	513	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	c	513	CLA	O1D-CGD-O2D-CED
32	L	102	LHG	O10-C23-O8-C6
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
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	L	101	LHG	C27-C28-C29-C30
32	l	102	LHG	C27-C28-C29-C30
27	C	506	CLA	C4-C3-C5-C6
27	c	506	CLA	C4-C3-C5-C6
27	B	601	CLA	C11-C10-C8-C7
27	B	610	CLA	C12-C13-C15-C16
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	506	CLA	C2-C3-C5-C6
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	Z	102	CLA	C11-C12-C13-C15
27	b	601	CLA	C11-C10-C8-C7
27	b	610	CLA	C12-C13-C15-C16
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	506	CLA	C2-C3-C5-C6
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	z	102	CLA	C11-C12-C13-C15
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

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Mol	Chain	Res	Type	Atoms
27	34	304	CLA	C11-C10-C8-C7
33	B	619	LMG	C21-C22-C23-C24
33	b	619	LMG	C21-C22-C23-C24
27	B	605	CLA	C11-C12-C13-C14
27	B	606	CLA	C11-C10-C8-C9
27	B	607	CLA	C14-C13-C15-C16
27	B	610	CLA	C14-C13-C15-C16
27	B	622	CLA	C6-C7-C8-C9
27	B	622	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	C	508	CLA	C11-C10-C8-C9
27	C	513	CLA	C11-C10-C8-C9
27	Z	102	CLA	C6-C7-C8-C9
27	W	103	CLA	C11-C12-C13-C14
27	W	103	CLA	C14-C13-C15-C16
27	b	605	CLA	C11-C12-C13-C14
27	b	606	CLA	C11-C10-C8-C9
27	b	607	CLA	C14-C13-C15-C16
27	b	610	CLA	C14-C13-C15-C16
27	b	622	CLA	C6-C7-C8-C9
27	b	622	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	c	508	CLA	C11-C10-C8-C9
27	c	513	CLA	C11-C10-C8-C9
27	z	102	CLA	C6-C7-C8-C9
27	w	103	CLA	C11-C12-C13-C14
27	w	103	CLA	C14-C13-C15-C16
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
27	11	303	CLA	CBA-CGA-O2A-C1
27	11	315	CLA	CBA-CGA-O2A-C1
27	12	303	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	12	307	CLA	CBA-CGA-O2A-C1
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
32	A	408	LHG	C32-C33-C34-C35
32	a	408	LHG	C32-C33-C34-C35
35	h	102	DGD	C5A-C6A-C7A-C8A
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
33	M	103	LMG	C16-C17-C18-C19
33	m	102	LMG	C16-C17-C18-C19
35	H	102	DGD	C5A-C6A-C7A-C8A
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
35	C	518	DGD	C5A-C6A-C7A-C8A
35	c	518	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
27	B	608	CLA	C13-C15-C16-C17
27	b	608	CLA	C13-C15-C16-C17
35	H	102	DGD	CCB-CDB-CEB-CFB
33	M	103	LMG	C29-C28-O8-C9
33	m	102	LMG	C29-C28-O8-C9
35	h	102	DGD	CCB-CDB-CEB-CFB
32	l	103	LHG	C30-C31-C32-C33
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
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
27	Z	102	CLA	C16-C17-C18-C20
27	z	102	CLA	C16-C17-C18-C20
27	C	513	CLA	C13-C15-C16-C17
27	c	513	CLA	C13-C15-C16-C17
32	L	101	LHG	O6-C4-C5-C6
32	l	102	LHG	O6-C4-C5-C6
32	B	621	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
32	L	102	LHG	C30-C31-C32-C33
32	b	621	LHG	C32-C33-C34-C35
33	D	408	LMG	C20-C21-C22-C23
35	c	517	DGD	C5A-C6A-C7A-C8A
35	c	518	DGD	C4A-C5A-C6A-C7A
33	B	618	LMG	C13-C14-C15-C16
33	b	618	LMG	C13-C14-C15-C16
33	d	408	LMG	C20-C21-C22-C23
35	C	517	DGD	C5A-C6A-C7A-C8A
35	C	518	DGD	C4A-C5A-C6A-C7A
27	B	606	CLA	C13-C15-C16-C17
27	b	606	CLA	C13-C15-C16-C17
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	611	CLA	CBA-CGA-O2A-C1
27	B	601	CLA	C3A-C2A-CAA-CBA
27	C	513	CLA	C3A-C2A-CAA-CBA
27	b	601	CLA	C3A-C2A-CAA-CBA
27	b	622	CLA	C3A-C2A-CAA-CBA
27	c	513	CLA	C3A-C2A-CAA-CBA
32	A	408	LHG	C12-C13-C14-C15
32	a	408	LHG	C12-C13-C14-C15
38	11	310	A86	O-C13-C14-C15
38	11	312	A86	O-C13-C14-C15
38	12	314	A86	O-C13-C14-C15
38	12	316	A86	O-C13-C14-C15
38	13	312	A86	O-C13-C14-C15
38	13	314	A86	O-C13-C14-C15
38	14	312	A86	O-C13-C14-C15
38	14	314	A86	O-C13-C14-C15
38	31	310	A86	O-C13-C14-C15
38	31	312	A86	O-C13-C14-C15
38	32	314	A86	O-C13-C14-C15
38	32	316	A86	O-C13-C14-C15
38	33	312	A86	O-C13-C14-C15
38	33	314	A86	O-C13-C14-C15
38	34	313	A86	O-C13-C14-C15
38	34	315	A86	O-C13-C14-C15
27	b	611	CLA	CBA-CGA-O2A-C1
30	L	103	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
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	q	301	LMG	O1-C7-C8-C9
35	C	517	DGD	C1G-C2G-C3G-O3G
35	c	517	DGD	C1G-C2G-C3G-O3G
30	A	406	SQD	C28-C29-C30-C31
30	a	406	SQD	C28-C29-C30-C31
30	l	101	SQD	C25-C26-C27-C28
32	l	103	LHG	C9-C10-C11-C12
36	D	407	PL9	C32-C33-C34-C36
36	d	407	PL9	C32-C33-C34-C36
32	L	102	LHG	C9-C10-C11-C12
33	D	408	LMG	C34-C35-C36-C37
33	W	101	LMG	C32-C33-C34-C35
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	505	CLA	O1D-CGD-O2D-CED
27	b	609	CLA	C5-C6-C7-C8
33	C	519	LMG	C28-C29-C30-C31
33	q	301	LMG	C28-C29-C30-C31
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
27	C	505	CLA	O1D-CGD-O2D-CED
27	W	102	CLA	O1D-CGD-O2D-CED
27	w	102	CLA	O1D-CGD-O2D-CED
32	B	621	LHG	O6-C4-C5-O7
32	L	101	LHG	O6-C4-C5-O7
32	b	621	LHG	O6-C4-C5-O7
32	l	102	LHG	O6-C4-C5-O7
35	H	102	DGD	C6A-C7A-C8A-C9A
35	h	102	DGD	C6A-C7A-C8A-C9A
27	C	502	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	c	502	CLA	O1A-CGA-O2A-C1
33	B	619	LMG	C19-C20-C21-C22
27	B	609	CLA	C2B-C3B-CAB-CBB
27	B	611	CLA	C2B-C3B-CAB-CBB
27	C	512	CLA	C2B-C3B-CAB-CBB
27	D	406	CLA	C2B-C3B-CAB-CBB
27	b	609	CLA	C2B-C3B-CAB-CBB
27	b	611	CLA	C2B-C3B-CAB-CBB
27	b	622	CLA	C2B-C3B-CAB-CBB
27	c	512	CLA	C2B-C3B-CAB-CBB
27	d	406	CLA	C2B-C3B-CAB-CBB
27	11	306	CLA	C2B-C3B-CAB-CBB
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
32	L	102	LHG	C29-C30-C31-C32
32	l	103	LHG	C29-C30-C31-C32
33	W	101	LMG	C22-C23-C24-C25
33	b	619	LMG	C19-C20-C21-C22
33	w	101	LMG	C22-C23-C24-C25
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
27	C	514	CLA	CBA-CGA-O2A-C1
27	c	514	CLA	CBA-CGA-O2A-C1
32	A	408	LHG	C8-C7-O7-C5
27	B	605	CLA	CBD-CGD-O2D-CED
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

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Mol	Chain	Res	Type	Atoms
38	34	316	A86	C10-C11-C13-C14
27	A	402	CLA	C2-C1-O2A-CGA
27	B	615	CLA	C2-C1-O2A-CGA
27	a	402	CLA	C2-C1-O2A-CGA
27	b	615	CLA	C2-C1-O2A-CGA
27	B	613	CLA	C8-C10-C11-C12
27	b	613	CLA	C8-C10-C11-C12
27	A	404	CLA	C11-C10-C8-C9
27	B	605	CLA	C6-C7-C8-C9
27	C	504	CLA	C11-C12-C13-C14
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	a	404	CLA	C11-C10-C8-C9
27	b	605	CLA	C6-C7-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	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	b	605	CLA	CBD-CGD-O2D-CED
32	L	102	LHG	C10-C11-C12-C13
32	L	101	LHG	C17-C18-C19-C20
32	l	103	LHG	C10-C11-C12-C13
33	B	618	LMG	C38-C39-C40-C41
33	C	519	LMG	C30-C31-C32-C33
33	b	618	LMG	C38-C39-C40-C41
33	d	408	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
33	q	301	LMG	C30-C31-C32-C33
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
27	D	402	CLA	C16-C17-C18-C19
27	d	402	CLA	C16-C17-C18-C19
29	A	405	BCR	C23-C24-C25-C26
29	A	405	BCR	C23-C24-C25-C30
29	A	409	BCR	C23-C24-C25-C26
29	A	409	BCR	C23-C24-C25-C30
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	F	101	BCR	C23-C24-C25-C30
29	H	101	BCR	C23-C24-C25-C26
29	Z	101	BCR	C1-C6-C7-C8
29	Z	101	BCR	C23-C24-C25-C26
29	Z	101	BCR	C23-C24-C25-C30
29	a	405	BCR	C23-C24-C25-C26
29	a	405	BCR	C23-C24-C25-C30
29	a	409	BCR	C23-C24-C25-C26
29	a	409	BCR	C23-C24-C25-C30
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	f	101	BCR	C23-C24-C25-C30
29	h	101	BCR	C23-C24-C25-C26
29	z	101	BCR	C1-C6-C7-C8
29	z	101	BCR	C23-C24-C25-C26
29	z	101	BCR	C23-C24-C25-C30
32	l	102	LHG	C17-C18-C19-C20
33	D	408	LMG	C39-C40-C41-C42
35	H	102	DGD	C3B-C4B-C5B-C6B
35	C	518	DGD	C4E-C5E-C6E-O5E
35	c	518	DGD	C4E-C5E-C6E-O5E
33	B	619	LMG	C17-C18-C19-C20
35	h	102	DGD	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
35	C	517	DGD	C6B-C7B-C8B-C9B
35	c	517	DGD	C6B-C7B-C8B-C9B
32	a	408	LHG	C8-C7-O7-C5
33	C	519	LMG	C11-C10-O7-C8
33	q	301	LMG	C11-C10-O7-C8
33	b	619	LMG	C17-C18-C19-C20
27	b	613	CLA	CBD-CGD-O2D-CED
35	C	517	DGD	C9A-CAA-CBA-CCA
35	c	517	DGD	C9A-CAA-CBA-CCA
33	12	301	LMG	C13-C14-C15-C16
33	32	301	LMG	C11-C12-C13-C14
32	L	102	LHG	O6-C4-C5-C6
32	l	103	LHG	O6-C4-C5-C6
33	C	519	LMG	C33-C34-C35-C36
33	q	301	LMG	C33-C34-C35-C36
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	612	CLA	C11-C10-C8-C7
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	508	CLA	C12-C13-C15-C16
27	C	510	CLA	C12-C13-C15-C16
27	C	514	CLA	C12-C13-C15-C16
27	D	402	CLA	C11-C10-C8-C7
27	D	405	CLA	C11-C12-C13-C15
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	612	CLA	C11-C10-C8-C7
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	508	CLA	C12-C13-C15-C16
27	c	510	CLA	C12-C13-C15-C16
27	c	514	CLA	C12-C13-C15-C16
27	d	402	CLA	C11-C10-C8-C7
27	d	405	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
27	z	102	CLA	C6-C7-C8-C10
27	11	303	CLA	C11-C12-C13-C15
27	11	307	CLA	C12-C13-C15-C16
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	12	311	CLA	C12-C13-C15-C16
27	13	301	CLA	C12-C13-C15-C16
27	13	305	CLA	C11-C12-C13-C15
27	13	309	CLA	C12-C13-C15-C16
27	14	302	CLA	C12-C13-C15-C16
27	14	305	CLA	C11-C12-C13-C15
27	14	309	CLA	C12-C13-C15-C16
27	31	303	CLA	C11-C12-C13-C15
27	31	307	CLA	C12-C13-C15-C16
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	32	311	CLA	C12-C13-C15-C16
27	33	301	CLA	C12-C13-C15-C16
27	33	305	CLA	C11-C12-C13-C15
27	33	309	CLA	C12-C13-C15-C16
27	34	302	CLA	C12-C13-C15-C16
27	34	306	CLA	C11-C12-C13-C15
27	34	310	CLA	C12-C13-C15-C16
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
27	B	613	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
33	12	301	LMG	C11-C12-C13-C14
27	B	604	CLA	CBA-CGA-O2A-C1
27	D	405	CLA	C2A-CAA-CBA-CGA
27	d	405	CLA	C2A-CAA-CBA-CGA
29	C	516	BCR	C35-C13-C14-C15
29	c	516	BCR	C35-C13-C14-C15
35	C	518	DGD	C1B-C2B-C3B-C4B
35	c	518	DGD	C1B-C2B-C3B-C4B
32	B	621	LHG	C34-C35-C36-C37
32	b	621	LHG	C34-C35-C36-C37
35	J	101	DGD	C4A-C5A-C6A-C7A
35	j	101	DGD	C4A-C5A-C6A-C7A
27	C	503	CLA	CBA-CGA-O2A-C1
27	b	604	CLA	CBA-CGA-O2A-C1
27	c	503	CLA	CBA-CGA-O2A-C1
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	601	CLA	CAD-CBD-CGD-O2D
27	B	613	CLA	CAD-CBD-CGD-O2D
27	C	513	CLA	CAD-CBD-CGD-O2D
27	C	514	CLA	CAD-CBD-CGD-O2D
27	W	102	CLA	CAD-CBD-CGD-O2D
27	W	103	CLA	CAD-CBD-CGD-O2D
27	b	601	CLA	CAD-CBD-CGD-O2D
27	b	613	CLA	CAD-CBD-CGD-O2D
27	c	513	CLA	CAD-CBD-CGD-O2D
27	c	514	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
28	A	403	PHO	CAD-CBD-CGD-O2D
28	a	403	PHO	CAD-CBD-CGD-O2D
27	C	509	CLA	C13-C15-C16-C17
27	D	402	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
27	c	509	CLA	C13-C15-C16-C17
27	d	401	CLA	C10-C11-C12-C13
27	d	402	CLA	C13-C15-C16-C17
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
27	C	504	CLA	C4-C3-C5-C6
27	c	504	CLA	C4-C3-C5-C6
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
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
38	34	303	A86	C12-C11-C13-O
27	C	514	CLA	O1A-CGA-O2A-C1
27	c	514	CLA	O1A-CGA-O2A-C1
37	V	201	HEM	C4C-C3C-CAC-CBC
37	v	201	HEM	C4C-C3C-CAC-CBC
35	C	518	DGD	O1A-C1A-O1G-C1G
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
32	L	102	LHG	C33-C34-C35-C36
32	l	103	LHG	C33-C34-C35-C36
27	B	609	CLA	CHA-CBD-CGD-O1D
27	B	609	CLA	CHA-CBD-CGD-O2D
27	B	610	CLA	CHA-CBD-CGD-O1D
27	B	612	CLA	CHA-CBD-CGD-O1D
27	B	612	CLA	CHA-CBD-CGD-O2D
27	B	615	CLA	CHA-CBD-CGD-O1D
27	C	503	CLA	CHA-CBD-CGD-O1D
27	C	503	CLA	CHA-CBD-CGD-O2D
27	C	507	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
27	C	508	CLA	CHA-CBD-CGD-O1D
27	C	509	CLA	CHA-CBD-CGD-O1D
27	C	509	CLA	CHA-CBD-CGD-O2D
27	C	510	CLA	CHA-CBD-CGD-O1D
27	C	510	CLA	CHA-CBD-CGD-O2D
27	C	512	CLA	CHA-CBD-CGD-O2D
27	b	609	CLA	CHA-CBD-CGD-O1D
27	b	609	CLA	CHA-CBD-CGD-O2D
27	b	610	CLA	CHA-CBD-CGD-O1D
27	b	612	CLA	CHA-CBD-CGD-O1D
27	b	612	CLA	CHA-CBD-CGD-O2D
27	b	615	CLA	CHA-CBD-CGD-O1D
27	c	503	CLA	CHA-CBD-CGD-O1D
27	c	503	CLA	CHA-CBD-CGD-O2D
27	c	507	CLA	CHA-CBD-CGD-O1D
27	c	508	CLA	CHA-CBD-CGD-O1D
27	c	509	CLA	CHA-CBD-CGD-O1D
27	c	509	CLA	CHA-CBD-CGD-O2D
27	c	510	CLA	CHA-CBD-CGD-O1D
27	c	510	CLA	CHA-CBD-CGD-O2D
27	c	512	CLA	CHA-CBD-CGD-O2D
27	11	303	CLA	CHA-CBD-CGD-O1D
27	11	303	CLA	CHA-CBD-CGD-O2D
27	11	305	CLA	CHA-CBD-CGD-O2D
27	11	308	CLA	CHA-CBD-CGD-O1D
27	11	308	CLA	CHA-CBD-CGD-O2D
27	12	307	CLA	CHA-CBD-CGD-O1D
27	12	307	CLA	CHA-CBD-CGD-O2D
27	12	309	CLA	CHA-CBD-CGD-O2D
27	12	312	CLA	CHA-CBD-CGD-O1D
27	12	312	CLA	CHA-CBD-CGD-O2D
27	13	305	CLA	CHA-CBD-CGD-O1D
27	13	305	CLA	CHA-CBD-CGD-O2D
27	13	307	CLA	CHA-CBD-CGD-O2D
27	13	310	CLA	CHA-CBD-CGD-O1D
27	13	310	CLA	CHA-CBD-CGD-O2D
27	14	305	CLA	CHA-CBD-CGD-O1D
27	14	305	CLA	CHA-CBD-CGD-O2D
27	14	307	CLA	CHA-CBD-CGD-O2D
27	14	310	CLA	CHA-CBD-CGD-O1D
27	14	310	CLA	CHA-CBD-CGD-O2D
27	31	303	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
27	31	303	CLA	CHA-CBD-CGD-O2D
27	31	305	CLA	CHA-CBD-CGD-O2D
27	31	308	CLA	CHA-CBD-CGD-O1D
27	31	308	CLA	CHA-CBD-CGD-O2D
27	32	307	CLA	CHA-CBD-CGD-O1D
27	32	307	CLA	CHA-CBD-CGD-O2D
27	32	309	CLA	CHA-CBD-CGD-O2D
27	32	312	CLA	CHA-CBD-CGD-O1D
27	32	312	CLA	CHA-CBD-CGD-O2D
27	33	305	CLA	CHA-CBD-CGD-O1D
27	33	305	CLA	CHA-CBD-CGD-O2D
27	33	307	CLA	CHA-CBD-CGD-O2D
27	33	310	CLA	CHA-CBD-CGD-O1D
27	33	310	CLA	CHA-CBD-CGD-O2D
27	34	306	CLA	CHA-CBD-CGD-O1D
27	34	306	CLA	CHA-CBD-CGD-O2D
27	34	308	CLA	CHA-CBD-CGD-O2D
27	34	311	CLA	CHA-CBD-CGD-O1D
27	34	311	CLA	CHA-CBD-CGD-O2D
27	c	510	CLA	C5-C6-C7-C8
27	33	303	CLA	C5-C6-C7-C8
27	B	611	CLA	O1A-CGA-O2A-C1
27	b	611	CLA	O1A-CGA-O2A-C1
35	c	518	DGD	O1A-C1A-O1G-C1G
29	A	409	BCR	C11-C10-C9-C8
29	a	409	BCR	C11-C10-C9-C8
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
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
32	L	102	LHG	C27-C28-C29-C30
32	l	103	LHG	C27-C28-C29-C30
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	11	301	CLA	C5-C6-C7-C8
27	13	303	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	14	303	CLA	C5-C6-C7-C8
27	32	305	CLA	C5-C6-C7-C8
28	D	403	PHO	C16-C17-C18-C20
38	11	313	A86	C10-C11-C13-O
38	11	316	A86	C10-C11-C13-O
38	11	316	A86	C13-C14-C15-O1
38	12	304	A86	C10-C11-C13-O
38	12	304	A86	C13-C14-C15-O1
38	12	317	A86	C10-C11-C13-O
38	13	302	A86	C10-C11-C13-O
38	13	302	A86	C13-C14-C15-O1
38	13	315	A86	C10-C11-C13-O
38	13	317	A86	C10-C11-C13-O
38	13	317	A86	C13-C14-C15-O1
38	14	315	A86	C10-C11-C13-O
38	31	313	A86	C10-C11-C13-O
38	31	316	A86	C10-C11-C13-O
38	31	316	A86	C13-C14-C15-O1
38	32	304	A86	C10-C11-C13-O
38	32	304	A86	C13-C14-C15-O1
38	32	317	A86	C10-C11-C13-O
38	33	302	A86	C10-C11-C13-O
38	33	302	A86	C13-C14-C15-O1
38	33	315	A86	C10-C11-C13-O
38	34	303	A86	C10-C11-C13-O
38	34	303	A86	C13-C14-C15-O1
38	34	316	A86	C10-C11-C13-O
33	W	101	LMG	C16-C17-C18-C19
33	w	101	LMG	C16-C17-C18-C19
27	12	305	CLA	C5-C6-C7-C8
27	34	304	CLA	C5-C6-C7-C8
27	D	401	CLA	C4-C3-C5-C6
27	d	401	CLA	C4-C3-C5-C6
27	31	301	CLA	C5-C6-C7-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
28	d	403	PHO	C16-C17-C18-C20
27	B	613	CLA	O1D-CGD-O2D-CED
27	C	503	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	c	503	CLA	O1A-CGA-O2A-C1
29	B	616	BCR	C11-C12-C13-C35
29	b	616	BCR	C11-C12-C13-C35
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
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	C	509	CLA	C1A-C2A-CAA-CBA
27	c	509	CLA	C1A-C2A-CAA-CBA
27	C	507	CLA	C16-C17-C18-C20
27	c	507	CLA	C16-C17-C18-C20
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
35	c	518	DGD	C6B-C7B-C8B-C9B
27	D	401	CLA	C2-C1-O2A-CGA
27	W	103	CLA	C2-C1-O2A-CGA
27	d	401	CLA	C2-C1-O2A-CGA
27	w	103	CLA	C2-C1-O2A-CGA
33	B	618	LMG	C19-C20-C21-C22
35	C	518	DGD	C6B-C7B-C8B-C9B
27	b	613	CLA	O1D-CGD-O2D-CED
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	b	621	LHG	C28-C29-C30-C31
33	b	618	LMG	C19-C20-C21-C22
35	c	518	DGD	CBB-CCB-CDB-CEB
32	B	621	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
35	C	518	DGD	CBB-CCB-CDB-CEB
27	13	305	CLA	C10-C11-C12-C13
27	B	608	CLA	C4B-C3B-CAB-CBB
27	W	102	CLA	C4B-C3B-CAB-CBB
27	b	608	CLA	C4B-C3B-CAB-CBB
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
32	A	408	LHG	C3-O3-P-O4
32	A	408	LHG	C4-O6-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	a	408	LHG	C3-O3-P-O4
32	a	408	LHG	C4-O6-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
27	z	102	CLA	CBD-CGD-O2D-CED
33	b	618	LMG	C18-C19-C20-C21
27	b	604	CLA	O1A-CGA-O2A-C1
33	B	618	LMG	C18-C19-C20-C21
33	12	301	LMG	C30-C31-C32-C33
27	C	508	CLA	C5-C6-C7-C8
27	D	405	CLA	C13-C15-C16-C17
27	c	508	CLA	C5-C6-C7-C8
27	d	405	CLA	C13-C15-C16-C17
37	E	101	HEM	C2A-CAA-CBA-CGA
37	f	102	HEM	C2A-CAA-CBA-CGA
27	B	604	CLA	O1A-CGA-O2A-C1
27	D	401	CLA	C16-C17-C18-C19
27	d	401	CLA	C16-C17-C18-C19
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	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	11	303	CLA	CAD-CBD-CGD-O1D
27	11	305	CLA	CAD-CBD-CGD-O1D
27	12	307	CLA	CAD-CBD-CGD-O1D
27	12	309	CLA	CAD-CBD-CGD-O1D
27	13	305	CLA	CAD-CBD-CGD-O1D
27	13	307	CLA	CAD-CBD-CGD-O1D
27	14	305	CLA	CAD-CBD-CGD-O1D
27	14	307	CLA	CAD-CBD-CGD-O1D
27	31	303	CLA	CAD-CBD-CGD-O1D
27	31	305	CLA	CAD-CBD-CGD-O1D
27	32	307	CLA	CAD-CBD-CGD-O1D
27	32	309	CLA	CAD-CBD-CGD-O1D
27	33	305	CLA	CAD-CBD-CGD-O1D
27	33	307	CLA	CAD-CBD-CGD-O1D
27	34	306	CLA	CAD-CBD-CGD-O1D
27	34	308	CLA	CAD-CBD-CGD-O1D
35	C	517	DGD	C4D-C5D-C6D-O5D
35	H	102	DGD	CCA-CDA-CEA-CFA
33	b	619	LMG	C22-C23-C24-C25
35	h	102	DGD	CCA-CDA-CEA-CFA
35	c	517	DGD	C4D-C5D-C6D-O5D
33	B	619	LMG	C22-C23-C24-C25
27	Z	102	CLA	CBD-CGD-O2D-CED
27	B	601	CLA	C12-C13-C15-C16
27	C	504	CLA	C11-C12-C13-C15
27	C	506	CLA	C11-C12-C13-C15
27	C	509	CLA	C6-C7-C8-C10
27	Z	102	CLA	C12-C13-C15-C16
27	b	601	CLA	C12-C13-C15-C16
27	c	504	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
27	c	506	CLA	C11-C12-C13-C15
27	c	509	CLA	C6-C7-C8-C10
27	z	102	CLA	C12-C13-C15-C16
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
27	33	311	CLA	C3A-C2A-CAA-CBA
27	34	312	CLA	C3A-C2A-CAA-CBA
28	A	403	PHO	C11-C10-C8-C7
28	a	403	PHO	C11-C10-C8-C7
32	L	101	LHG	C23-C24-C25-C26
32	L	102	LHG	O6-C4-C5-O7
32	l	103	LHG	O6-C4-C5-O7
33	32	301	LMG	C16-C17-C18-C19
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
35	C	517	DGD	O6D-C5D-C6D-O5D
35	c	517	DGD	O6D-C5D-C6D-O5D
32	L	102	LHG	C35-C36-C37-C38
32	l	102	LHG	C23-C24-C25-C26
32	l	103	LHG	C35-C36-C37-C38
35	C	518	DGD	C7B-C8B-C9B-CAB
35	c	518	DGD	C7B-C8B-C9B-CAB
27	C	514	CLA	C16-C17-C18-C19
27	c	514	CLA	C16-C17-C18-C19
35	C	518	DGD	C1A-C2A-C3A-C4A
35	c	518	DGD	C1A-C2A-C3A-C4A
33	b	618	LMG	C16-C17-C18-C19
33	w	101	LMG	C38-C39-C40-C41
35	C	517	DGD	C2D-C1D-O3G-C3G
35	c	517	DGD	C2D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
33	B	618	LMG	C16-C17-C18-C19
33	W	101	LMG	C38-C39-C40-C41
35	h	102	DGD	C5B-C6B-C7B-C8B
28	A	403	PHO	C5-C6-C7-C8
36	D	404	PL9	C30-C29-C31-C32
36	d	404	PL9	C30-C29-C31-C32
35	H	102	DGD	C5B-C6B-C7B-C8B
27	D	401	CLA	C2-C3-C5-C6
27	d	401	CLA	C2-C3-C5-C6
27	B	612	CLA	C11-C10-C8-C9
27	B	622	CLA	C11-C12-C13-C14
27	C	502	CLA	C14-C13-C15-C16
27	C	508	CLA	C14-C13-C15-C16
27	D	405	CLA	C11-C12-C13-C14
27	Z	102	CLA	C14-C13-C15-C16
27	b	612	CLA	C11-C10-C8-C9
27	b	622	CLA	C11-C12-C13-C14
27	c	502	CLA	C14-C13-C15-C16
27	c	508	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
28	a	403	PHO	C5-C6-C7-C8
35	J	101	DGD	CDB-CEB-CFB-CGB
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
35	j	101	DGD	CDB-CEB-CFB-CGB
32	L	102	LHG	C12-C13-C14-C15
32	l	103	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
33	w	101	LMG	C21-C22-C23-C24
33	w	101	LMG	C36-C37-C38-C39
33	W	101	LMG	C21-C22-C23-C24
33	W	101	LMG	C36-C37-C38-C39
27	B	610	CLA	C2B-C3B-CAB-CBB
27	C	506	CLA	C2B-C3B-CAB-CBB
27	C	507	CLA	C2B-C3B-CAB-CBB
27	C	513	CLA	C2B-C3B-CAB-CBB
27	M	102	CLA	C2B-C3B-CAB-CBB
27	b	610	CLA	C2B-C3B-CAB-CBB
27	c	506	CLA	C2B-C3B-CAB-CBB
27	c	507	CLA	C2B-C3B-CAB-CBB
27	c	513	CLA	C2B-C3B-CAB-CBB
27	m	101	CLA	C2B-C3B-CAB-CBB
27	11	301	CLA	C2B-C3B-CAB-CBB
27	11	303	CLA	C2B-C3B-CAB-CBB
27	11	305	CLA	C2B-C3B-CAB-CBB
27	11	307	CLA	C2B-C3B-CAB-CBB
27	12	305	CLA	C2B-C3B-CAB-CBB
27	12	307	CLA	C2B-C3B-CAB-CBB
27	12	309	CLA	C2B-C3B-CAB-CBB
27	12	310	CLA	C2B-C3B-CAB-CBB
27	12	311	CLA	C2B-C3B-CAB-CBB
27	13	303	CLA	C2B-C3B-CAB-CBB
27	13	305	CLA	C2B-C3B-CAB-CBB
27	13	307	CLA	C2B-C3B-CAB-CBB
27	13	308	CLA	C2B-C3B-CAB-CBB
27	13	309	CLA	C2B-C3B-CAB-CBB
27	14	303	CLA	C2B-C3B-CAB-CBB
27	14	305	CLA	C2B-C3B-CAB-CBB
27	14	307	CLA	C2B-C3B-CAB-CBB
27	14	308	CLA	C2B-C3B-CAB-CBB
27	14	309	CLA	C2B-C3B-CAB-CBB
27	31	301	CLA	C2B-C3B-CAB-CBB
27	31	303	CLA	C2B-C3B-CAB-CBB
27	31	305	CLA	C2B-C3B-CAB-CBB
27	31	306	CLA	C2B-C3B-CAB-CBB
27	31	307	CLA	C2B-C3B-CAB-CBB
27	32	305	CLA	C2B-C3B-CAB-CBB
27	32	307	CLA	C2B-C3B-CAB-CBB
27	32	309	CLA	C2B-C3B-CAB-CBB
27	32	310	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
27	32	311	CLA	C2B-C3B-CAB-CBB
27	33	303	CLA	C2B-C3B-CAB-CBB
27	33	305	CLA	C2B-C3B-CAB-CBB
27	33	307	CLA	C2B-C3B-CAB-CBB
27	33	308	CLA	C2B-C3B-CAB-CBB
27	33	309	CLA	C2B-C3B-CAB-CBB
27	34	304	CLA	C2B-C3B-CAB-CBB
27	34	306	CLA	C2B-C3B-CAB-CBB
27	34	308	CLA	C2B-C3B-CAB-CBB
27	34	309	CLA	C2B-C3B-CAB-CBB
27	34	310	CLA	C2B-C3B-CAB-CBB
27	C	513	CLA	C10-C11-C12-C13
27	c	513	CLA	C10-C11-C12-C13
27	11	315	CLA	O1D-CGD-O2D-CED
27	32	303	CLA	O1D-CGD-O2D-CED
37	E	101	HEM	C3A-C2A-CAA-CBA
27	B	615	CLA	C5-C6-C7-C8
27	b	615	CLA	C5-C6-C7-C8
27	12	303	CLA	O1D-CGD-O2D-CED
27	13	301	CLA	O1D-CGD-O2D-CED
30	l	101	SQD	C24-C25-C26-C27
32	b	621	LHG	C29-C30-C31-C32
35	H	102	DGD	O2G-C1B-C2B-C3B
35	h	102	DGD	O2G-C1B-C2B-C3B
32	B	621	LHG	C29-C30-C31-C32
27	14	302	CLA	O1D-CGD-O2D-CED
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
30	L	103	SQD	C24-C25-C26-C27
35	H	102	DGD	C4A-C5A-C6A-C7A
35	h	102	DGD	C4A-C5A-C6A-C7A
33	b	619	LMG	O10-C28-O8-C9
27	33	301	CLA	O1D-CGD-O2D-CED
27	B	608	CLA	CBD-CGD-O2D-CED
33	B	619	LMG	O10-C28-O8-C9
27	34	302	CLA	O1D-CGD-O2D-CED
35	C	517	DGD	C8A-C9A-CAA-CBA
33	32	301	LMG	C13-C14-C15-C16
38	11	313	A86	C12-C11-C13-C14
38	12	317	A86	C12-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
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
35	c	517	DGD	C8A-C9A-CAA-CBA
27	B	605	CLA	O1D-CGD-O2D-CED
27	31	315	CLA	O1D-CGD-O2D-CED
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
27	b	605	CLA	O1D-CGD-O2D-CED
29	H	101	BCR	C23-C24-C25-C30
29	h	101	BCR	C23-C24-C25-C30
27	Z	102	CLA	O1D-CGD-O2D-CED
27	z	102	CLA	O1D-CGD-O2D-CED
27	z	102	CLA	C5-C6-C7-C8
27	13	301	CLA	C13-C15-C16-C17
27	33	301	CLA	C13-C15-C16-C17
37	f	102	HEM	C3A-C2A-CAA-CBA
33	B	619	LMG	C32-C33-C34-C35
33	b	619	LMG	C32-C33-C34-C35
27	b	608	CLA	CBD-CGD-O2D-CED
32	L	102	LHG	C4-O6-P-O3
32	l	103	LHG	C4-O6-P-O3
33	12	301	LMG	C7-C8-C9-O8
27	C	511	CLA	C11-C12-C13-C15
27	c	511	CLA	C11-C12-C13-C15
32	l	102	LHG	C10-C11-C12-C13
33	B	618	LMG	C20-C21-C22-C23
33	b	618	LMG	C20-C21-C22-C23
35	C	518	DGD	C5B-C6B-C7B-C8B
27	C	509	CLA	C6-C7-C8-C9
27	c	509	CLA	C6-C7-C8-C9
27	B	606	CLA	C8-C10-C11-C12
29	C	520	BCR	C9-C10-C11-C12
29	c	519	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	B	603	CLA	C16-C17-C18-C20
27	b	603	CLA	C16-C17-C18-C20
32	L	101	LHG	C10-C11-C12-C13
35	c	518	DGD	C5B-C6B-C7B-C8B
27	b	606	CLA	C8-C10-C11-C12
32	L	101	LHG	C30-C31-C32-C33
32	l	102	LHG	C30-C31-C32-C33
27	B	614	CLA	C13-C15-C16-C17
27	C	509	CLA	CBA-CGA-O2A-C1
27	c	509	CLA	CBA-CGA-O2A-C1
27	b	605	CLA	C8-C10-C11-C12
27	b	614	CLA	C13-C15-C16-C17
30	L	103	SQD	C11-C12-C13-C14
33	12	301	LMG	C15-C16-C17-C18
27	34	302	CLA	C3-C5-C6-C7
30	l	101	SQD	C11-C12-C13-C14
27	D	401	CLA	C16-C17-C18-C20
27	d	401	CLA	C16-C17-C18-C20
32	A	408	LHG	C24-C23-O8-C6
32	a	408	LHG	C24-C23-O8-C6
33	C	519	LMG	C29-C28-O8-C9
33	q	301	LMG	C29-C28-O8-C9
27	11	315	CLA	C3-C5-C6-C7
27	13	301	CLA	C3-C5-C6-C7
27	B	601	CLA	CAA-CBA-CGA-O2A
27	b	601	CLA	CAA-CBA-CGA-O2A
35	C	517	DGD	C8B-C9B-CAB-CBB
35	c	517	DGD	C8B-C9B-CAB-CBB
27	B	605	CLA	C8-C10-C11-C12
30	B	620	SQD	O10-C23-O48-C46
30	b	620	SQD	O10-C23-O48-C46
35	H	102	DGD	C2B-C3B-C4B-C5B
35	h	102	DGD	C2B-C3B-C4B-C5B
27	B	603	CLA	C4B-C3B-CAB-CBB
27	b	603	CLA	C4B-C3B-CAB-CBB
27	11	303	CLA	C4B-C3B-CAB-CBB
27	12	307	CLA	C4B-C3B-CAB-CBB
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

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Mol	Chain	Res	Type	Atoms
27	34	306	CLA	C4B-C3B-CAB-CBB
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	J	101	DGD	C3A-C4A-C5A-C6A
35	j	101	DGD	C3A-C4A-C5A-C6A
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
27	C	509	CLA	C10-C11-C12-C13
27	c	509	CLA	C10-C11-C12-C13
32	A	408	LHG	C31-C32-C33-C34
32	a	408	LHG	C31-C32-C33-C34
27	32	311	CLA	CAA-CBA-CGA-O1A
27	B	622	CLA	O1A-CGA-O2A-C1
30	B	620	SQD	C12-C13-C14-C15
30	b	620	SQD	C12-C13-C14-C15
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	33	306	CLA	CAA-CBA-CGA-O2A
27	34	307	CLA	CAA-CBA-CGA-O2A
27	b	612	CLA	C5-C6-C7-C8
27	b	622	CLA	O1A-CGA-O2A-C1
27	B	612	CLA	C5-C6-C7-C8
27	C	514	CLA	C10-C11-C12-C13
27	c	514	CLA	C10-C11-C12-C13
27	33	301	CLA	C8-C10-C11-C12
27	11	304	CLA	CAA-CBA-CGA-O1A
27	11	304	CLA	CAA-CBA-CGA-O2A
27	12	308	CLA	CAA-CBA-CGA-O1A
27	13	306	CLA	CAA-CBA-CGA-O1A
27	14	306	CLA	CAA-CBA-CGA-O1A
27	31	304	CLA	CAA-CBA-CGA-O1A
27	32	308	CLA	CAA-CBA-CGA-O1A
27	33	306	CLA	CAA-CBA-CGA-O1A
27	34	307	CLA	CAA-CBA-CGA-O1A
37	E	101	HEM	CAD-CBD-CGD-O1D
37	f	102	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
27	A	404	CLA	C2-C1-O2A-CGA
27	B	610	CLA	C2-C1-O2A-CGA
27	C	506	CLA	C2-C1-O2A-CGA
27	C	511	CLA	C2-C1-O2A-CGA
27	a	404	CLA	C2-C1-O2A-CGA
27	b	610	CLA	C2-C1-O2A-CGA
27	c	511	CLA	C2-C1-O2A-CGA
27	31	315	CLA	C8-C10-C11-C12
27	34	302	CLA	C8-C10-C11-C12
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
27	C	511	CLA	C2A-CAA-CBA-CGA
27	c	511	CLA	C2A-CAA-CBA-CGA
33	12	301	LMG	O7-C8-C9-O8
33	W	101	LMG	C34-C35-C36-C37
35	C	518	DGD	C8B-C9B-CAB-CBB
35	c	518	DGD	C8B-C9B-CAB-CBB
27	C	507	CLA	C3A-C2A-CAA-CBA
27	c	507	CLA	C3A-C2A-CAA-CBA
33	w	101	LMG	C34-C35-C36-C37
27	12	303	CLA	C8-C10-C11-C12
28	A	403	PHO	C13-C15-C16-C17
35	C	517	DGD	C2A-C3A-C4A-C5A
35	c	517	DGD	C2A-C3A-C4A-C5A
36	D	404	PL9	C4-C3-C7-C8
36	d	404	PL9	C4-C3-C7-C8
27	B	605	CLA	C11-C10-C8-C9
27	b	605	CLA	C11-C10-C8-C9
33	12	301	LMG	O1-C7-C8-C9
32	L	101	LHG	C35-C36-C37-C38
32	l	102	LHG	C35-C36-C37-C38
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
27	B	603	CLA	C16-C17-C18-C19
27	b	603	CLA	C16-C17-C18-C19
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
27	33	310	CLA	CAA-CBA-CGA-O1A
35	j	101	DGD	O1A-C1A-O1G-C1G
27	12	303	CLA	CBD-CGD-O2D-CED
35	j	101	DGD	C3B-C4B-C5B-C6B
27	13	310	CLA	CAA-CBA-CGA-O1A
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
27	C	510	CLA	C6-C7-C8-C10
27	W	102	CLA	C11-C12-C13-C15
27	c	510	CLA	C6-C7-C8-C10
27	w	102	CLA	C11-C12-C13-C15
35	J	101	DGD	C3B-C4B-C5B-C6B
27	c	509	CLA	O1A-CGA-O2A-C1
35	J	101	DGD	O1A-C1A-O1G-C1G
29	c	515	BCR	C19-C20-C21-C22
27	C	509	CLA	O1A-CGA-O2A-C1
33	D	408	LMG	C15-C16-C17-C18
27	31	315	CLA	CBD-CGD-O2D-CED
33	d	408	LMG	C15-C16-C17-C18
27	Z	102	CLA	C2A-CAA-CBA-CGA
27	z	102	CLA	C2A-CAA-CBA-CGA
33	B	618	LMG	C11-C12-C13-C14
33	b	618	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
37	E	101	HEM	CAA-CBA-CGA-O1A
37	f	102	HEM	CAA-CBA-CGA-O1A
32	L	101	LHG	C9-C10-C11-C12
32	l	102	LHG	C9-C10-C11-C12
27	34	302	CLA	CBD-CGD-O2D-CED
37	E	101	HEM	CAD-CBD-CGD-O2D
37	f	102	HEM	CAD-CBD-CGD-O2D
27	W	102	CLA	C4-C3-C5-C6
27	w	102	CLA	C4-C3-C5-C6
32	B	621	LHG	C14-C15-C16-C17
32	b	621	LHG	C14-C15-C16-C17
33	D	408	LMG	C28-C29-C30-C31
33	d	408	LMG	C28-C29-C30-C31
27	32	303	CLA	CBD-CGD-O2D-CED
27	33	301	CLA	CBD-CGD-O2D-CED
36	D	404	PL9	C12-C11-C9-C8
36	d	404	PL9	C12-C11-C9-C8
27	B	603	CLA	C2B-C3B-CAB-CBB
27	W	102	CLA	C2B-C3B-CAB-CBB
27	b	603	CLA	C2B-C3B-CAB-CBB
27	w	102	CLA	C2B-C3B-CAB-CBB
27	11	315	CLA	C2B-C3B-CAB-CBB
27	12	303	CLA	C2B-C3B-CAB-CBB
27	13	301	CLA	C2B-C3B-CAB-CBB
27	14	302	CLA	C2B-C3B-CAB-CBB
27	31	315	CLA	C2B-C3B-CAB-CBB
27	32	303	CLA	C2B-C3B-CAB-CBB
27	33	301	CLA	C2B-C3B-CAB-CBB
27	34	302	CLA	C2B-C3B-CAB-CBB
27	11	315	CLA	CBD-CGD-O2D-CED
27	13	301	CLA	CBD-CGD-O2D-CED
27	14	302	CLA	CBD-CGD-O2D-CED
38	11	310	A86	C13-C14-C15-C16
38	11	313	A86	C13-C14-C15-C16
38	12	314	A86	C13-C14-C15-C16
38	12	317	A86	C13-C14-C15-C16
38	13	312	A86	C13-C14-C15-C16
38	13	315	A86	C13-C14-C15-C16
38	14	312	A86	C13-C14-C15-C16
38	14	315	A86	C13-C14-C15-C16
38	31	310	A86	C13-C14-C15-C16
38	31	313	A86	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
38	32	314	A86	C13-C14-C15-C16
38	32	317	A86	C13-C14-C15-C16
38	33	312	A86	C13-C14-C15-C16
38	33	315	A86	C13-C14-C15-C16
38	34	313	A86	C13-C14-C15-C16
38	34	316	A86	C13-C14-C15-C16
30	L	103	SQD	C9-C10-C11-C12
30	l	101	SQD	C9-C10-C11-C12
27	b	601	CLA	CBA-CGA-O2A-C1
33	C	519	LMG	C35-C36-C37-C38
33	12	301	LMG	C31-C32-C33-C34
29	C	515	BCR	C19-C20-C21-C22
33	q	301	LMG	C35-C36-C37-C38
27	C	514	CLA	C16-C17-C18-C20
33	B	619	LMG	C36-C37-C38-C39
36	D	407	PL9	C39-C41-C42-C43
36	d	407	PL9	C39-C41-C42-C43
38	12	304	A86	C10-C11-C13-C14
38	13	317	A86	C10-C11-C13-C14
38	33	302	A86	C10-C11-C13-C14
33	b	619	LMG	C36-C37-C38-C39
35	H	102	DGD	C9B-CAB-CBB-CCB
35	h	102	DGD	C9B-CAB-CBB-CCB
27	B	601	CLA	O1A-CGA-O2A-C1
27	b	601	CLA	O1A-CGA-O2A-C1
27	b	608	CLA	O1D-CGD-O2D-CED
27	c	514	CLA	C16-C17-C18-C20
27	B	601	CLA	CBA-CGA-O2A-C1
30	L	103	SQD	C19-C20-C21-C22
30	l	101	SQD	C19-C20-C21-C22
37	E	101	HEM	CAA-CBA-CGA-O2A
37	f	102	HEM	CAA-CBA-CGA-O2A
33	B	618	LMG	C34-C35-C36-C37
35	C	518	DGD	CCB-CDB-CEB-CFB
35	c	518	DGD	CCB-CDB-CEB-CFB
27	A	404	CLA	O1A-CGA-O2A-C1
27	a	404	CLA	O1A-CGA-O2A-C1
29	B	616	BCR	C23-C24-C25-C30
29	B	617	BCR	C23-C24-C25-C30
29	B	623	BCR	C23-C24-C25-C26
29	B	623	BCR	C23-C24-C25-C30
29	C	516	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
29	C	516	BCR	C23-C24-C25-C30
29	b	616	BCR	C23-C24-C25-C30
29	b	617	BCR	C23-C24-C25-C30
29	b	623	BCR	C23-C24-C25-C26
29	b	623	BCR	C23-C24-C25-C30
29	c	516	BCR	C23-C24-C25-C26
29	c	516	BCR	C23-C24-C25-C30
33	b	618	LMG	C34-C35-C36-C37
28	D	403	PHO	O1D-CGD-O2D-CED
28	d	403	PHO	O1D-CGD-O2D-CED
28	D	403	PHO	CAA-CBA-CGA-O2A
28	d	403	PHO	CAA-CBA-CGA-O2A
35	H	102	DGD	C1G-C2G-C3G-O3G
35	h	102	DGD	C1G-C2G-C3G-O3G
36	D	407	PL9	C15-C14-C16-C17
36	d	407	PL9	C15-C14-C16-C17
29	A	409	BCR	C17-C18-C19-C20
29	a	409	BCR	C17-C18-C19-C20
27	B	608	CLA	O1D-CGD-O2D-CED
33	C	519	LMG	C16-C17-C18-C19
33	q	301	LMG	C16-C17-C18-C19
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	310	CLA	CAA-CBA-CGA-O2A
27	31	308	CLA	CAA-CBA-CGA-O2A
27	32	312	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	C2A-CAA-CBA-CGA
27	b	605	CLA	C2A-CAA-CBA-CGA
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
27	A	404	CLA	CBA-CGA-O2A-C1
27	a	404	CLA	CBA-CGA-O2A-C1
27	C	507	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
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	622	CLA	CBA-CGA-O2A-C1
33	32	301	LMG	C2-C1-O1-C7
27	B	611	CLA	C2A-CAA-CBA-CGA
27	b	611	CLA	C2A-CAA-CBA-CGA
35	H	102	DGD	C4B-C5B-C6B-C7B
27	b	622	CLA	CBA-CGA-O2A-C1
29	Z	101	BCR	C16-C17-C18-C36
29	z	101	BCR	C16-C17-C18-C36
35	h	102	DGD	C4B-C5B-C6B-C7B
27	B	604	CLA	C4-C3-C5-C6
27	b	604	CLA	C4-C3-C5-C6
27	C	505	CLA	C5-C6-C7-C8
27	c	505	CLA	C5-C6-C7-C8
27	13	308	CLA	CAA-CBA-CGA-O2A
27	14	308	CLA	CAA-CBA-CGA-O2A
27	31	306	CLA	CAA-CBA-CGA-O2A
27	33	308	CLA	CAA-CBA-CGA-O2A
27	C	504	CLA	C2-C3-C5-C6
27	W	102	CLA	C2-C3-C5-C6
27	c	504	CLA	C2-C3-C5-C6
27	w	102	CLA	C2-C3-C5-C6
35	J	101	DGD	O1G-C1A-C2A-C3A
35	j	101	DGD	O1G-C1A-C2A-C3A

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Mol	Chain	Res	Type	Atoms
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	11	306	CLA	CAA-CBA-CGA-O2A
27	12	310	CLA	CAA-CBA-CGA-O2A
27	32	310	CLA	CAA-CBA-CGA-O2A
27	34	309	CLA	CAA-CBA-CGA-O2A
33	w	101	LMG	C39-C40-C41-C42
27	C	502	CLA	CAA-CBA-CGA-O2A
27	c	502	CLA	CAA-CBA-CGA-O2A
32	B	621	LHG	C10-C11-C12-C13
32	b	621	LHG	C10-C11-C12-C13
33	W	101	LMG	C39-C40-C41-C42
27	C	502	CLA	CAD-CBD-CGD-O2D
27	C	504	CLA	CAD-CBD-CGD-O2D
27	Z	102	CLA	CAD-CBD-CGD-O2D
27	c	502	CLA	CAD-CBD-CGD-O2D
27	c	504	CLA	CAD-CBD-CGD-O2D
27	z	102	CLA	CAD-CBD-CGD-O2D
27	11	302	CLA	CAD-CBD-CGD-O2D
27	11	307	CLA	CAD-CBD-CGD-O2D
27	12	306	CLA	CAD-CBD-CGD-O2D
27	12	311	CLA	CAD-CBD-CGD-O2D
27	13	304	CLA	CAD-CBD-CGD-O2D
27	13	309	CLA	CAD-CBD-CGD-O2D
27	14	304	CLA	CAD-CBD-CGD-O2D
27	14	309	CLA	CAD-CBD-CGD-O2D
27	31	302	CLA	CAD-CBD-CGD-O2D
27	31	307	CLA	CAD-CBD-CGD-O2D
27	32	306	CLA	CAD-CBD-CGD-O2D
27	32	311	CLA	CAD-CBD-CGD-O2D
27	33	304	CLA	CAD-CBD-CGD-O2D
27	33	309	CLA	CAD-CBD-CGD-O2D
27	34	305	CLA	CAD-CBD-CGD-O2D
27	34	310	CLA	CAD-CBD-CGD-O2D
32	A	408	LHG	C16-C17-C18-C19
32	a	408	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
35	C	518	DGD	O1B-C1B-O2G-C2G
35	c	518	DGD	O1B-C1B-O2G-C2G
33	w	101	LMG	O10-C28-O8-C9
27	B	605	CLA	C13-C15-C16-C17
27	b	605	CLA	C13-C15-C16-C17
27	c	506	CLA	C2-C1-O2A-CGA
30	B	620	SQD	C24-C25-C26-C27
27	A	404	CLA	CAA-CBA-CGA-O2A
27	a	404	CLA	CAA-CBA-CGA-O2A
27	w	103	CLA	CAA-CBA-CGA-O2A
28	D	403	PHO	CBD-CGD-O2D-CED
28	d	403	PHO	CBD-CGD-O2D-CED
30	b	620	SQD	C24-C25-C26-C27
36	D	407	PL9	C28-C29-C31-C32
36	d	407	PL9	C28-C29-C31-C32
27	W	103	CLA	CAA-CBA-CGA-O2A
38	11	314	A86	C5-C6-C8-C9
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
36	D	407	PL9	C29-C31-C32-C33
36	d	407	PL9	C29-C31-C32-C33
27	c	513	CLA	C15-C16-C17-C18
27	12	310	CLA	CAA-CBA-CGA-O1A
27	13	308	CLA	CAA-CBA-CGA-O1A
27	14	308	CLA	CAA-CBA-CGA-O1A
27	31	306	CLA	CAA-CBA-CGA-O1A
33	W	101	LMG	O10-C28-O8-C9
27	C	513	CLA	C15-C16-C17-C18
27	C	509	CLA	C3-C5-C6-C7
27	11	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	504	CLA	O2A-C1-C2-C3
27	C	510	CLA	O2A-C1-C2-C3
27	c	504	CLA	O2A-C1-C2-C3
27	c	510	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
28	A	403	PHO	O2A-C1-C2-C3
28	a	403	PHO	O2A-C1-C2-C3
27	D	402	CLA	C4C-C3C-CAC-CBC
27	d	402	CLA	C4C-C3C-CAC-CBC
27	c	509	CLA	C3-C5-C6-C7
27	B	607	CLA	CHA-CBD-CGD-O1D
27	C	507	CLA	CHA-CBD-CGD-O2D
27	C	508	CLA	CHA-CBD-CGD-O2D
27	C	513	CLA	CHA-CBD-CGD-O2D
27	b	607	CLA	CHA-CBD-CGD-O1D
27	c	507	CLA	CHA-CBD-CGD-O2D
27	c	508	CLA	CHA-CBD-CGD-O2D
27	c	513	CLA	CHA-CBD-CGD-O2D
29	M	101	BCR	C19-C20-C21-C22
29	m	103	BCR	C19-C20-C21-C22
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
27	d	401	CLA	CBD-CGD-O2D-CED
35	C	518	DGD	O1G-C1G-C2G-O2G
35	c	518	DGD	O1G-C1G-C2G-O2G
27	11	301	CLA	C8-C10-C11-C12
32	l	102	LHG	C11-C12-C13-C14
33	D	408	LMG	C16-C17-C18-C19
33	d	408	LMG	C16-C17-C18-C19
27	13	303	CLA	C8-C10-C11-C12
27	14	303	CLA	C8-C10-C11-C12
27	31	301	CLA	C8-C10-C11-C12
27	32	305	CLA	C8-C10-C11-C12
27	33	303	CLA	C8-C10-C11-C12
28	D	403	PHO	CHA-CBD-CGD-O1D
28	d	403	PHO	CHA-CBD-CGD-O1D
27	12	305	CLA	C8-C10-C11-C12
27	34	304	CLA	C8-C10-C11-C12
27	B	605	CLA	CBA-CGA-O2A-C1
27	b	605	CLA	CBA-CGA-O2A-C1
32	L	101	LHG	C11-C12-C13-C14
27	A	404	CLA	C11-C10-C8-C7
27	B	604	CLA	C11-C10-C8-C7
27	B	622	CLA	C11-C12-C13-C15
27	a	404	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
27	b	604	CLA	C11-C10-C8-C7
27	b	622	CLA	C11-C12-C13-C15
27	12	313	CLA	CAA-CBA-CGA-O1A
35	h	102	DGD	CDB-CEB-CFB-CGB
32	l	103	LHG	C11-C10-C9-C8
35	H	102	DGD	CDB-CEB-CFB-CGB
27	32	313	CLA	CAA-CBA-CGA-O1A
32	L	102	LHG	C11-C10-C9-C8
30	A	406	SQD	C5-C6-S-O8
30	a	406	SQD	C5-C6-S-O8
27	D	401	CLA	CBD-CGD-O2D-CED
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
27	W	103	CLA	CAA-CBA-CGA-O1A
27	w	103	CLA	CAA-CBA-CGA-O1A
27	11	309	CLA	CAA-CBA-CGA-O1A
27	14	311	CLA	CAA-CBA-CGA-O1A
38	12	316	A86	C-C1-C24-C25
38	34	315	A86	C-C1-C24-C25
27	C	506	CLA	C10-C11-C12-C13
30	A	406	SQD	C30-C31-C32-C33
27	B	608	CLA	C4-C3-C5-C6
27	b	608	CLA	C4-C3-C5-C6
30	a	406	SQD	C30-C31-C32-C33
27	c	506	CLA	C10-C11-C12-C13
30	A	406	SQD	C35-C36-C37-C38
30	a	406	SQD	C35-C36-C37-C38
32	B	621	LHG	C11-C12-C13-C14
32	b	621	LHG	C11-C12-C13-C14
33	B	618	LMG	C37-C38-C39-C40
33	C	519	LMG	C39-C40-C41-C42
33	b	618	LMG	C37-C38-C39-C40
33	q	301	LMG	C39-C40-C41-C42
28	D	403	PHO	C8-C10-C11-C12
28	d	403	PHO	C8-C10-C11-C12
33	32	301	LMG	C31-C32-C33-C34
32	A	408	LHG	C18-C19-C20-C21
32	a	408	LHG	C18-C19-C20-C21
27	C	502	CLA	CAA-CBA-CGA-O1A
27	c	502	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
27	B	605	CLA	C10-C11-C12-C13
27	b	605	CLA	C10-C11-C12-C13
32	L	102	LHG	C17-C18-C19-C20
27	a	404	CLA	CAA-CBA-CGA-O1A
32	l	103	LHG	C17-C18-C19-C20
27	A	404	CLA	CAA-CBA-CGA-O1A
32	l	102	LHG	C34-C35-C36-C37
32	L	101	LHG	C16-C17-C18-C19
32	l	102	LHG	C16-C17-C18-C19
35	C	518	DGD	CCA-CDA-CEA-CFA
35	c	518	DGD	CCA-CDA-CEA-CFA
32	L	101	LHG	C34-C35-C36-C37
33	C	519	LMG	C34-C35-C36-C37
33	q	301	LMG	C34-C35-C36-C37
33	12	301	LMG	C16-C17-C18-C19
35	j	101	DGD	CCA-CDA-CEA-CFA
27	B	607	CLA	CAD-CBD-CGD-O1D
27	b	607	CLA	CAD-CBD-CGD-O1D
27	11	307	CLA	CAD-CBD-CGD-O1D
27	12	311	CLA	CAD-CBD-CGD-O1D
27	13	309	CLA	CAD-CBD-CGD-O1D
27	14	309	CLA	CAD-CBD-CGD-O1D
27	31	307	CLA	CAD-CBD-CGD-O1D
27	32	311	CLA	CAD-CBD-CGD-O1D
27	33	309	CLA	CAD-CBD-CGD-O1D
27	34	310	CLA	CAD-CBD-CGD-O1D
27	c	508	CLA	CAA-CBA-CGA-O2A
27	B	607	CLA	C8-C10-C11-C12
27	B	607	CLA	C10-C11-C12-C13
27	b	607	CLA	C8-C10-C11-C12
27	b	607	CLA	C10-C11-C12-C13
35	J	101	DGD	CCA-CDA-CEA-CFA
27	B	605	CLA	O1A-CGA-O2A-C1
27	C	504	CLA	C3-C5-C6-C7
27	C	506	CLA	CAA-CBA-CGA-O2A
27	C	508	CLA	CAA-CBA-CGA-O2A
27	C	514	CLA	CAA-CBA-CGA-O2A
27	c	506	CLA	CAA-CBA-CGA-O2A
27	c	514	CLA	CAA-CBA-CGA-O2A
27	b	605	CLA	O1A-CGA-O2A-C1
33	M	103	LMG	C8-C9-O8-C28
27	Z	102	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
27	c	511	CLA	CAA-CBA-CGA-O2A
27	z	102	CLA	CAA-CBA-CGA-O2A
27	c	504	CLA	C3-C5-C6-C7
33	d	408	LMG	O9-C10-C11-C12
33	m	102	LMG	C8-C9-O8-C28
36	D	407	PL9	C12-C11-C9-C10
36	d	407	PL9	C12-C11-C9-C10
38	13	314	A86	C-C1-C24-C25
27	B	604	CLA	C11-C12-C13-C15
27	B	610	CLA	C11-C10-C8-C7
27	B	610	CLA	C11-C12-C13-C15
27	C	502	CLA	C12-C13-C15-C16
27	b	604	CLA	C11-C12-C13-C15
27	b	610	CLA	C11-C10-C8-C7
27	b	610	CLA	C11-C12-C13-C15
27	c	502	CLA	C12-C13-C15-C16
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
33	D	408	LMG	O9-C10-C11-C12
35	C	517	DGD	O1B-C1B-C2B-C3B
27	11	309	CLA	CAA-CBA-CGA-O2A
27	13	311	CLA	CAA-CBA-CGA-O2A
27	13	304	CLA	O1D-CGD-O2D-CED
27	C	511	CLA	CAA-CBA-CGA-O2A
27	11	303	CLA	CAA-CBA-CGA-O2A
27	12	307	CLA	CAA-CBA-CGA-O2A
27	13	305	CLA	CAA-CBA-CGA-O2A
27	14	305	CLA	CAA-CBA-CGA-O2A
27	31	303	CLA	CAA-CBA-CGA-O2A
27	32	307	CLA	CAA-CBA-CGA-O2A
27	33	305	CLA	CAA-CBA-CGA-O2A
27	34	306	CLA	CAA-CBA-CGA-O2A
29	B	617	BCR	C17-C18-C19-C20
29	C	516	BCR	C17-C18-C19-C20
29	b	617	BCR	C17-C18-C19-C20
29	c	516	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
38	11	310	A86	C2-C1-C24-C25
38	12	314	A86	C2-C1-C24-C25
38	13	312	A86	C2-C1-C24-C25
38	14	312	A86	C2-C1-C24-C25
38	31	310	A86	C2-C1-C24-C25
38	33	312	A86	C2-C1-C24-C25
38	34	313	A86	C2-C1-C24-C25
27	C	506	CLA	CAA-CBA-CGA-O1A
27	c	506	CLA	CAA-CBA-CGA-O1A
35	c	517	DGD	O1B-C1B-C2B-C3B
27	31	309	CLA	CAA-CBA-CGA-O2A
29	Z	101	BCR	C19-C20-C21-C22
29	z	101	BCR	C19-C20-C21-C22
33	b	619	LMG	C20-C21-C22-C23
38	11	316	A86	O-C13-C14-C15
38	12	304	A86	O-C13-C14-C15
38	13	302	A86	O-C13-C14-C15
38	13	317	A86	O-C13-C14-C15
38	31	316	A86	O-C13-C14-C15
38	32	304	A86	O-C13-C14-C15
38	33	302	A86	O-C13-C14-C15
38	34	303	A86	O-C13-C14-C15
35	C	518	DGD	O6D-C1D-O3G-C3G
35	c	518	DGD	O6D-C1D-O3G-C3G
27	11	302	CLA	O1D-CGD-O2D-CED
27	12	306	CLA	O1D-CGD-O2D-CED
27	33	304	CLA	O1D-CGD-O2D-CED
27	34	305	CLA	O1D-CGD-O2D-CED
27	B	602	CLA	C13-C15-C16-C17
27	b	602	CLA	C13-C15-C16-C17
33	B	619	LMG	C20-C21-C22-C23
27	C	511	CLA	CAA-CBA-CGA-O1A
27	c	511	CLA	CAA-CBA-CGA-O1A
30	A	406	SQD	O49-C7-C8-C9
30	a	406	SQD	O49-C7-C8-C9
36	D	407	PL9	C44-C46-C47-C48
36	d	407	PL9	C44-C46-C47-C48
27	12	313	CLA	CAA-CBA-CGA-O2A
27	14	311	CLA	CAA-CBA-CGA-O2A
27	32	313	CLA	CAA-CBA-CGA-O2A
27	33	311	CLA	CAA-CBA-CGA-O2A
27	34	312	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
36	D	407	PL9	C31-C32-C33-C34
36	d	407	PL9	C31-C32-C33-C34
27	32	306	CLA	O1D-CGD-O2D-CED
35	H	102	DGD	C8A-C9A-CAA-CBA
27	12	305	CLA	CAA-CBA-CGA-O2A
27	13	303	CLA	CAA-CBA-CGA-O2A
27	14	303	CLA	CAA-CBA-CGA-O2A
27	31	301	CLA	CAA-CBA-CGA-O2A
27	32	305	CLA	CAA-CBA-CGA-O2A
27	33	303	CLA	CAA-CBA-CGA-O2A
27	34	304	CLA	CAA-CBA-CGA-O2A
27	C	508	CLA	CAA-CBA-CGA-O1A
27	Z	102	CLA	CAA-CBA-CGA-O1A
27	c	508	CLA	CAA-CBA-CGA-O1A
35	h	102	DGD	C8A-C9A-CAA-CBA
27	z	102	CLA	CAA-CBA-CGA-O1A
33	B	619	LMG	O10-C28-C29-C30

There are no ring outliers.

251 monomers are involved in 639 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	31	306	CLA	1	0
27	13	303	CLA	9	0
30	L	103	SQD	3	0
27	33	309	CLA	2	0
27	C	507	CLA	6	0
33	D	408	LMG	1	0
27	C	506	CLA	1	0
27	C	504	CLA	3	0
27	12	308	CLA	3	0
27	B	609	CLA	2	0
27	13	310	CLA	1	0
27	12	307	CLA	3	0
27	c	512	CLA	2	0
27	B	614	CLA	4	0
27	12	303	CLA	5	0
33	b	619	LMG	1	0
27	13	307	CLA	2	0
34	C	501	OEX	1	0
33	w	101	LMG	4	0
36	d	407	PL9	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	13	305	CLA	3	0
30	b	620	SQD	1	0
38	33	302	A86	10	0
27	D	401	CLA	4	0
29	c	519	BCR	2	0
33	M	103	LMG	2	0
27	34	308	CLA	2	0
33	12	301	LMG	3	0
34	c	501	OEX	1	0
27	C	505	CLA	1	0
27	c	513	CLA	3	0
27	11	315	CLA	4	0
31	A	407	BCT	1	0
38	11	314	A86	3	0
27	b	615	CLA	3	0
27	31	308	CLA	1	0
30	l	101	SQD	3	0
38	13	314	A86	2	0
27	B	613	CLA	2	0
27	A	404	CLA	7	0
27	b	611	CLA	2	0
27	34	310	CLA	2	0
27	B	601	CLA	6	0
27	32	306	CLA	2	0
27	13	309	CLA	2	0
27	c	509	CLA	6	0
38	12	315	A86	9	0
38	13	302	A86	9	0
29	a	405	BCR	1	0
36	D	407	PL9	4	0
27	c	505	CLA	2	0
27	34	305	CLA	1	0
29	B	617	BCR	2	0
27	31	305	CLA	2	0
29	B	623	BCR	2	0
38	13	315	A86	5	0
27	c	504	CLA	2	0
38	12	304	A86	7	0
27	32	308	CLA	3	0
27	14	309	CLA	2	0
38	32	316	A86	4	0
38	11	316	A86	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	14	315	A86	5	0
29	Z	101	BCR	2	0
27	31	315	CLA	3	0
27	B	622	CLA	2	0
27	32	309	CLA	1	0
29	b	617	BCR	3	0
38	32	317	A86	3	0
30	B	620	SQD	1	0
27	C	502	CLA	2	0
38	34	314	A86	9	0
29	B	616	BCR	3	0
27	b	614	CLA	5	0
27	13	308	CLA	1	0
27	B	610	CLA	2	0
27	a	404	CLA	6	0
27	33	310	CLA	1	0
27	32	312	CLA	1	0
27	c	511	CLA	4	0
27	m	101	CLA	2	0
27	34	309	CLA	1	0
32	A	408	LHG	6	0
38	34	315	A86	3	0
29	z	101	BCR	2	0
27	33	305	CLA	3	0
29	a	409	BCR	1	0
27	d	405	CLA	7	0
27	13	304	CLA	2	0
27	b	609	CLA	2	0
38	32	318	A86	2	0
27	B	611	CLA	3	0
27	w	102	CLA	3	0
27	32	307	CLA	3	0
27	11	307	CLA	2	0
27	12	311	CLA	2	0
27	C	510	CLA	2	0
33	B	618	LMG	4	0
29	M	101	BCR	2	0
29	A	409	BCR	2	0
27	B	606	CLA	3	0
27	b	605	CLA	3	0
27	12	310	CLA	2	0
38	33	314	A86	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B	604	CLA	4	0
27	31	304	CLA	2	0
27	c	510	CLA	3	0
27	b	606	CLA	4	0
27	34	311	CLA	1	0
36	D	404	PL9	3	0
31	a	407	BCT	1	0
33	m	102	LMG	3	0
35	h	102	DGD	3	0
27	C	503	CLA	3	0
27	C	508	CLA	2	0
27	32	311	CLA	2	0
27	14	308	CLA	1	0
27	34	304	CLA	9	0
27	31	303	CLA	3	0
29	C	516	BCR	3	0
33	d	408	LMG	1	0
27	31	307	CLA	2	0
27	c	508	CLA	2	0
29	c	515	BCR	4	0
38	31	313	A86	5	0
27	b	603	CLA	1	0
27	11	303	CLA	3	0
27	C	512	CLA	1	0
27	32	303	CLA	4	0
27	c	503	CLA	3	0
27	33	303	CLA	11	0
27	B	608	CLA	2	0
27	33	307	CLA	2	0
27	14	307	CLA	2	0
27	c	514	CLA	3	0
27	d	406	CLA	1	0
32	L	102	LHG	1	0
27	13	306	CLA	1	0
27	b	601	CLA	3	0
27	B	615	CLA	4	0
33	q	301	LMG	1	0
37	V	201	HEM	2	0
33	32	301	LMG	3	0
27	11	301	CLA	8	0
27	34	302	CLA	4	0
27	14	302	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	b	622	CLA	2	0
38	33	316	A86	2	0
27	32	310	CLA	2	0
27	A	402	CLA	1	0
27	M	102	CLA	1	0
27	b	604	CLA	7	0
27	11	304	CLA	2	0
29	C	515	BCR	2	0
29	H	101	BCR	3	0
38	13	316	A86	3	0
38	31	314	A86	2	0
27	B	602	CLA	7	0
27	b	613	CLA	4	0
38	14	301	A86	3	0
38	13	317	A86	6	0
27	31	301	CLA	9	0
37	E	101	HEM	2	0
27	14	305	CLA	3	0
37	f	102	HEM	2	0
27	b	610	CLA	2	0
29	c	516	BCR	2	0
38	31	312	A86	4	0
38	14	316	A86	2	0
38	34	303	A86	7	0
27	D	405	CLA	5	0
27	B	605	CLA	2	0
33	B	619	LMG	2	0
36	d	404	PL9	2	0
29	b	623	BCR	1	0
27	d	401	CLA	4	0
27	B	607	CLA	3	0
27	w	103	CLA	2	0
27	34	306	CLA	3	0
38	12	317	A86	5	0
27	C	511	CLA	5	0
35	H	102	DGD	5	0
29	f	101	BCR	2	0
38	34	301	A86	3	0
27	C	514	CLA	3	0
27	b	608	CLA	2	0
27	a	402	CLA	1	0
38	34	316	A86	4	0

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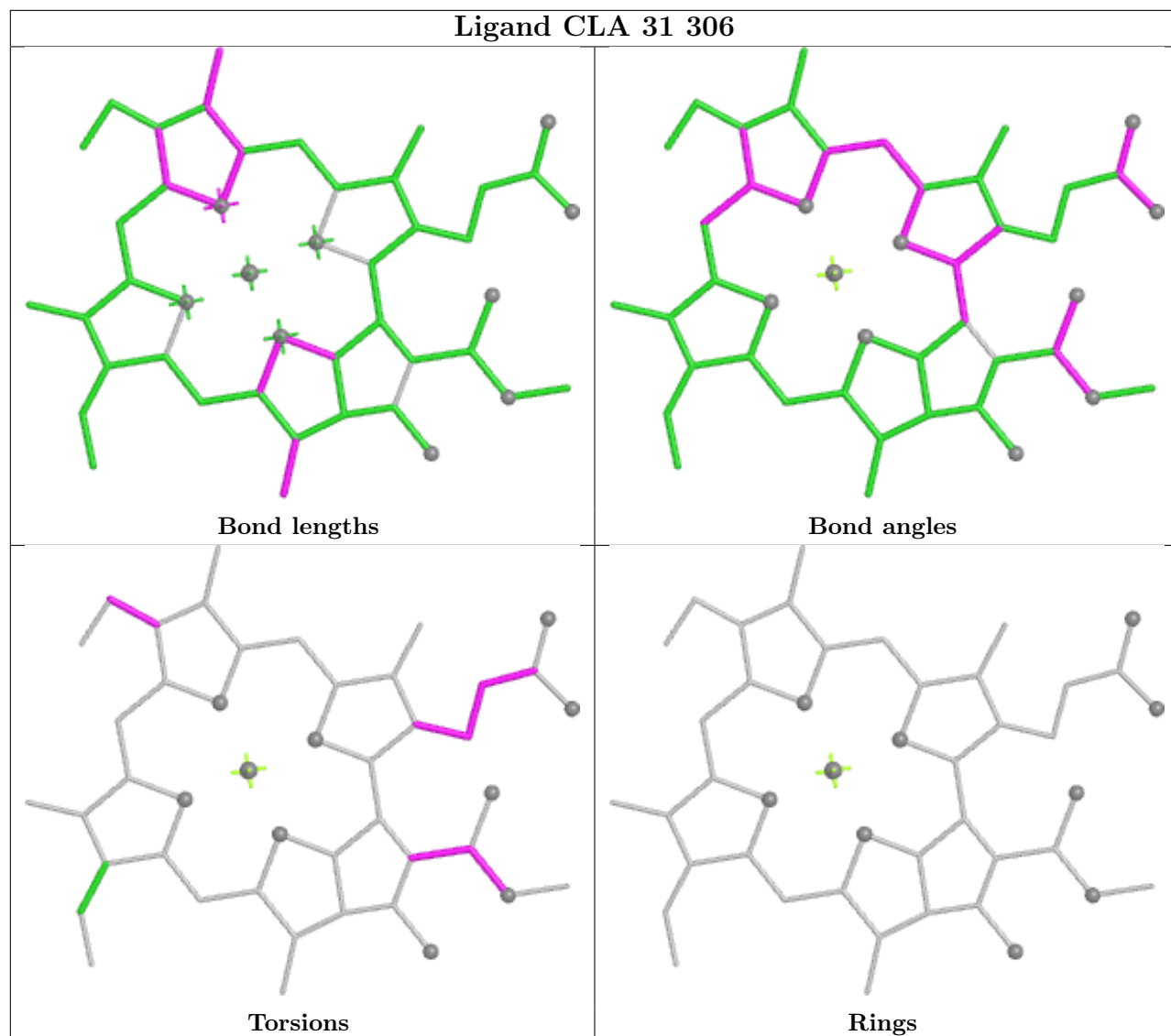
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33	C	519	LMG	2	0
27	c	507	CLA	5	0
27	32	305	CLA	8	0
27	11	305	CLA	2	0
27	14	303	CLA	7	0
38	31	311	A86	9	0
38	11	312	A86	3	0
29	m	103	BCR	3	0
37	v	201	HEM	2	0
28	D	403	PHO	2	0
27	B	612	CLA	4	0
27	C	509	CLA	6	0
27	14	304	CLA	2	0
33	b	618	LMG	3	0
35	j	101	DGD	2	0
27	d	402	CLA	3	0
38	14	313	A86	9	0
27	12	306	CLA	1	0
27	b	607	CLA	2	0
27	Z	102	CLA	2	0
38	13	313	A86	9	0
38	14	314	A86	4	0
29	h	101	BCR	3	0
32	a	408	LHG	6	0
38	12	316	A86	4	0
27	13	301	CLA	3	0
27	11	308	CLA	1	0
33	W	101	LMG	4	0
38	31	316	A86	9	0
27	12	305	CLA	9	0
32	l	102	LHG	3	0
38	11	311	A86	9	0
27	D	402	CLA	2	0
27	z	102	CLA	2	0
27	C	513	CLA	4	0
27	D	406	CLA	1	0
38	32	315	A86	9	0
27	14	310	CLA	1	0
38	11	313	A86	5	0
27	12	312	CLA	1	0
38	33	315	A86	5	0

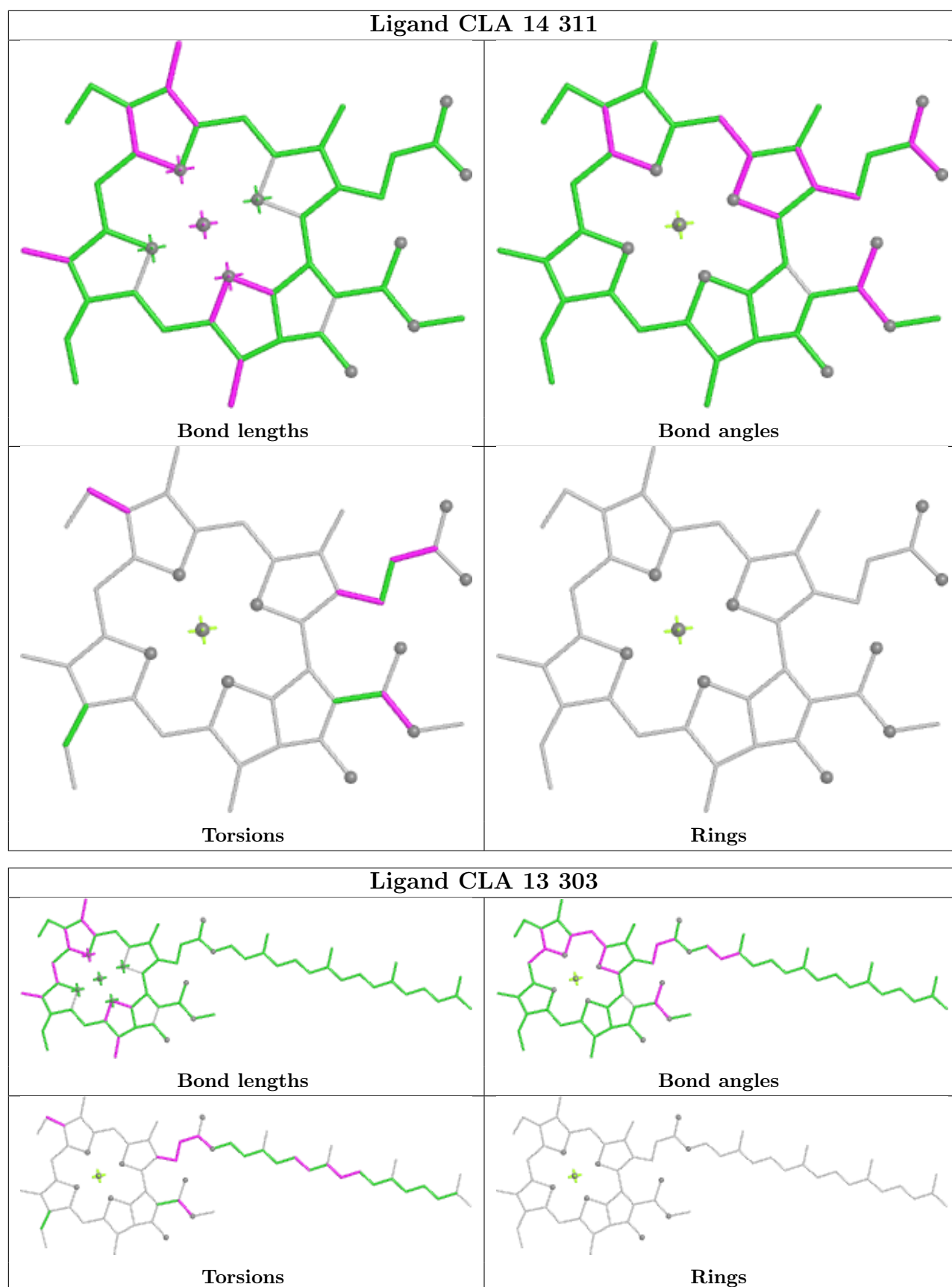
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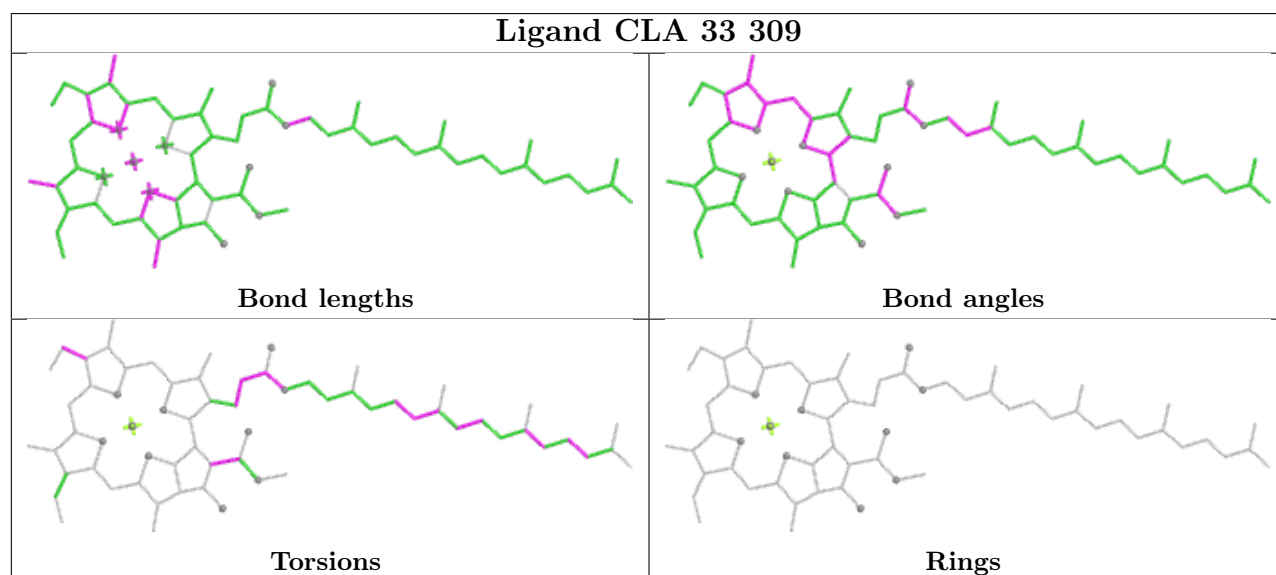
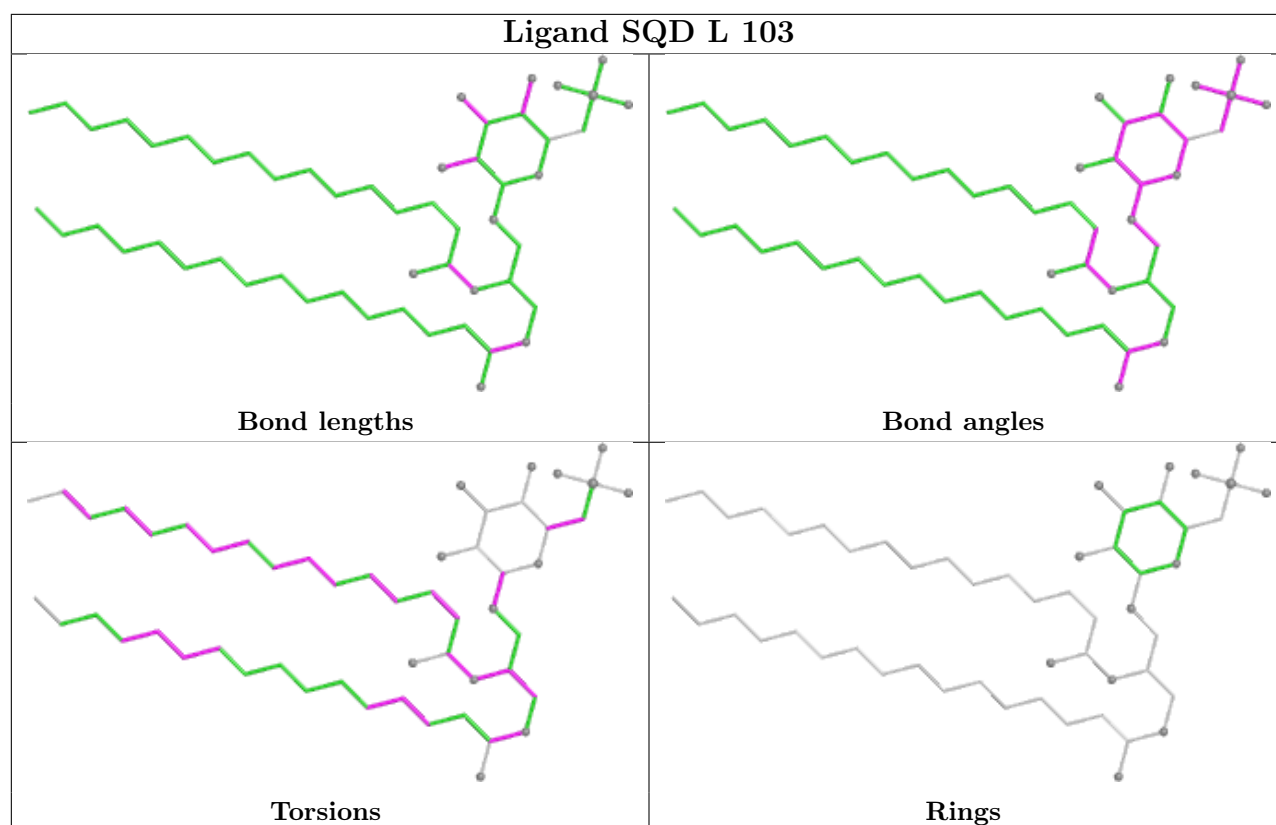
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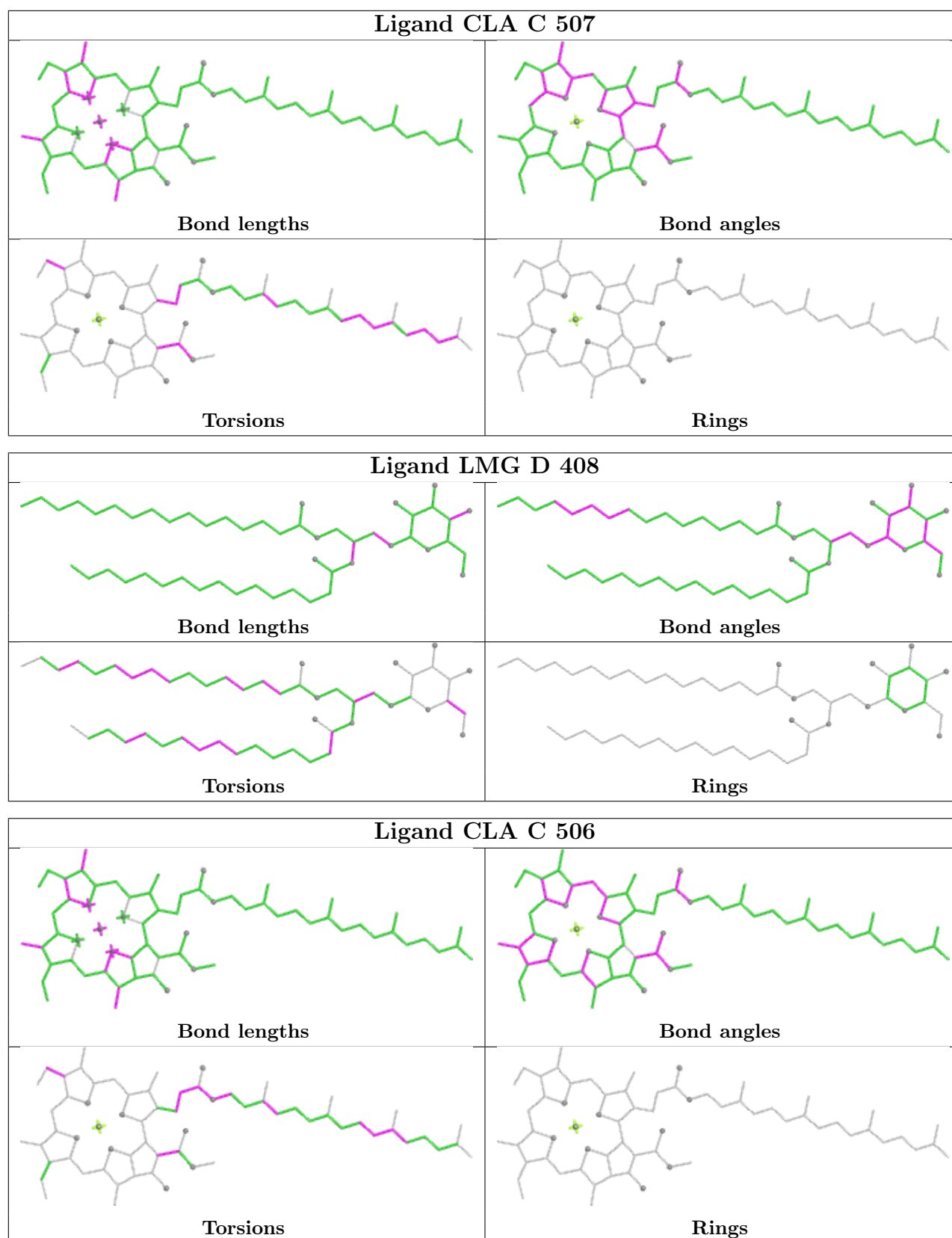
Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	33	313	A86	9	0
27	31	302	CLA	2	0
38	32	304	A86	7	0
27	B	603	CLA	1	0
27	c	502	CLA	4	0
27	11	306	CLA	1	0
32	l	103	LHG	1	0
27	33	306	CLA	2	0
27	33	301	CLA	5	0
27	W	103	CLA	3	0
27	33	304	CLA	2	0
32	L	101	LHG	6	0
27	12	309	CLA	2	0
29	F	101	BCR	2	0
27	b	612	CLA	4	0
27	33	308	CLA	1	0
29	C	520	BCR	1	0
27	11	302	CLA	2	0
28	d	403	PHO	2	0
27	b	602	CLA	6	0
27	W	102	CLA	4	0

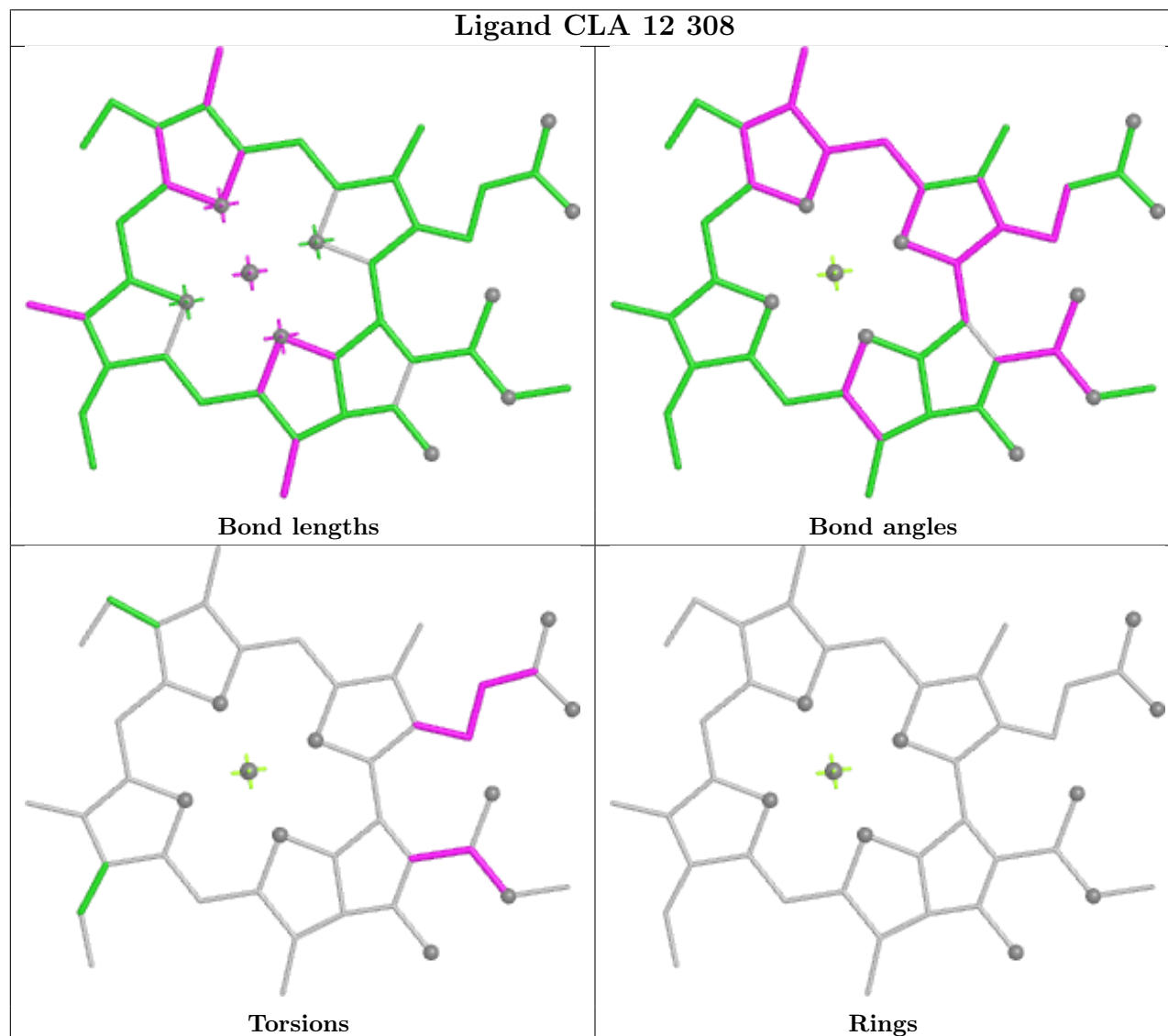
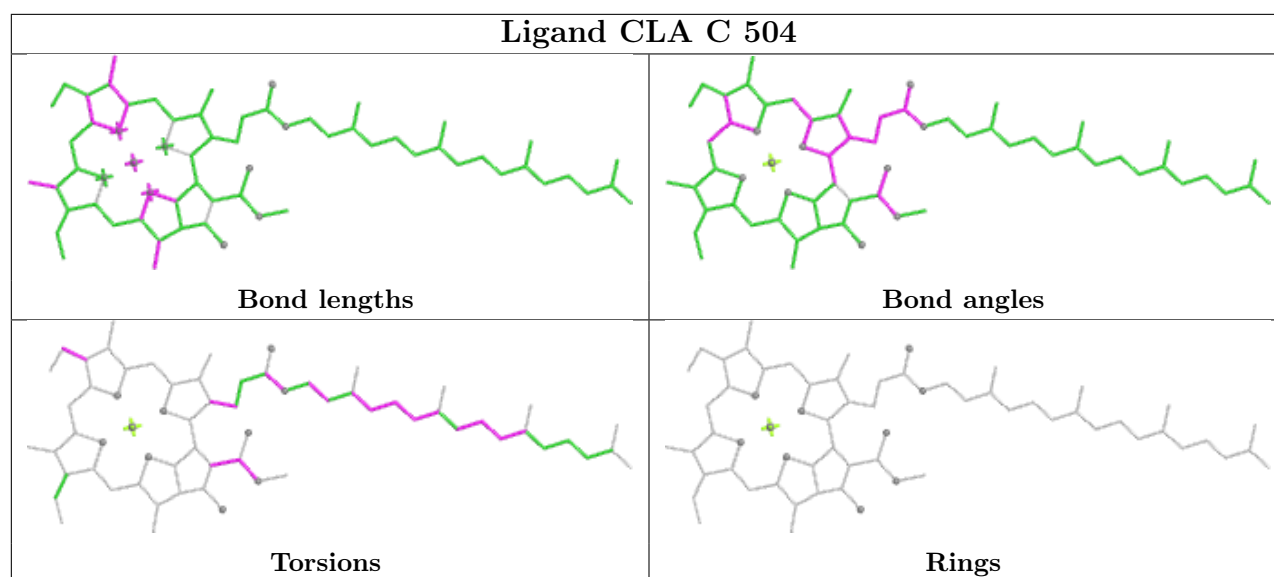
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

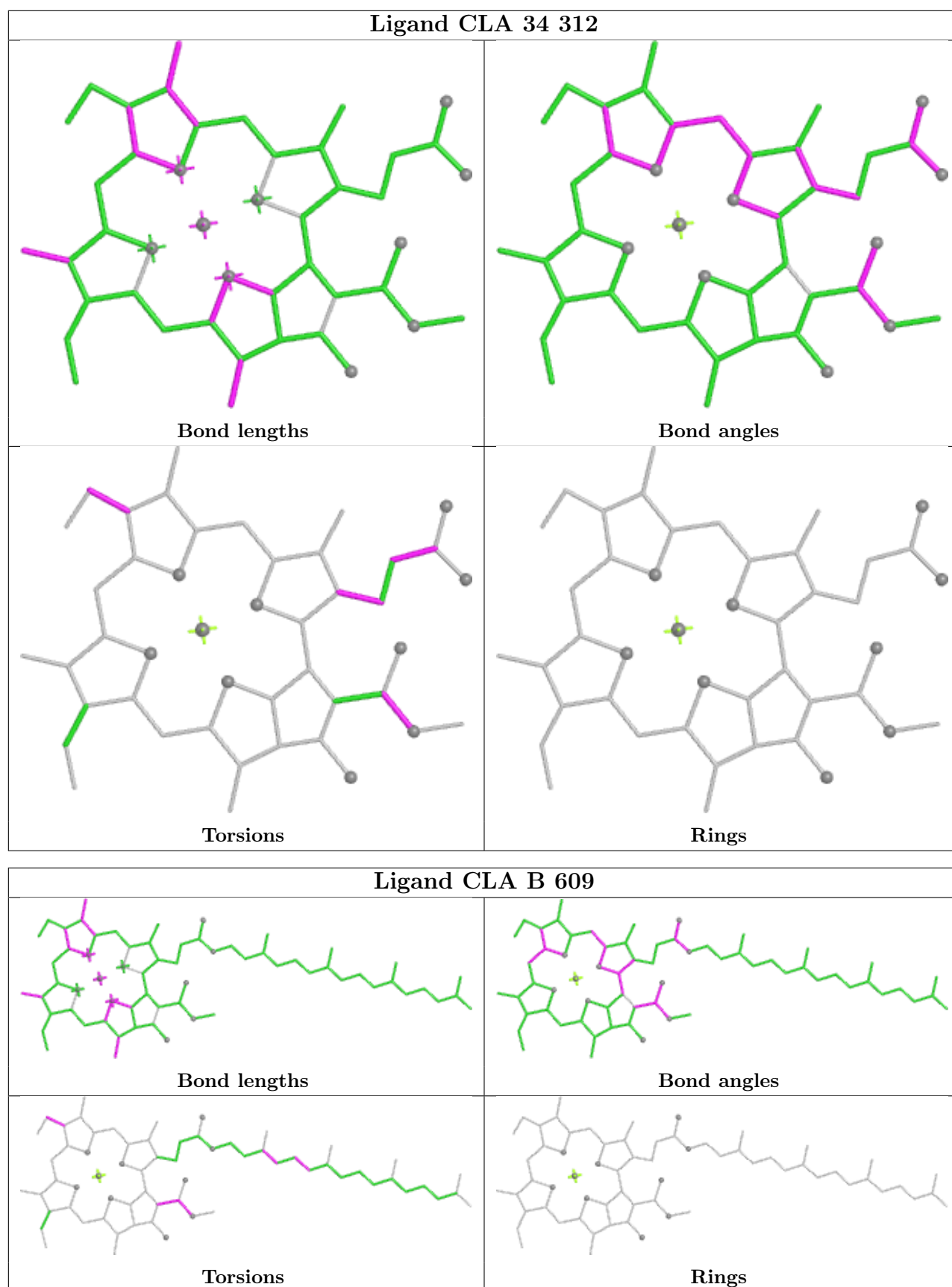


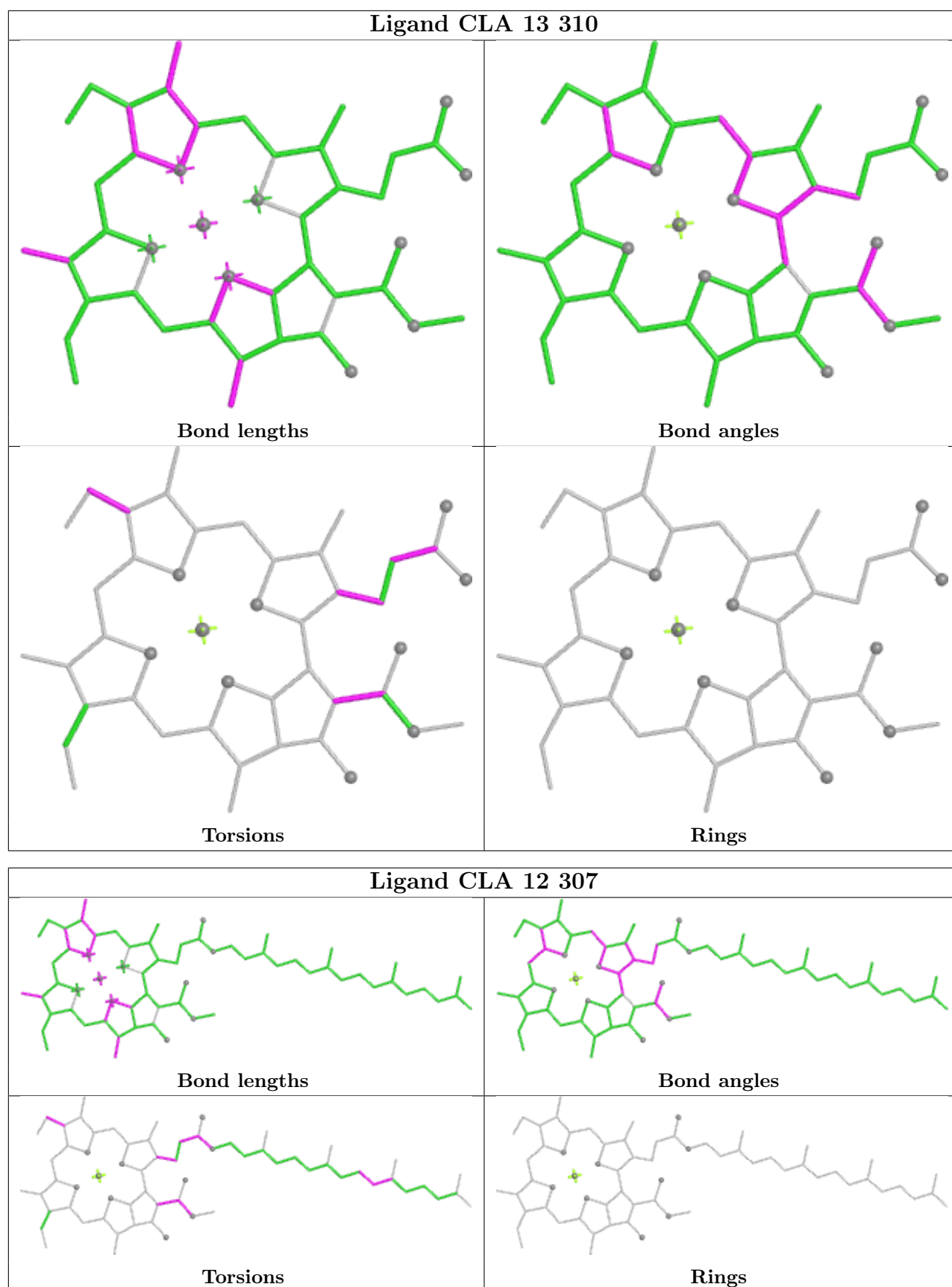


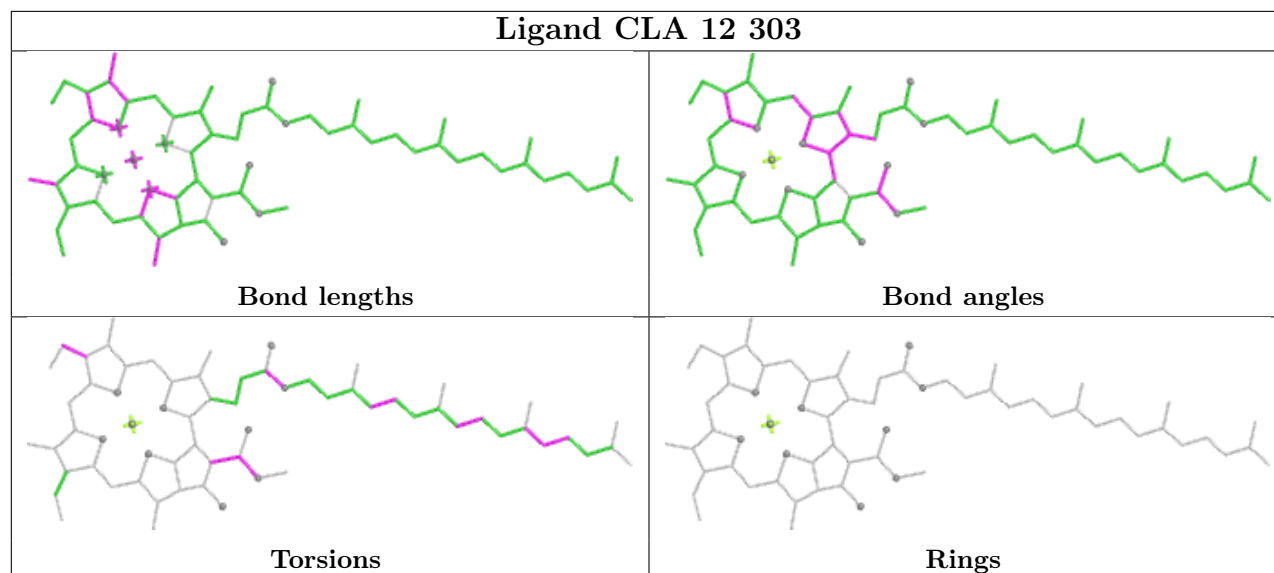
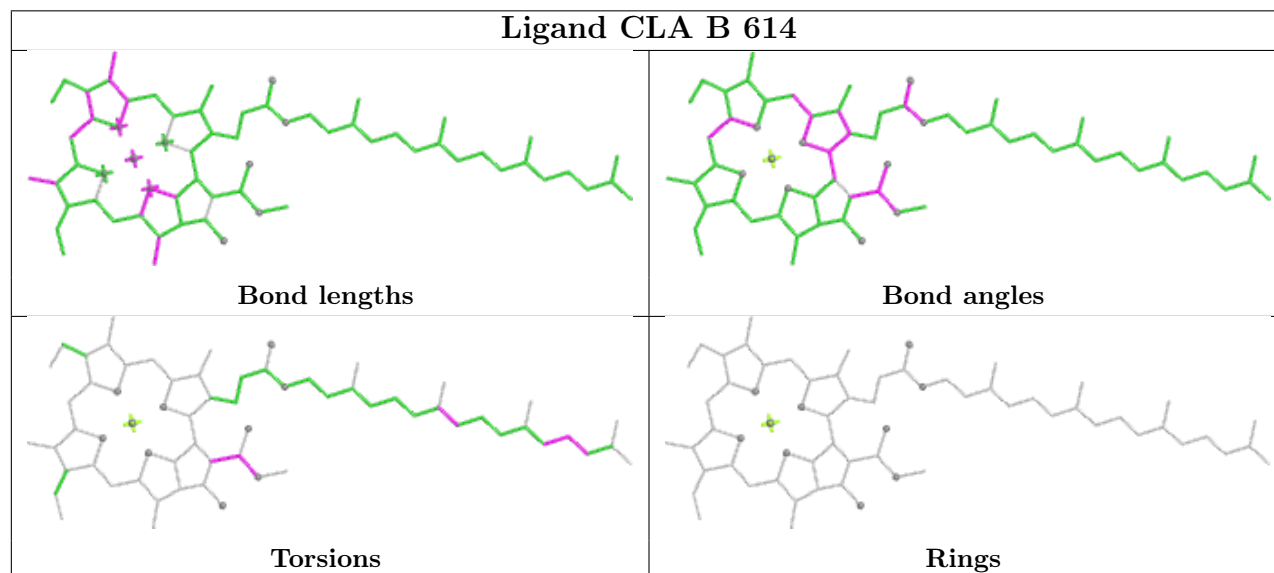
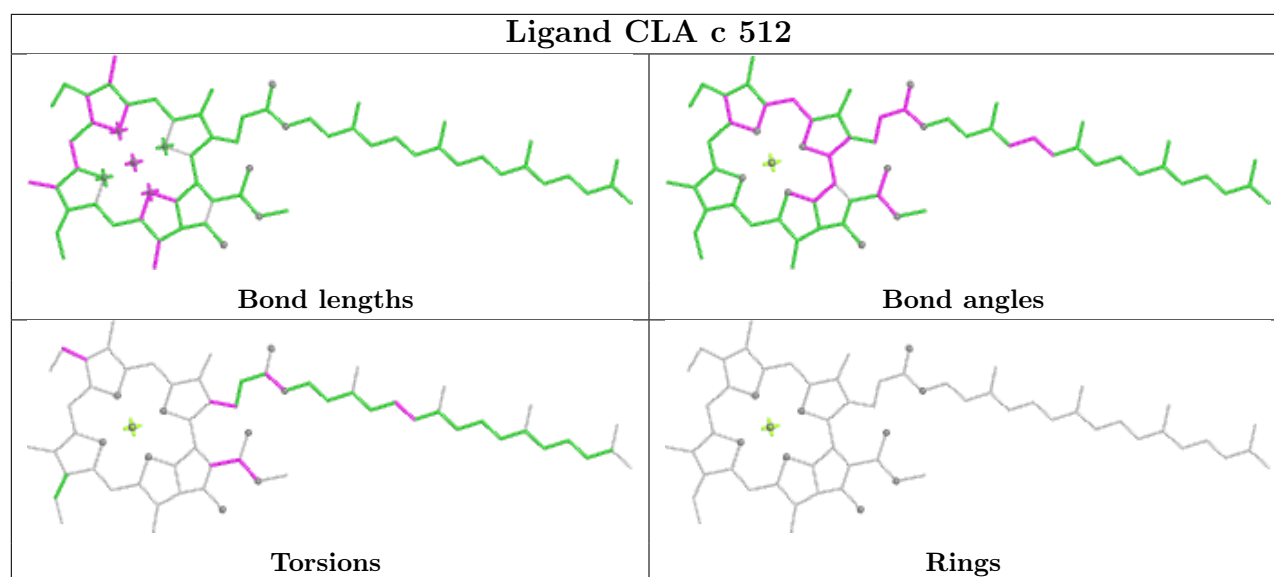


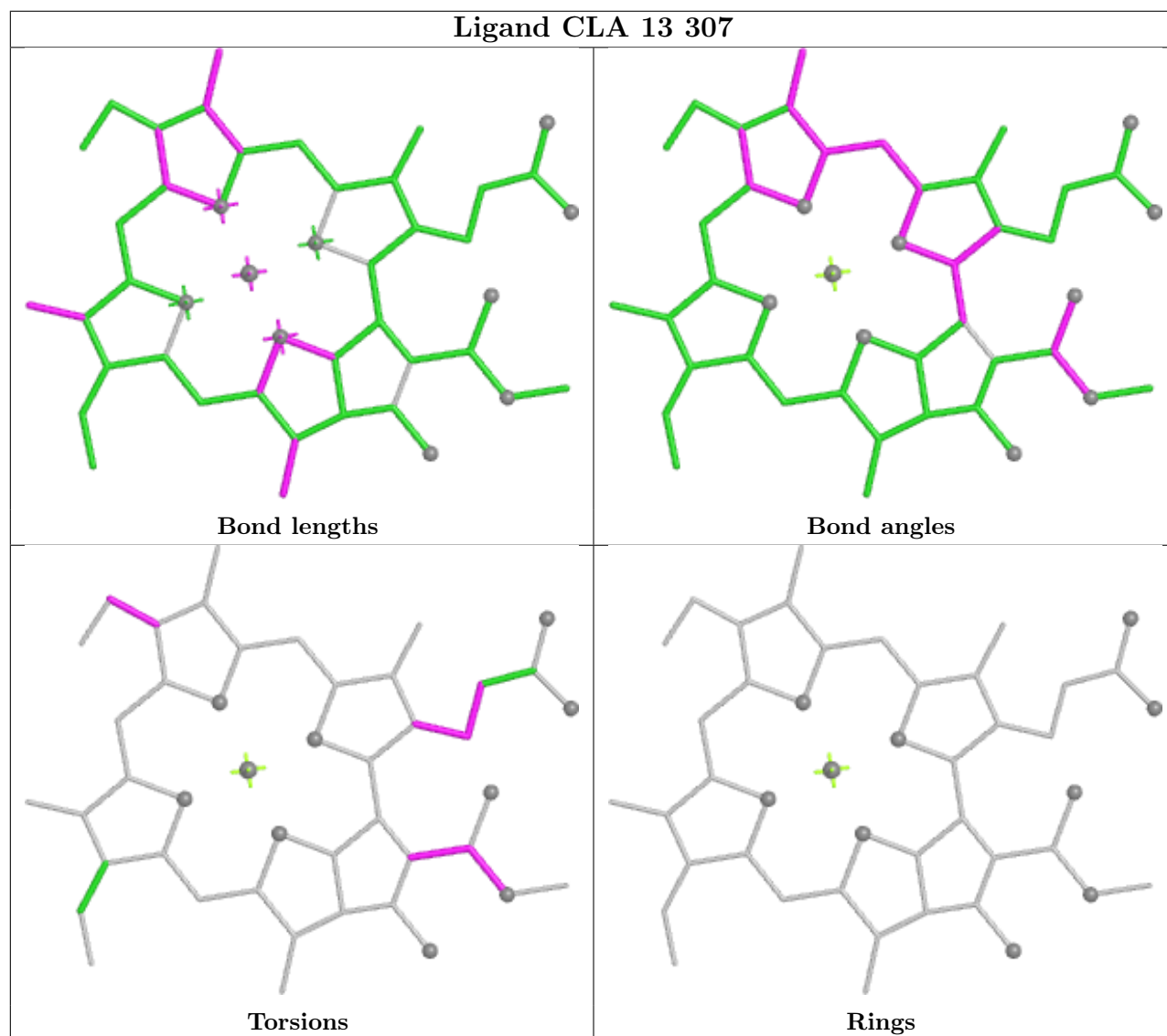
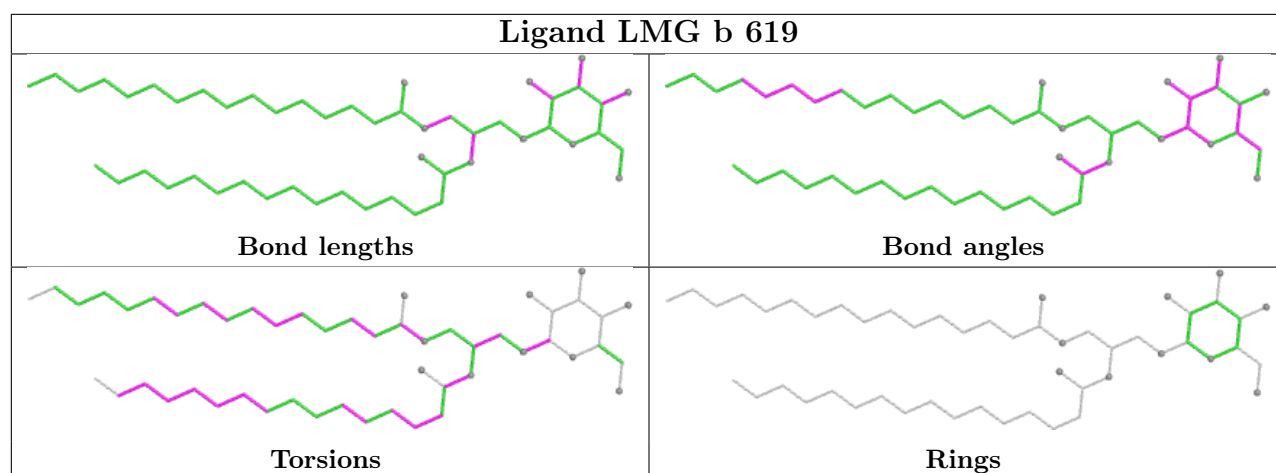


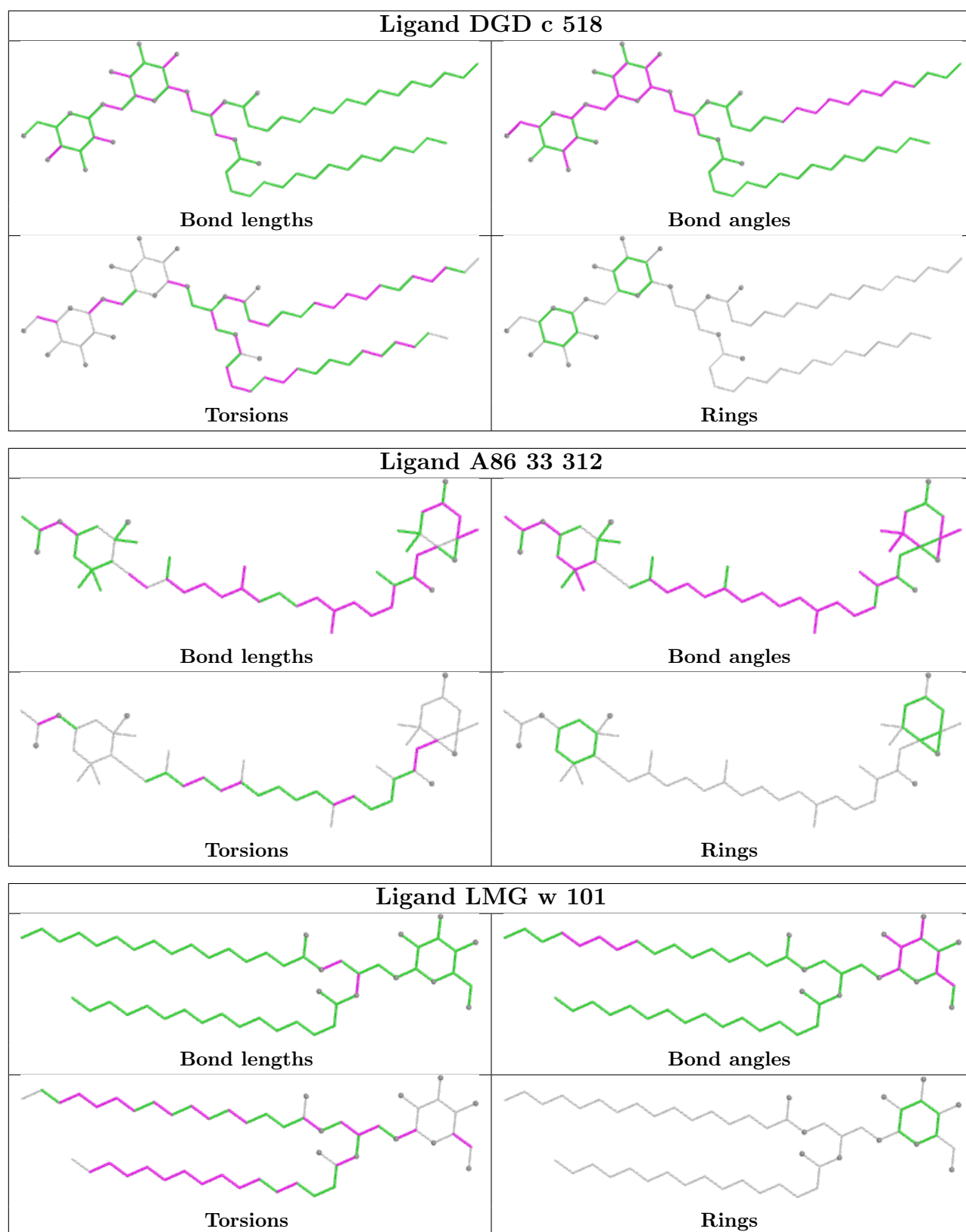


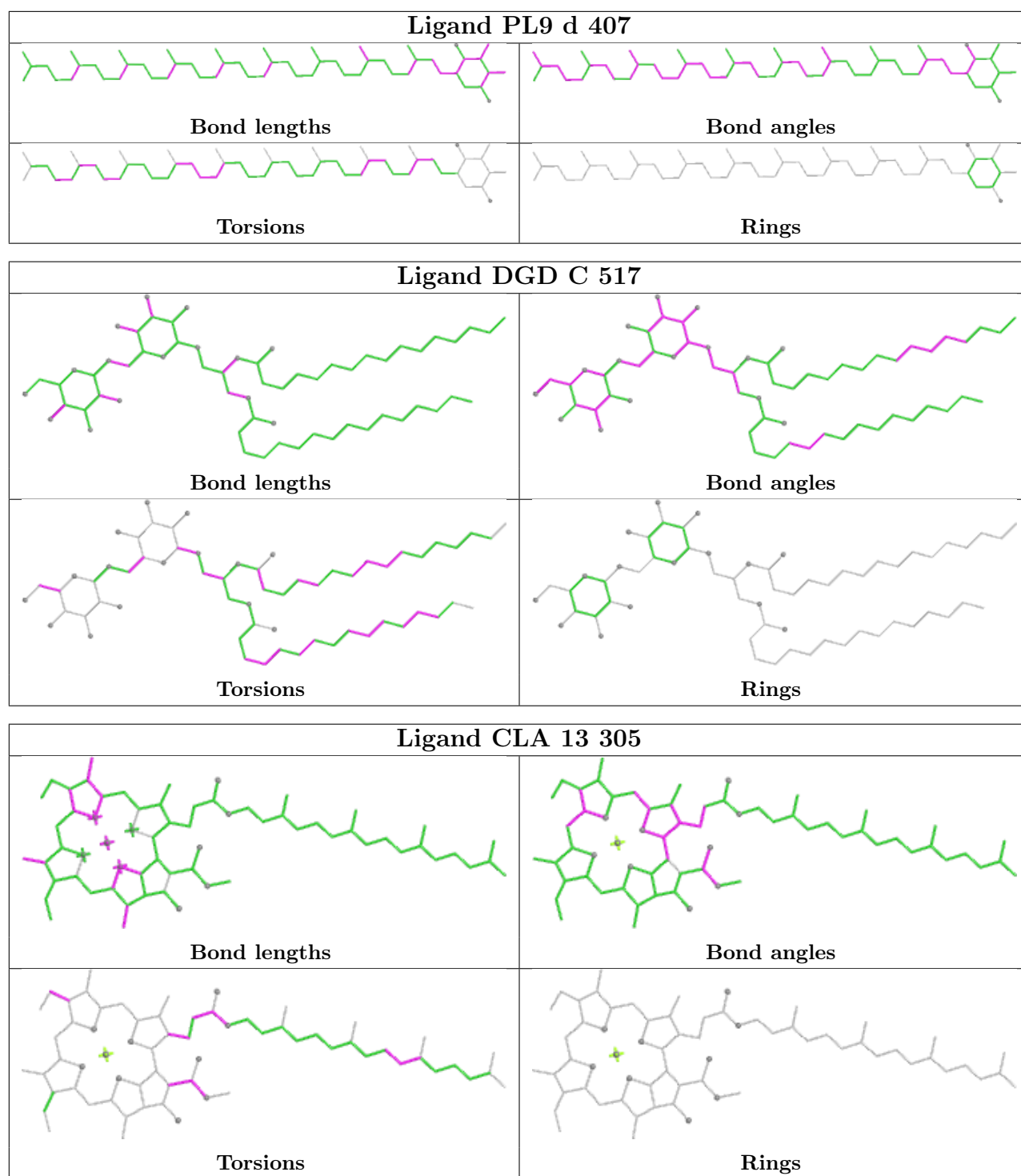




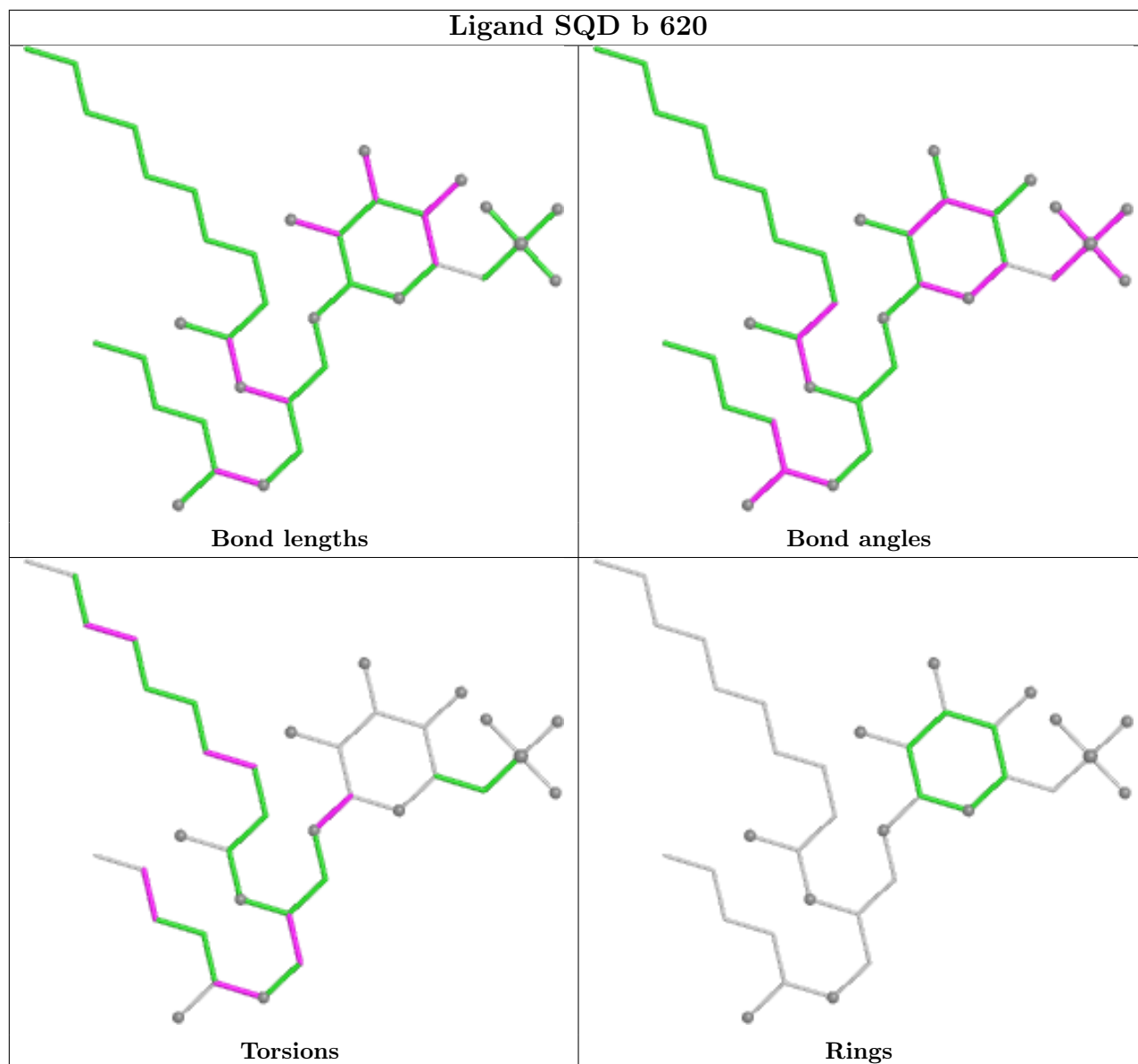




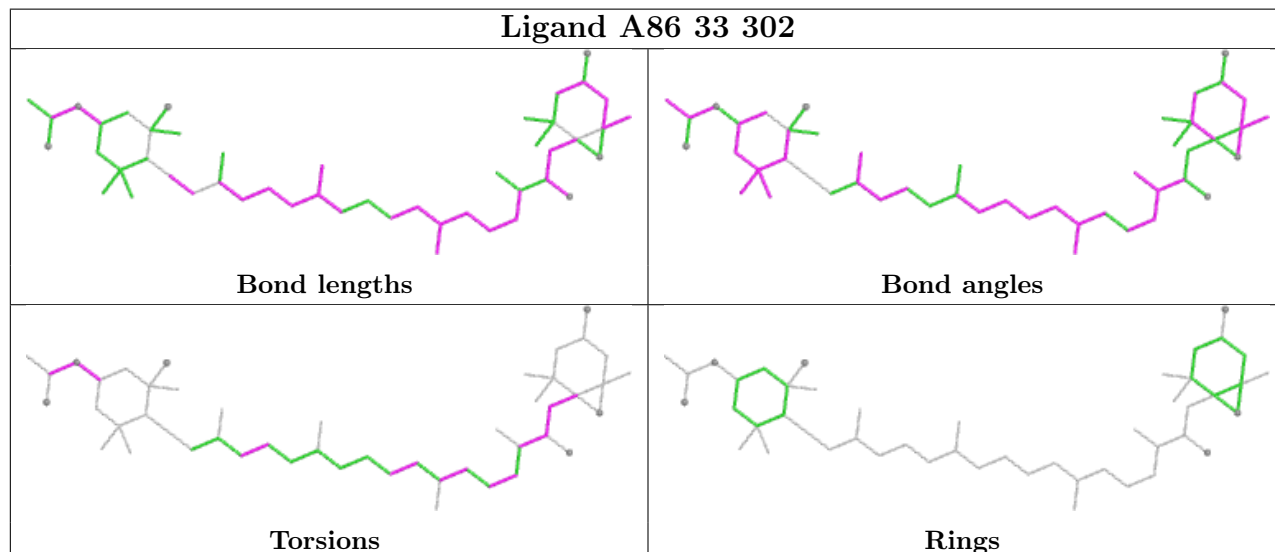


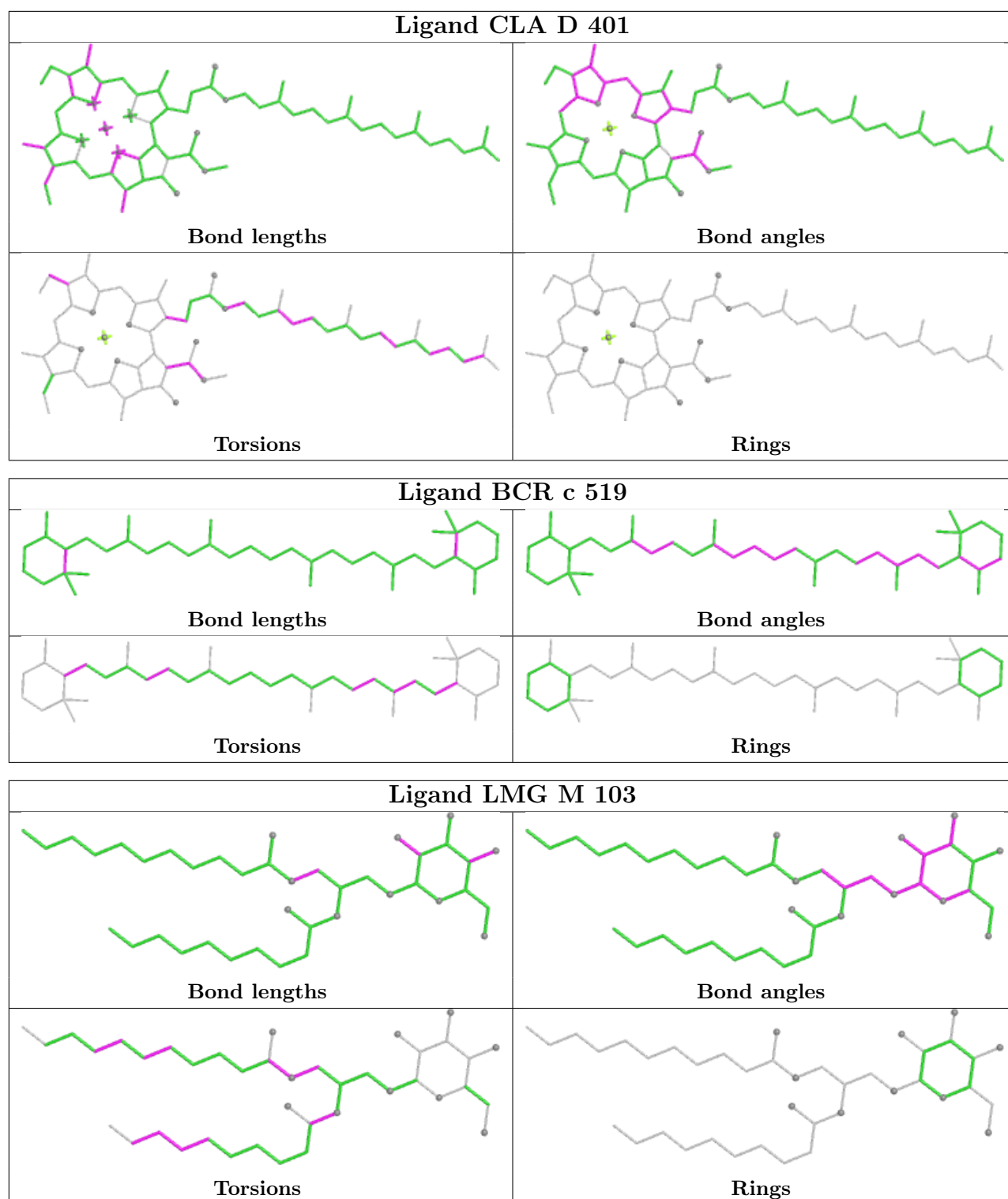


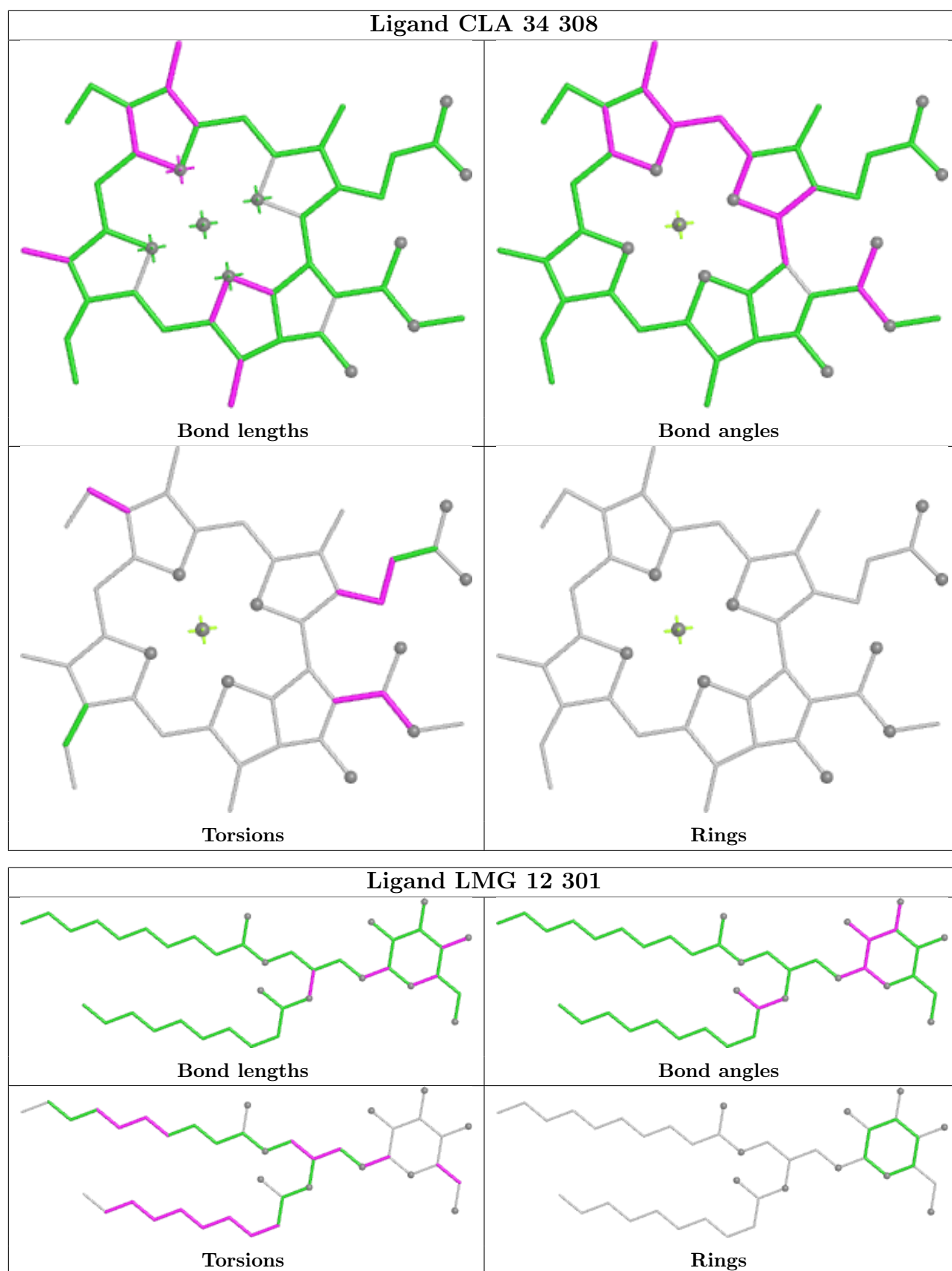
Ligand SQD b 620

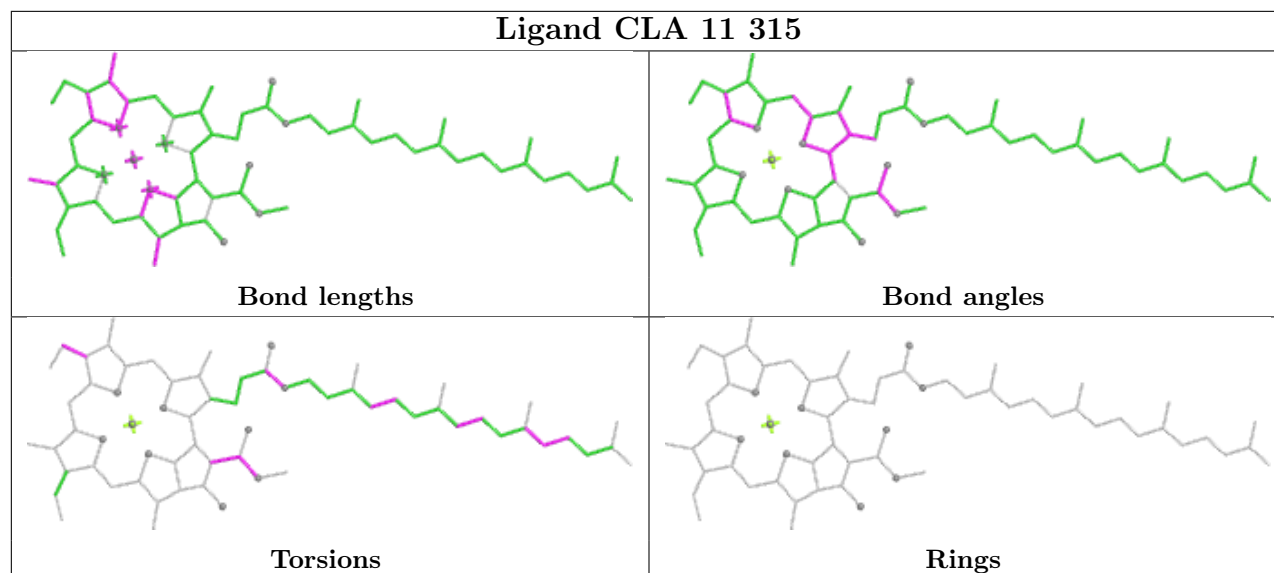
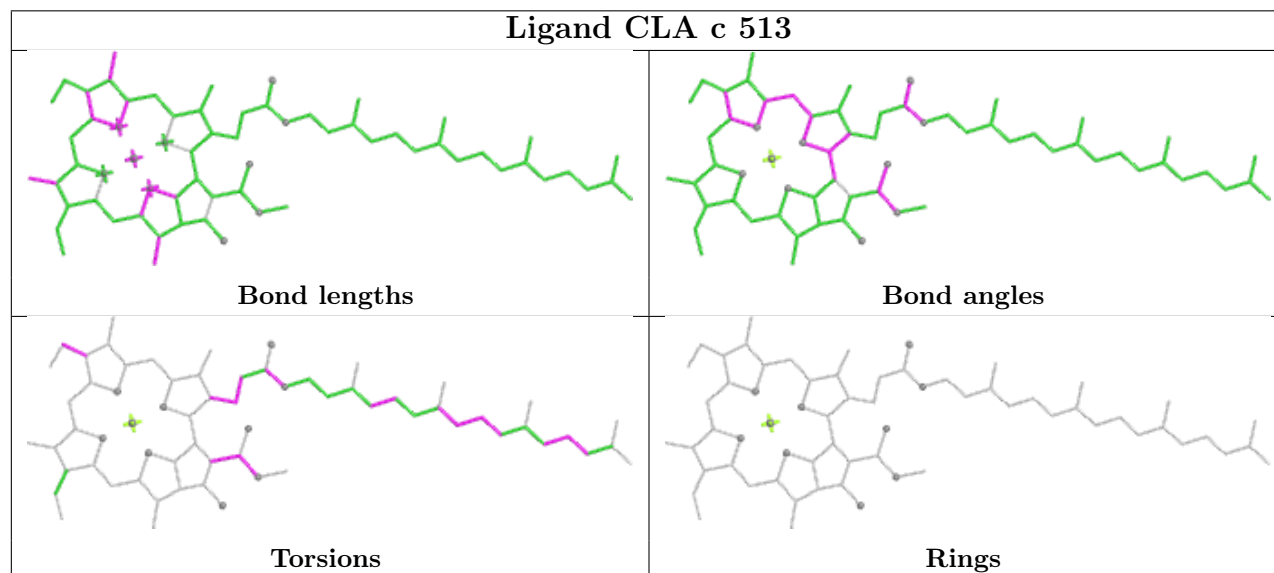
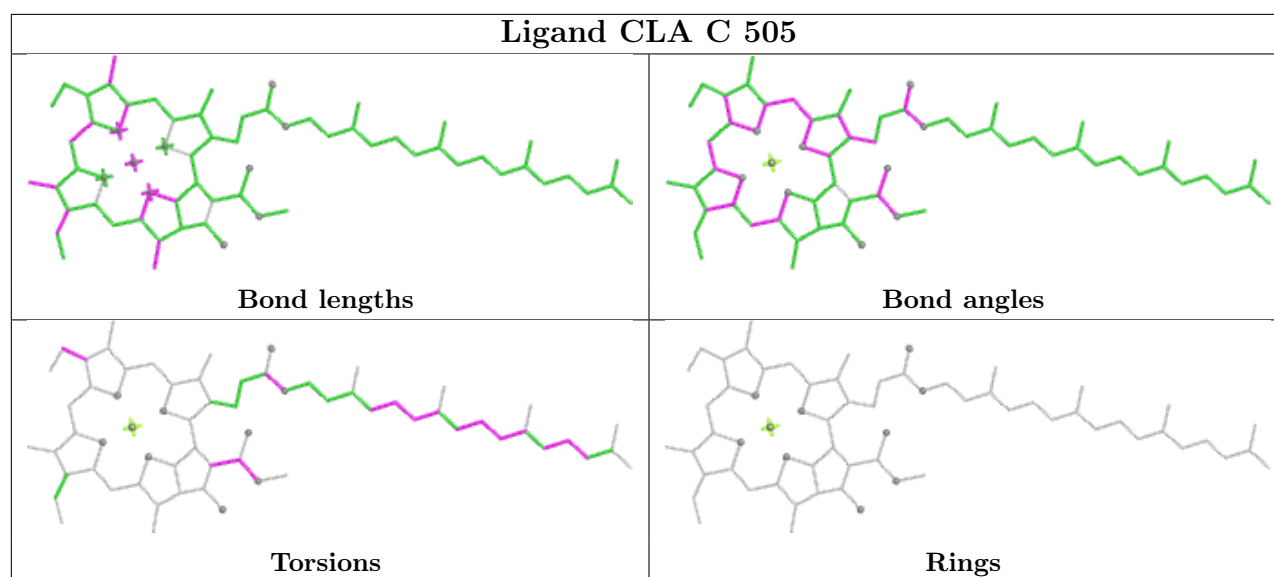


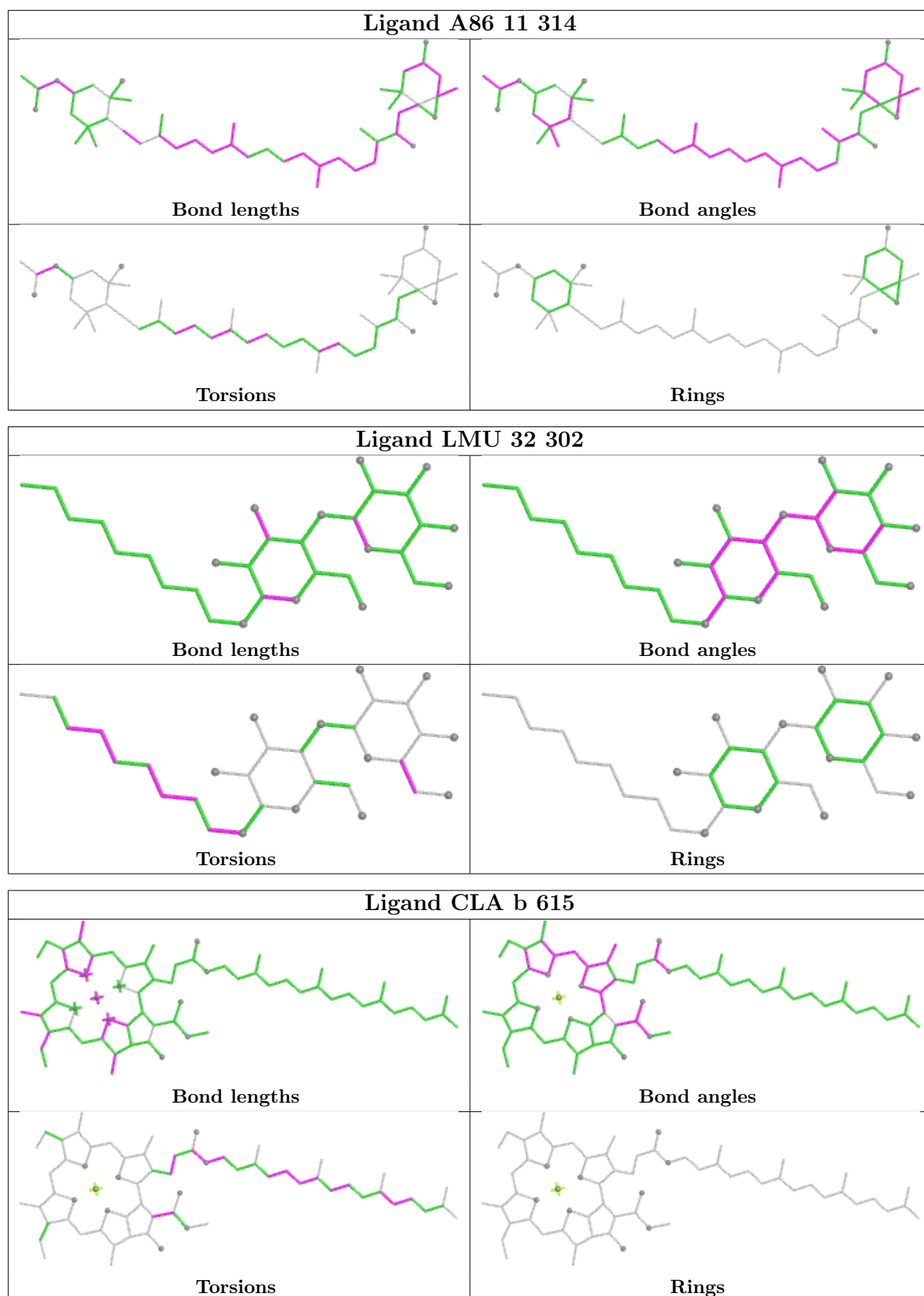
Ligand A86 33 302

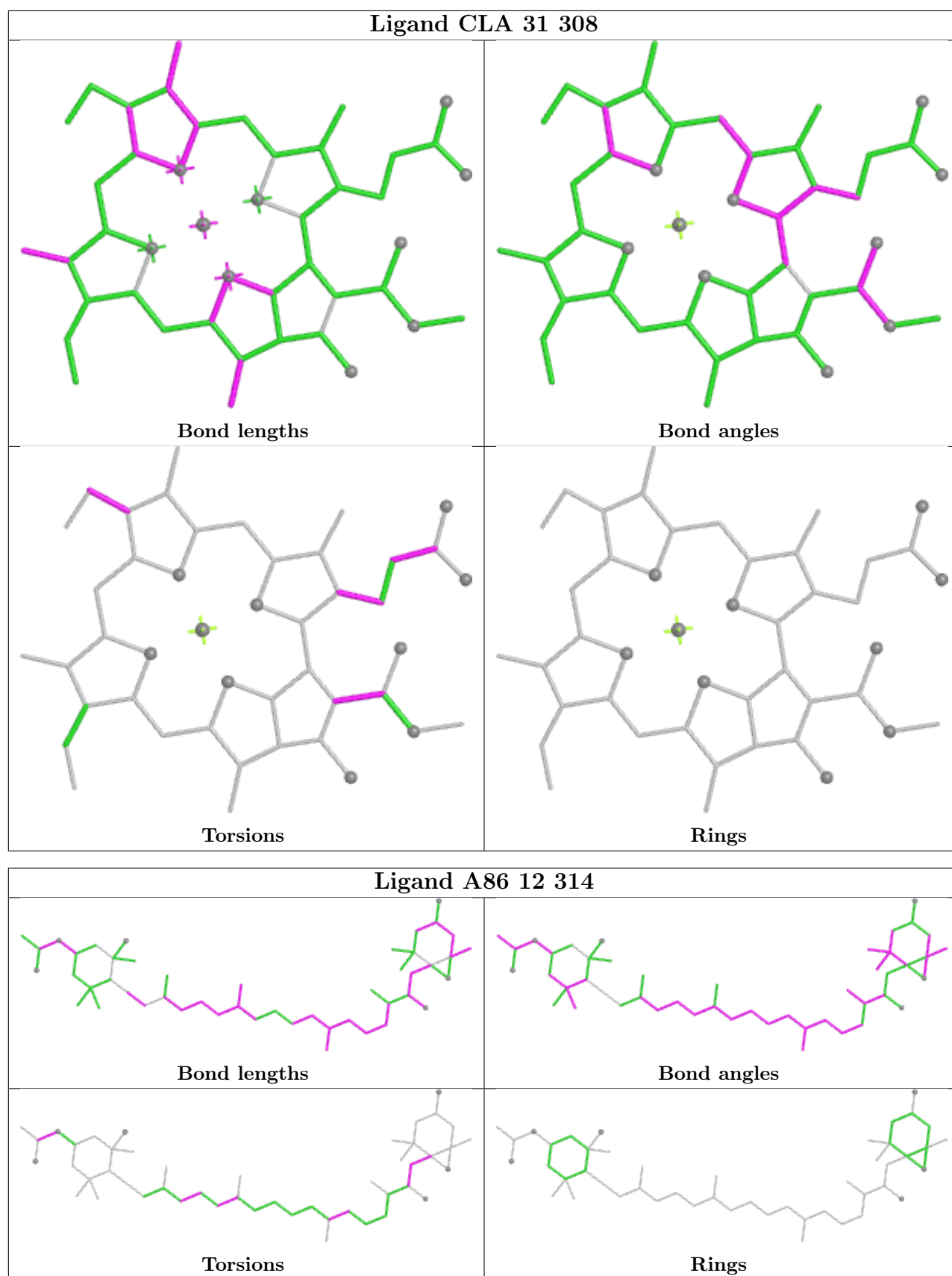


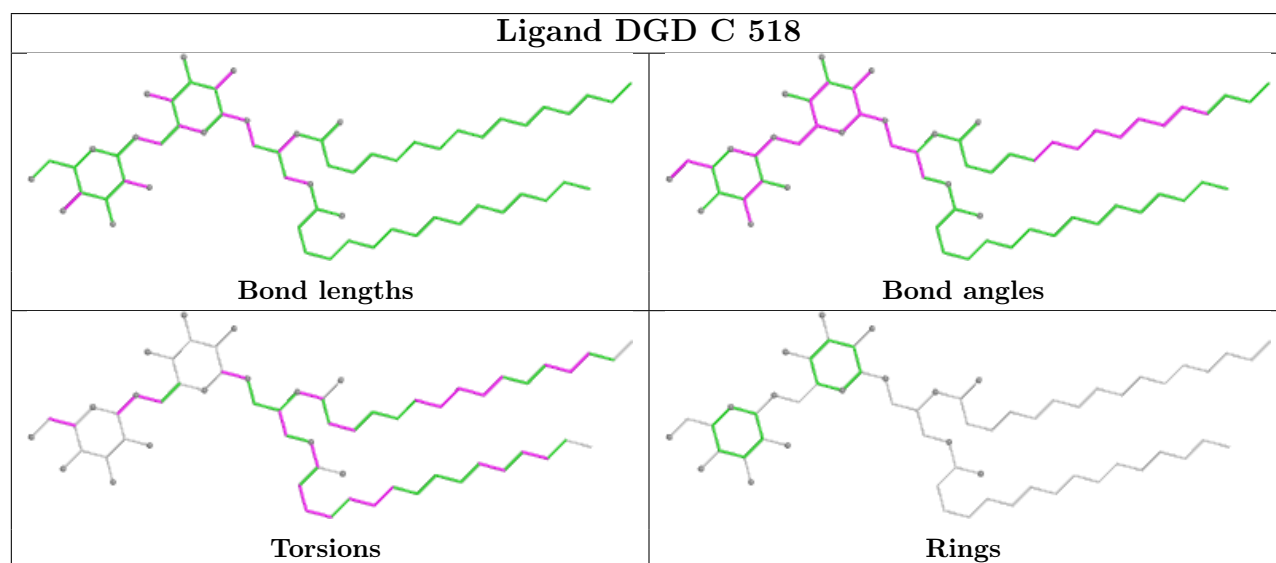
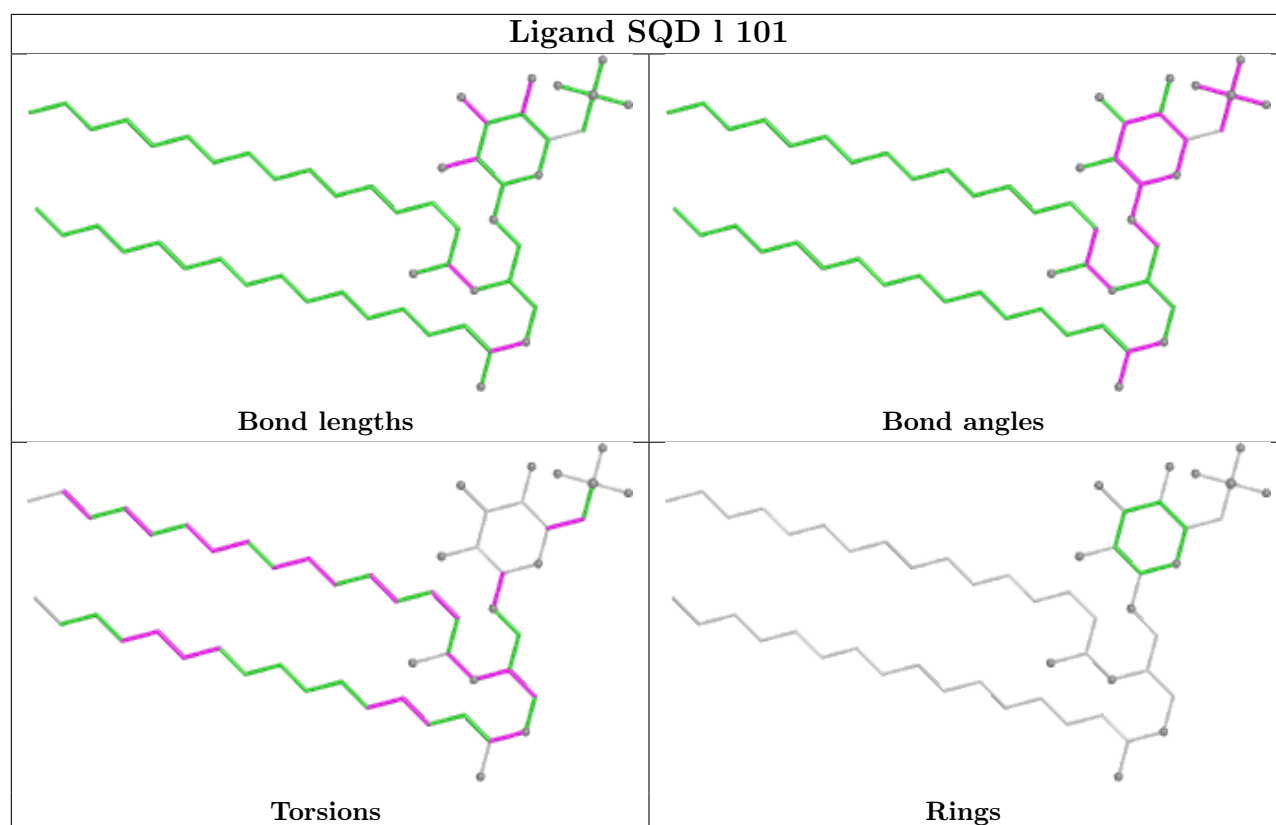


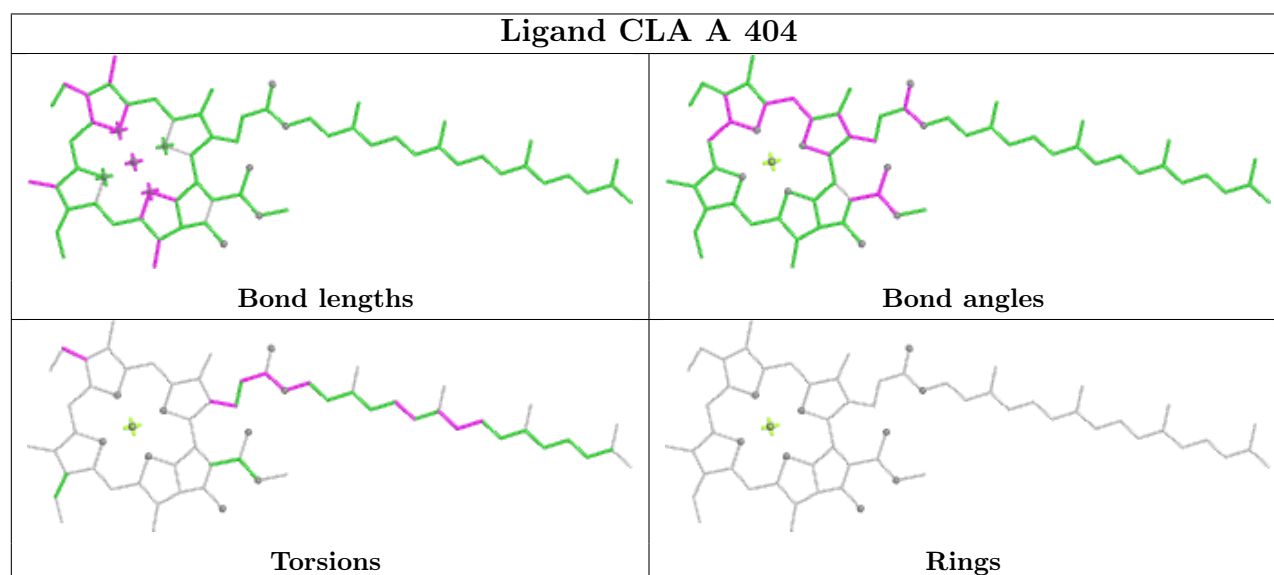
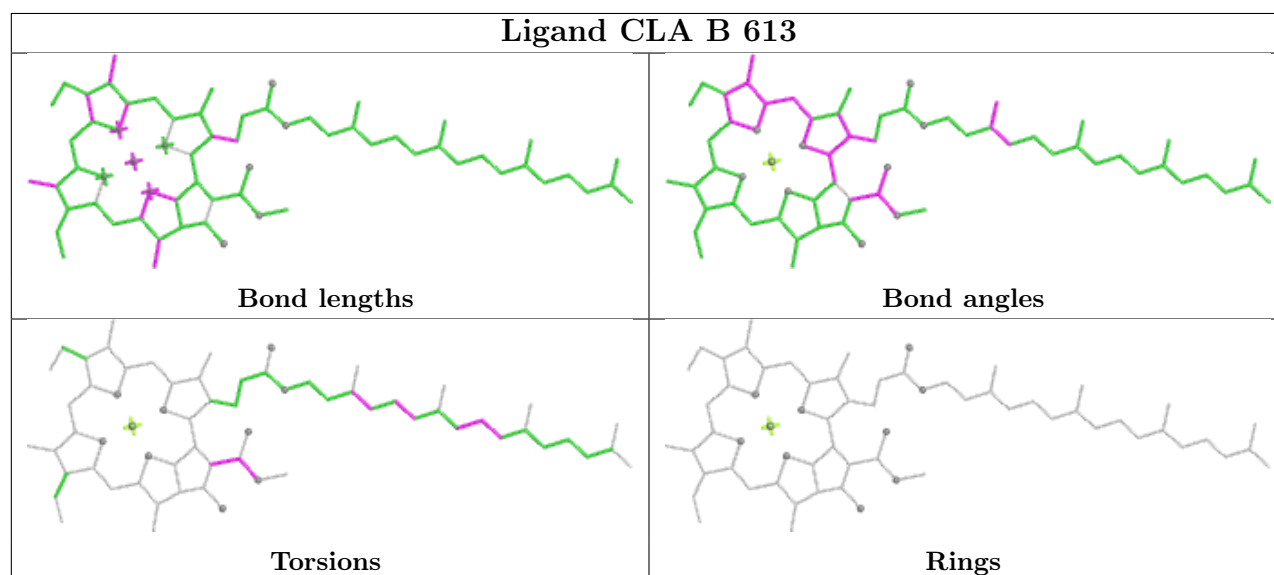
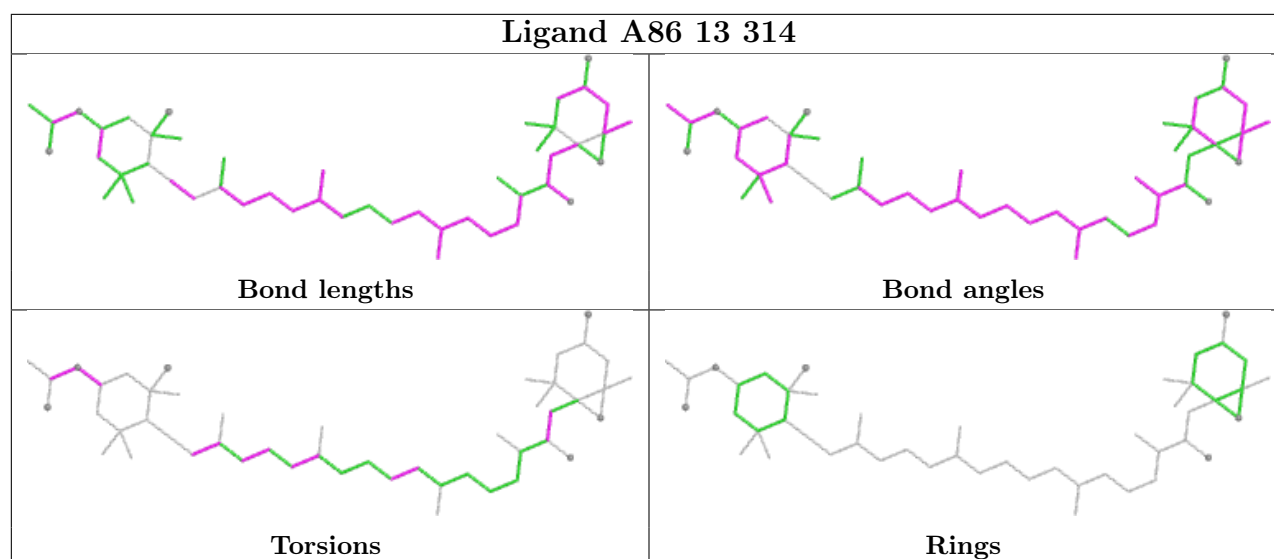


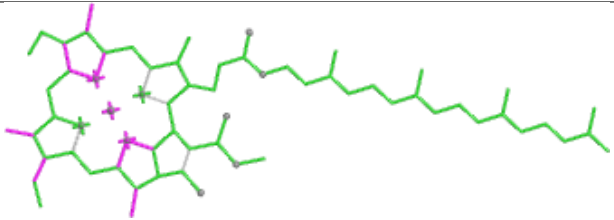
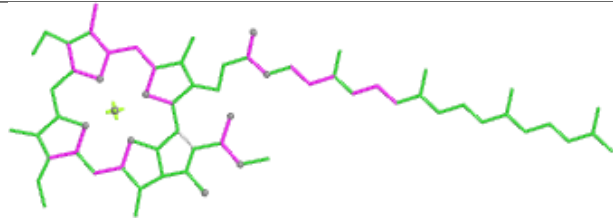
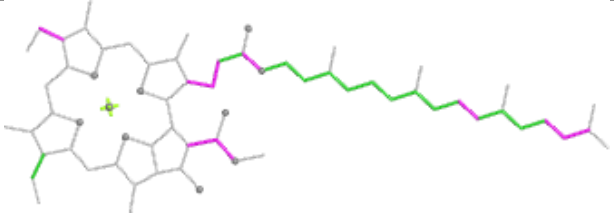
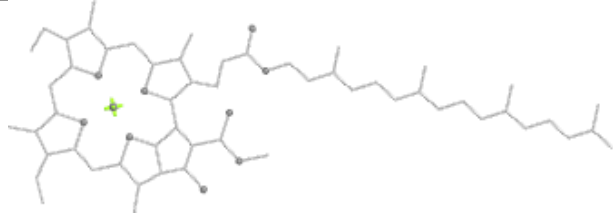


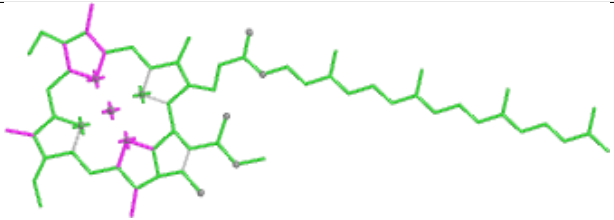
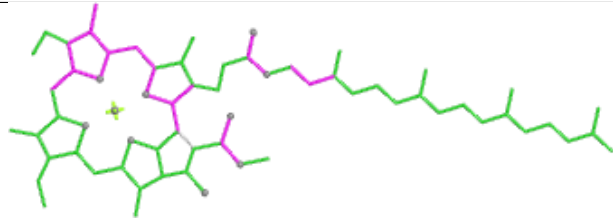
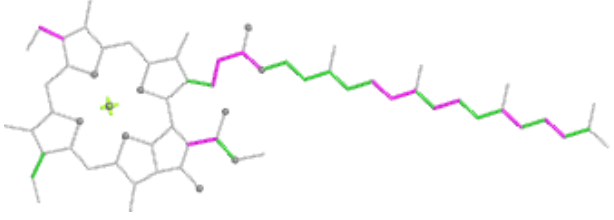
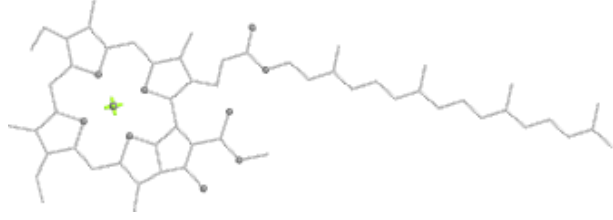


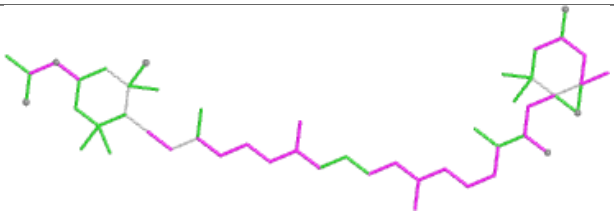
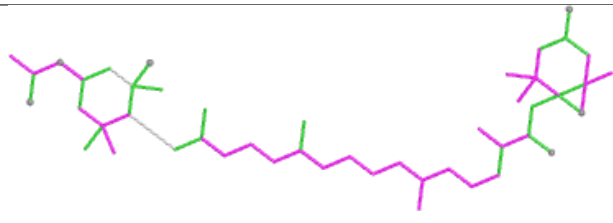
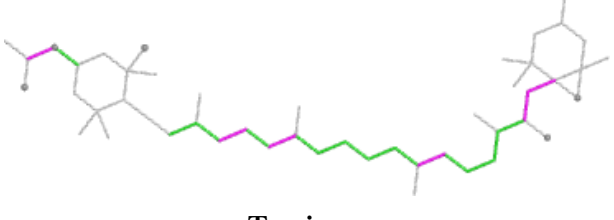
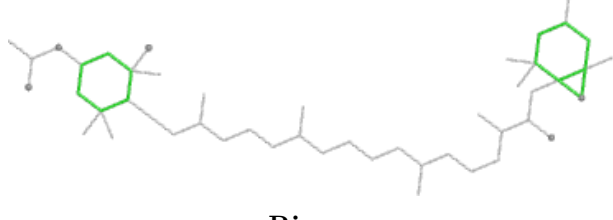


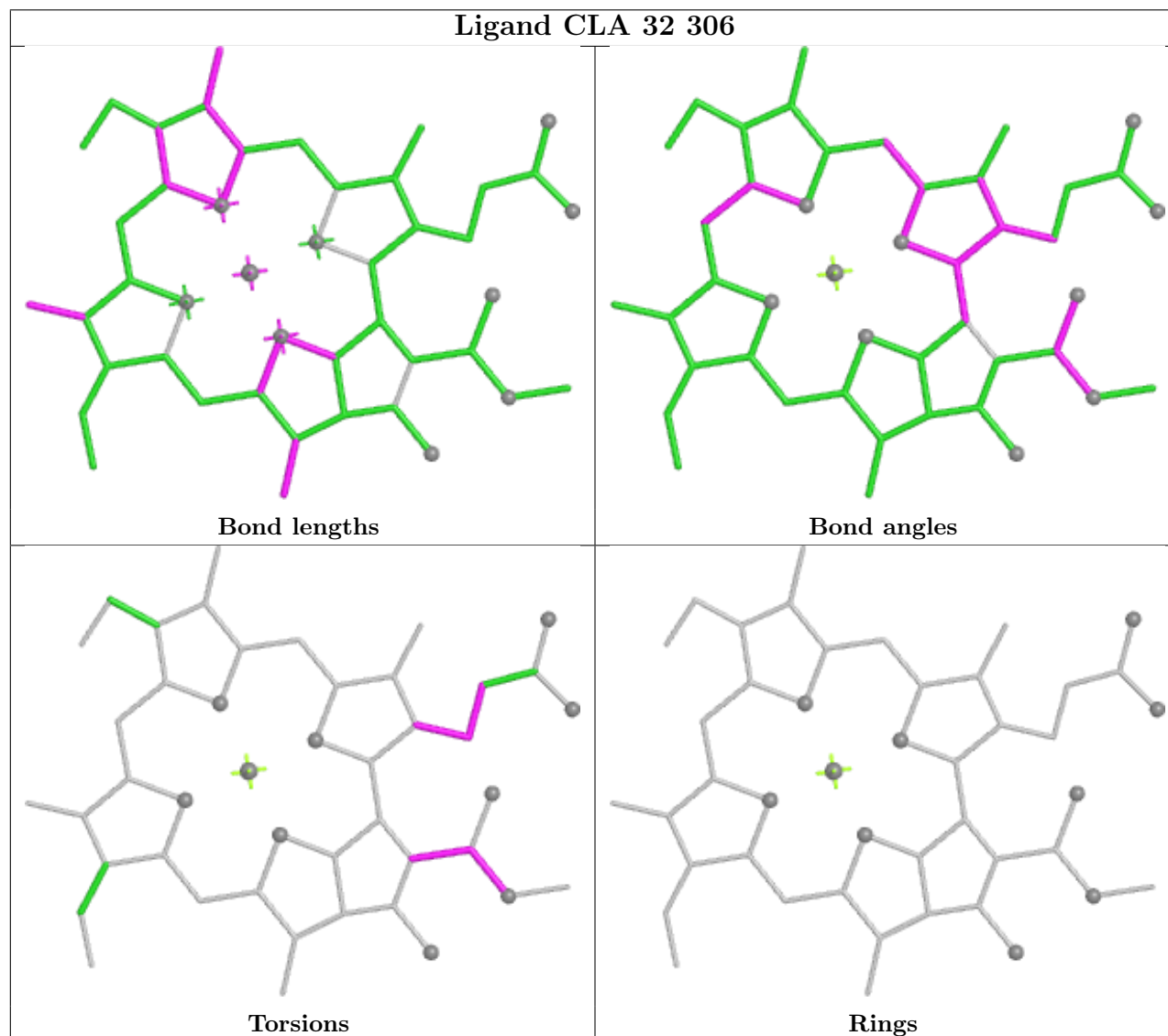
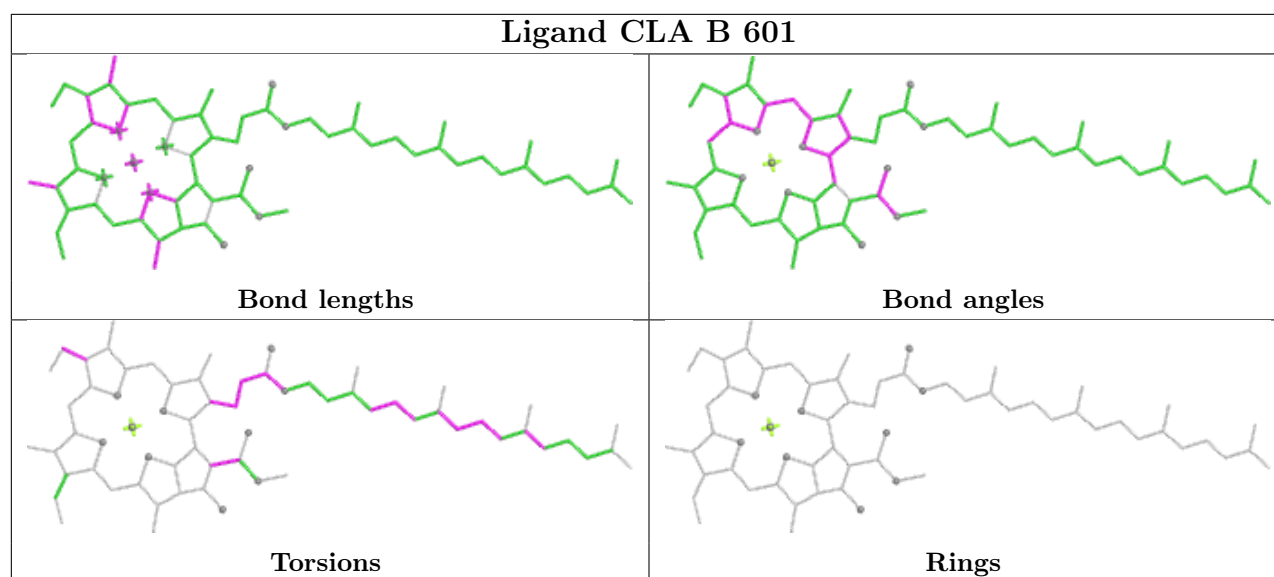


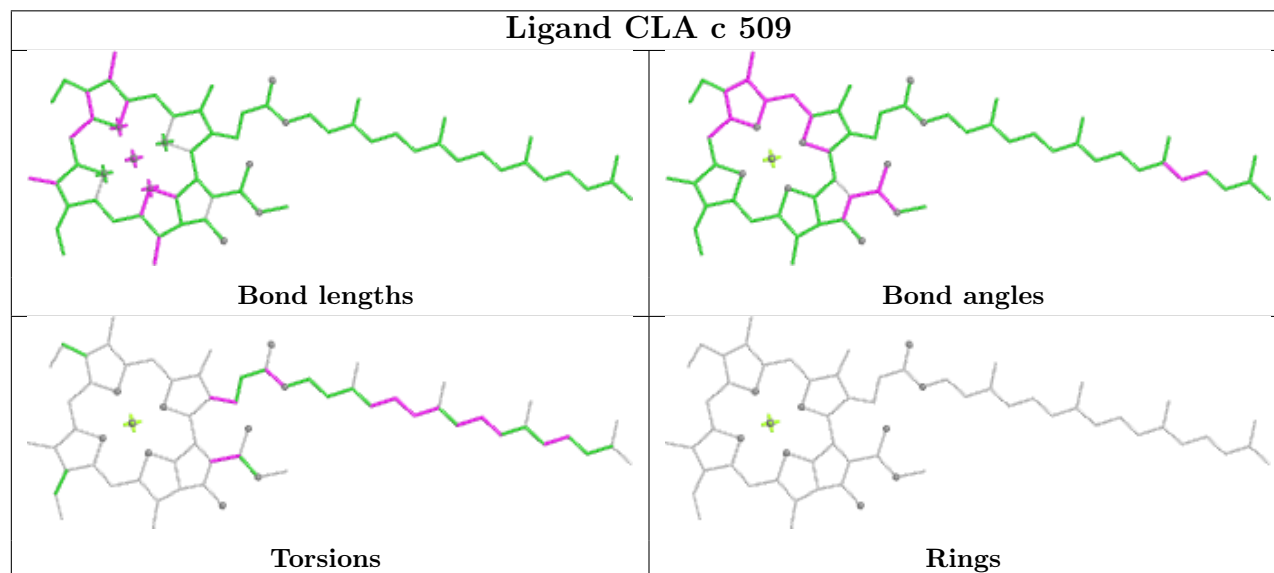
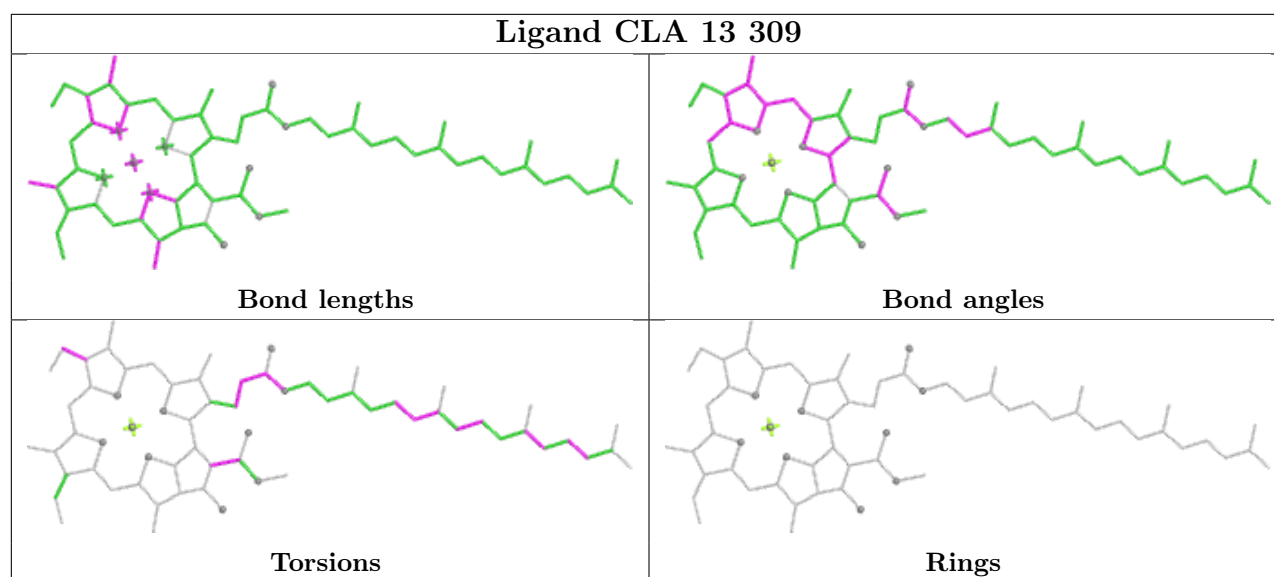


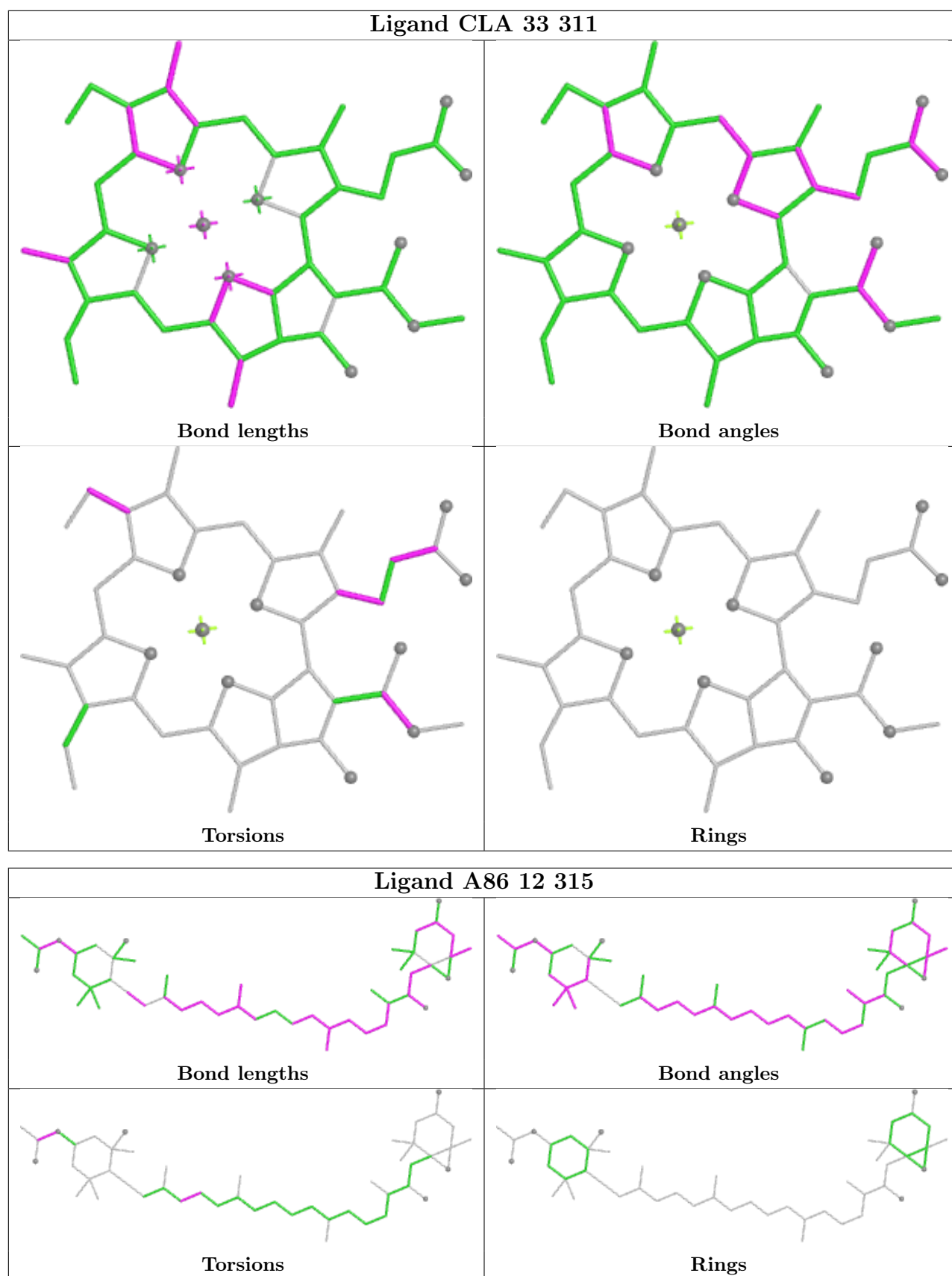
Ligand CLA b 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

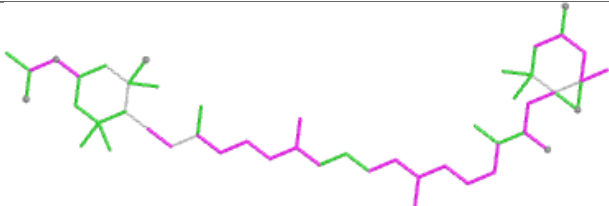
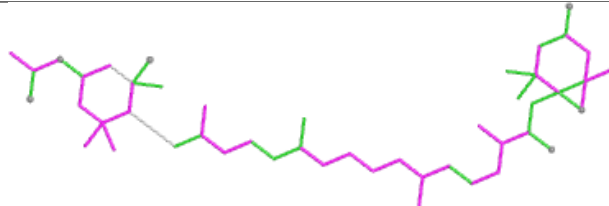
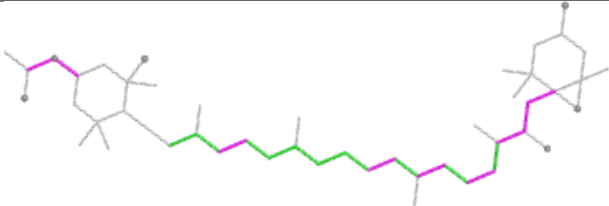
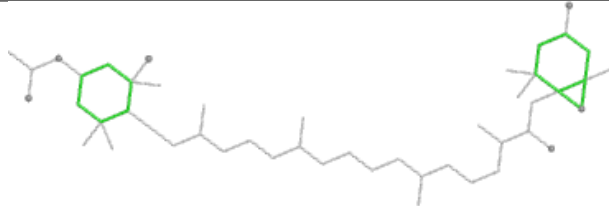
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Bond lengths	Bond angles
	
Torsions	Rings

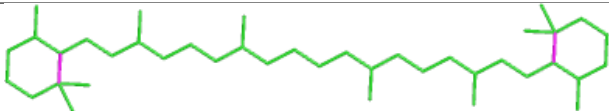
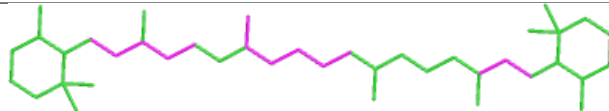
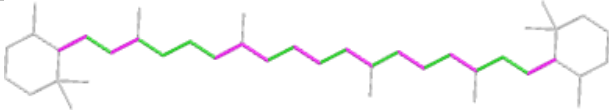
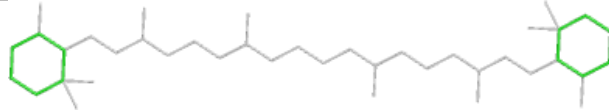
Ligand A86 13 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

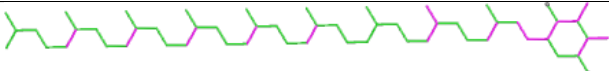
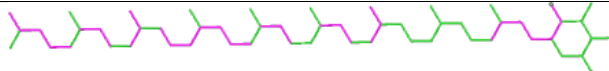
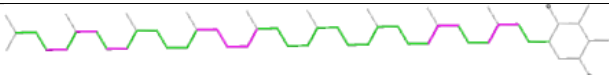
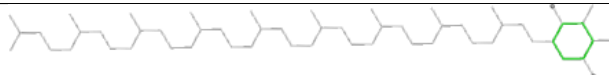


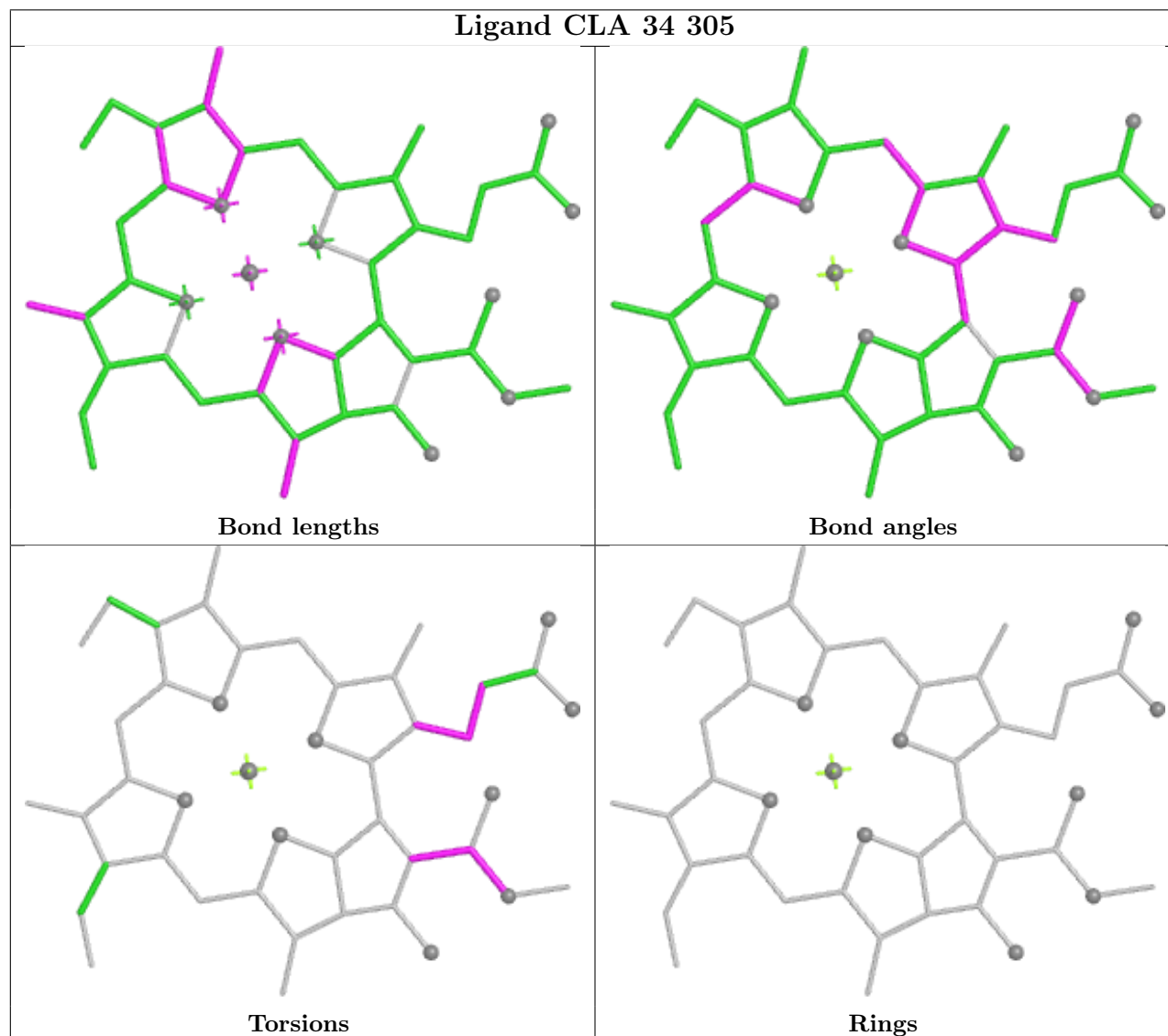
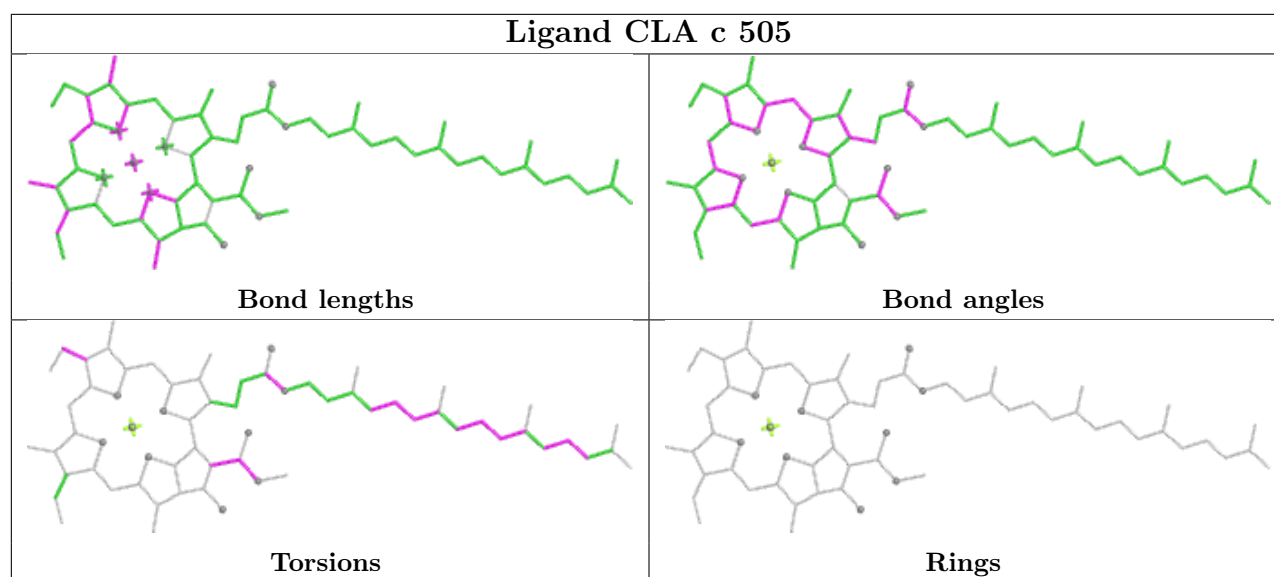


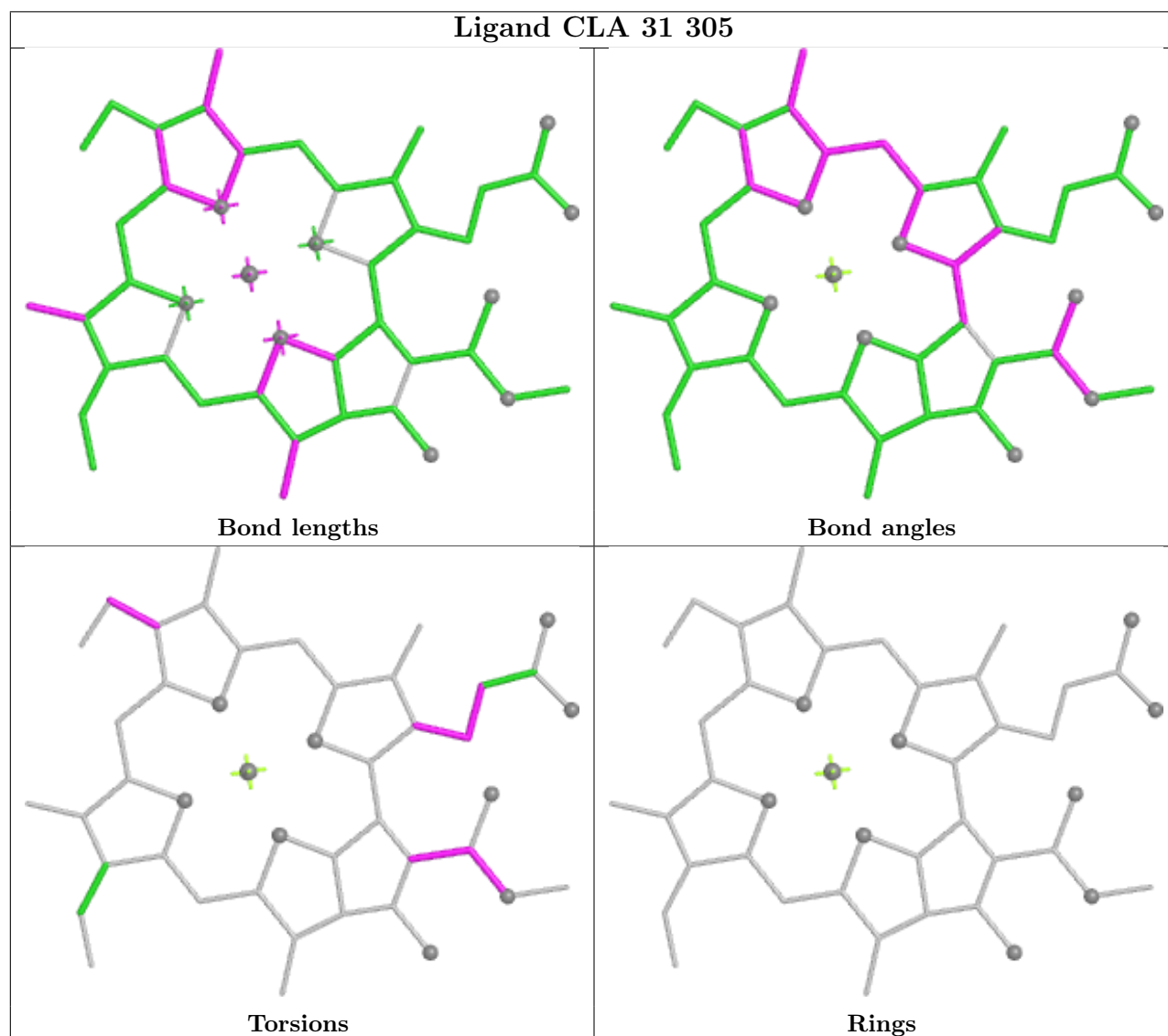
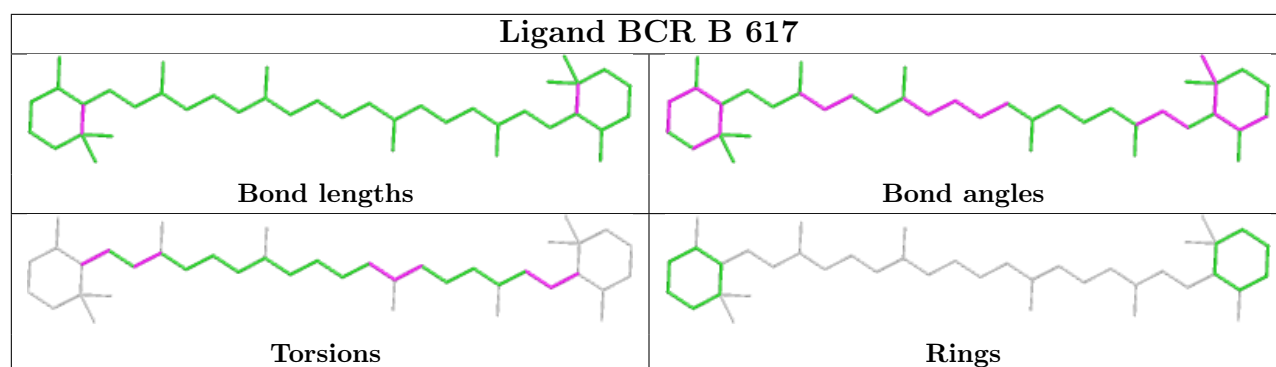


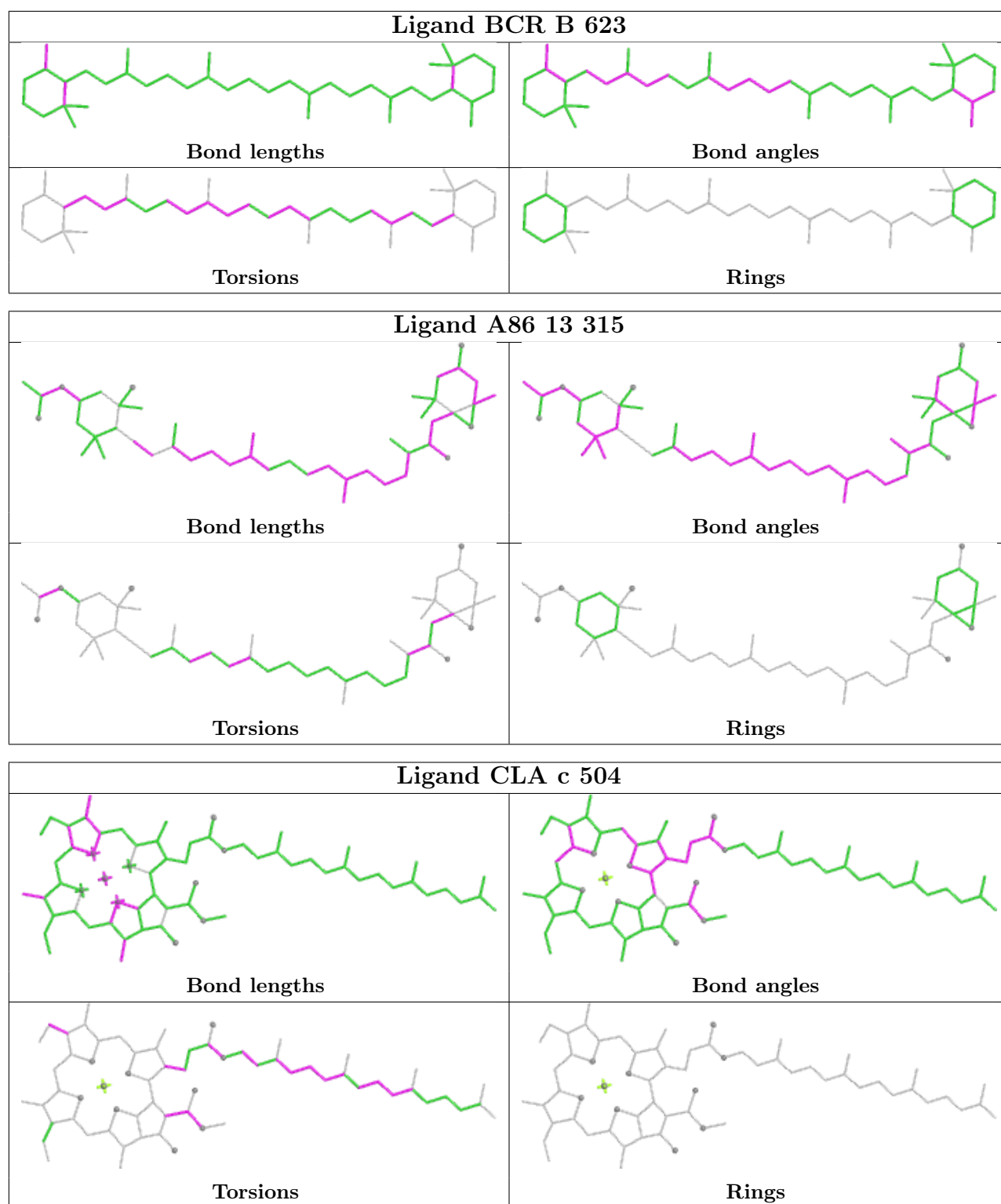
Ligand A86 13 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

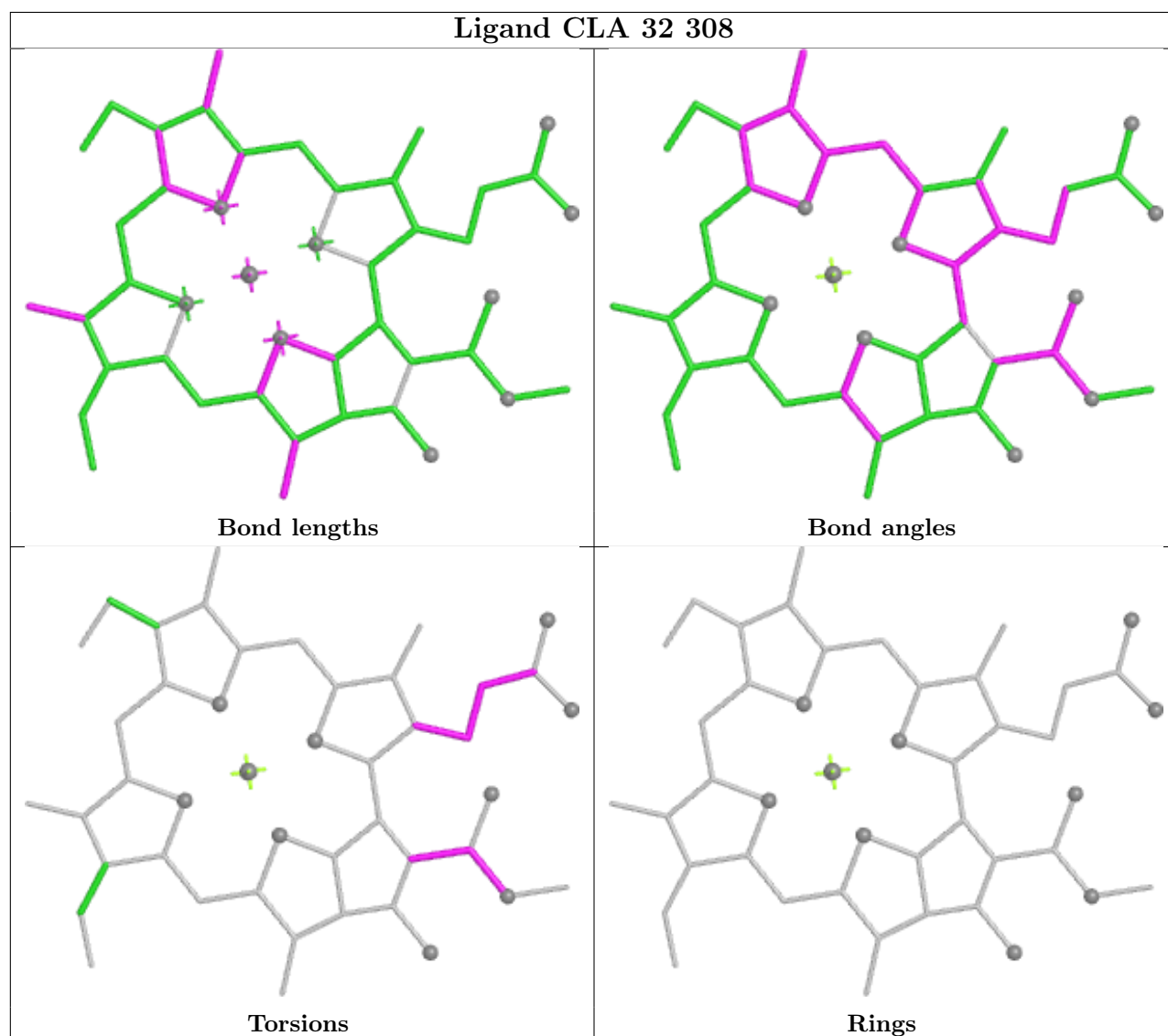
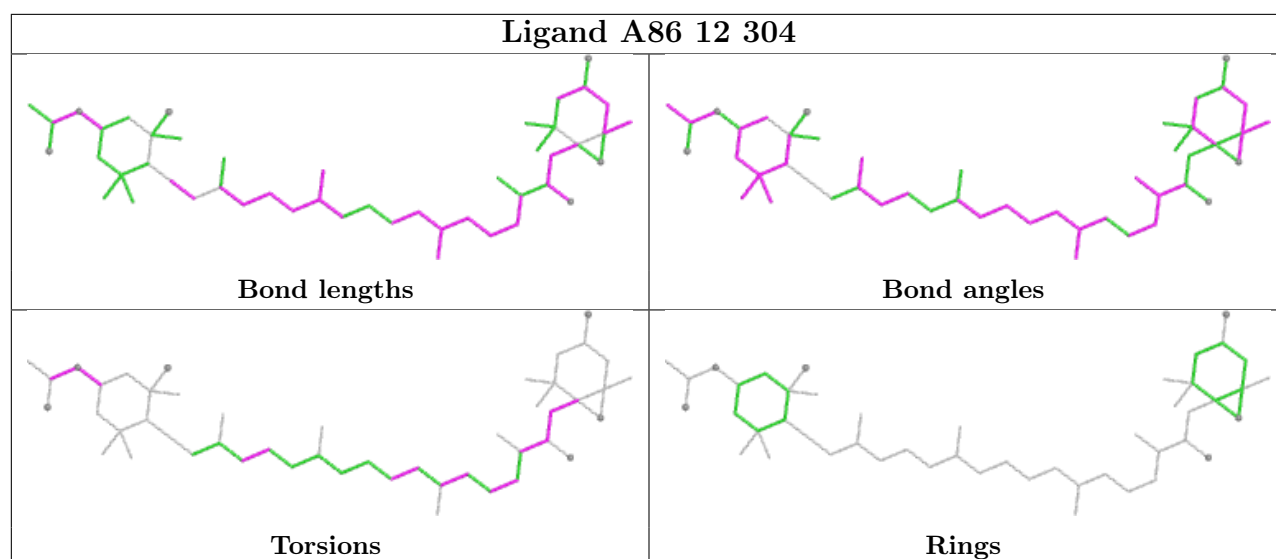
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Bond lengths	Bond angles
	
Torsions	Rings

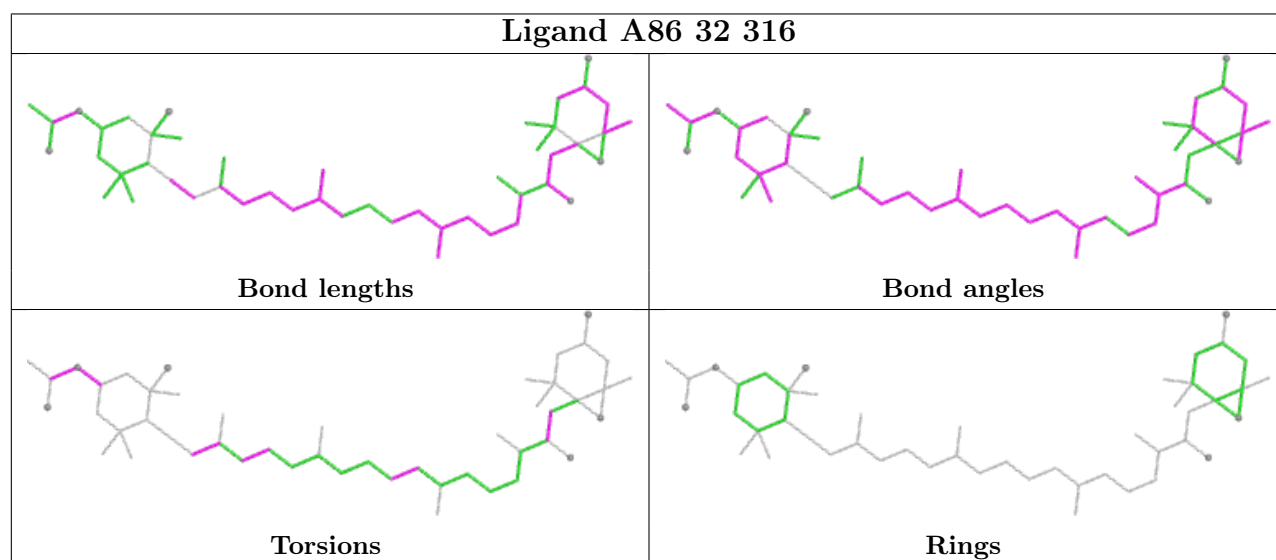
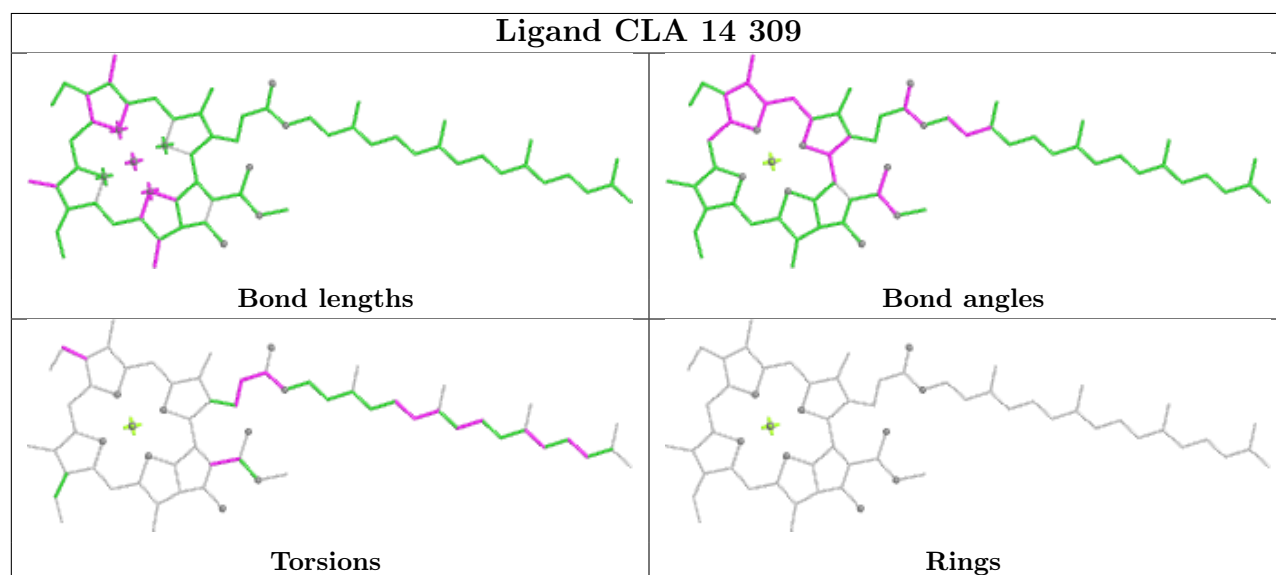
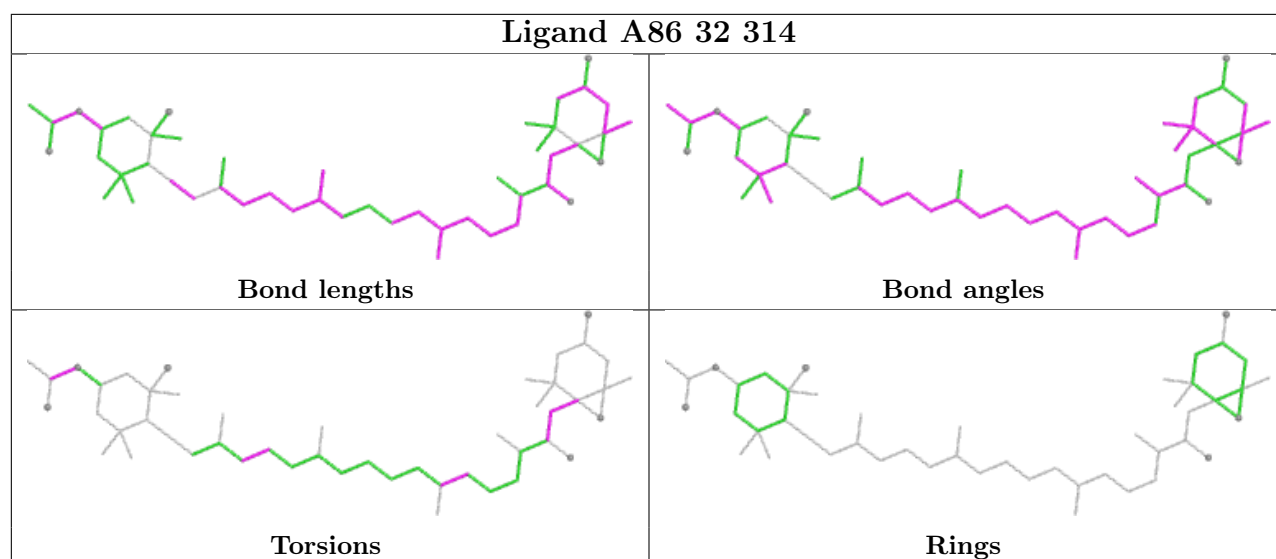
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Bond lengths	Bond angles
	
Torsions	Rings

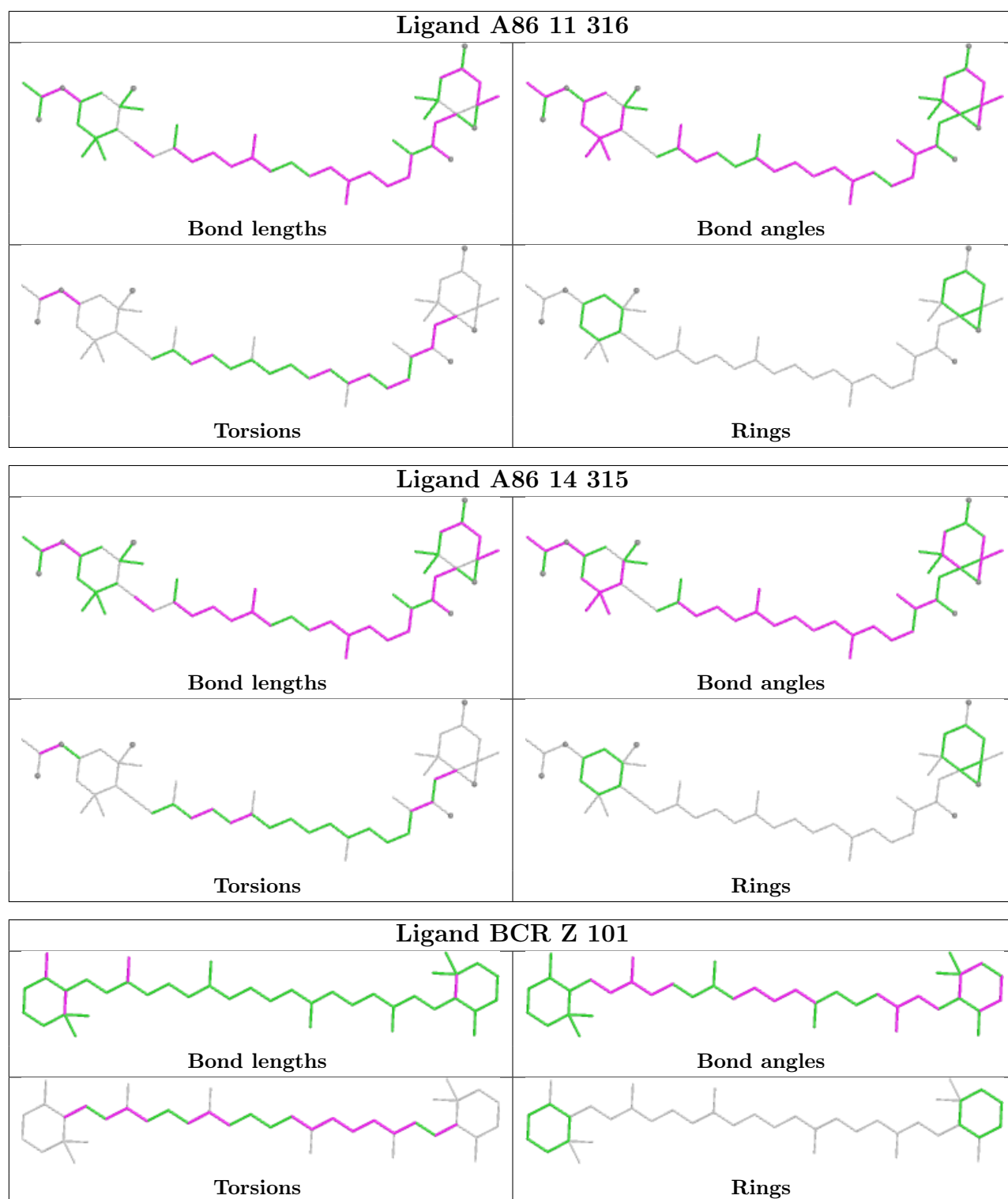


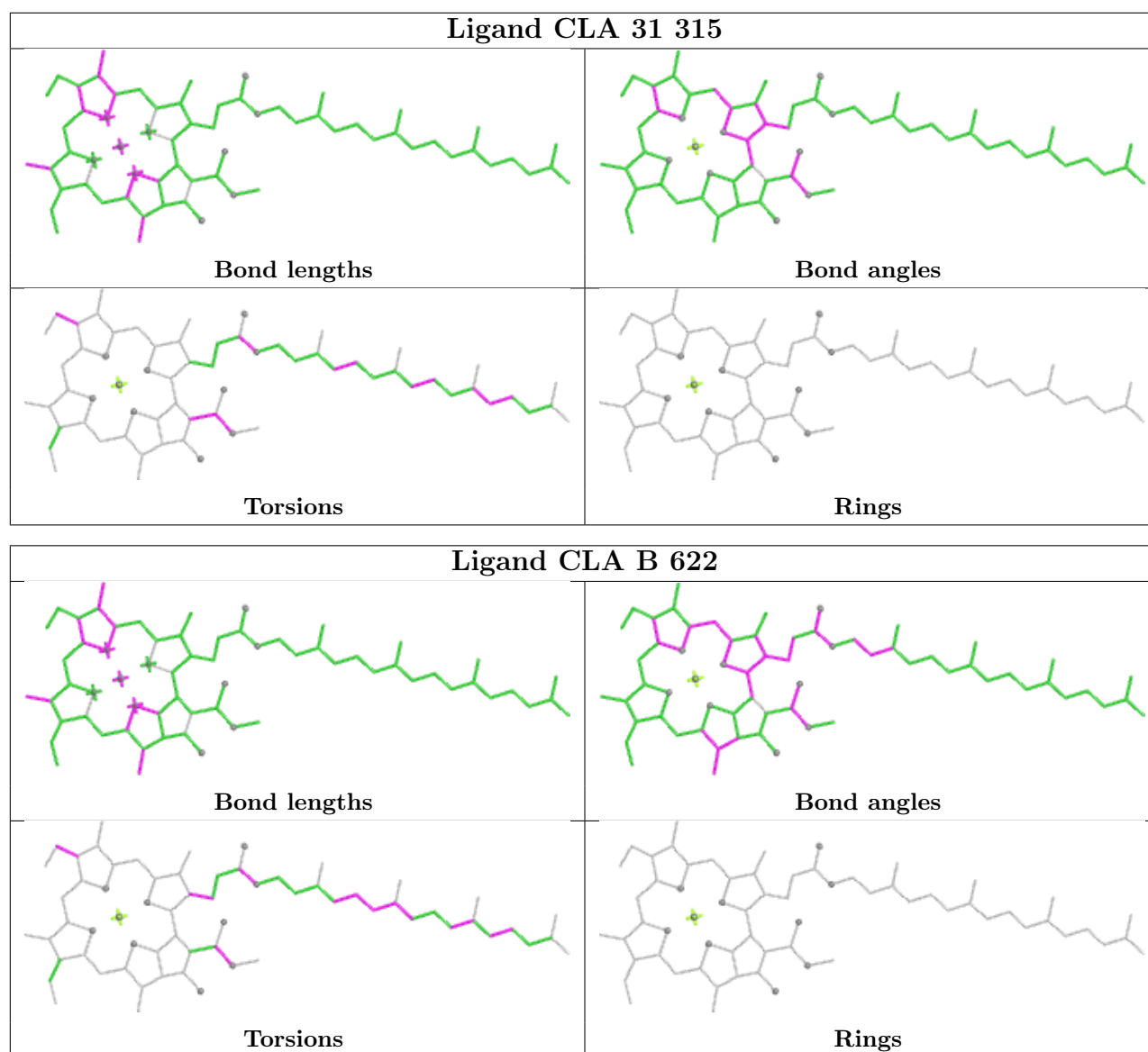


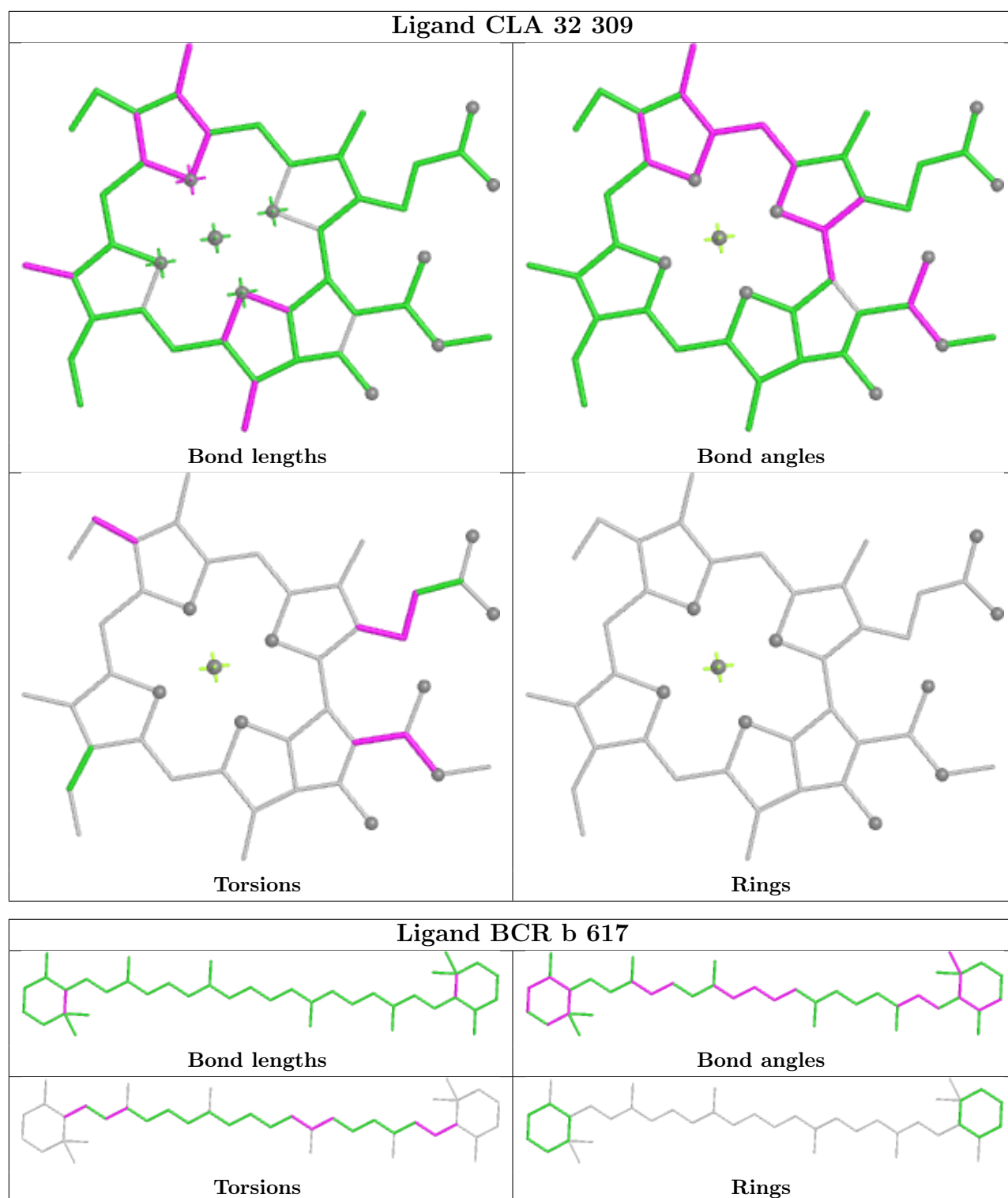


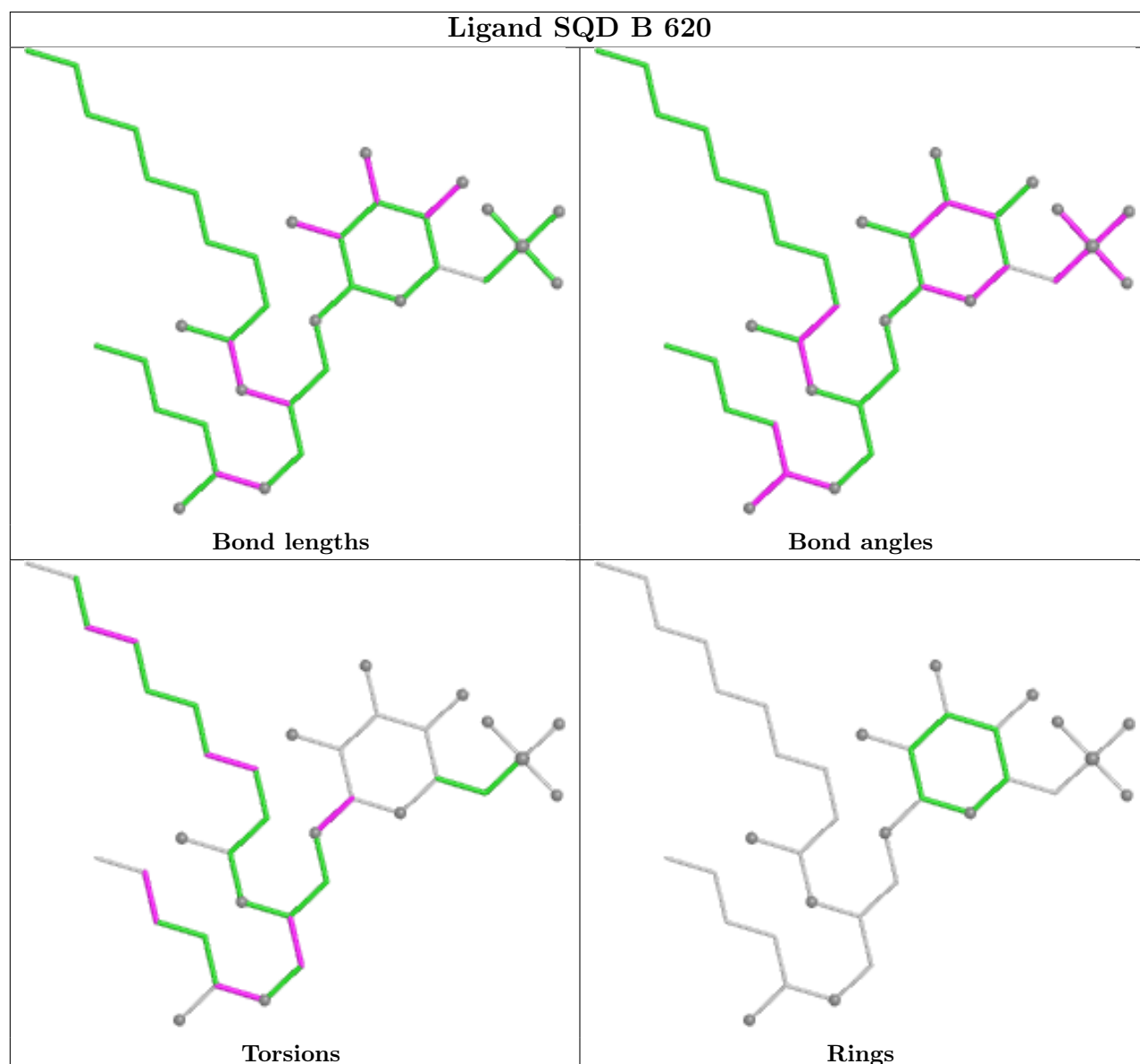
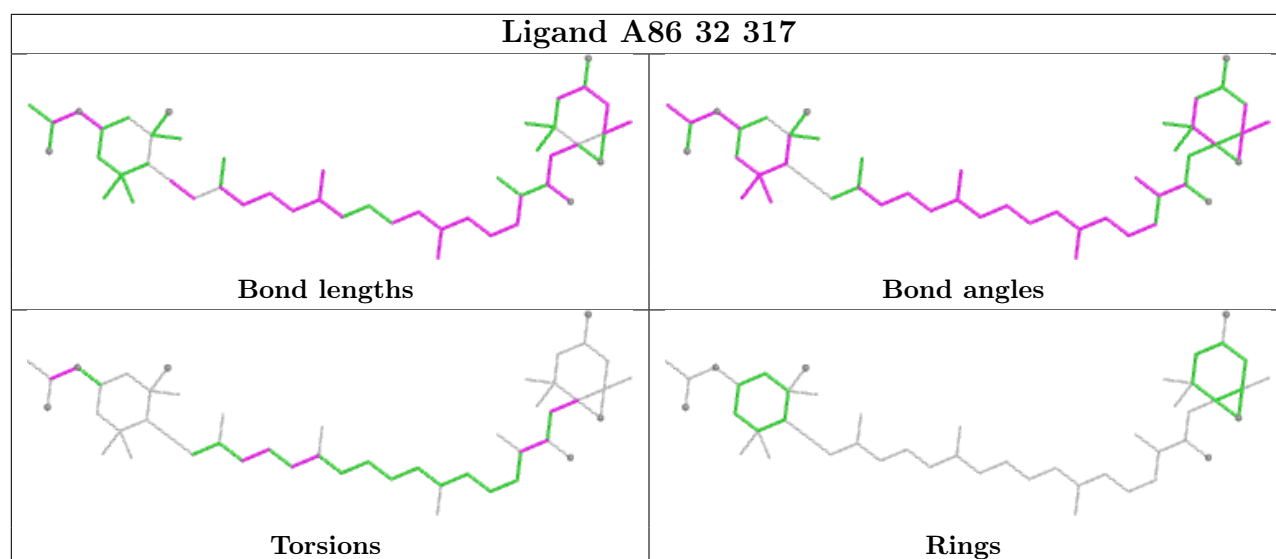


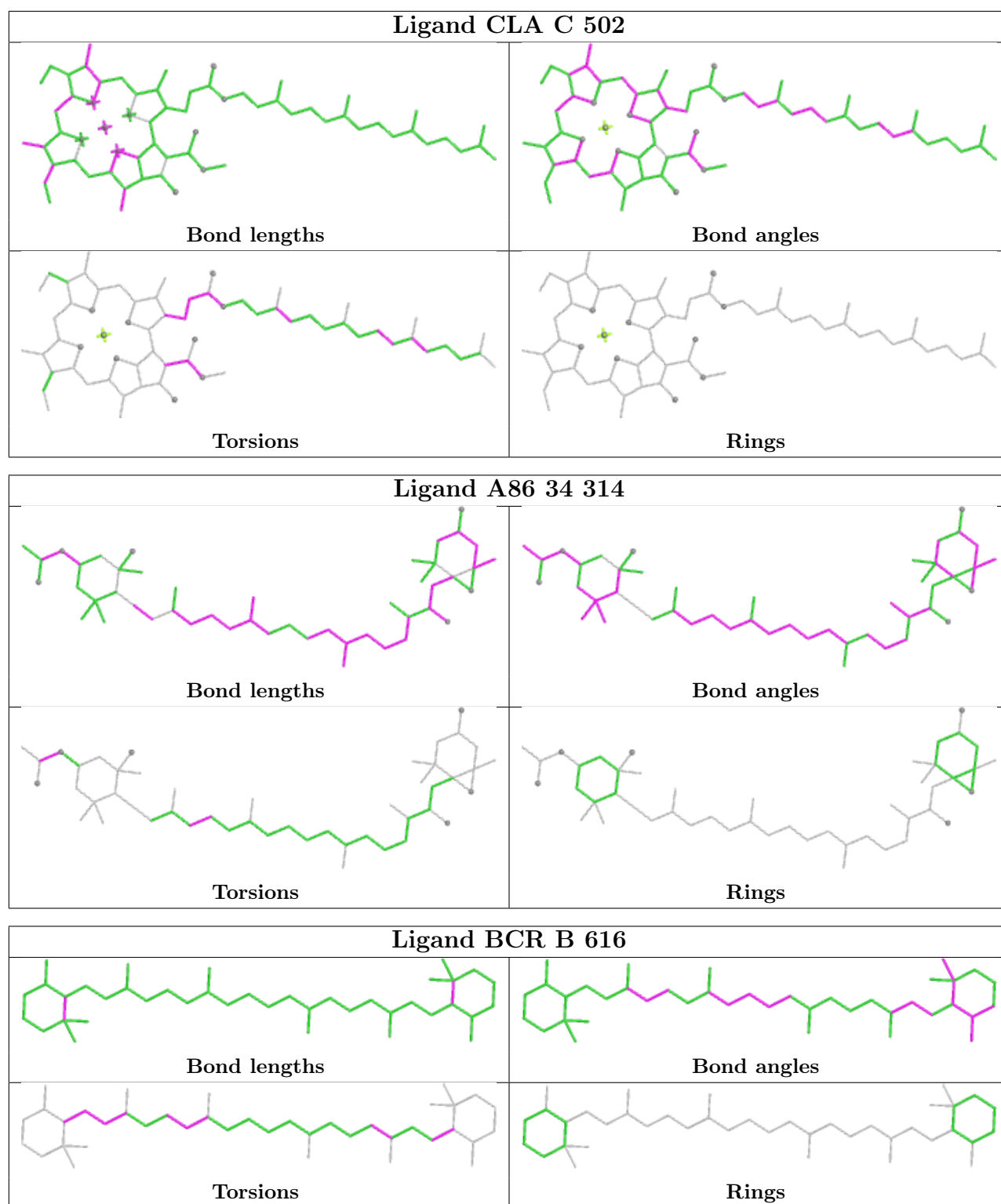




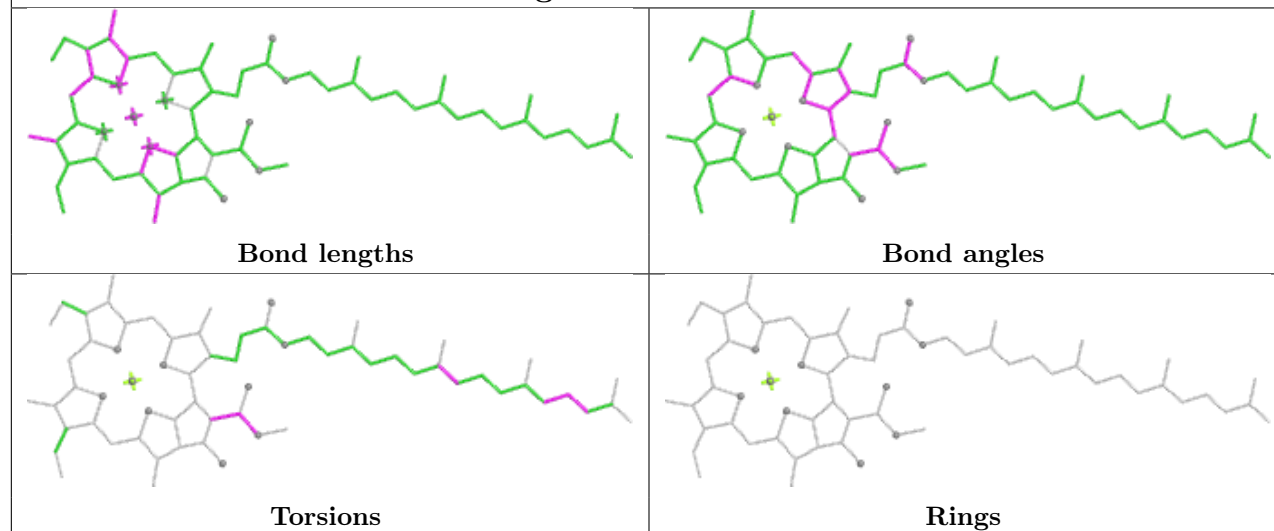




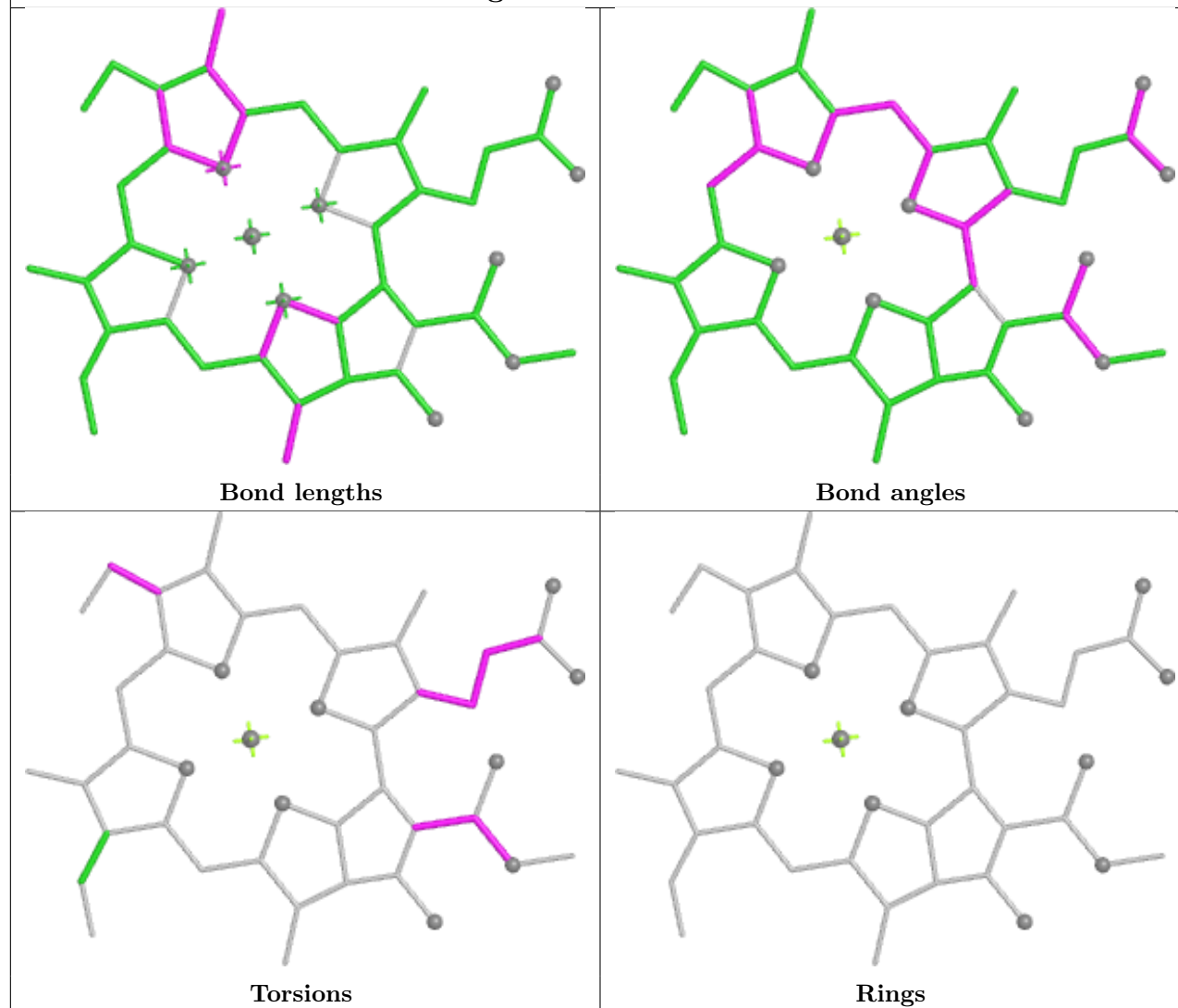


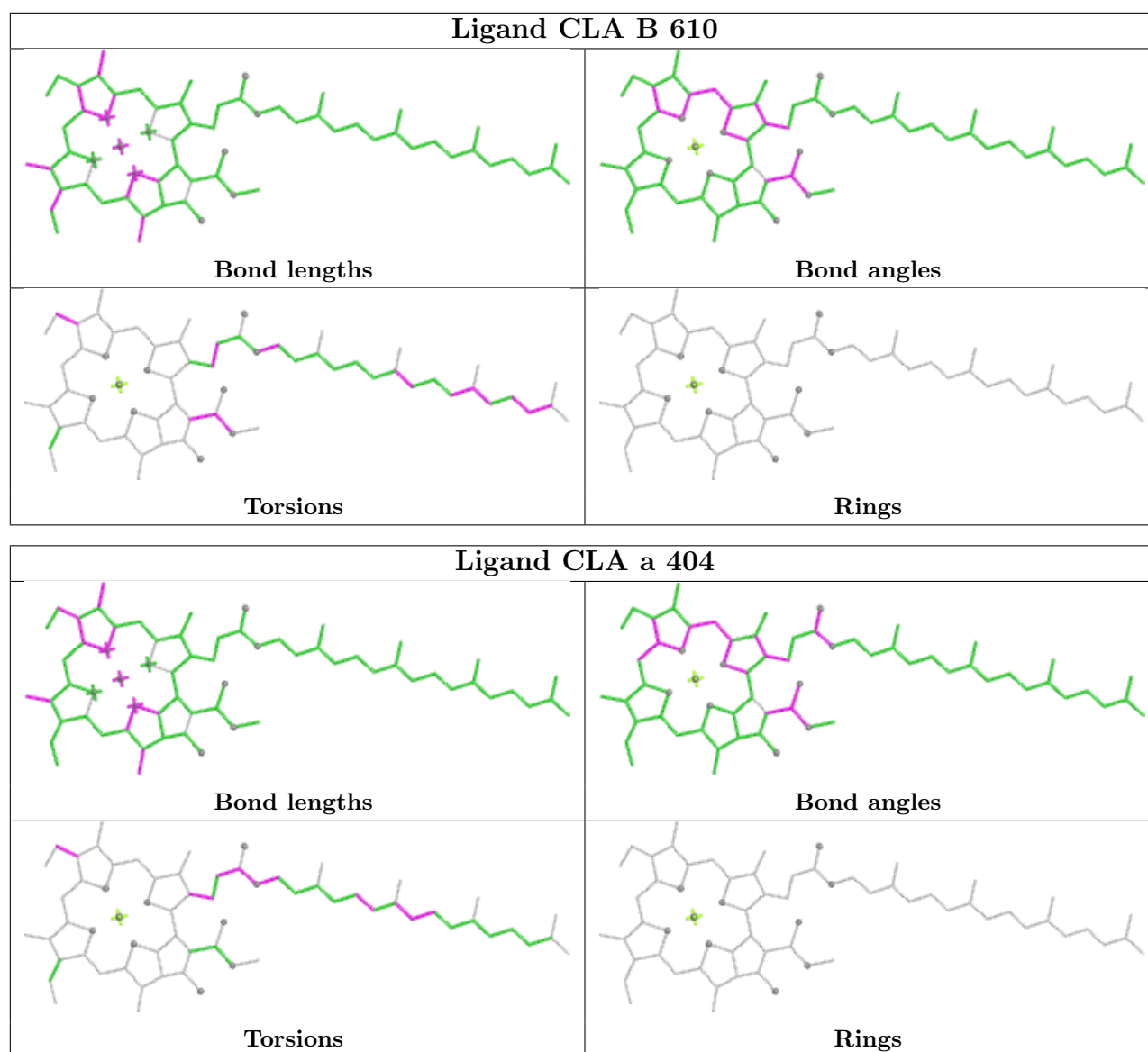


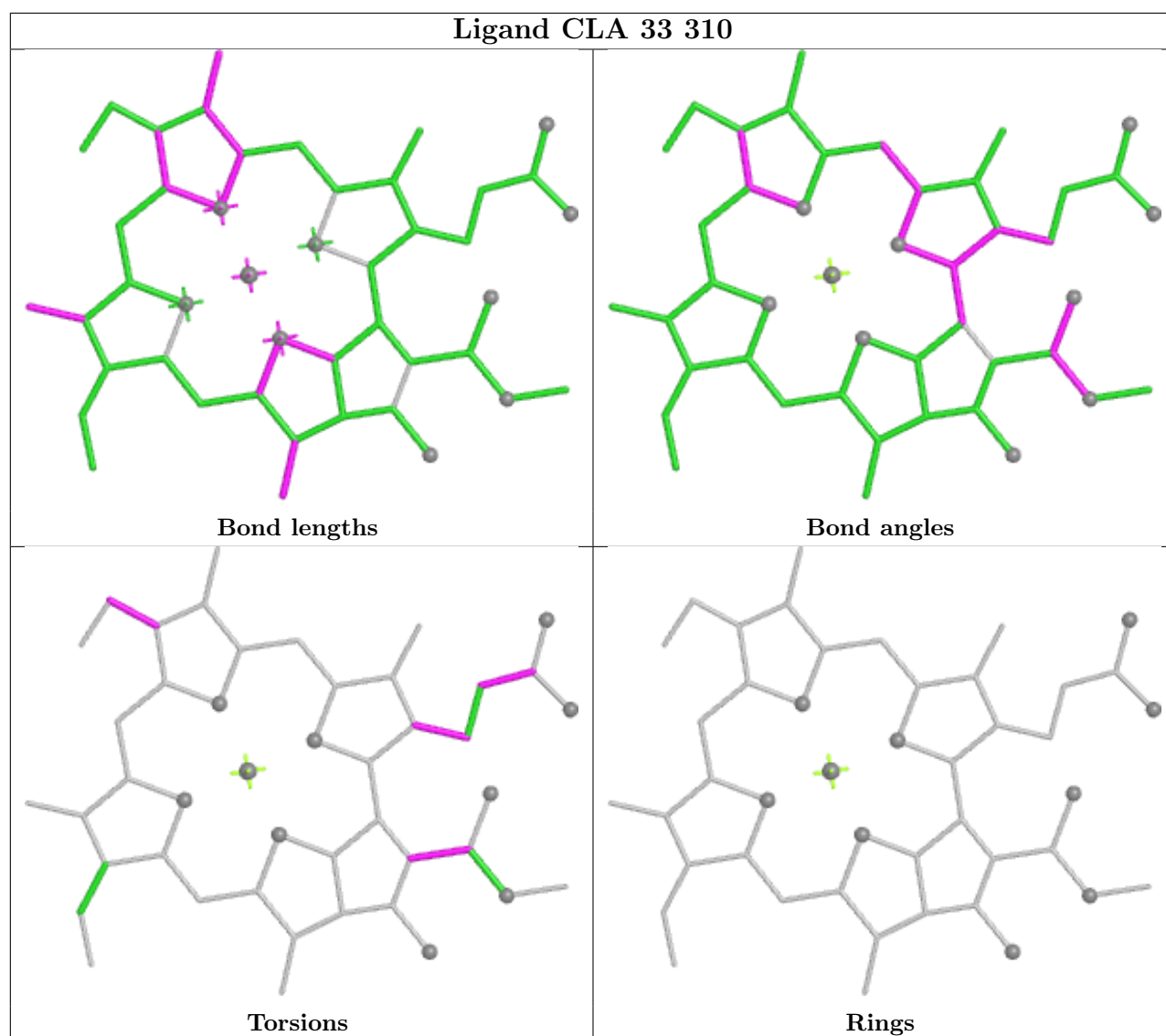
Ligand CLA b 614

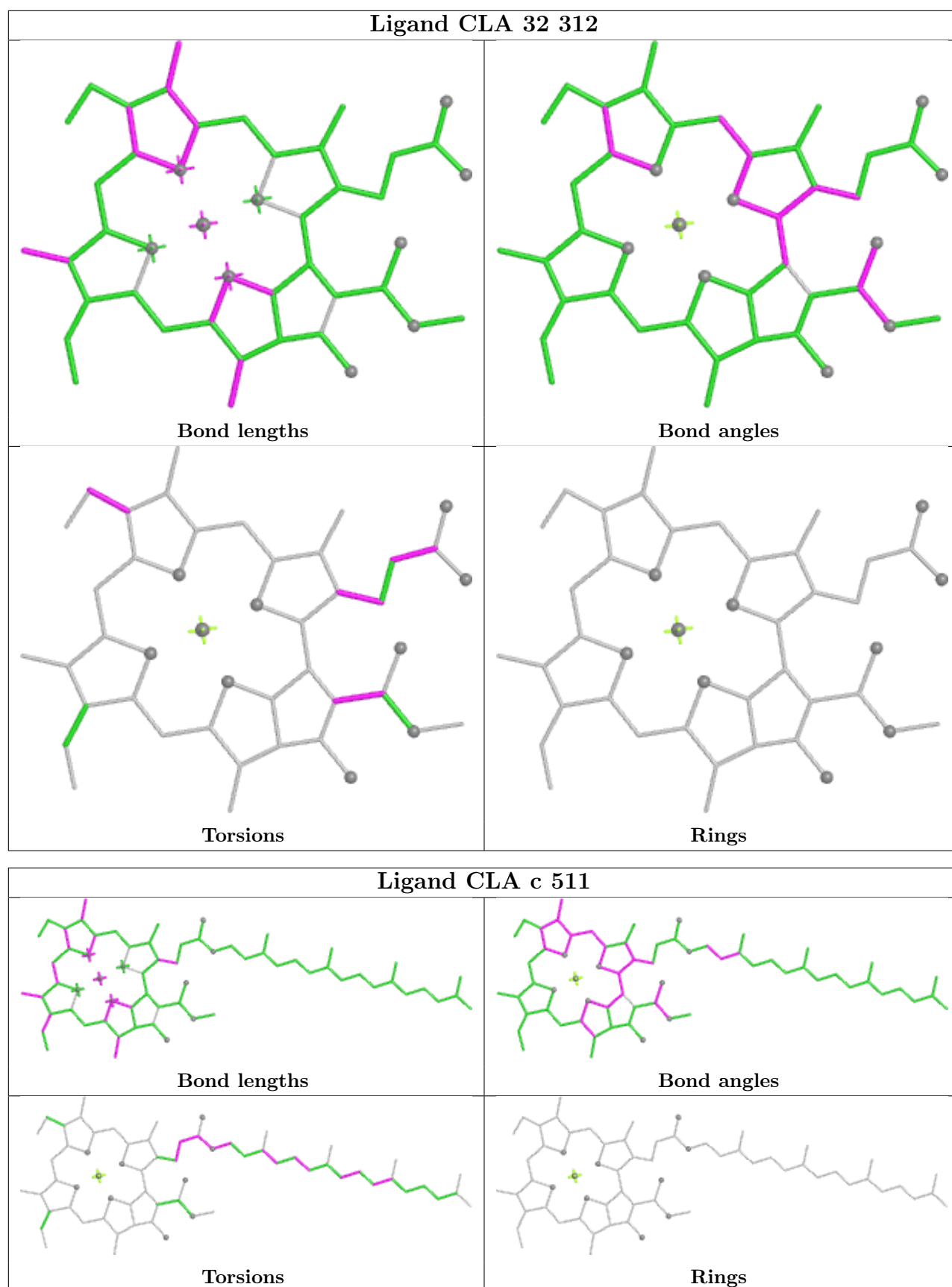


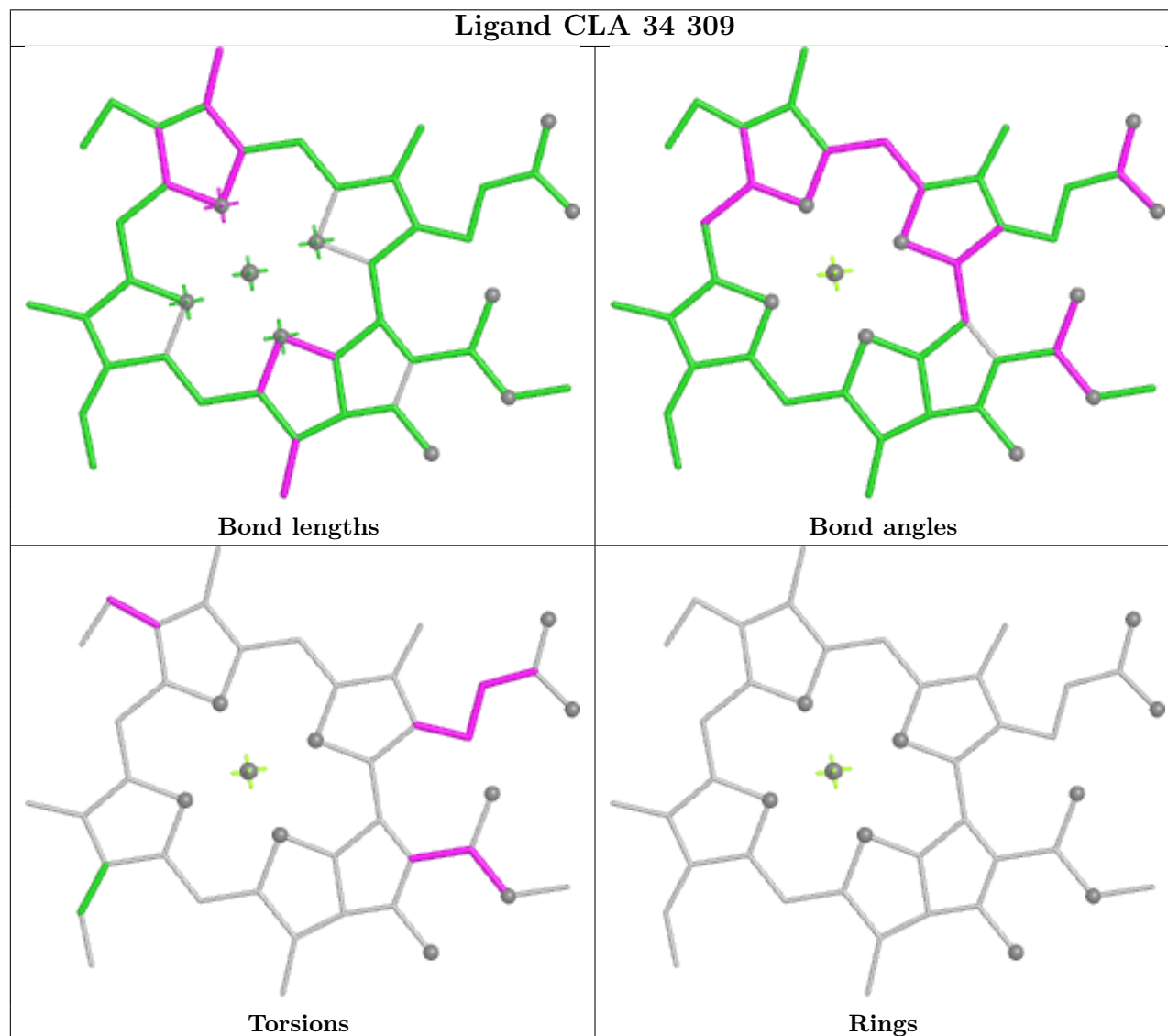
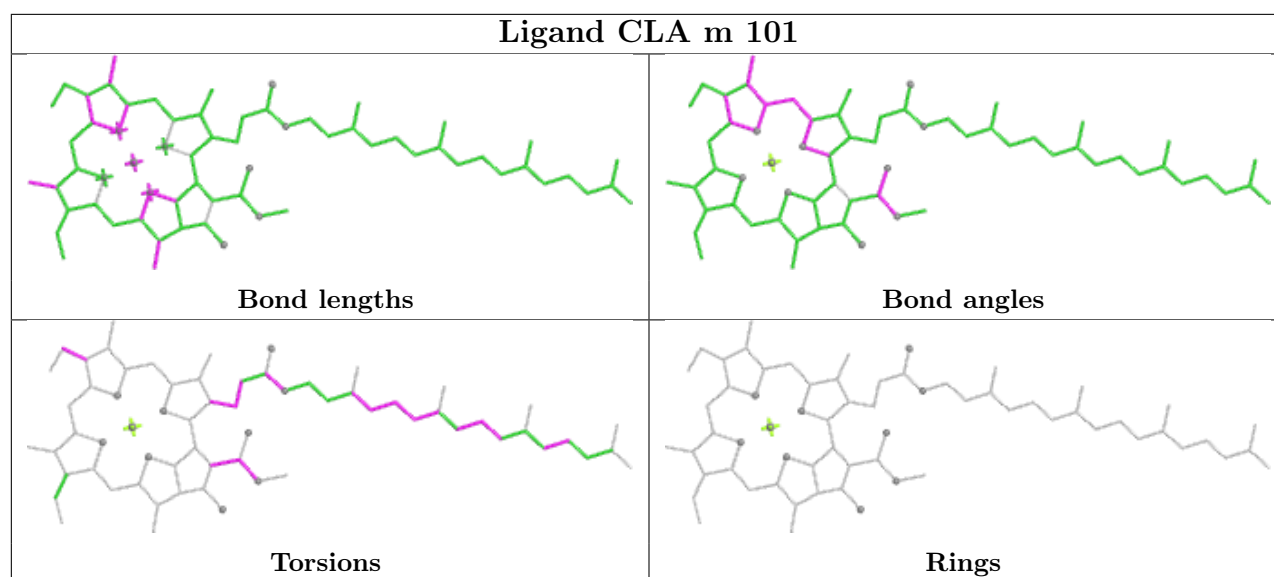
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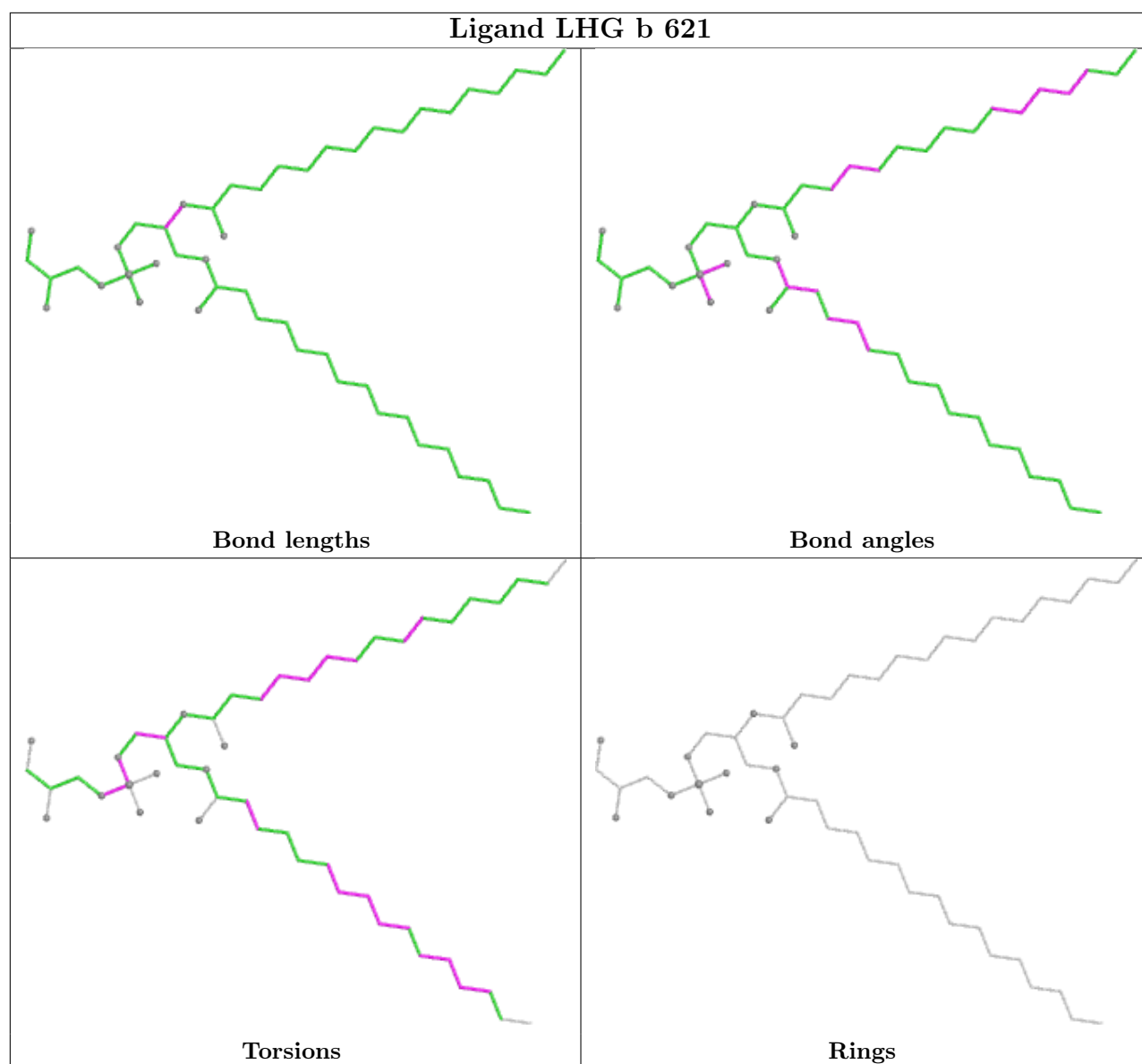


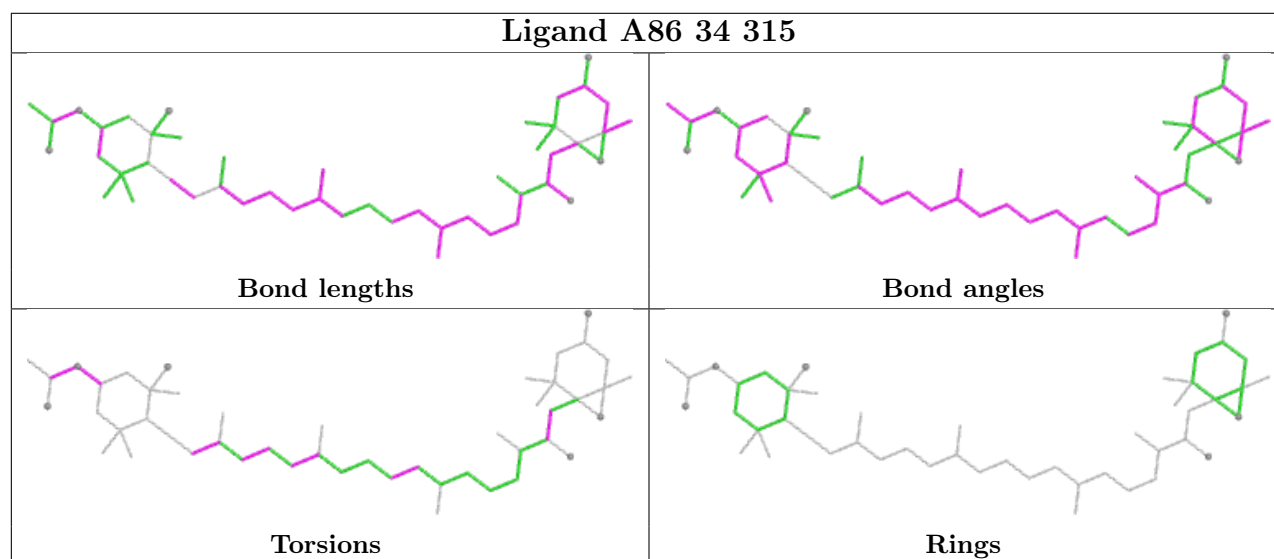
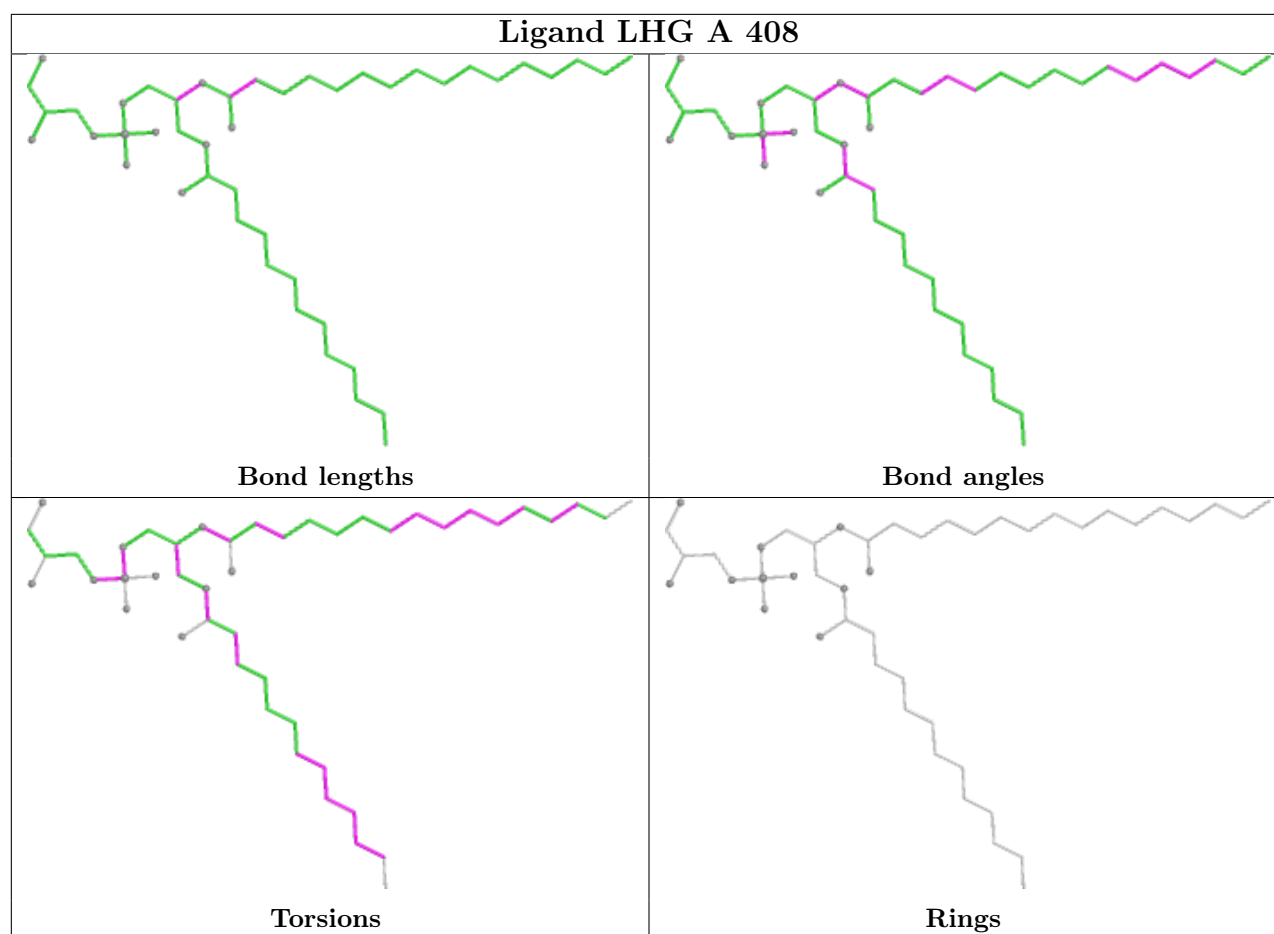


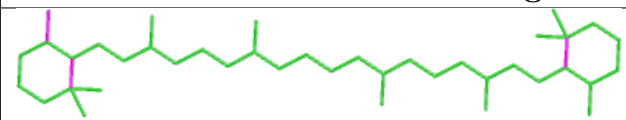
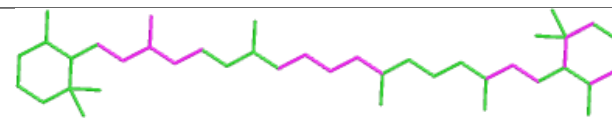
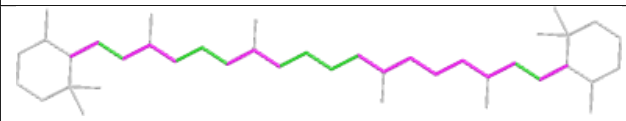
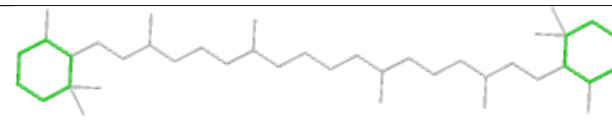


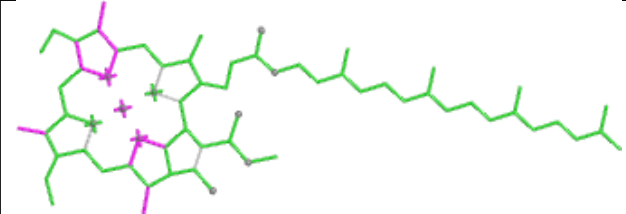
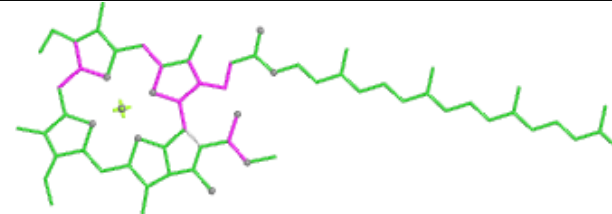
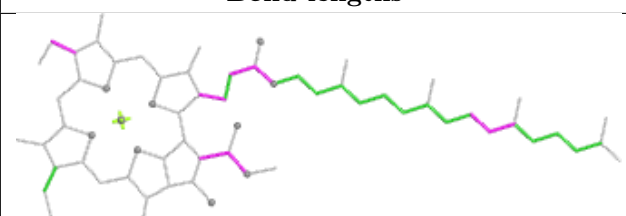
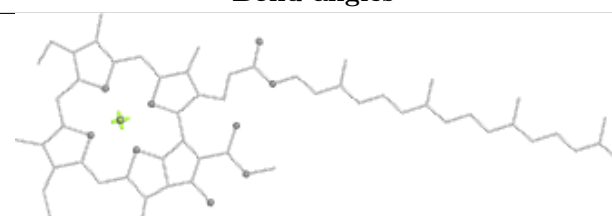


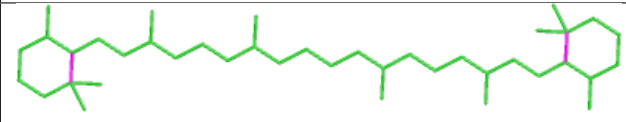
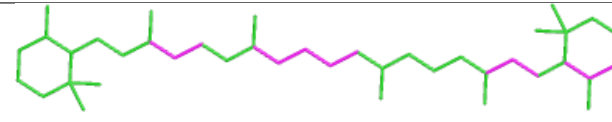
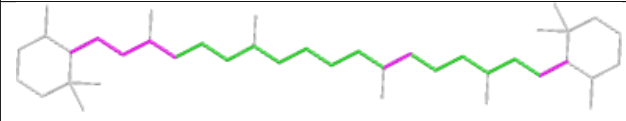
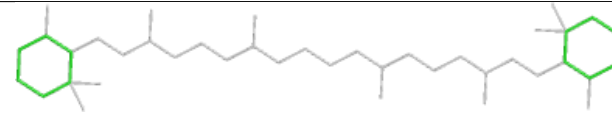


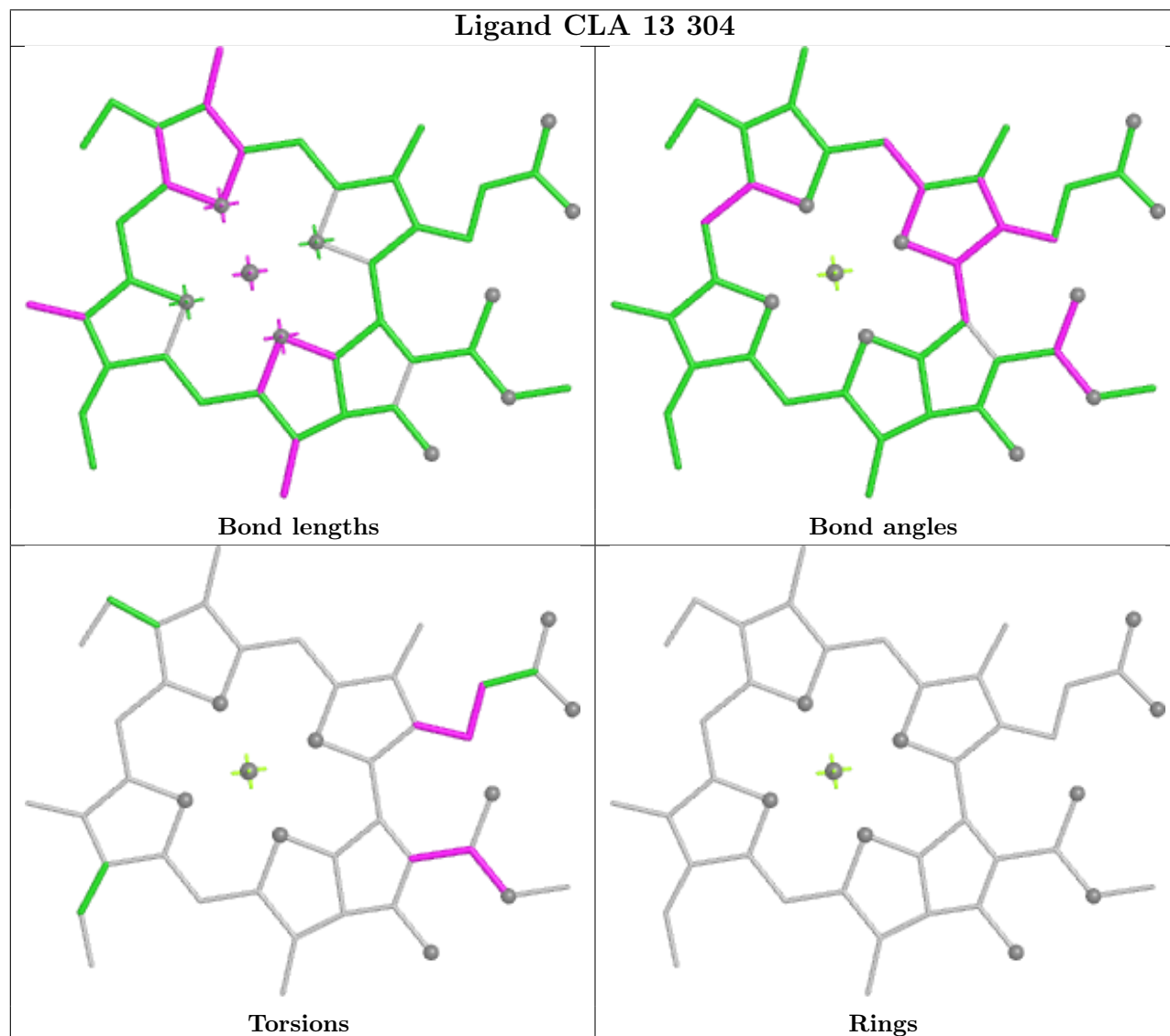
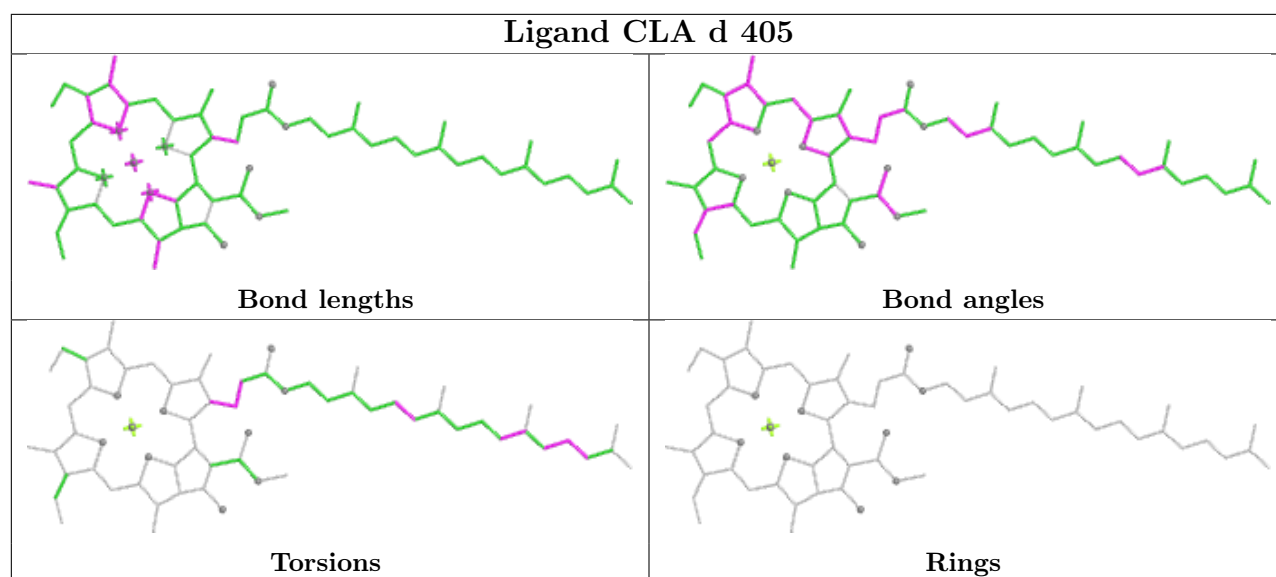


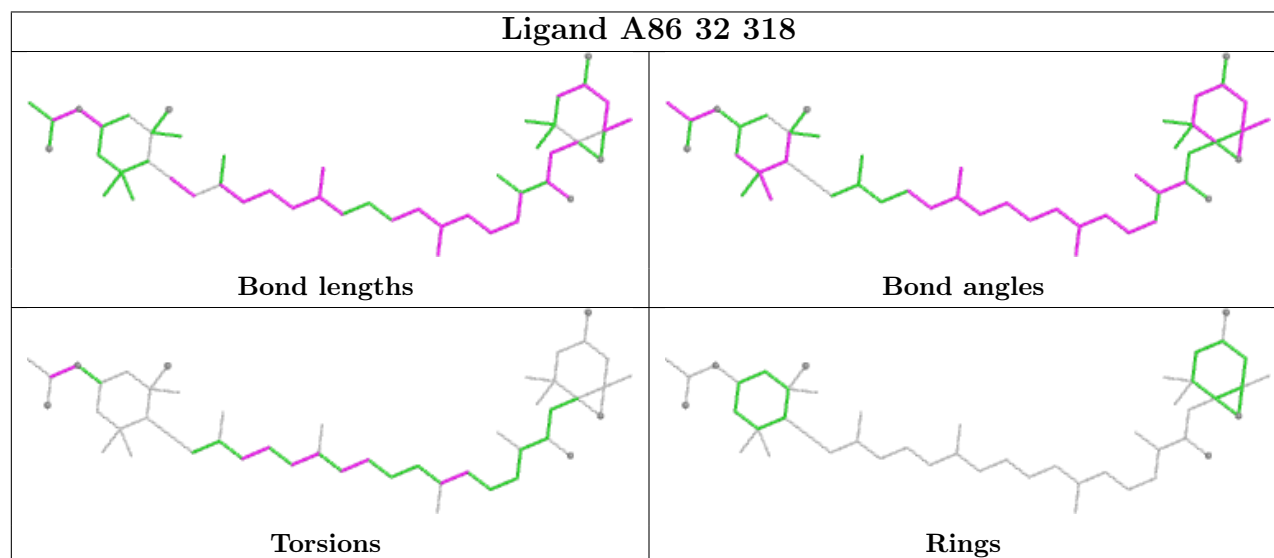
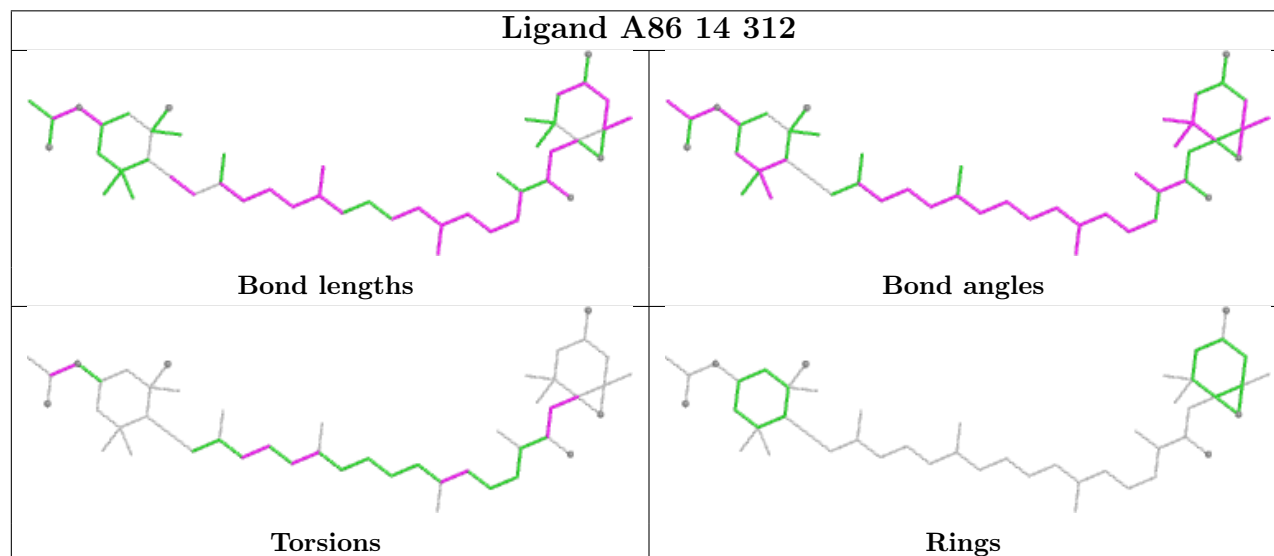
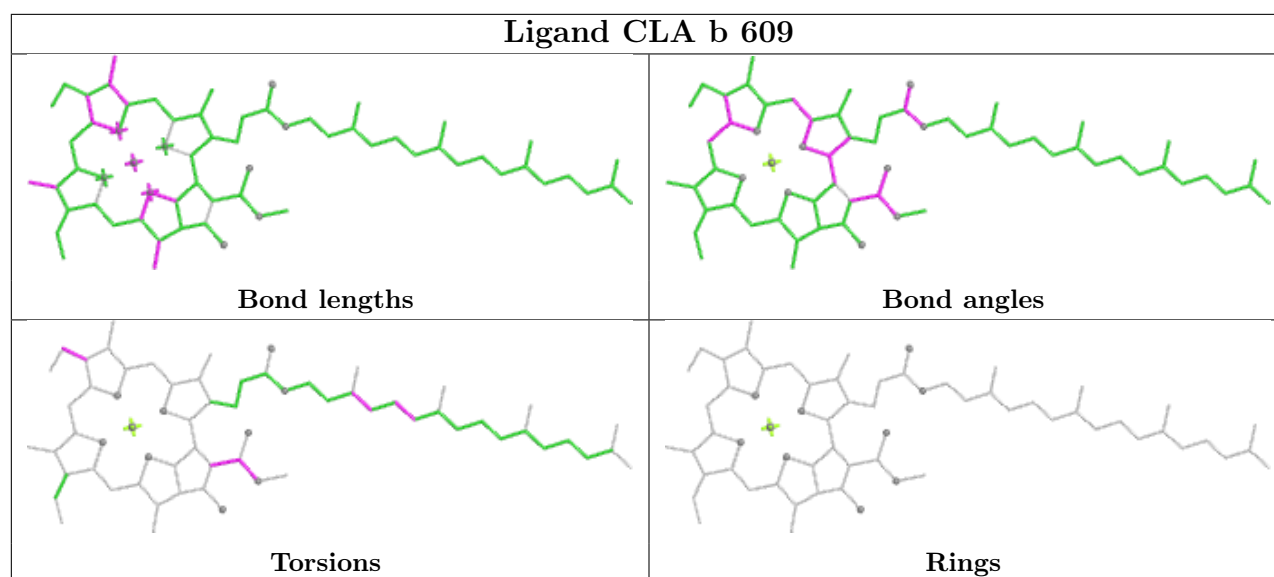


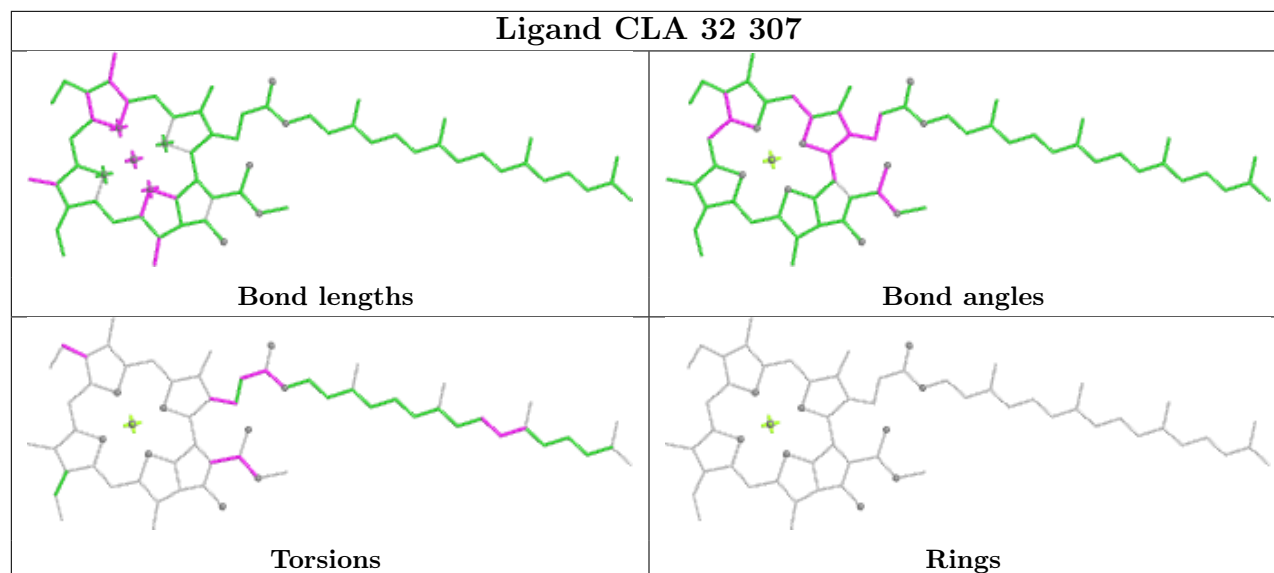
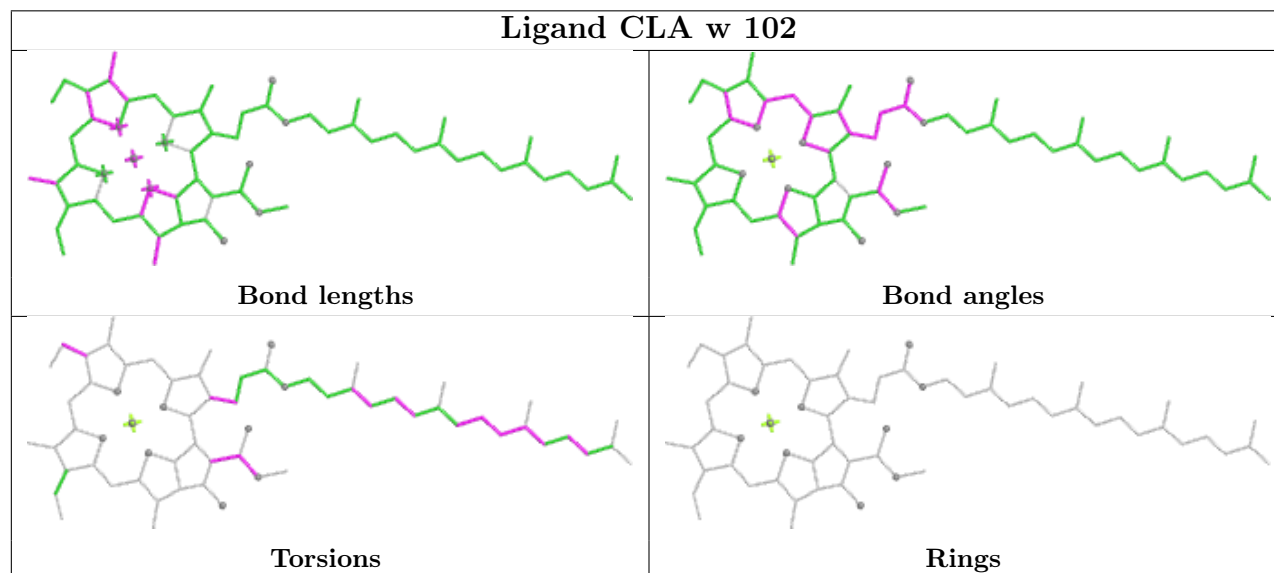
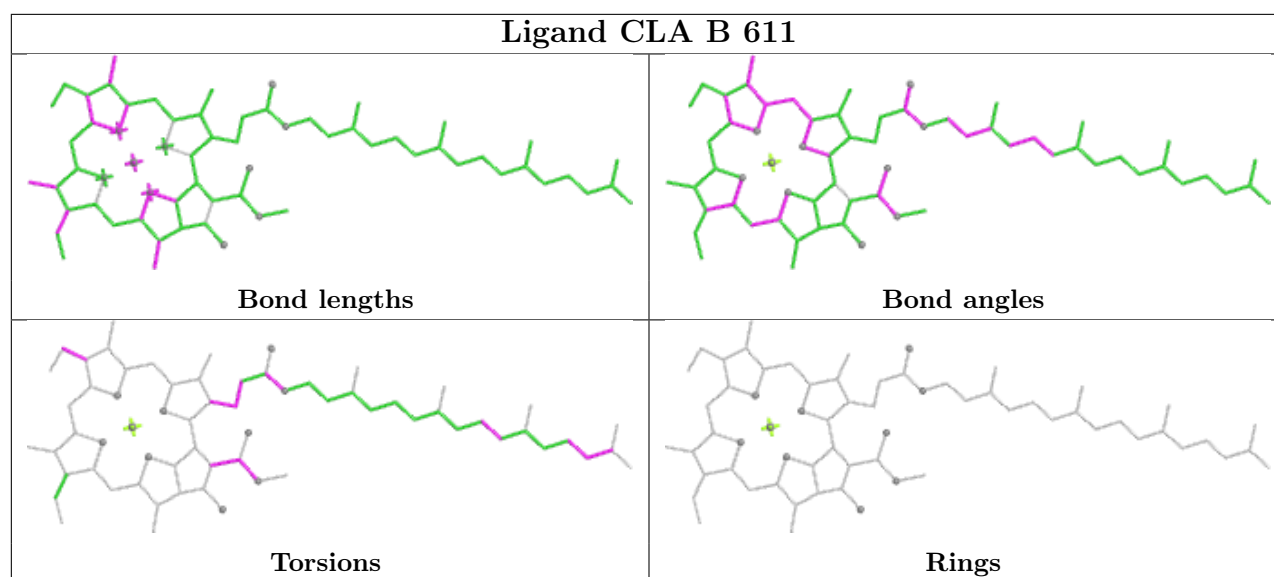
Ligand BCR z 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

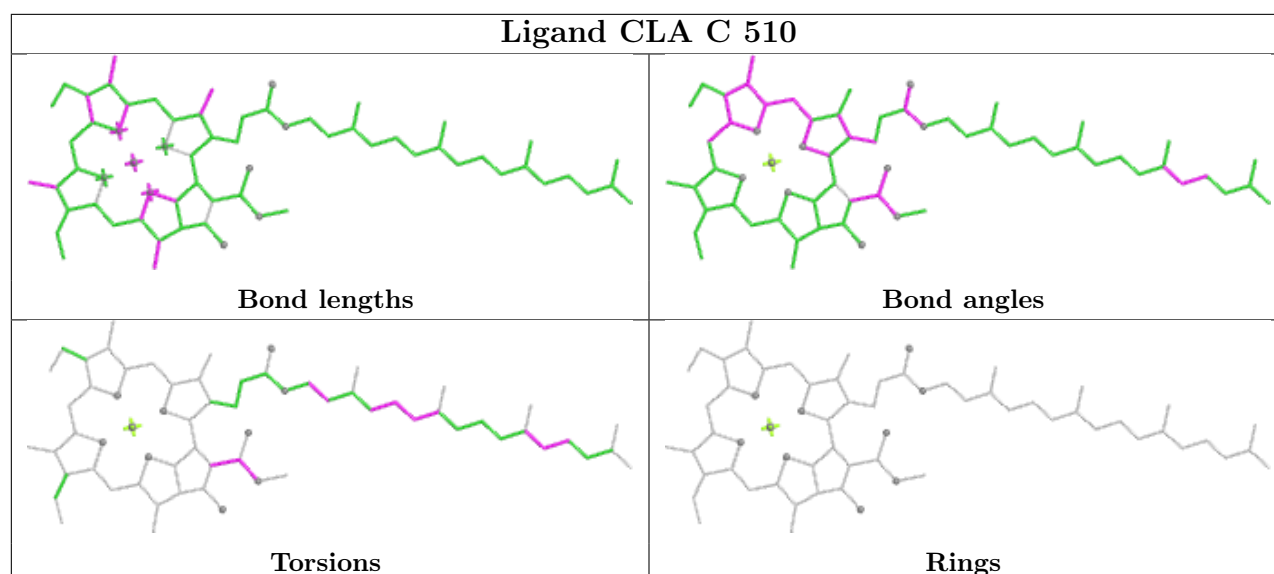
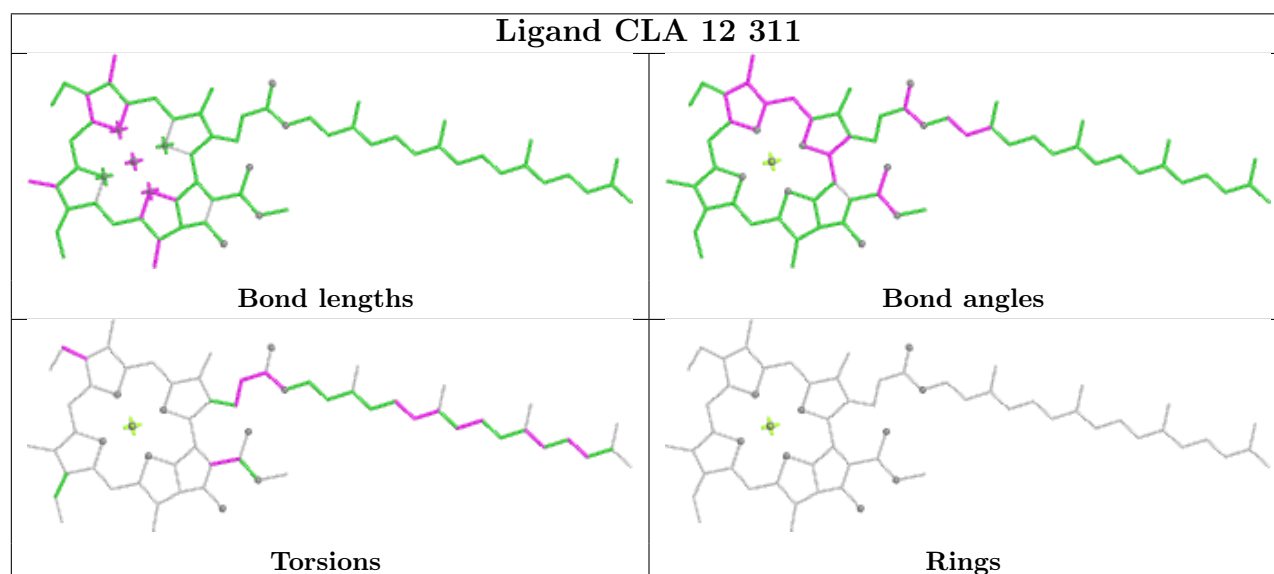
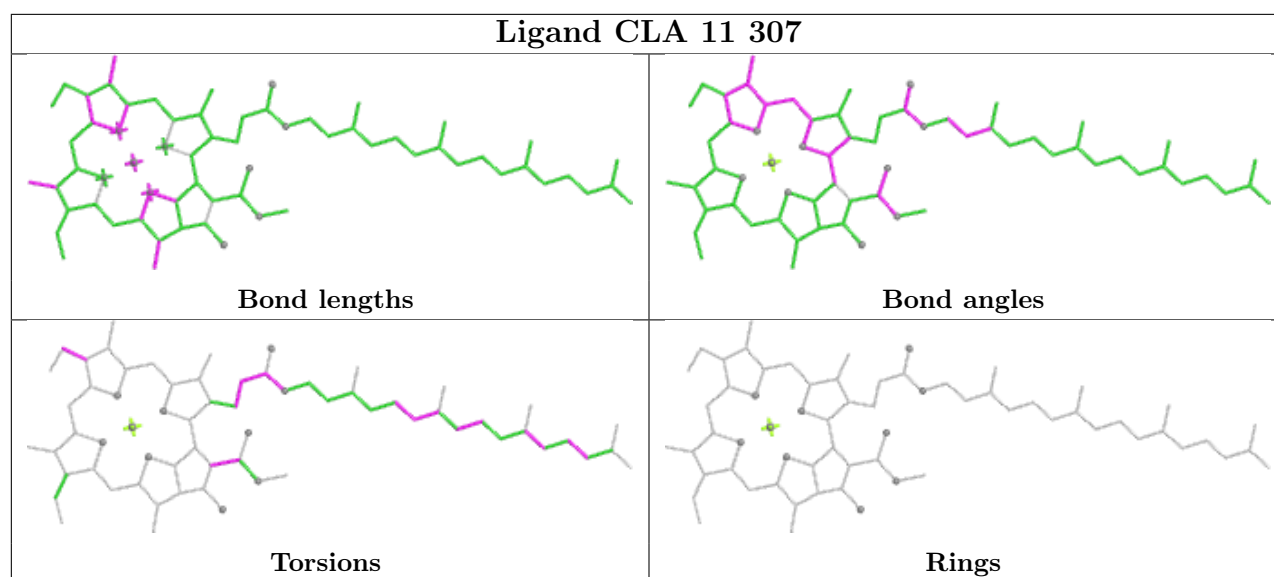
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Bond lengths	Bond angles
	
Torsions	Rings

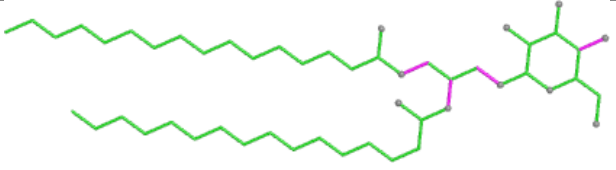
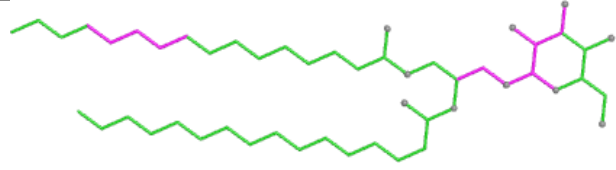
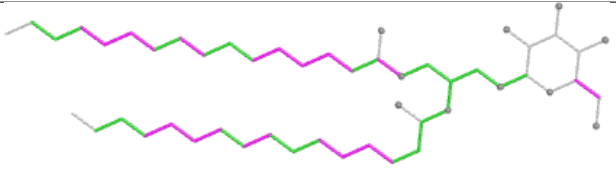
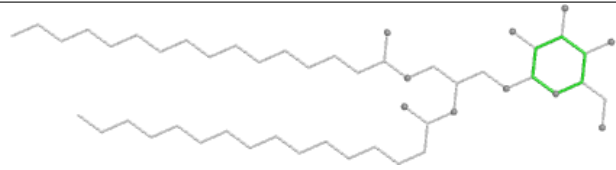
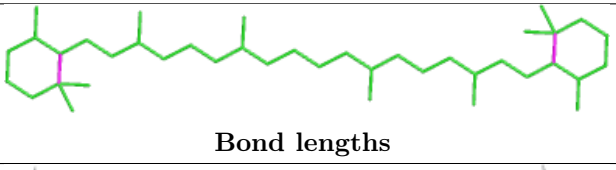
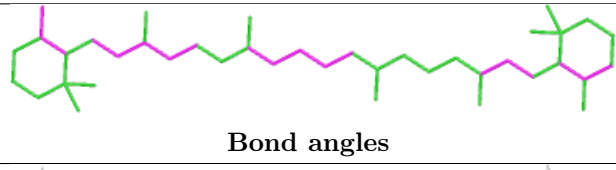
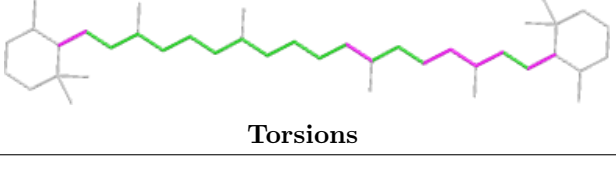
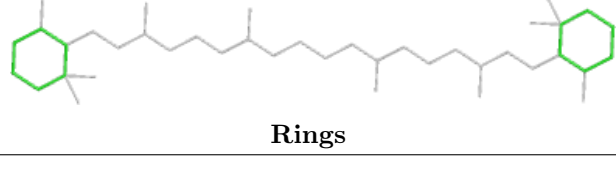
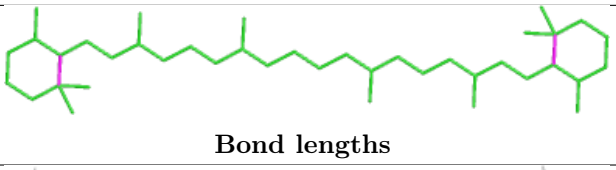
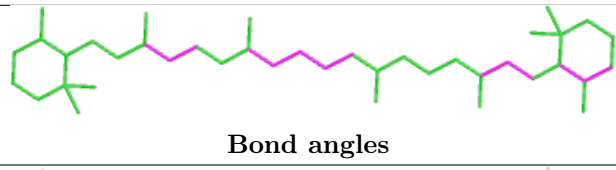
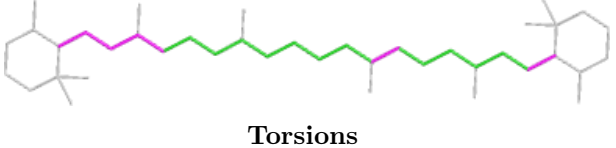
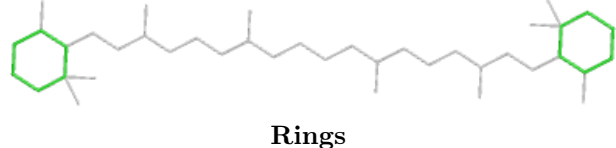
Ligand BCR a 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

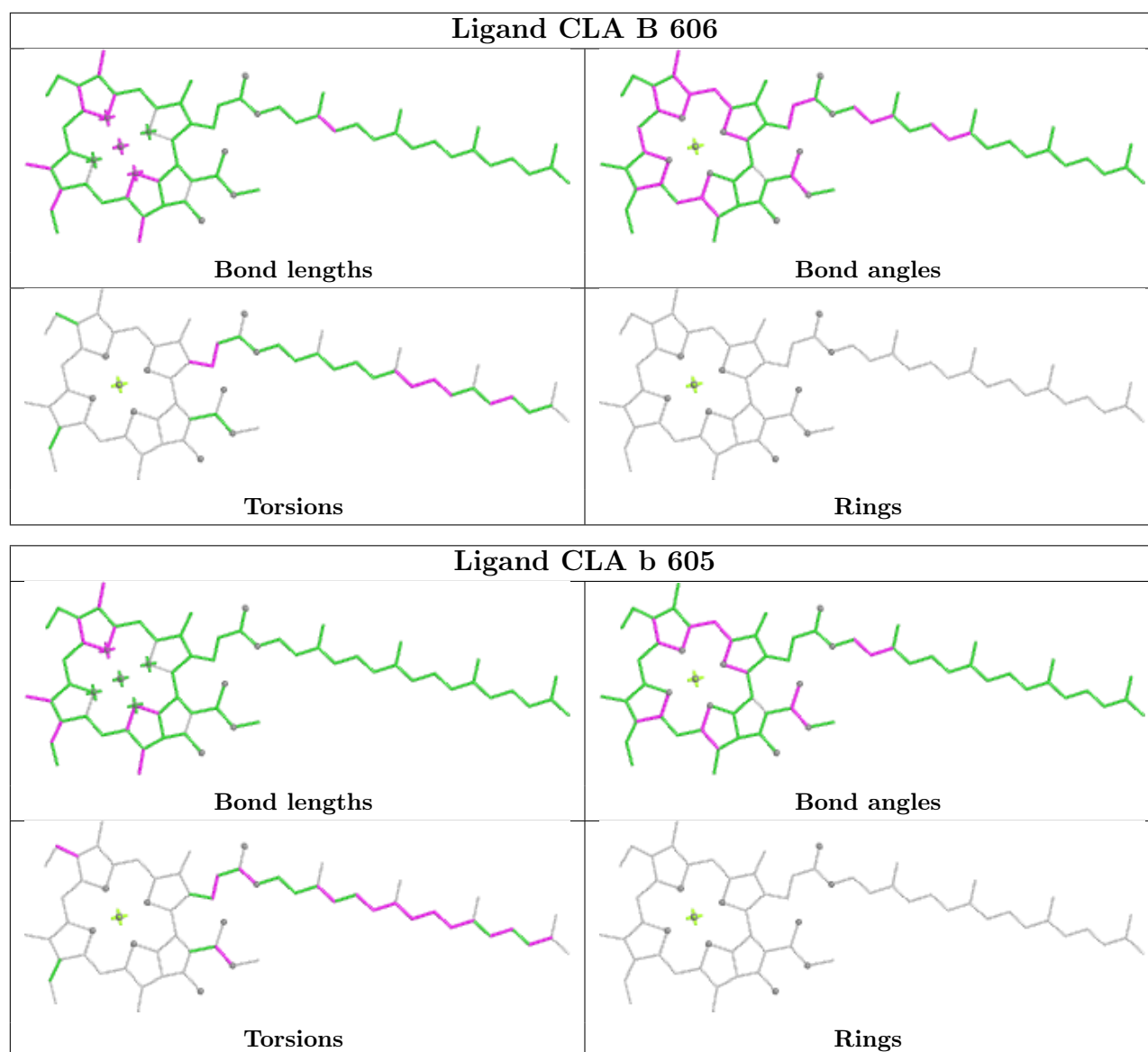


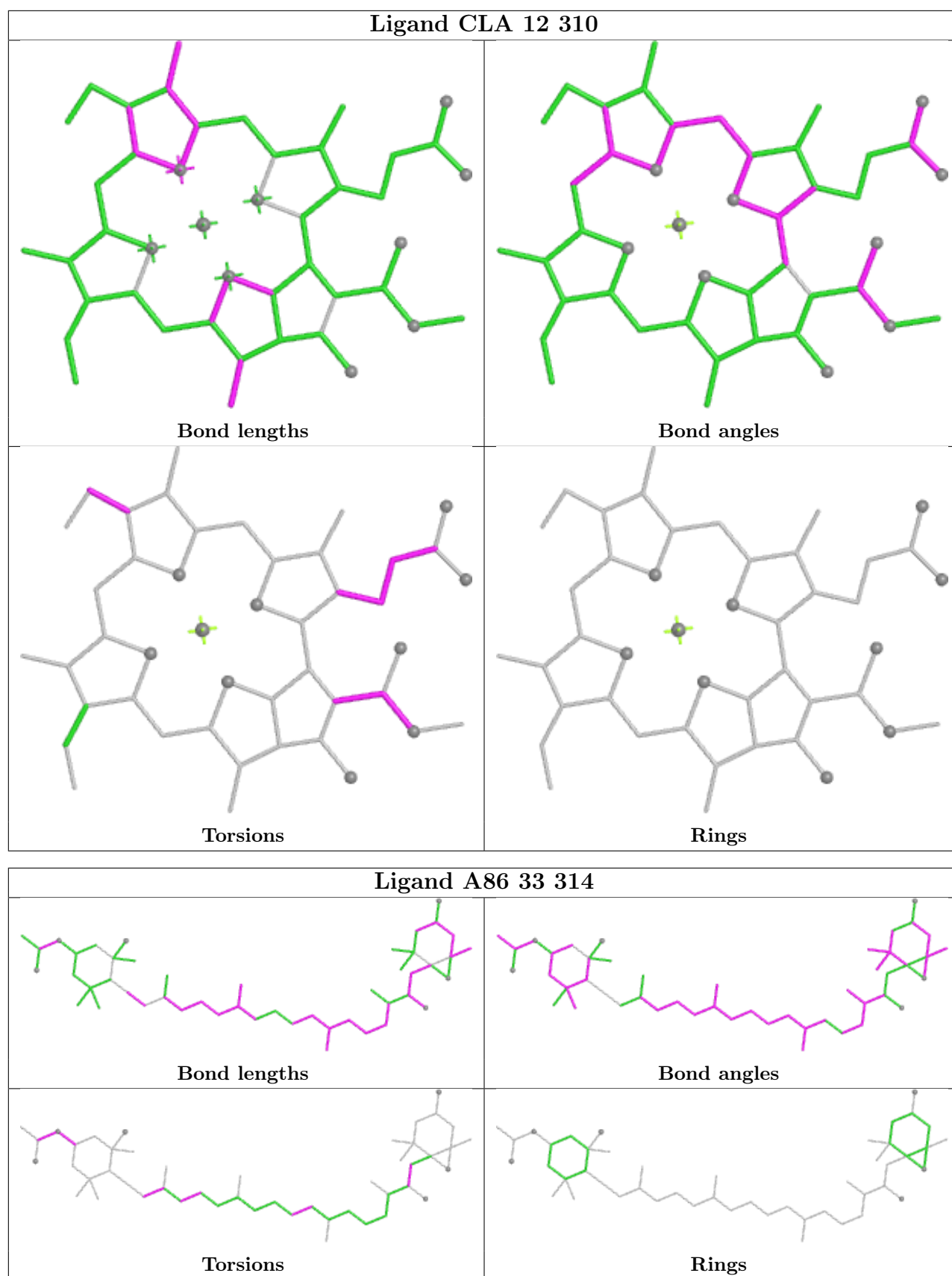


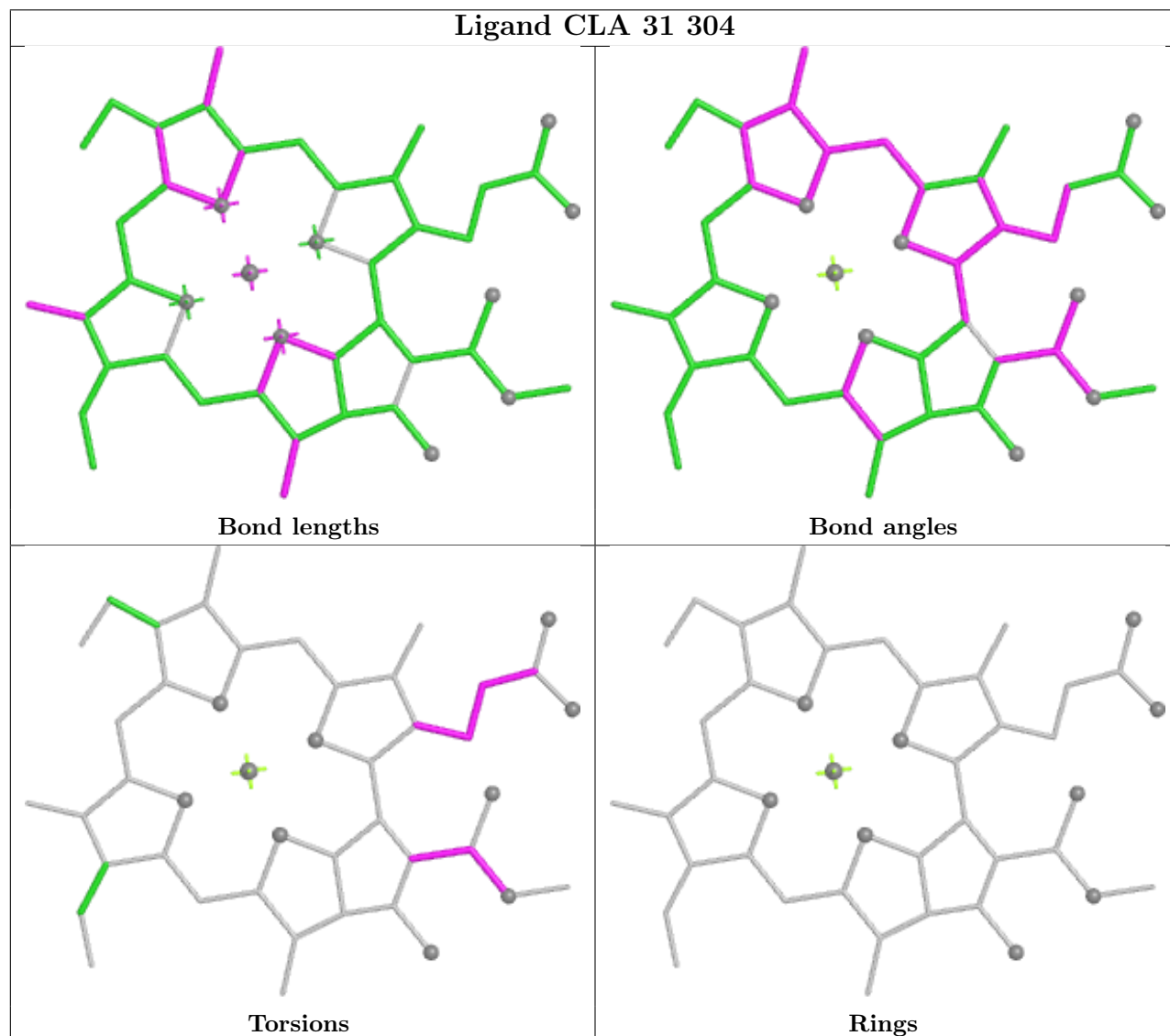
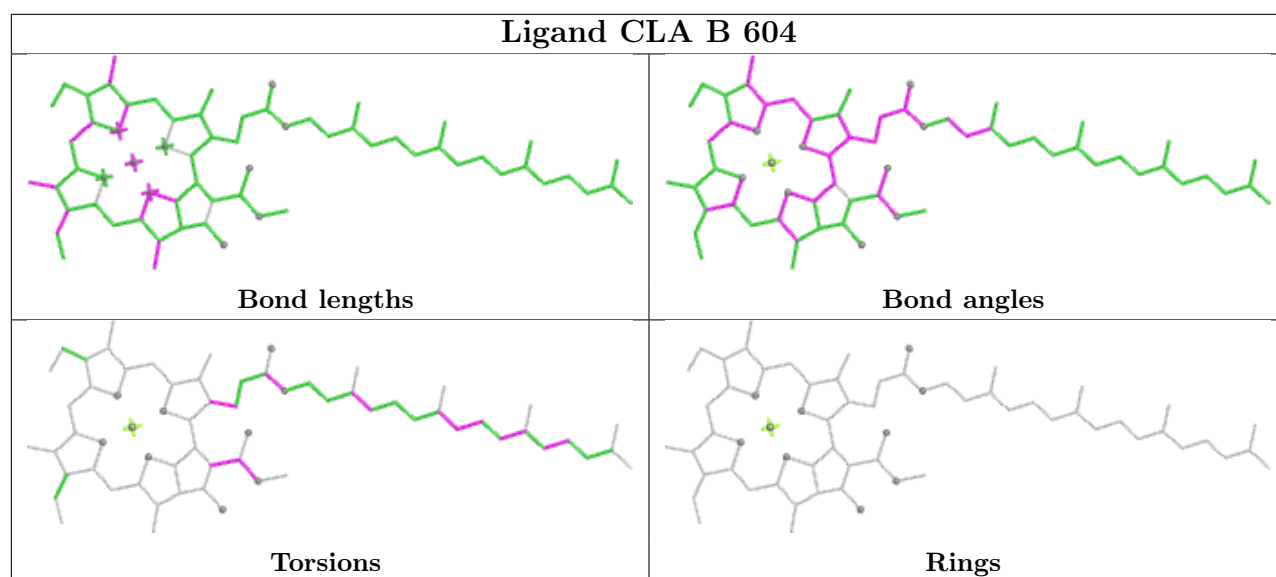




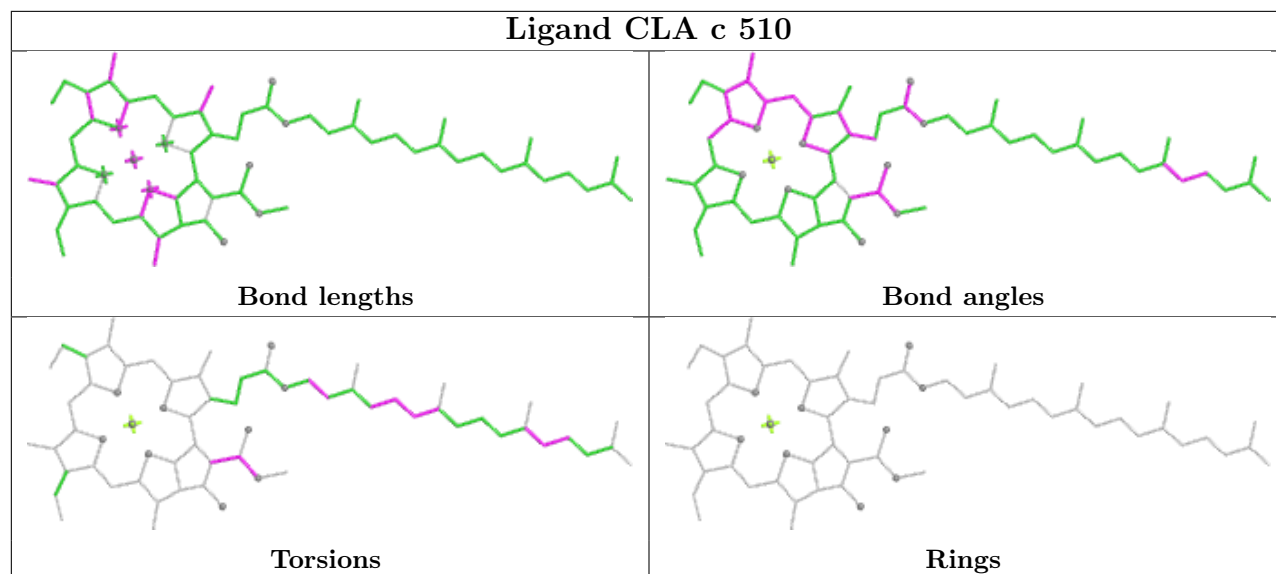
Ligand LMG B 618			
			
Bond lengths	Bond angles		
			
Torsions	Rings		
Ligand BCR M 101			
			
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Bond lengths	Bond angles		
			
Torsions	Rings		



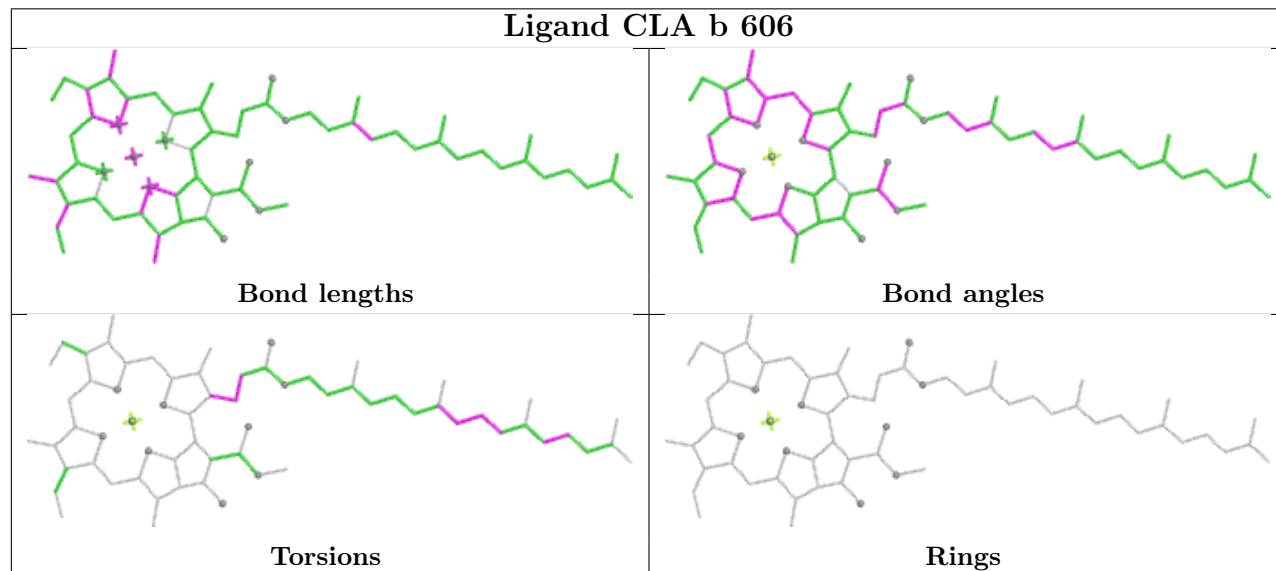


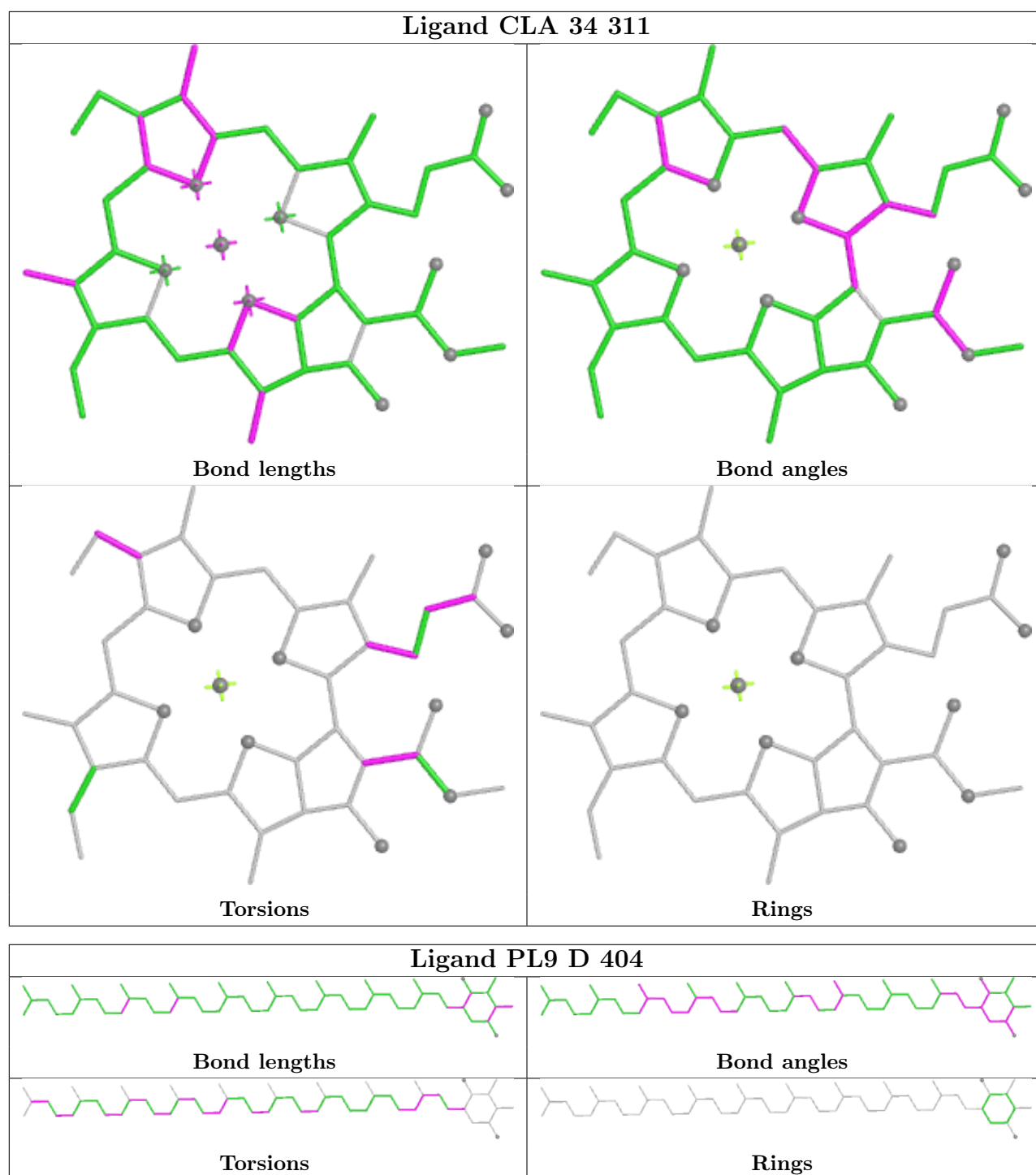


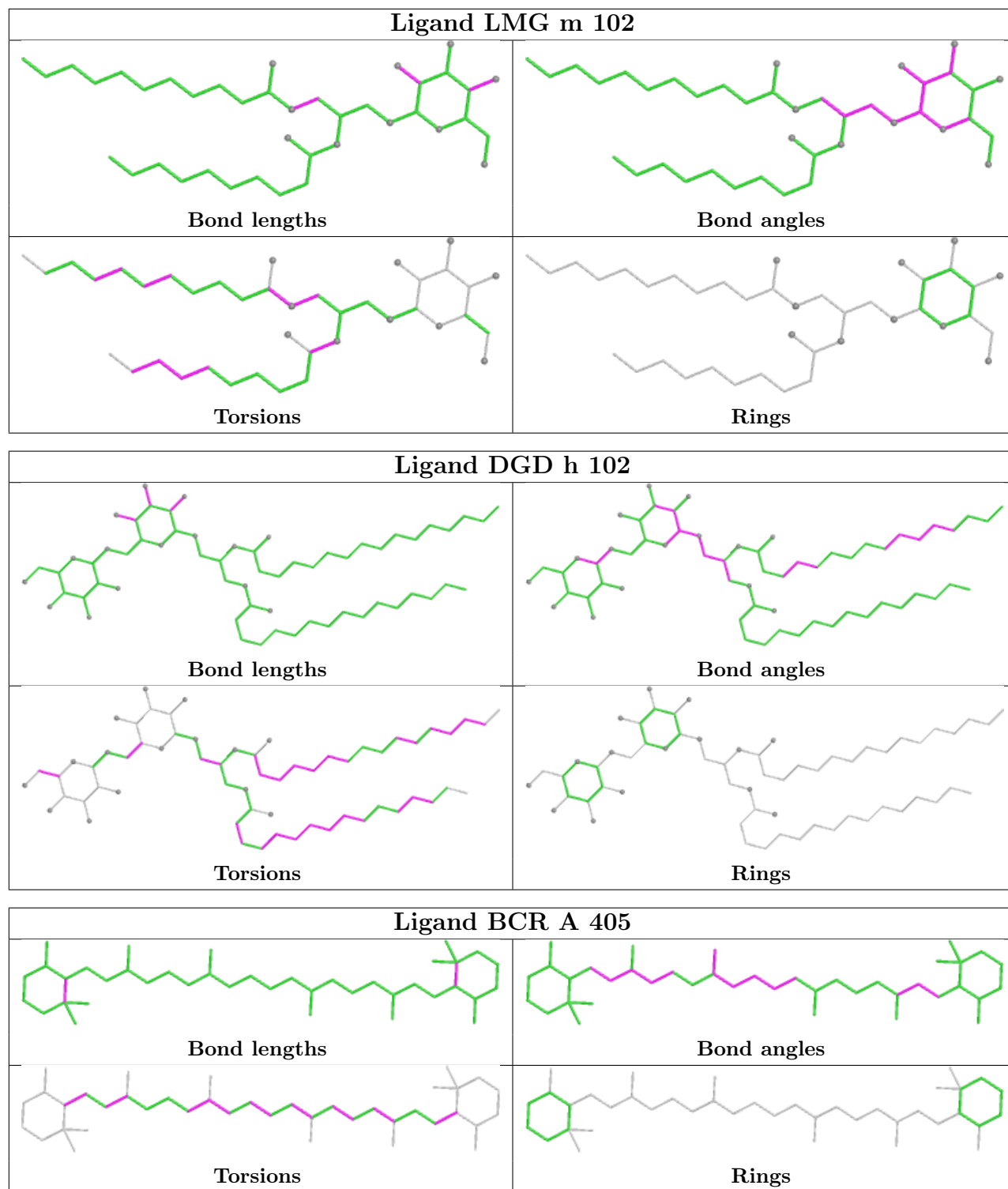
Ligand CLA c 510

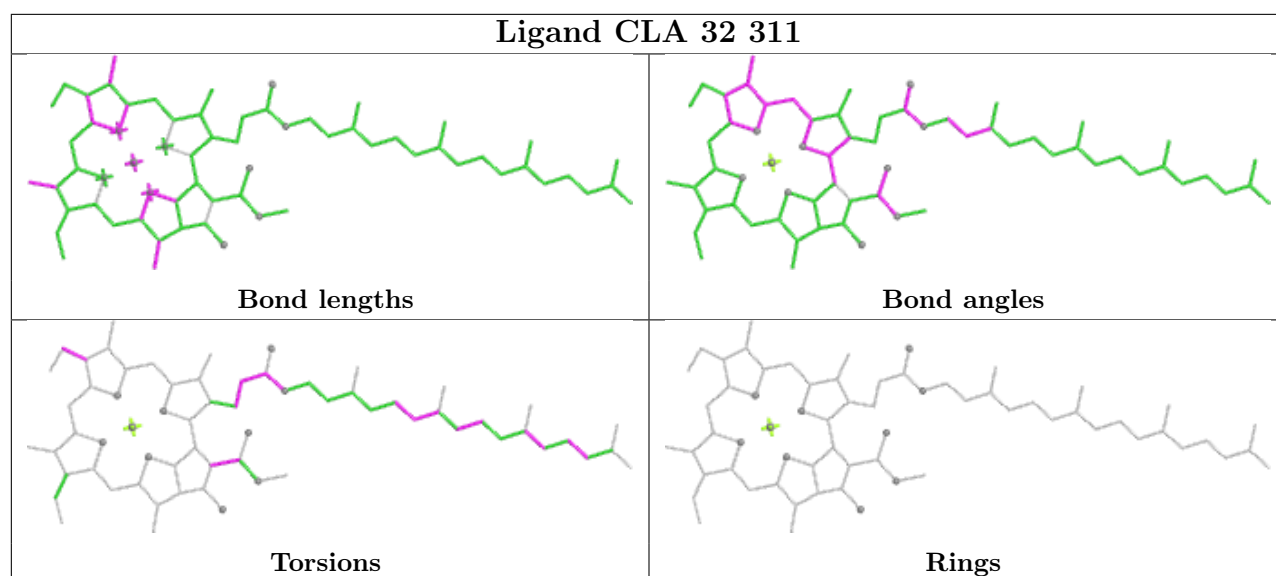
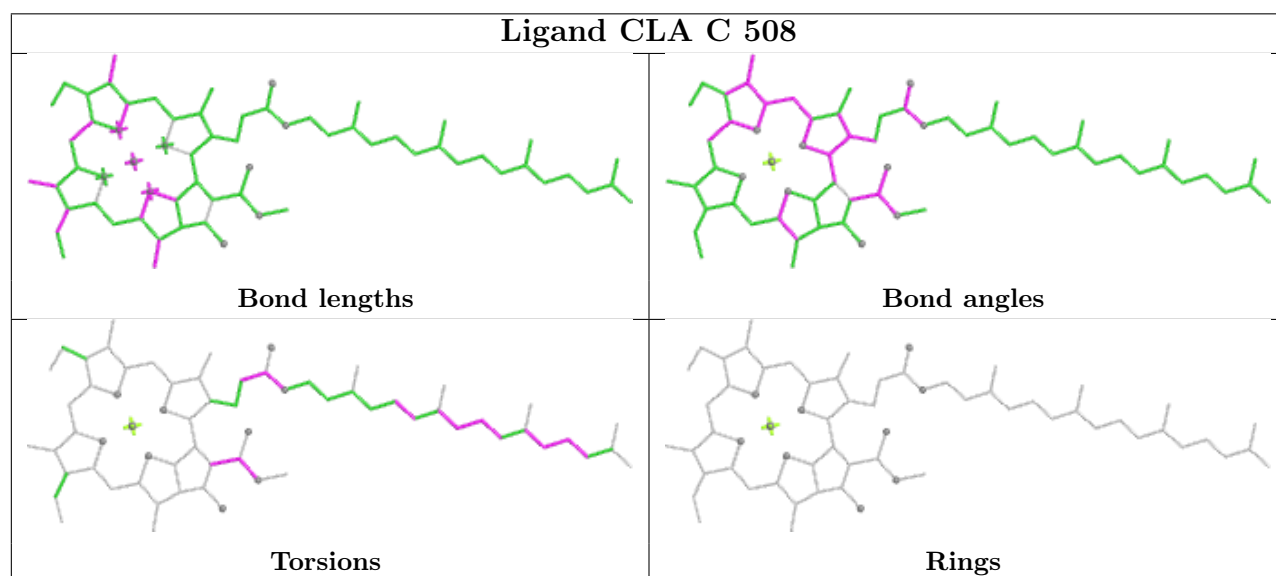
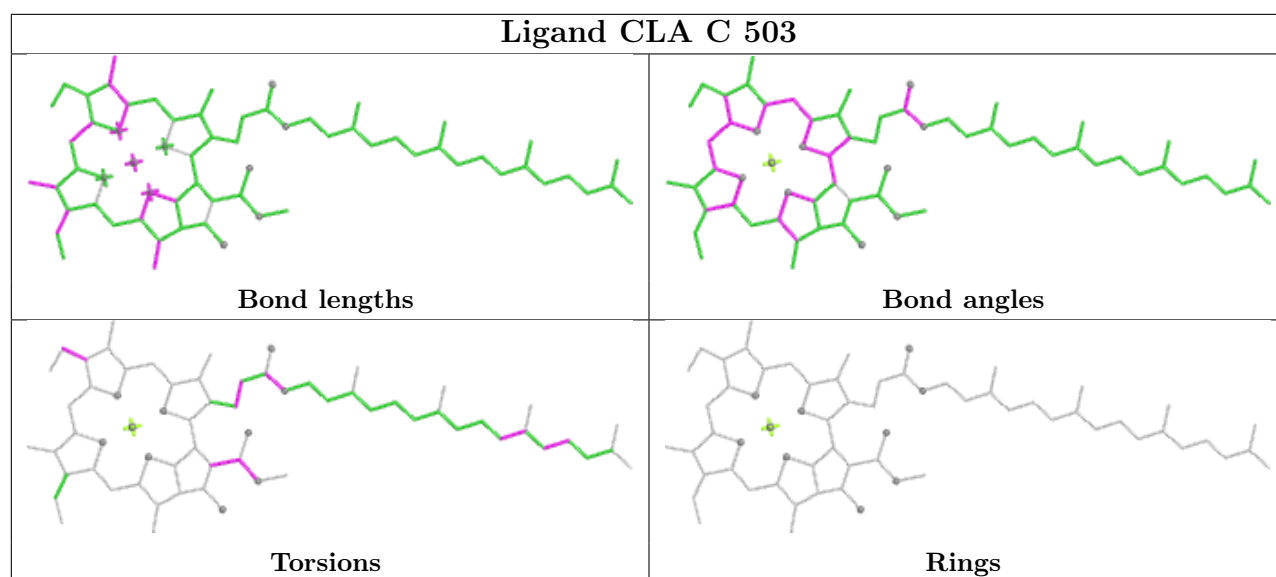


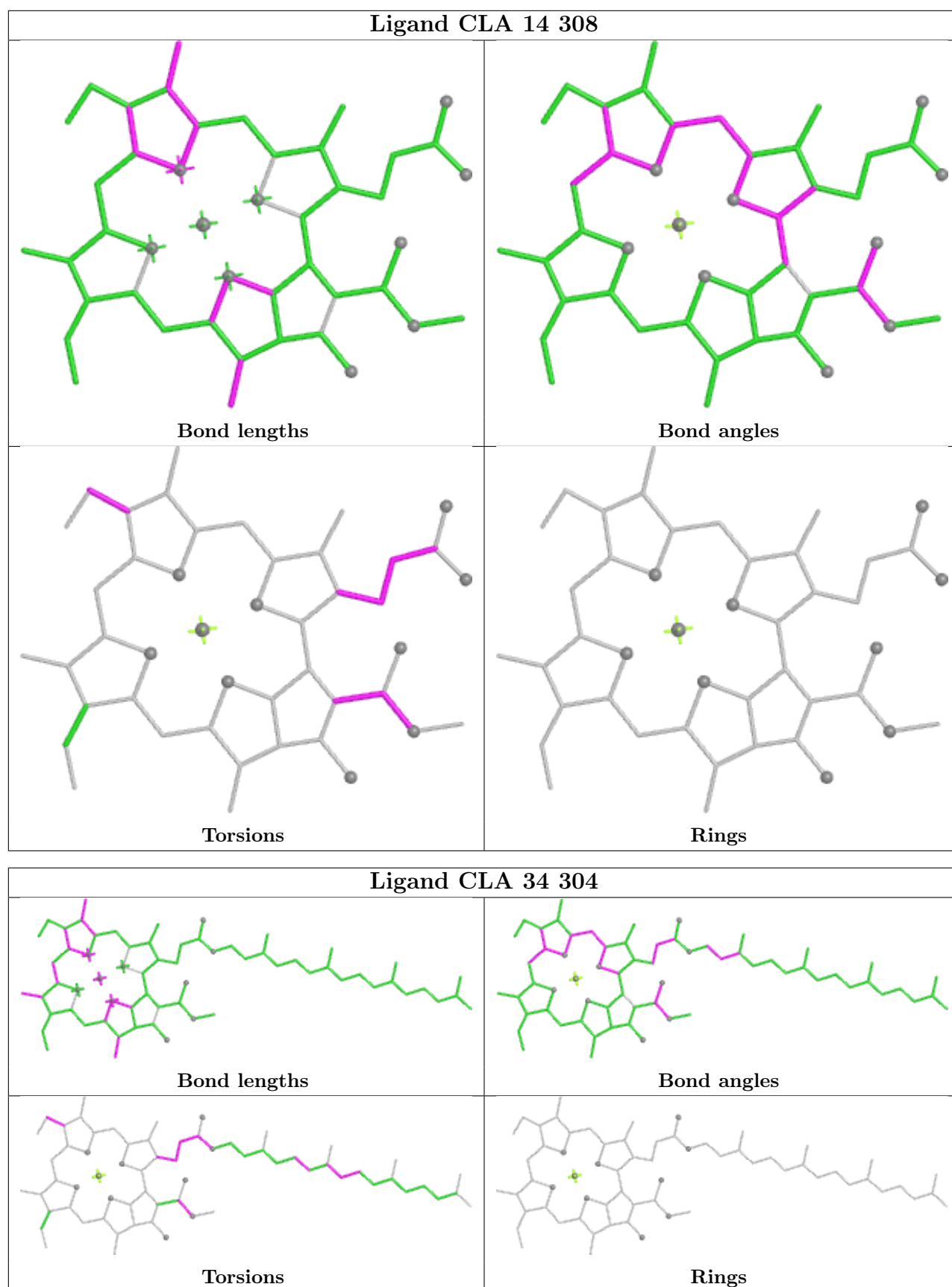
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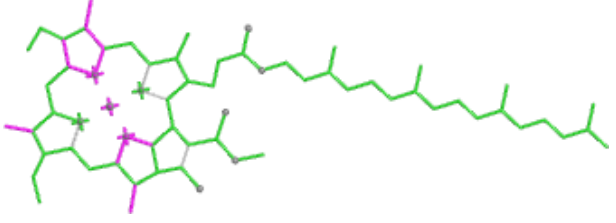
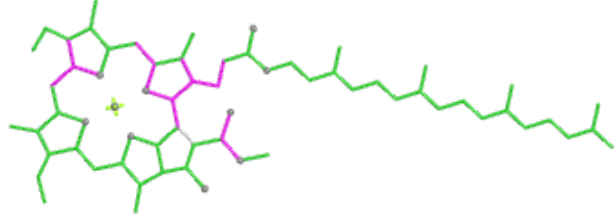
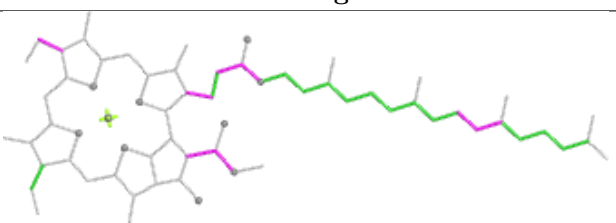
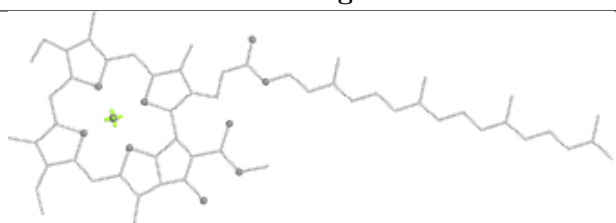
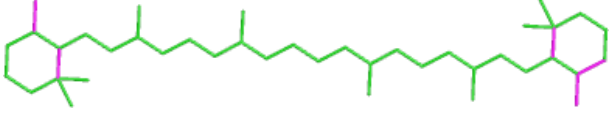
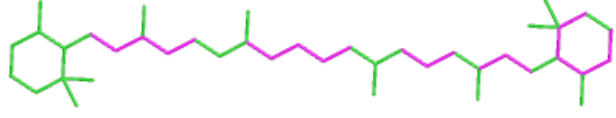
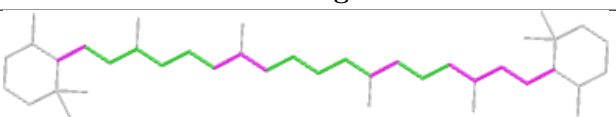
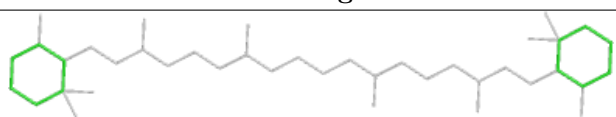
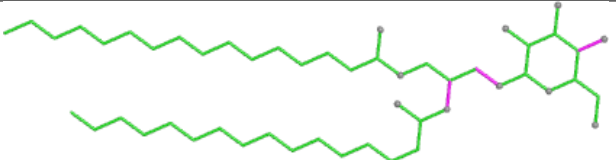
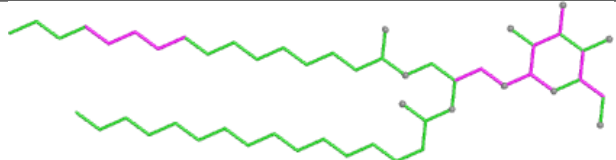
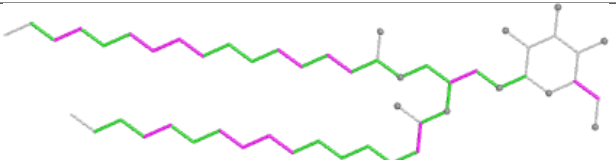
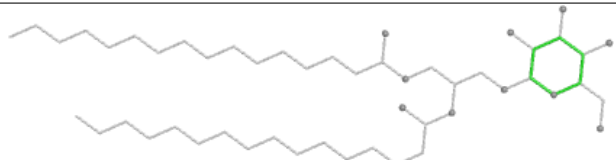


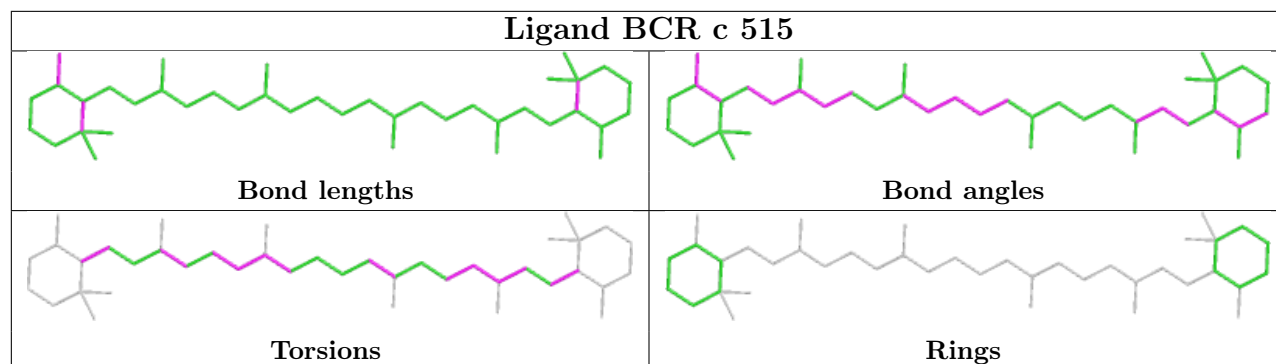
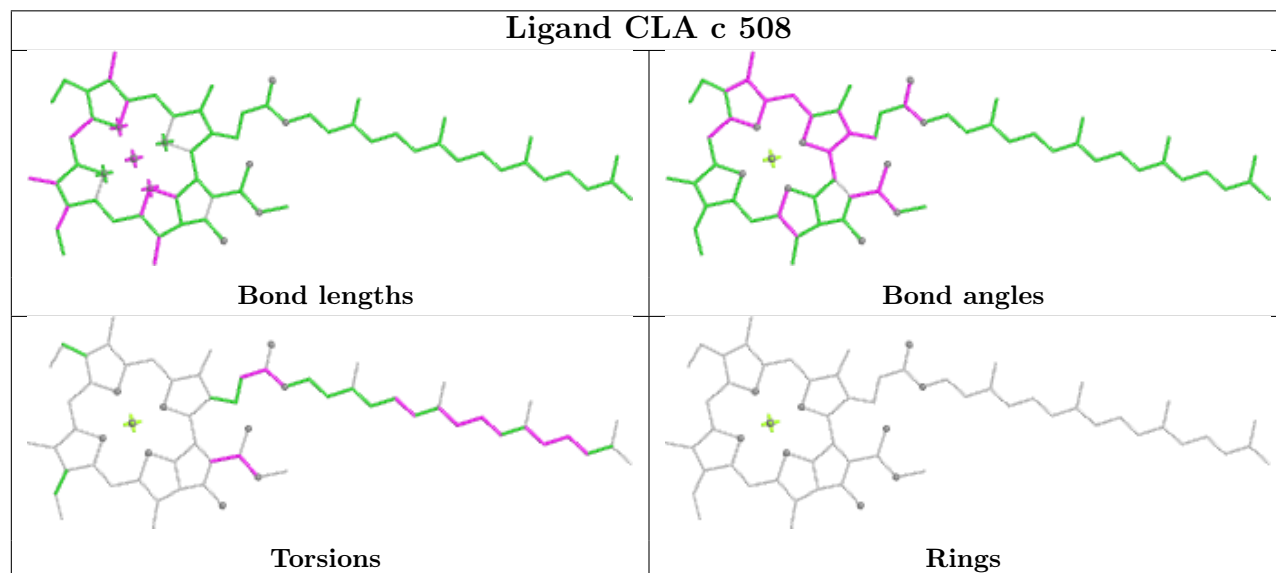
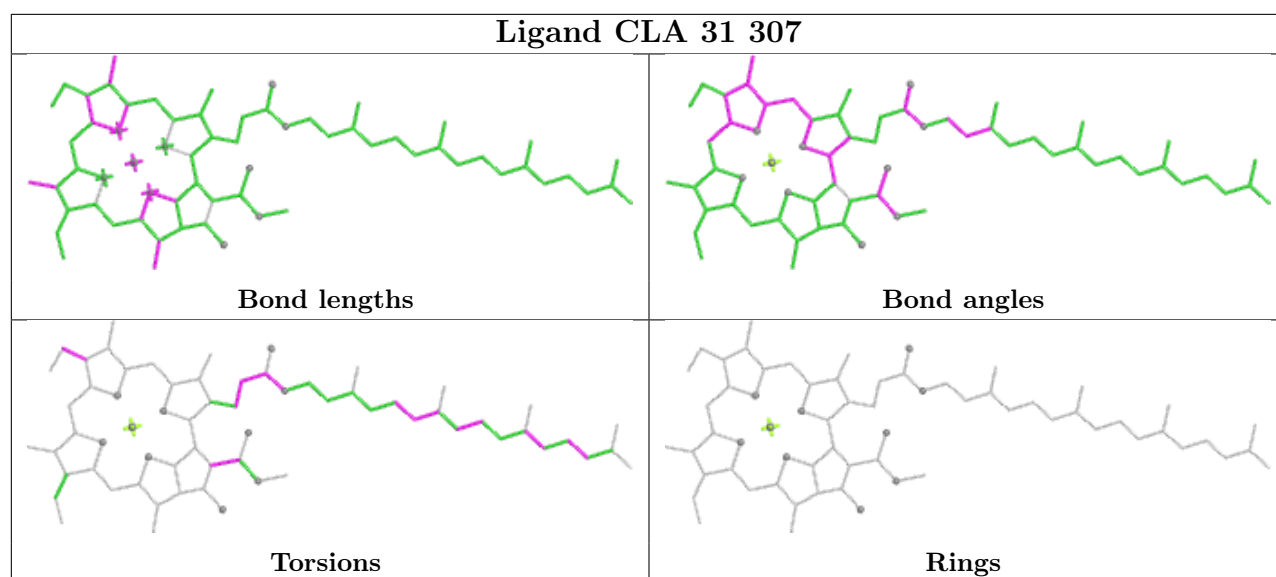


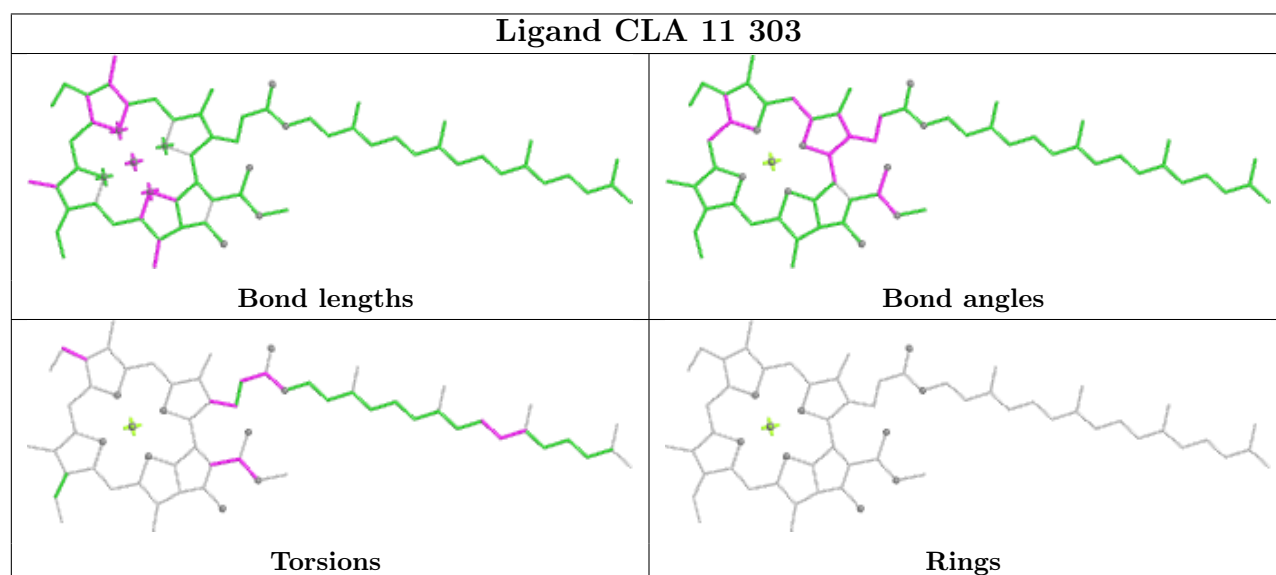
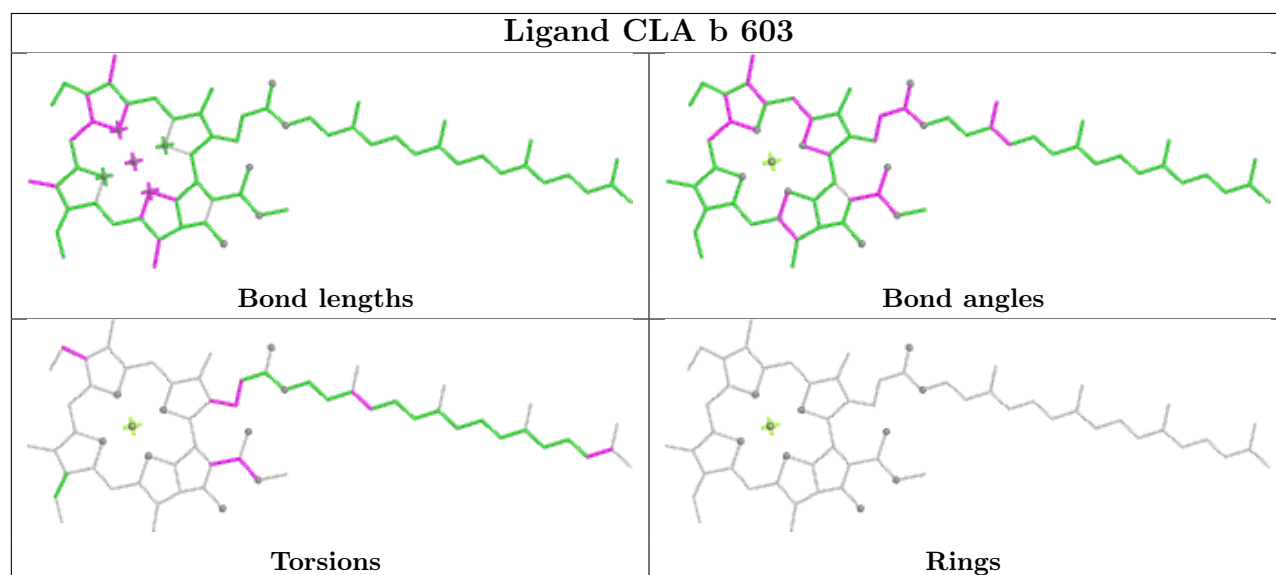
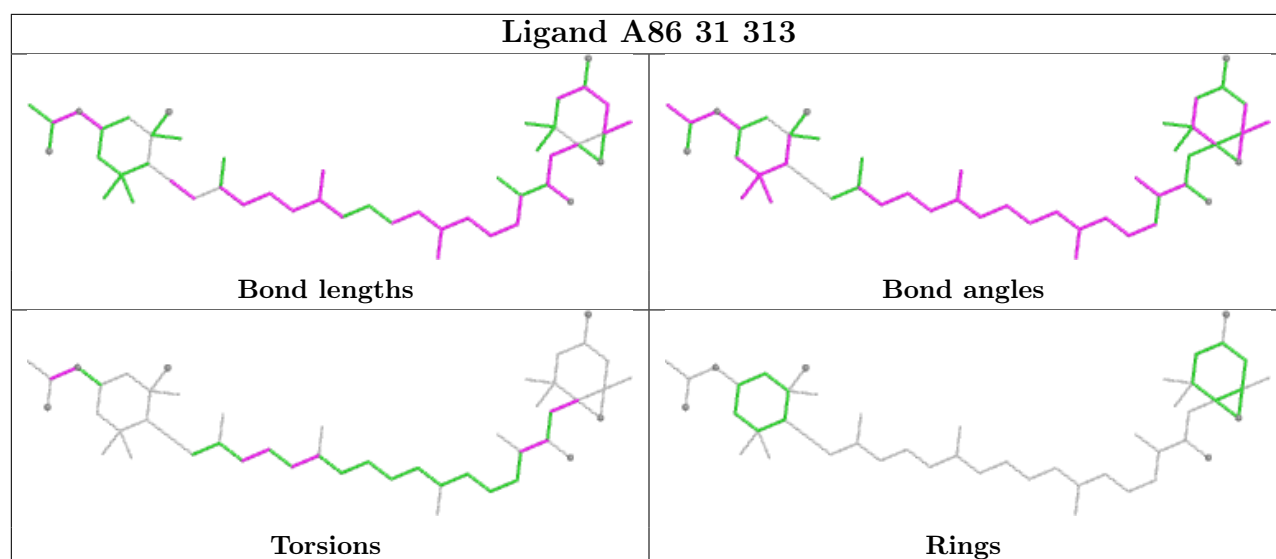


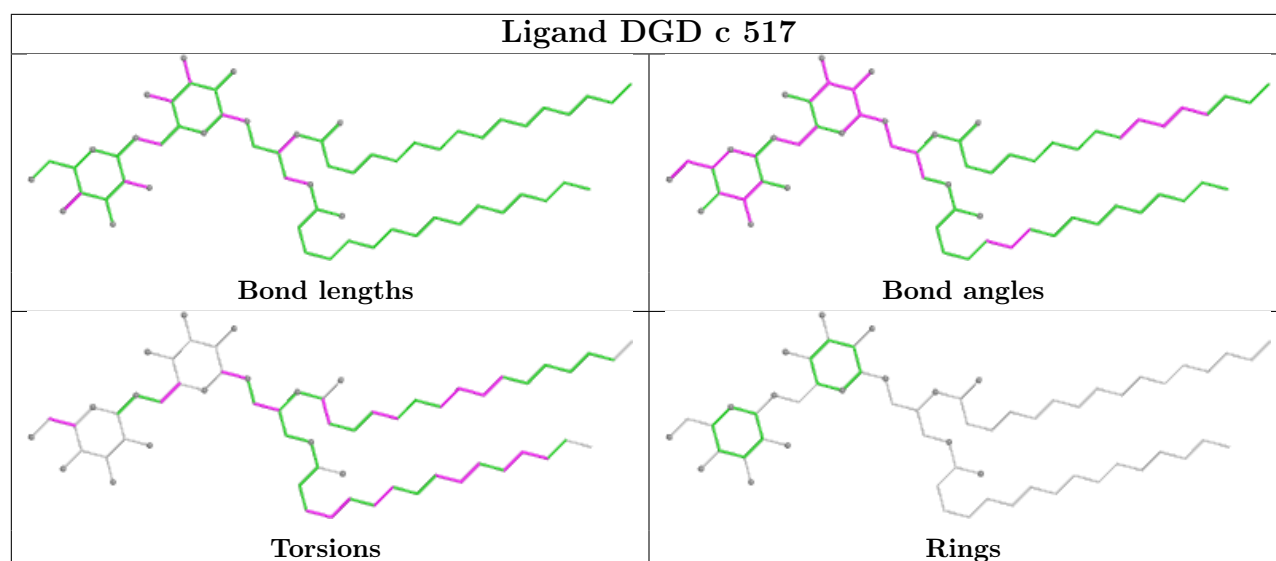
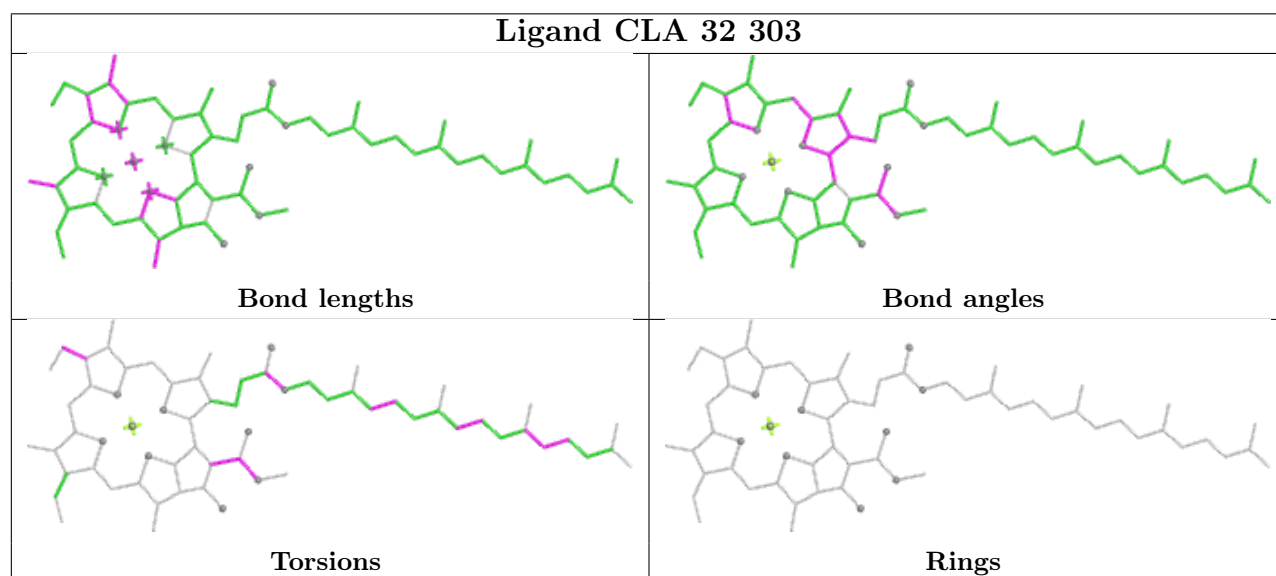
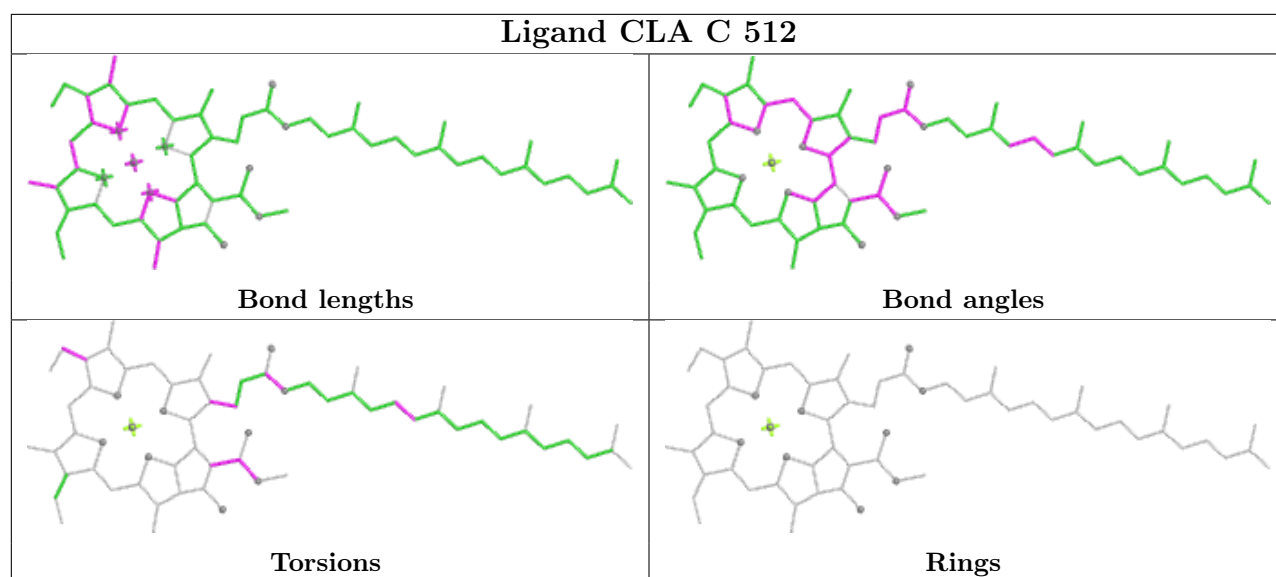


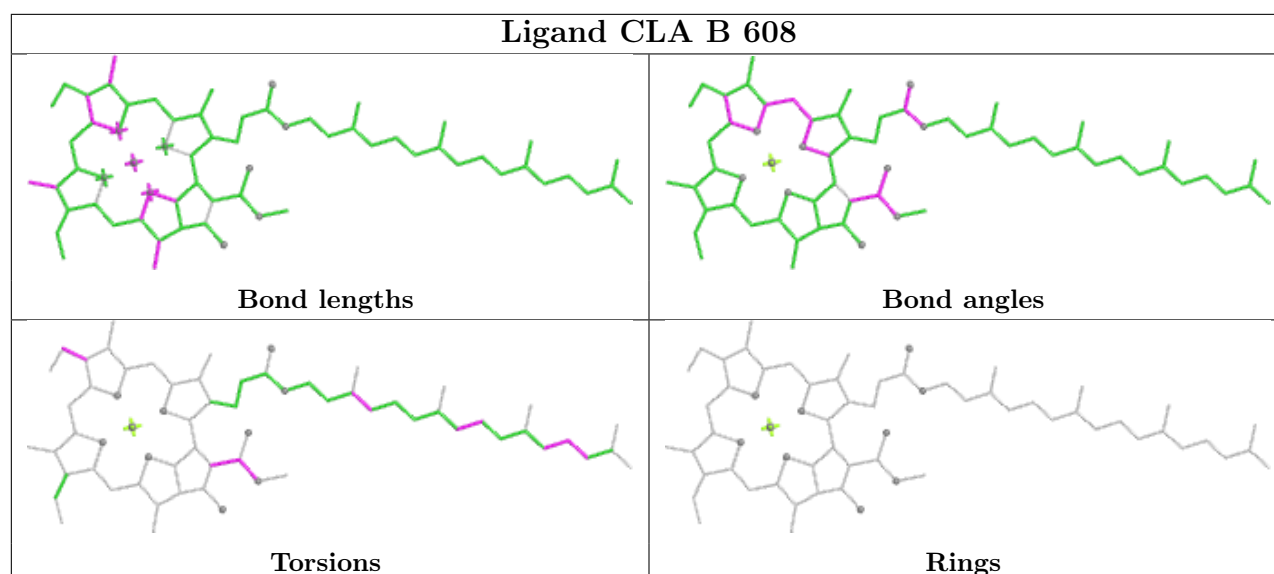
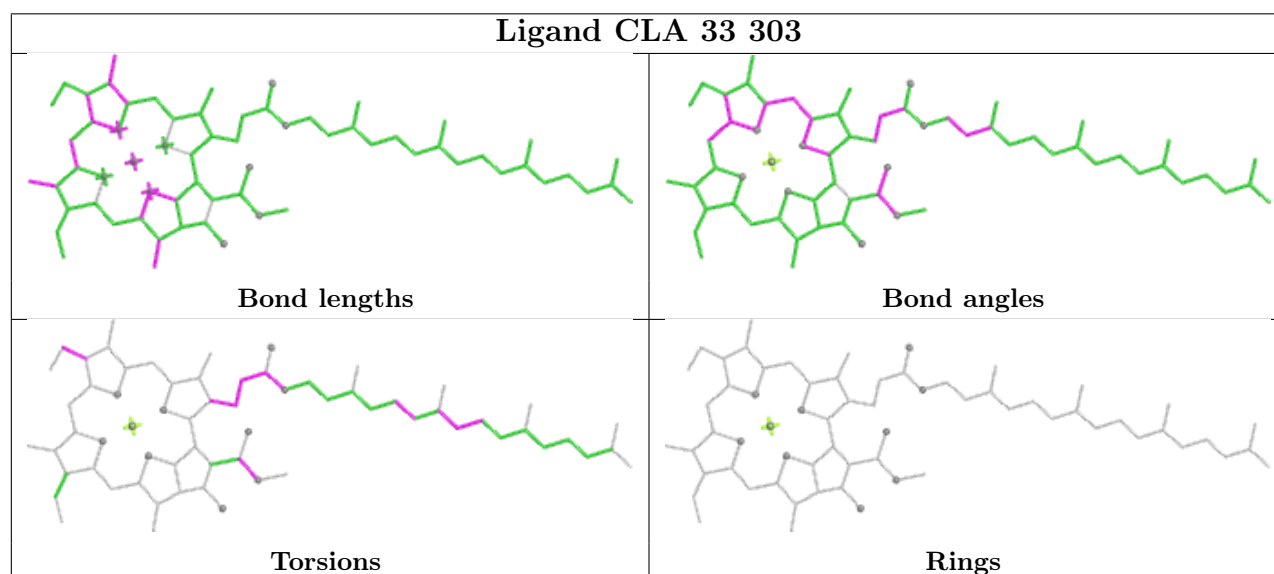
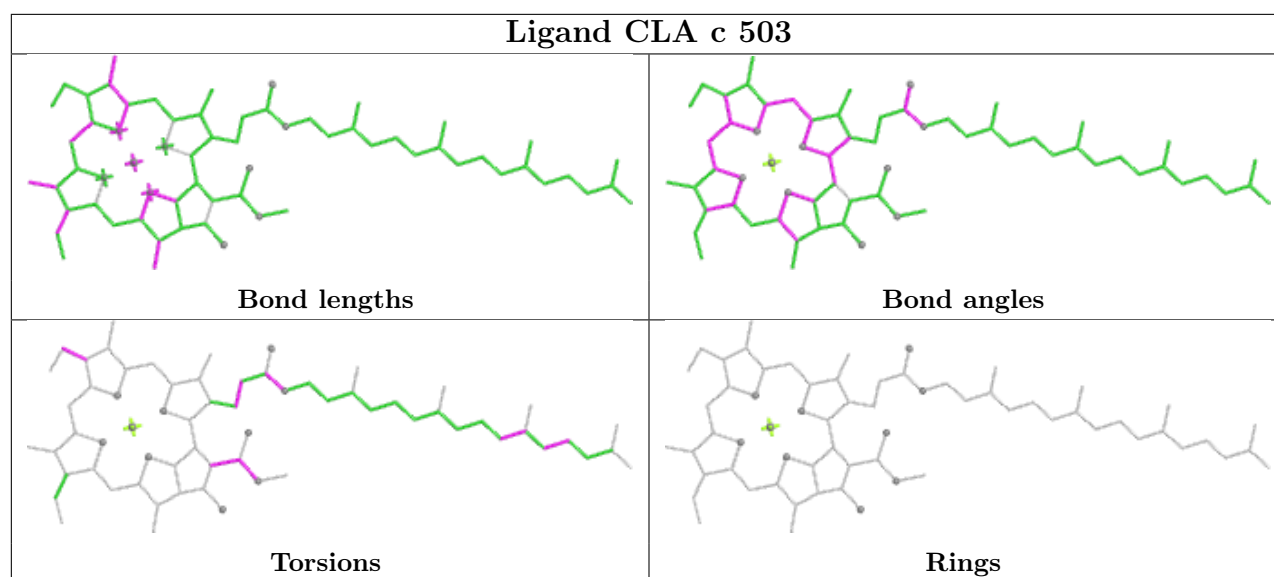


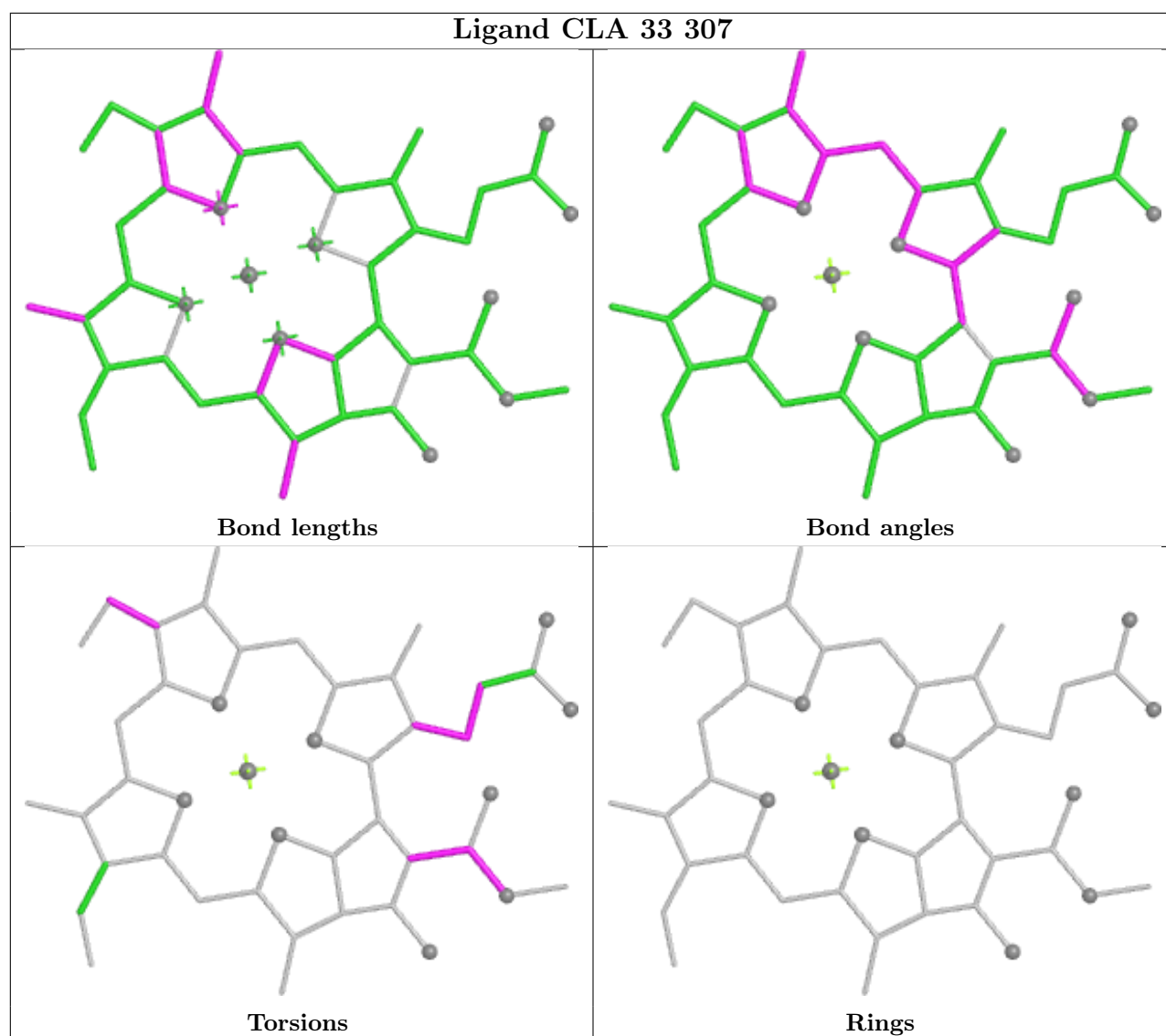
Ligand CLA 31 303	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 516	
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 Bond lengths	 Bond angles
 Torsions	 Rings

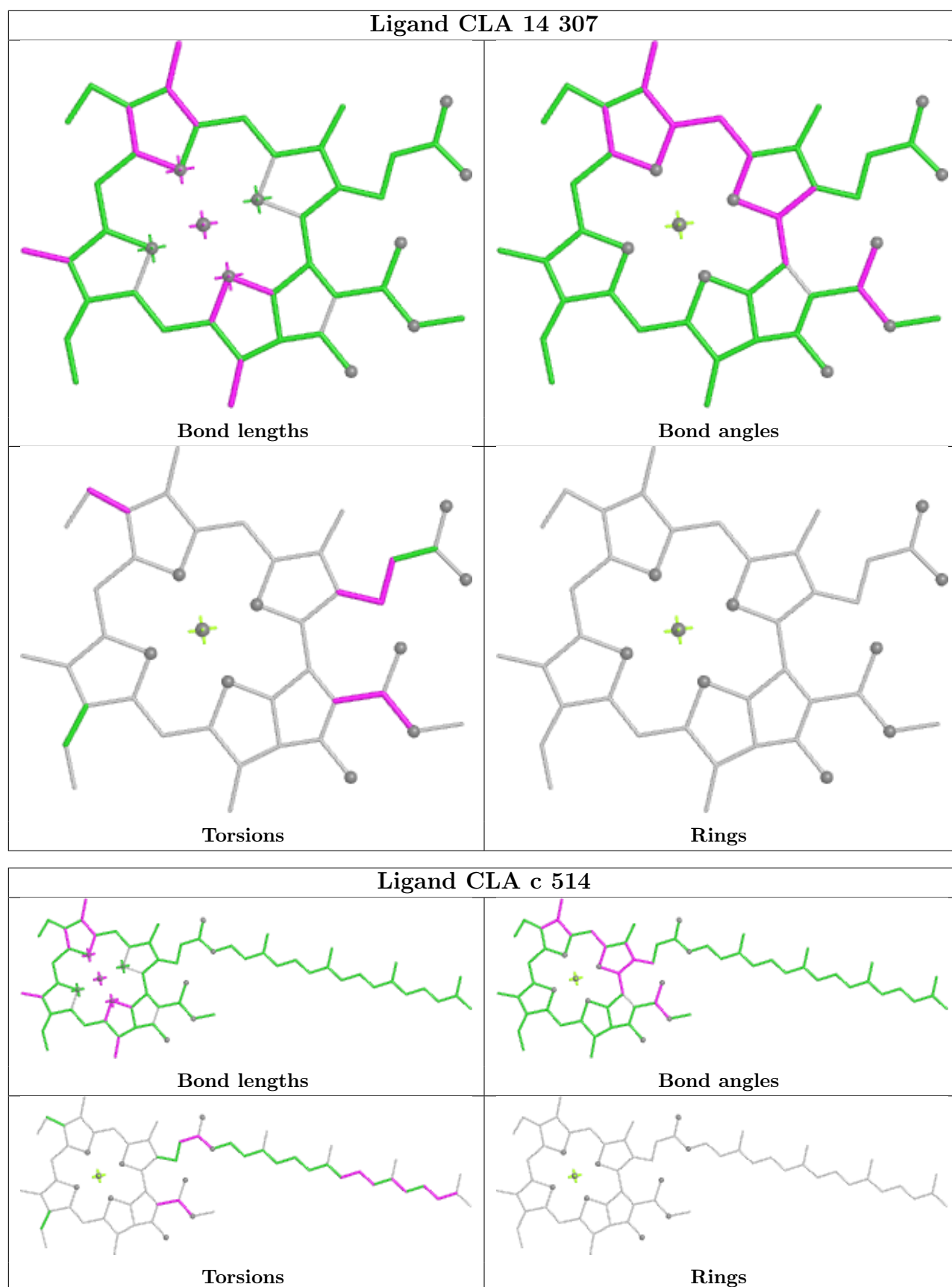


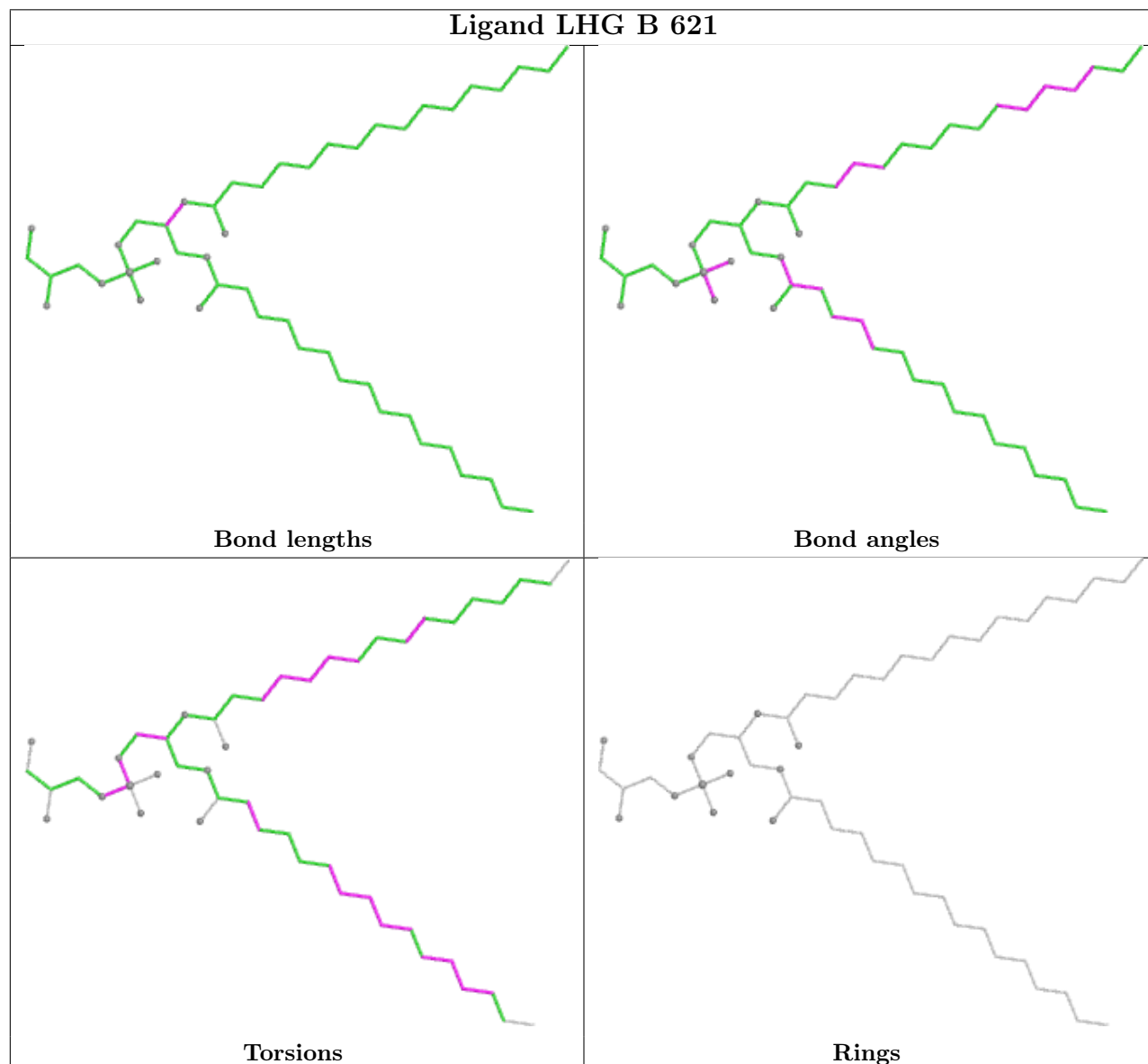
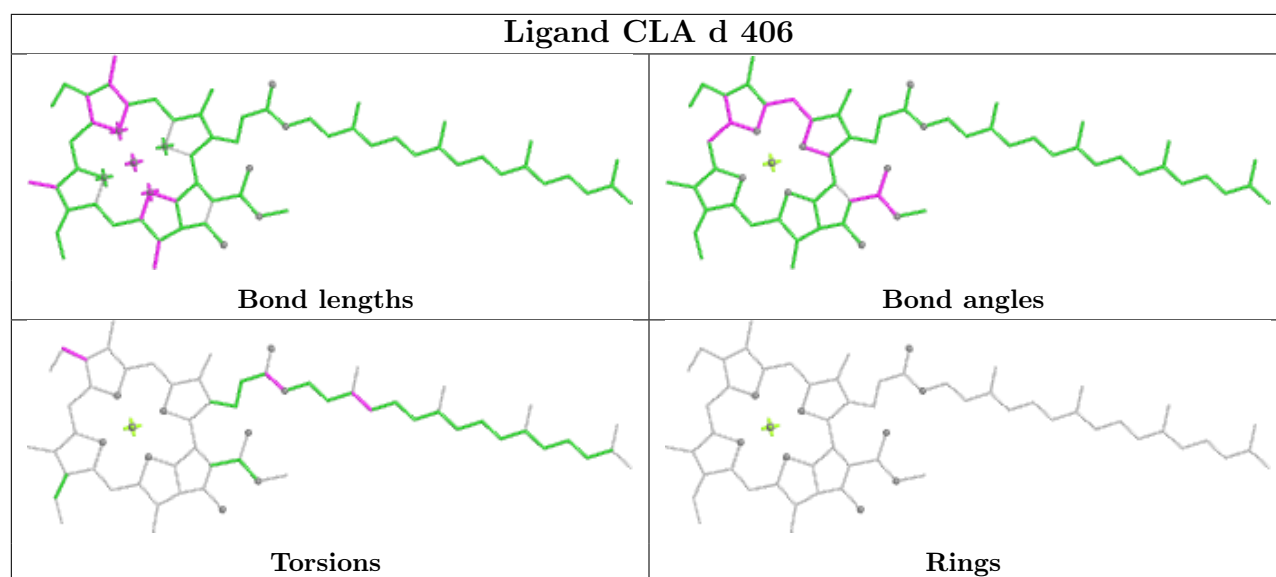


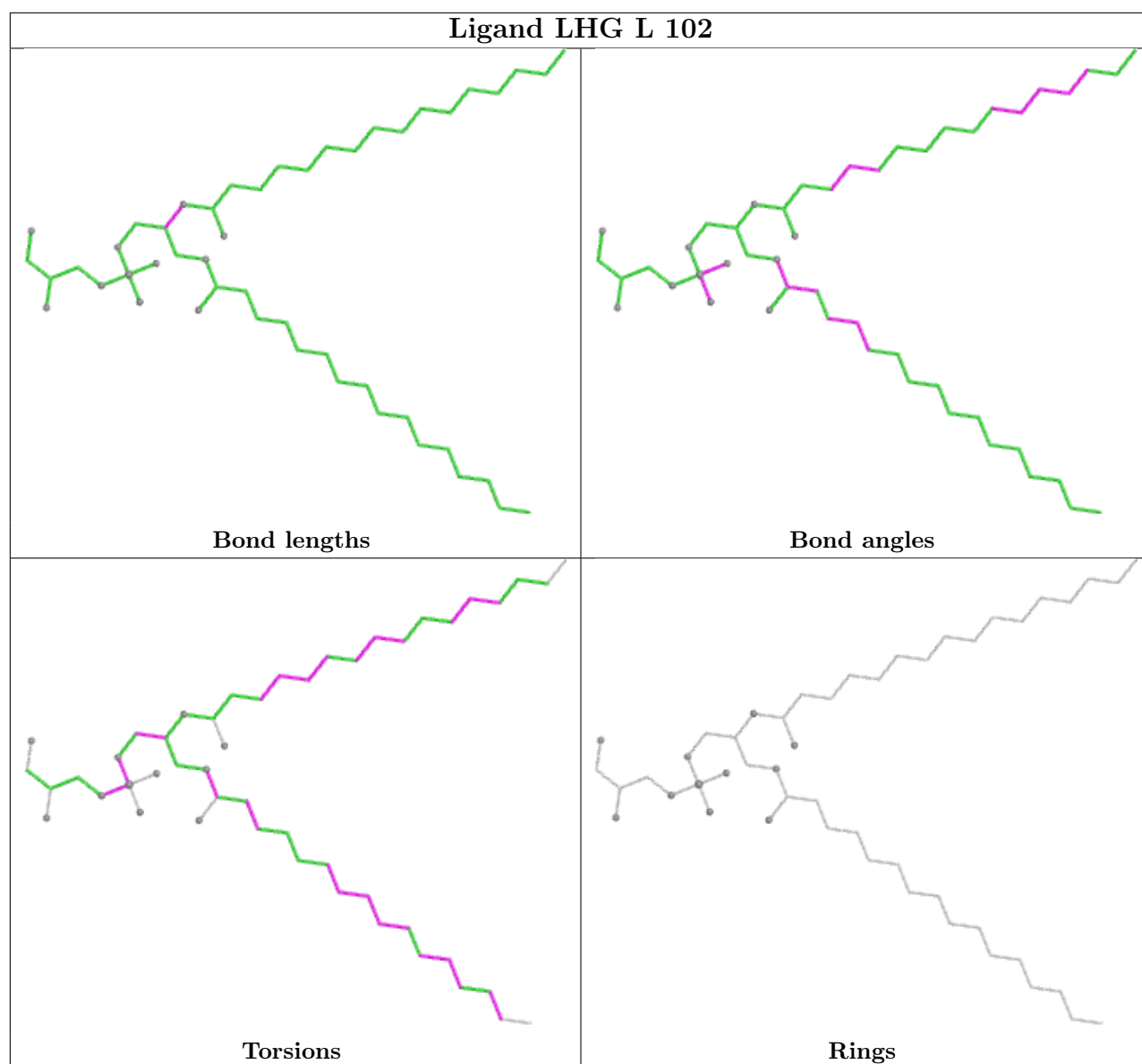


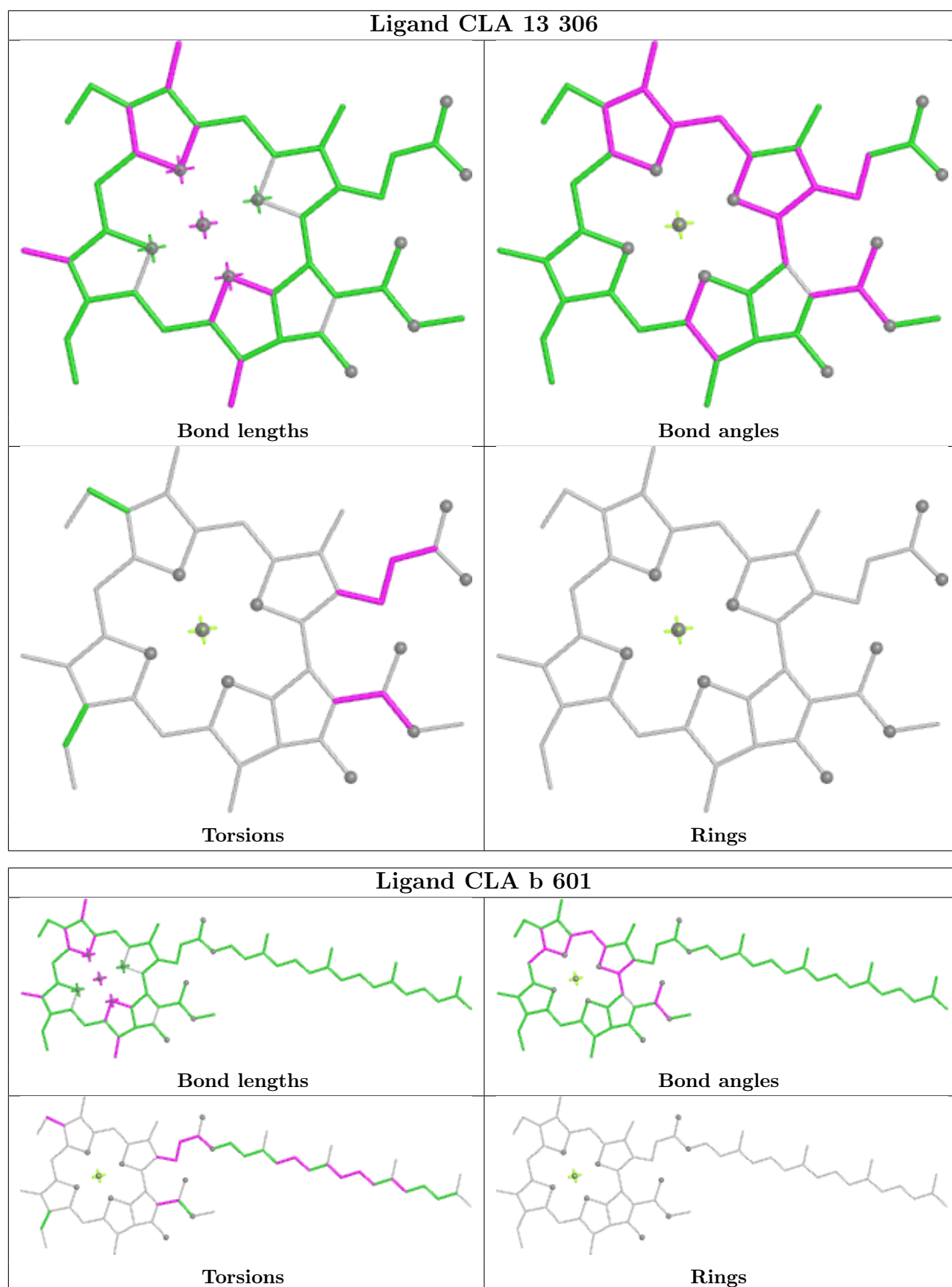


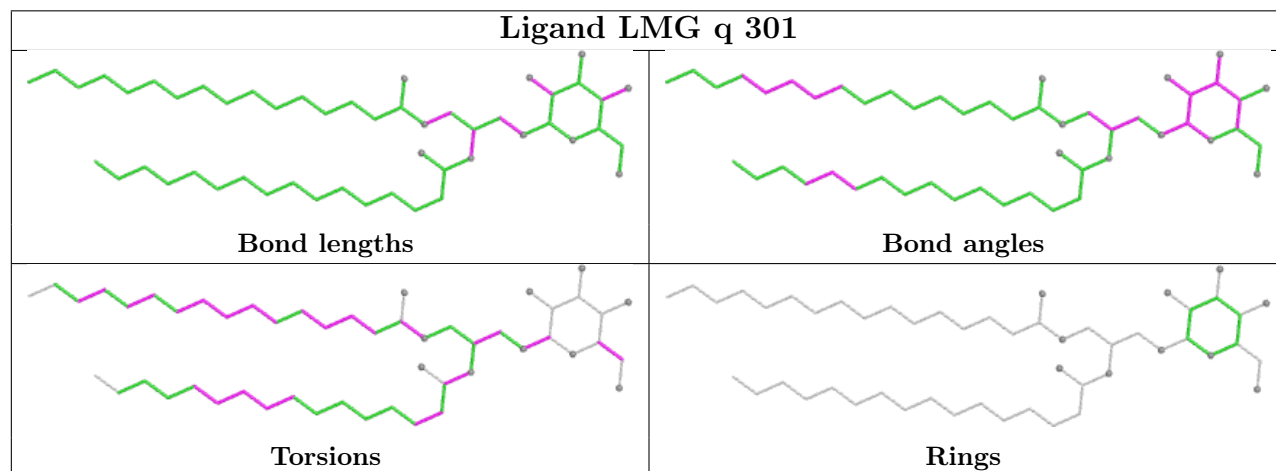
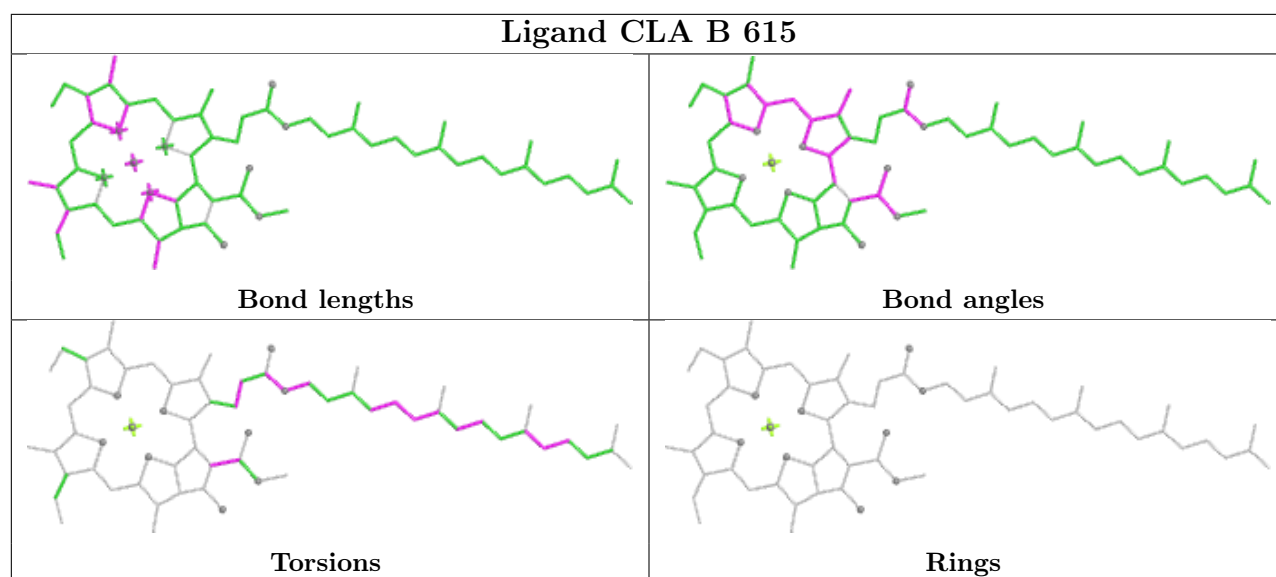


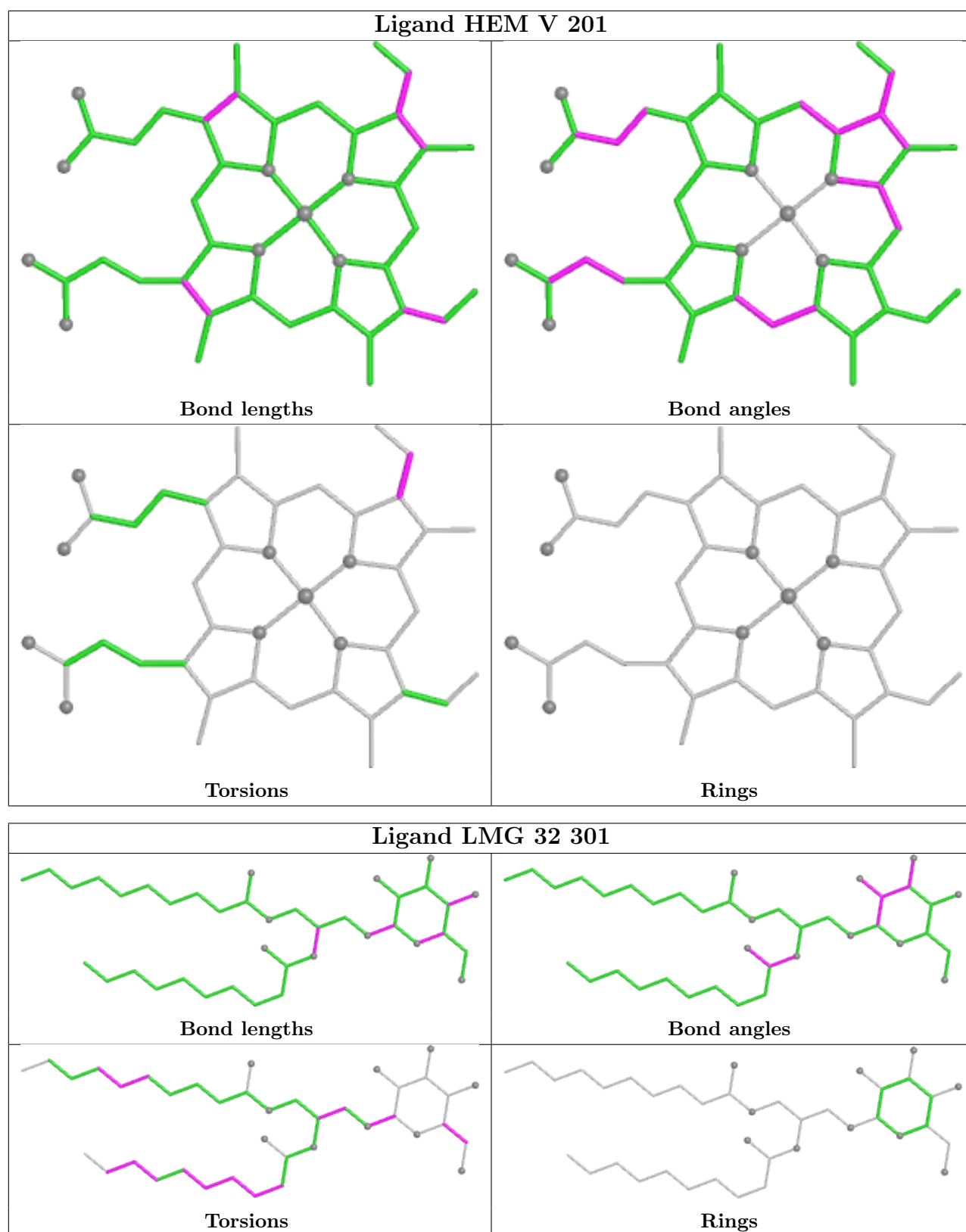


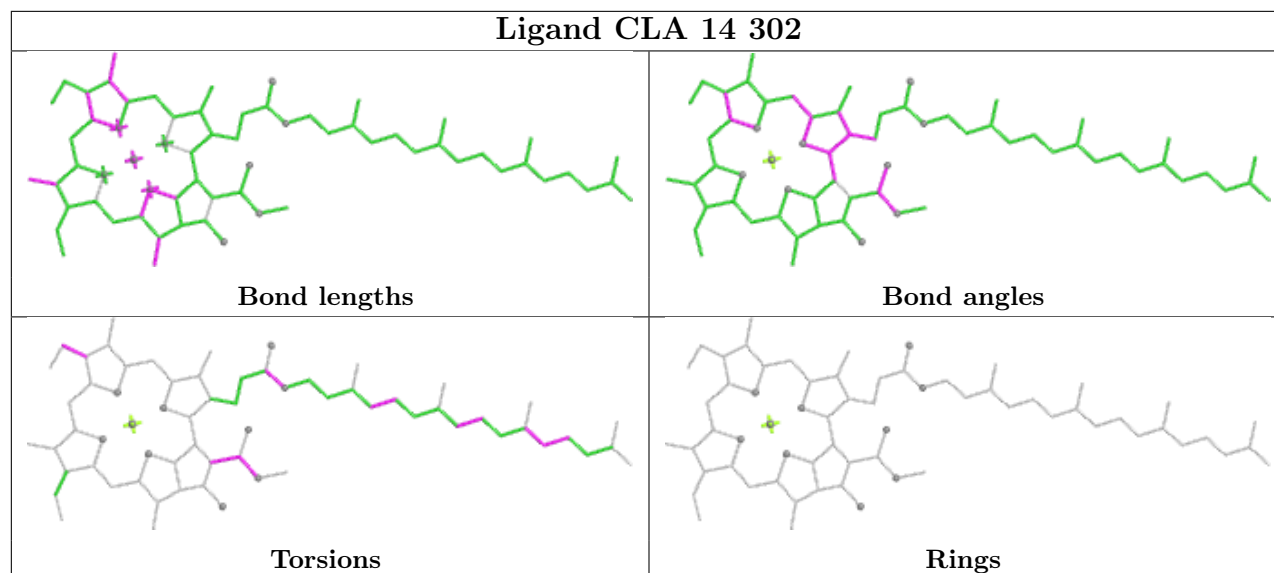
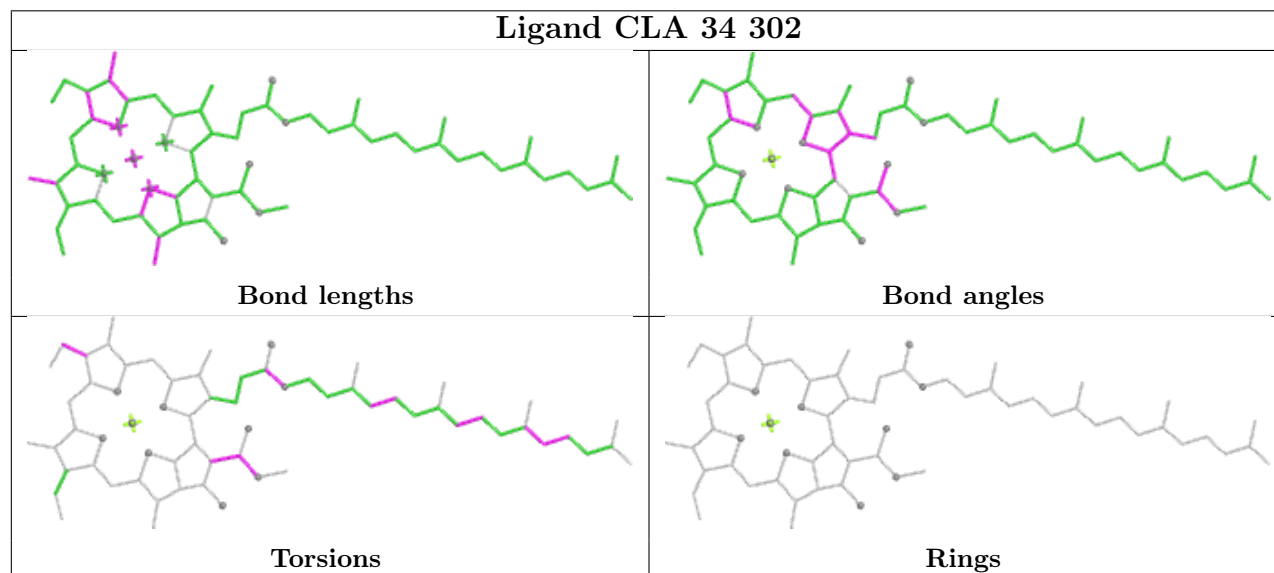
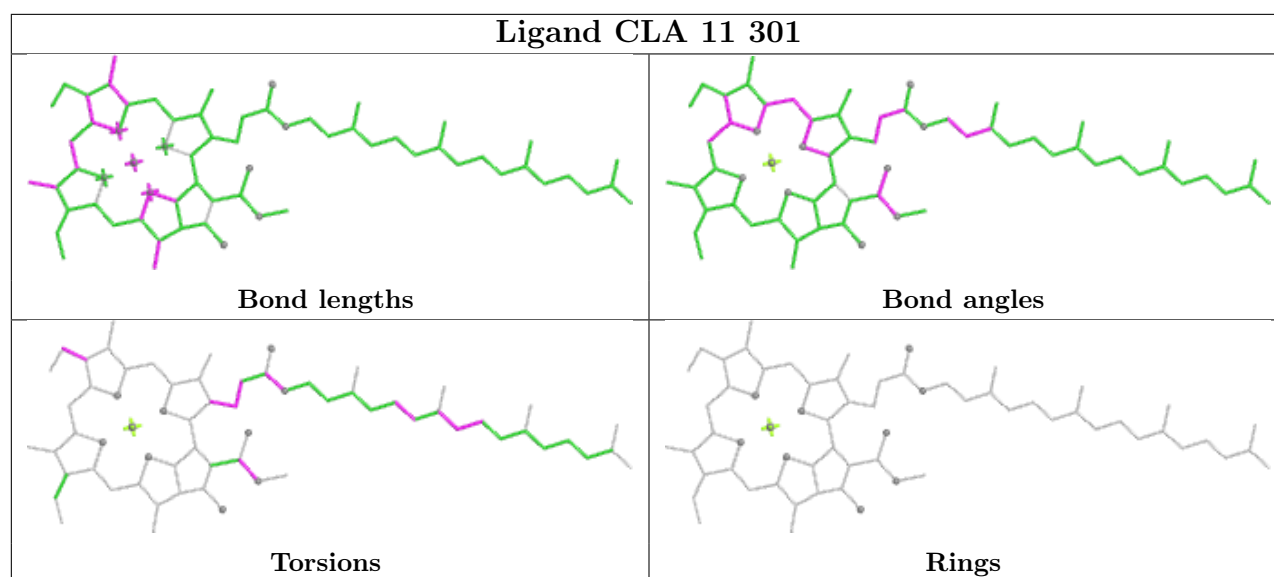


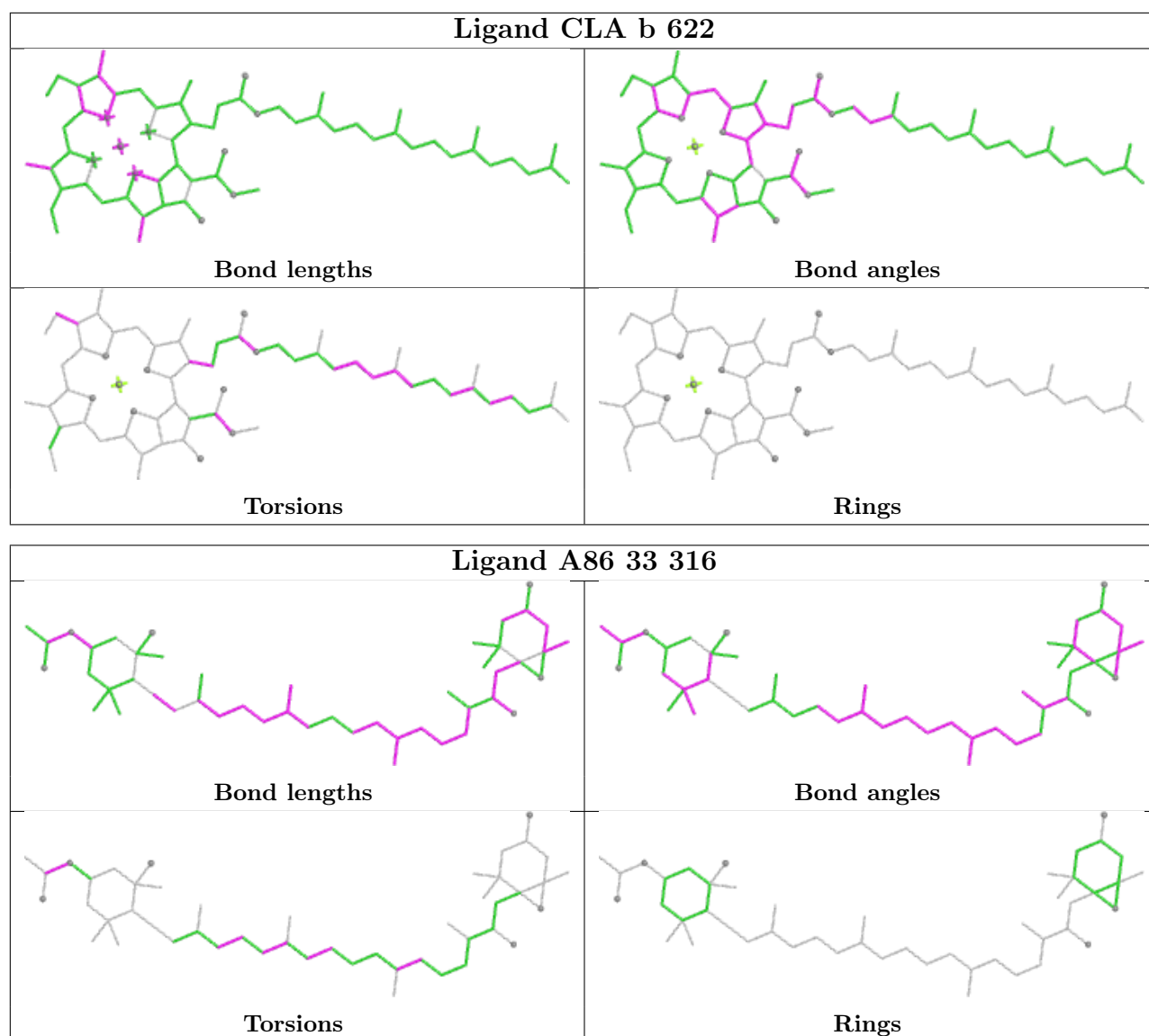


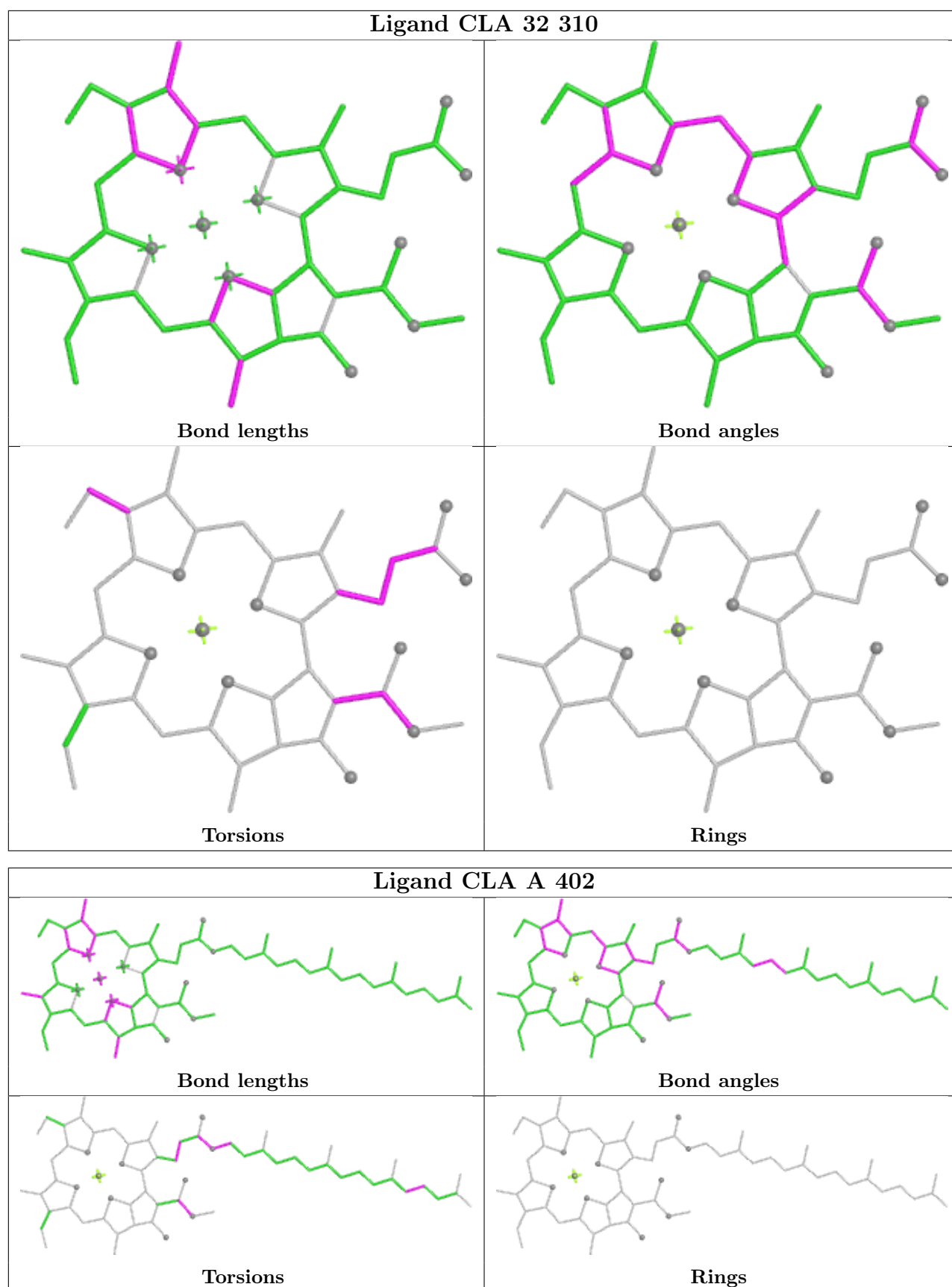


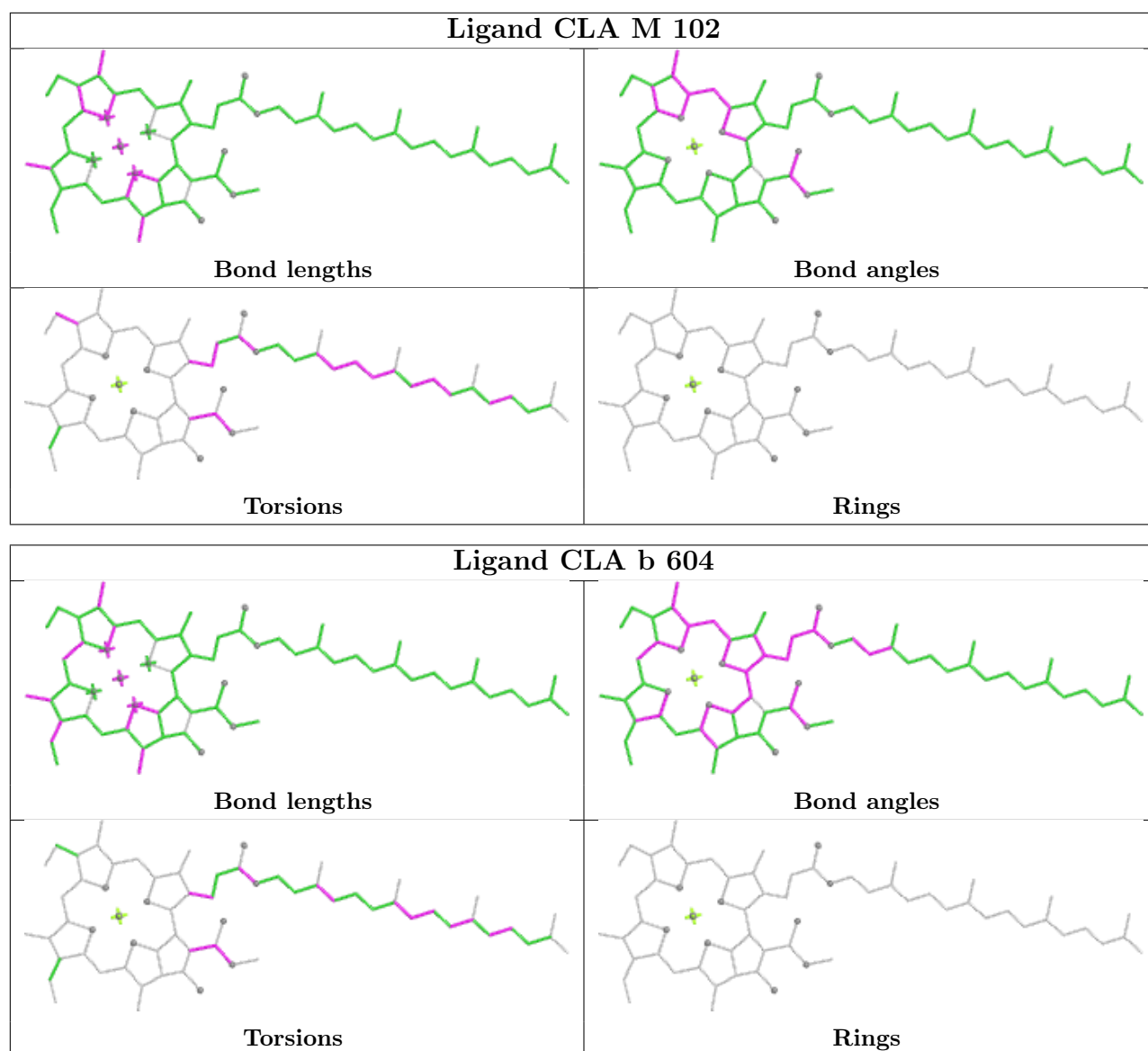


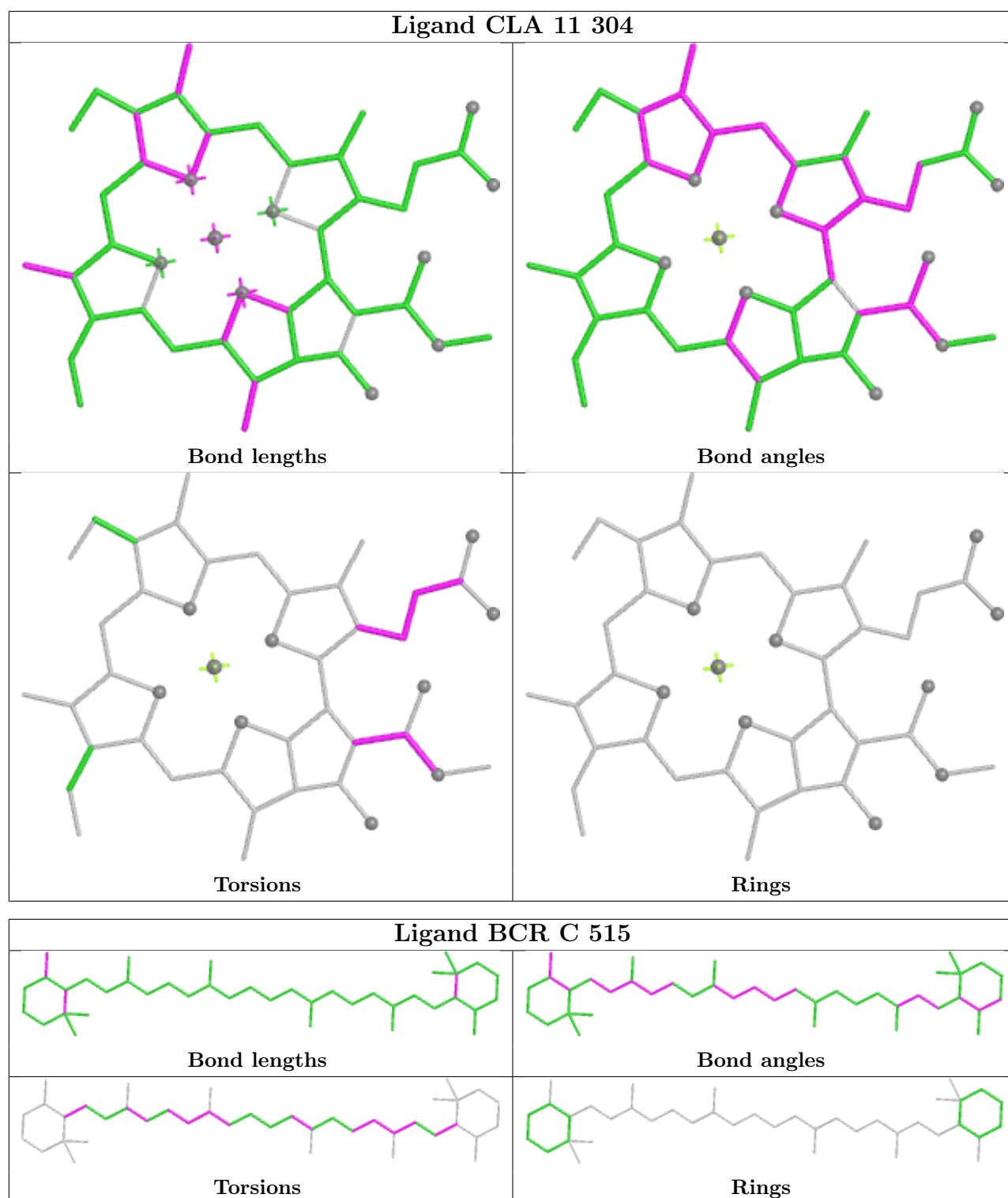


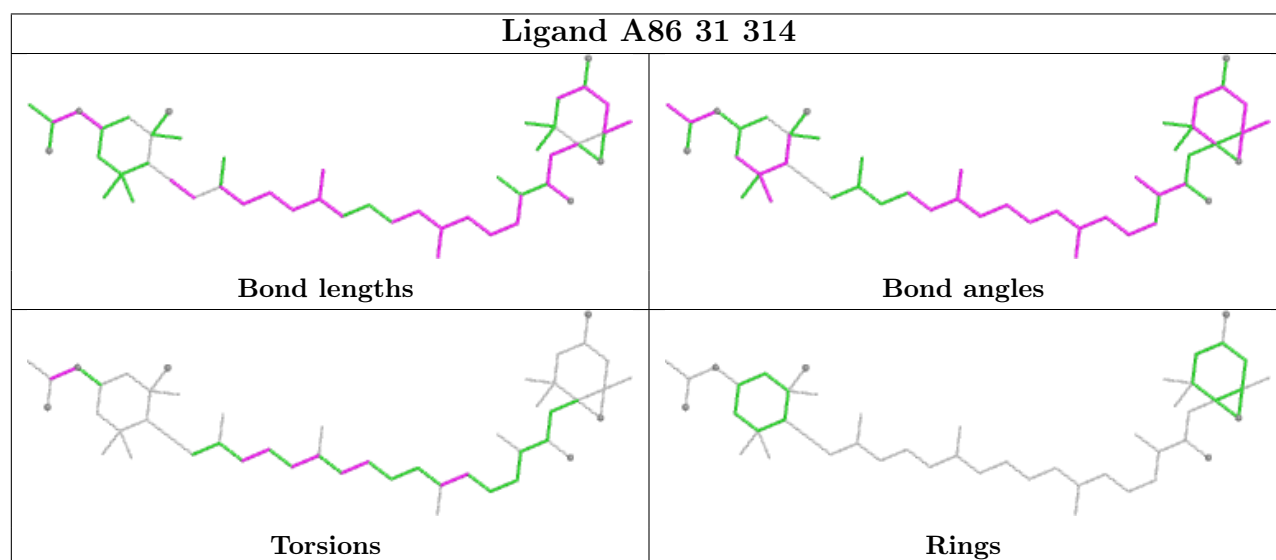
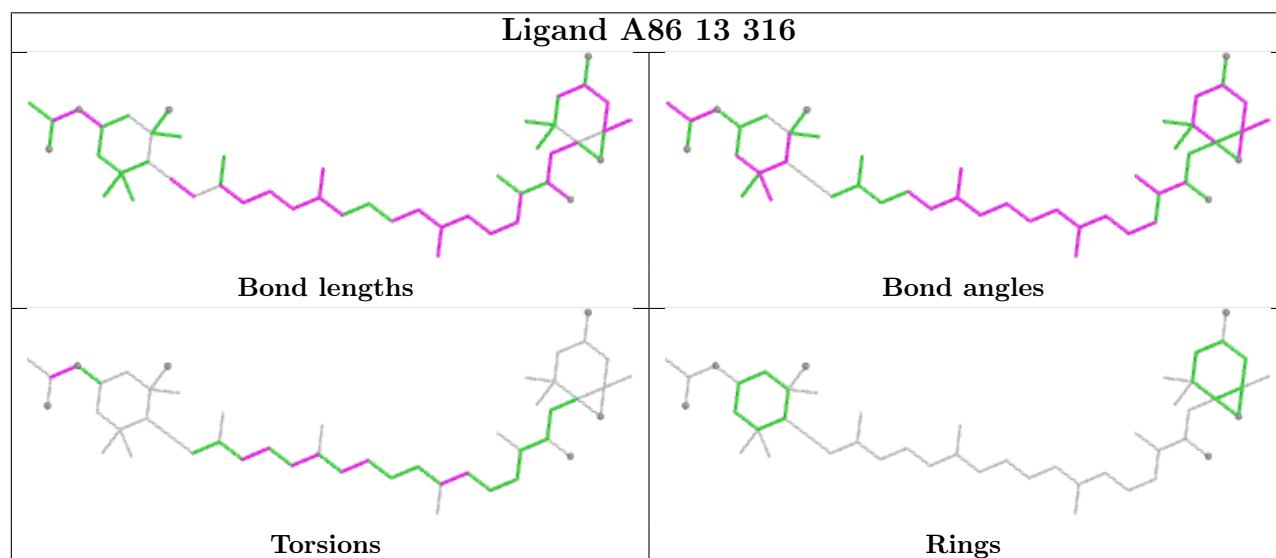
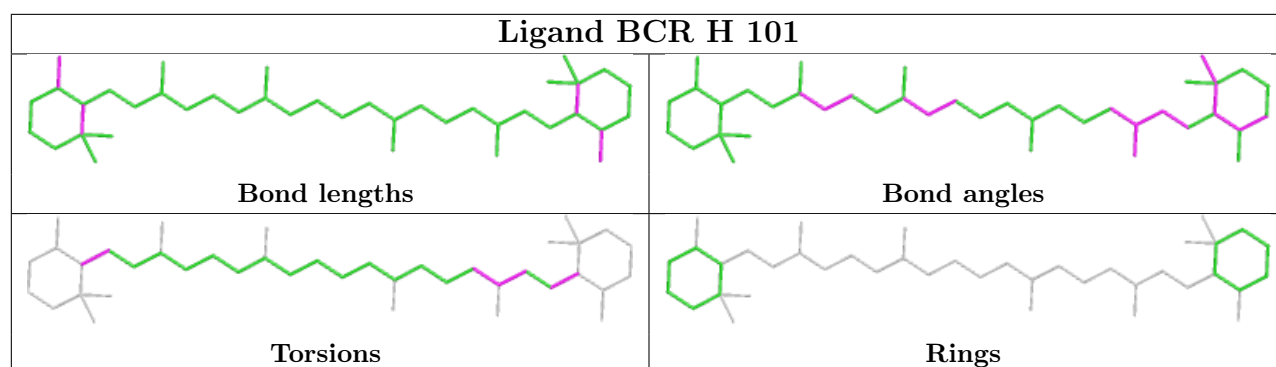


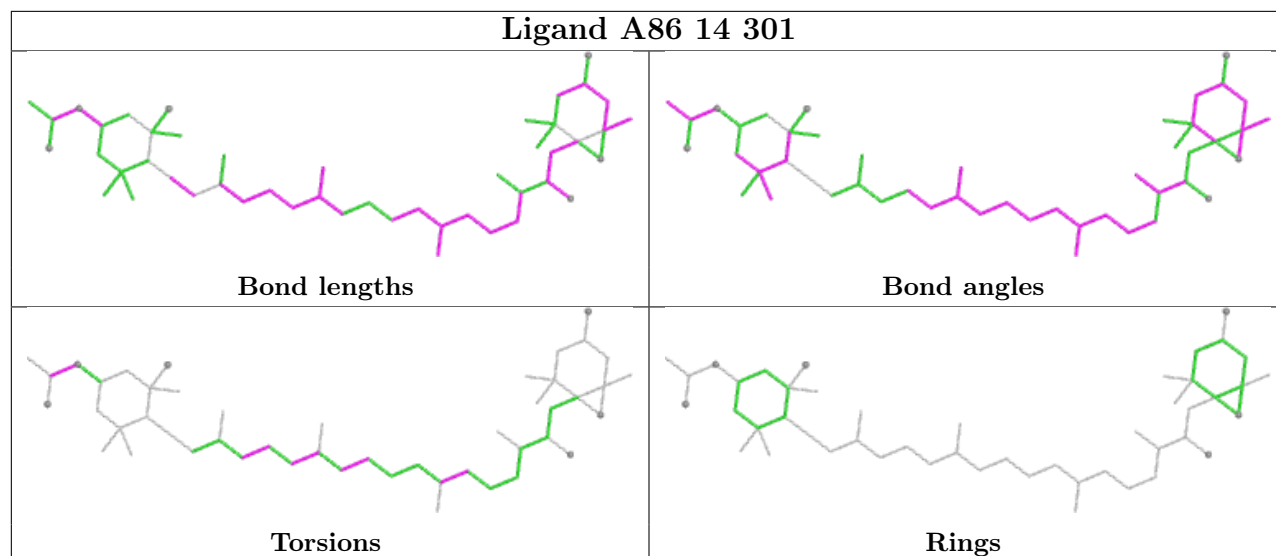
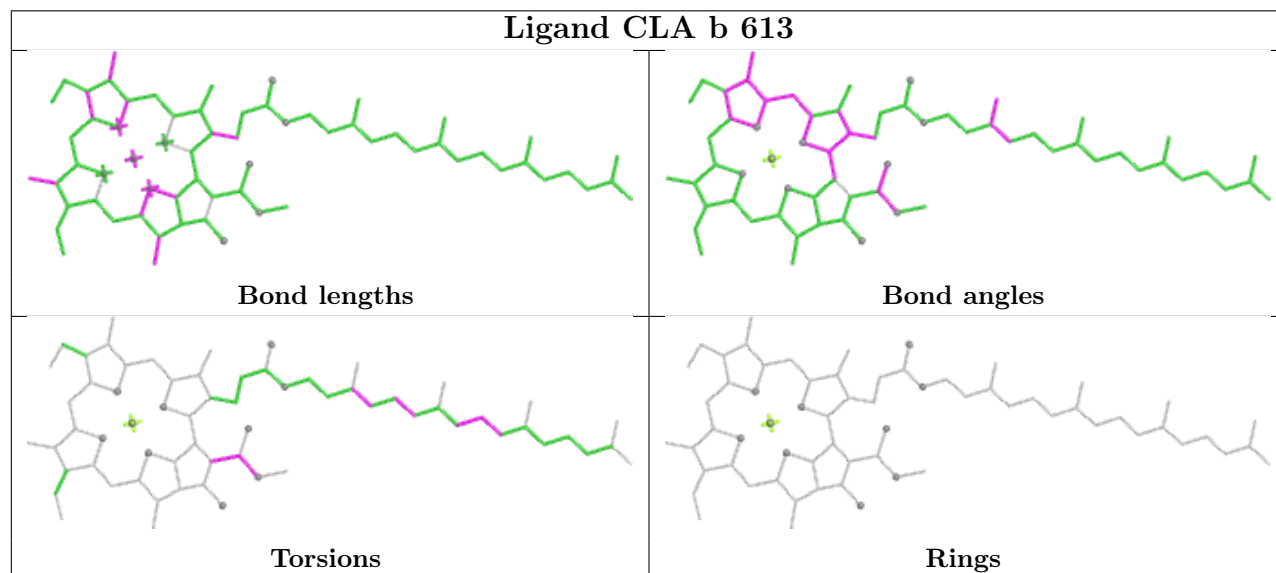
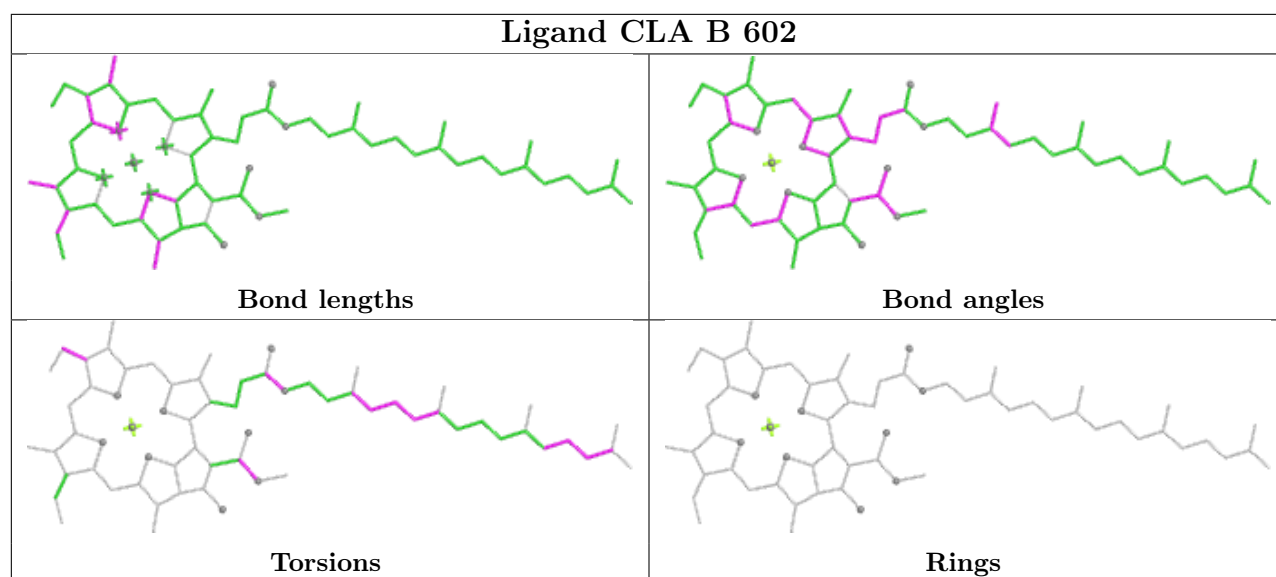


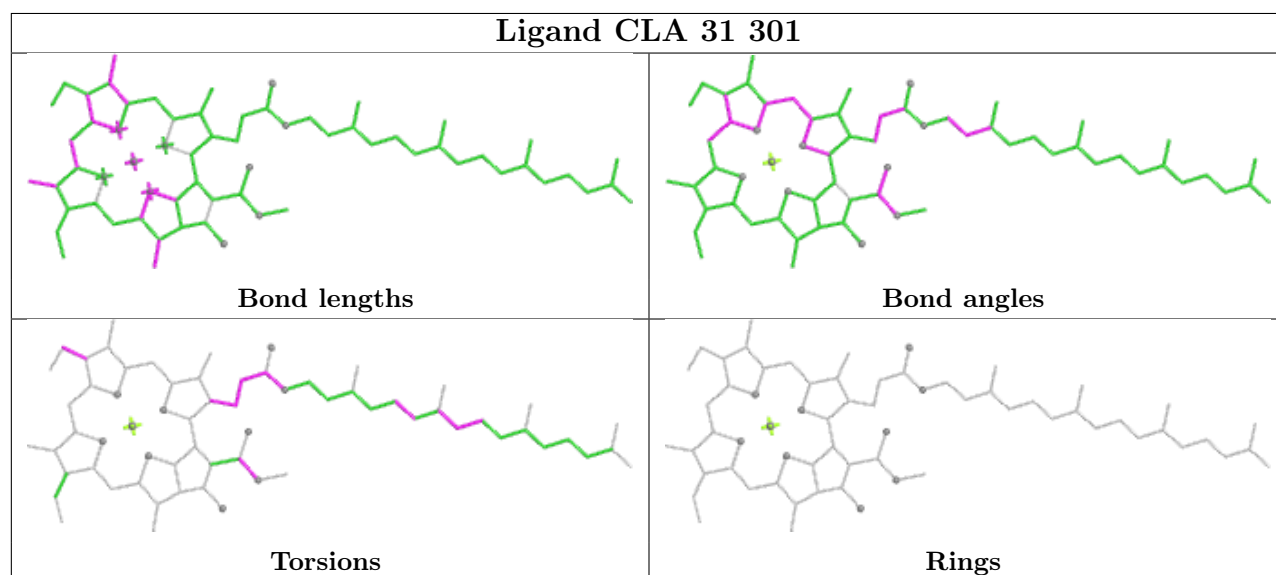
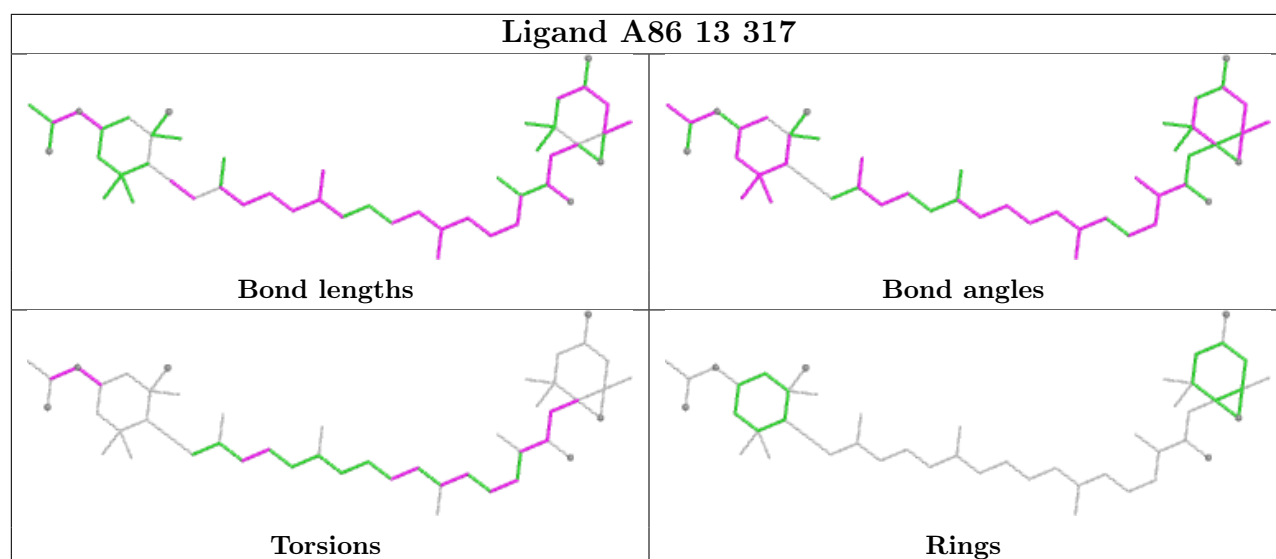


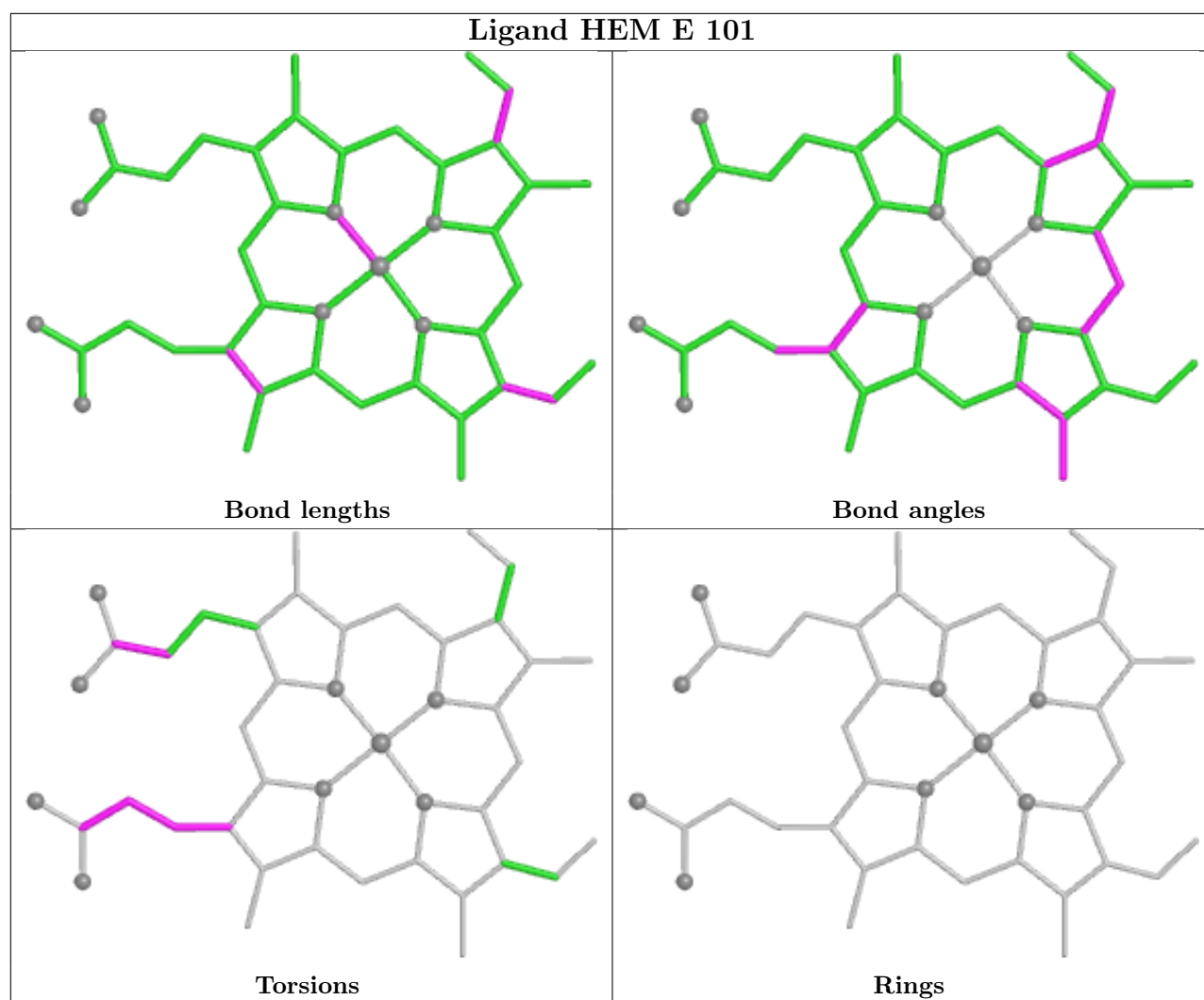


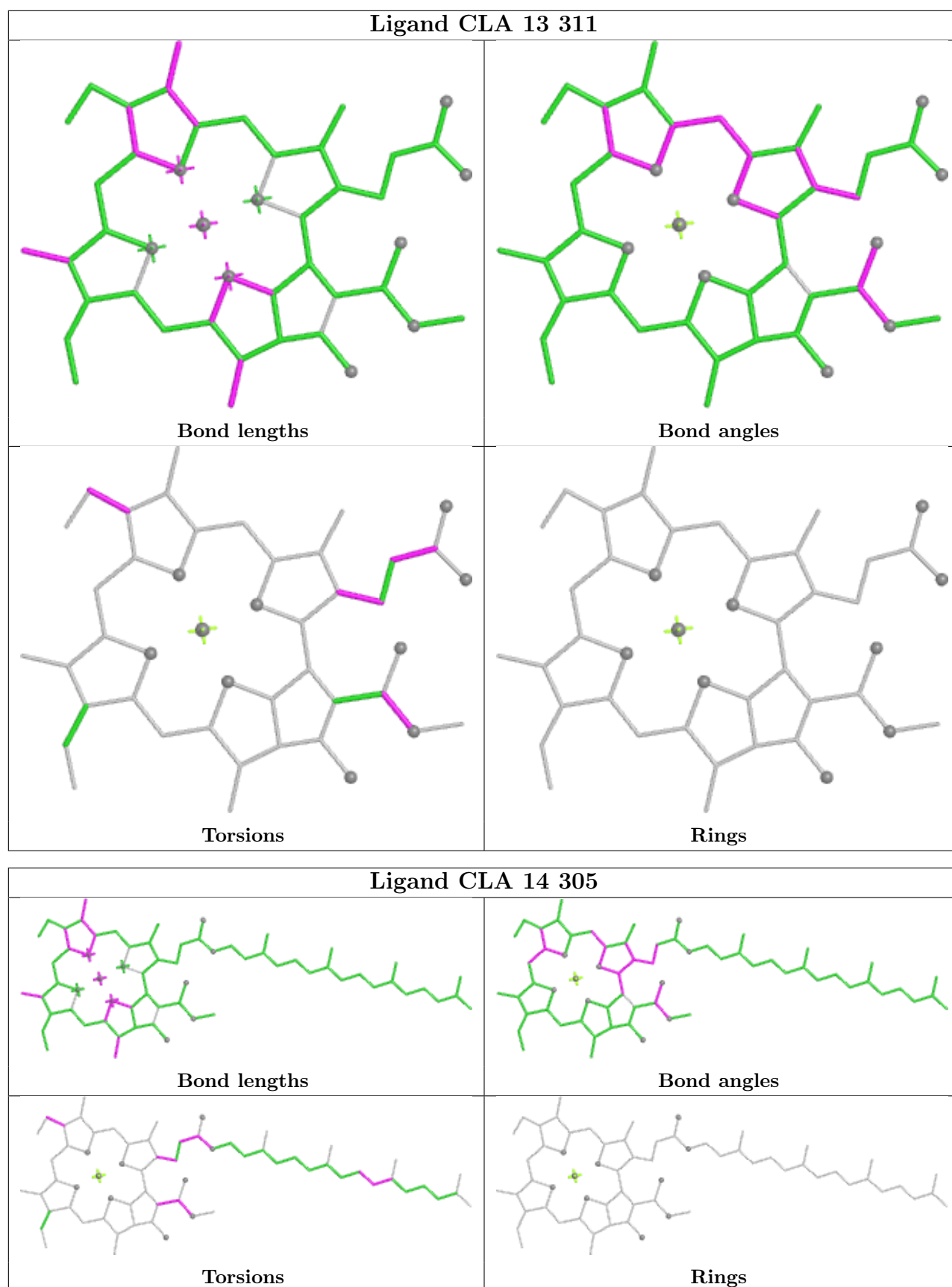




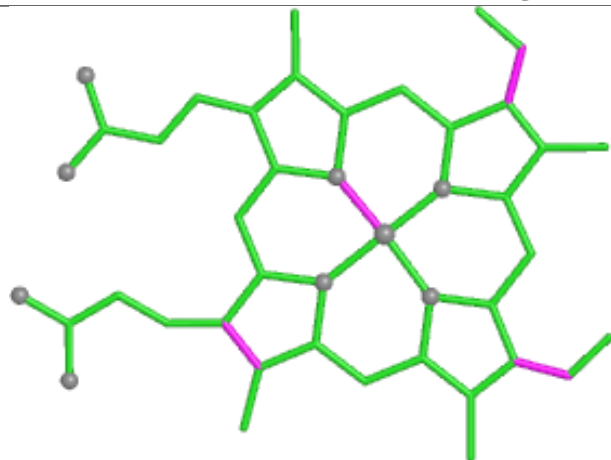




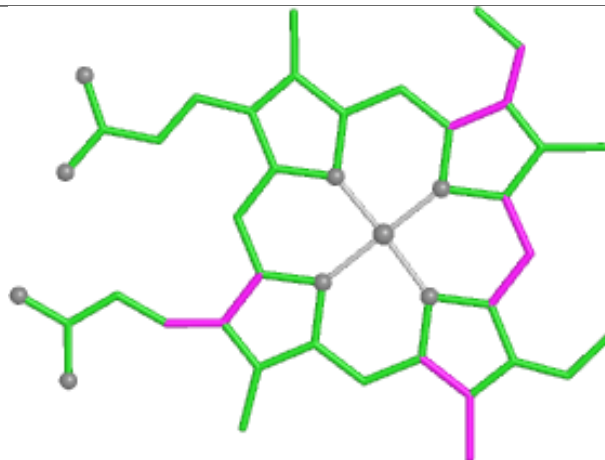




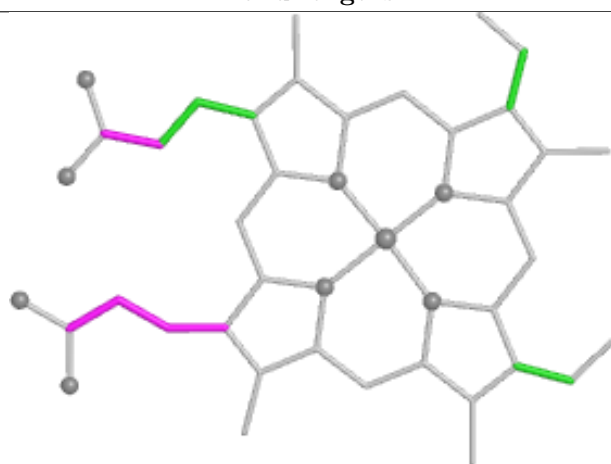
Ligand HEM f 102



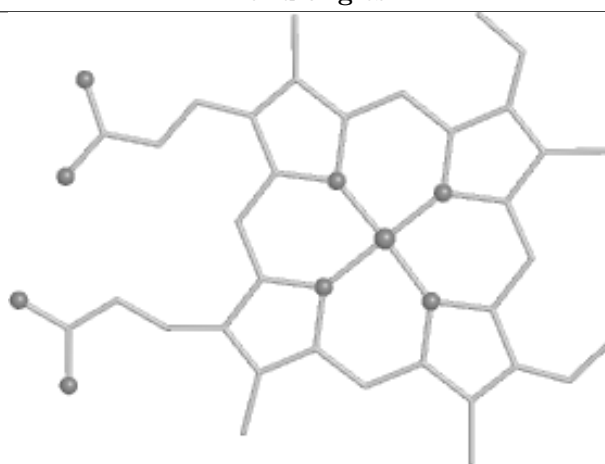
Bond lengths



Bond angles

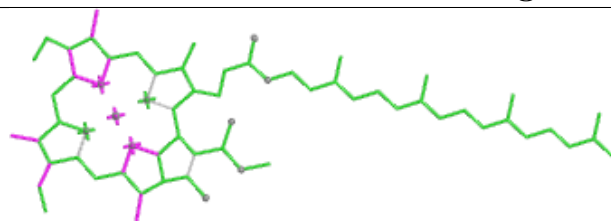


Torsions

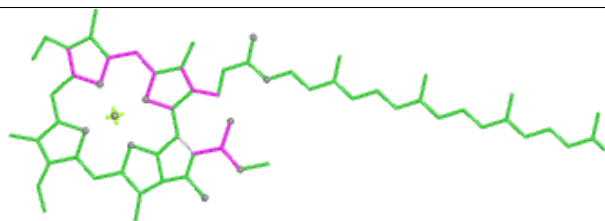


Rings

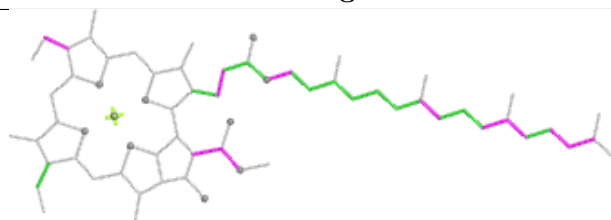
Ligand CLA b 610



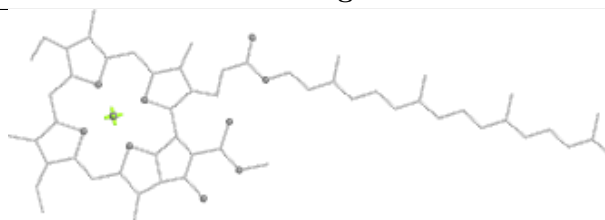
Bond lengths



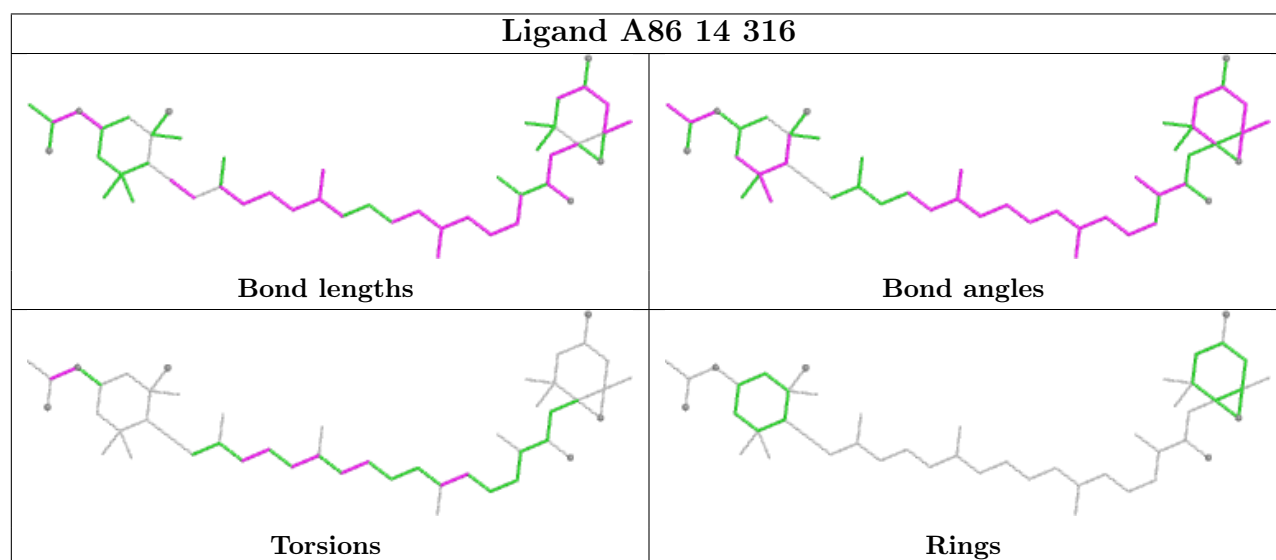
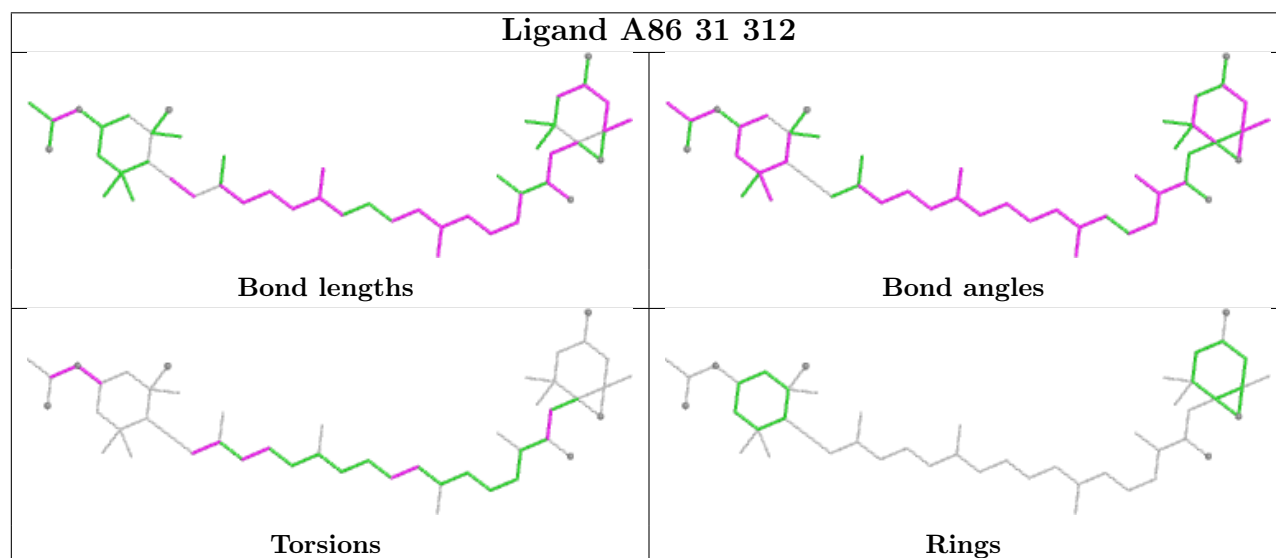
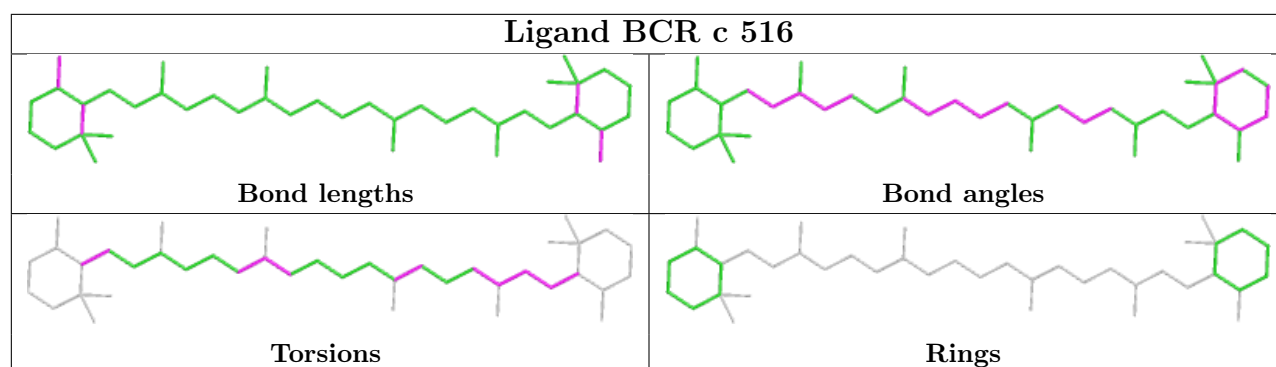
Bond angles

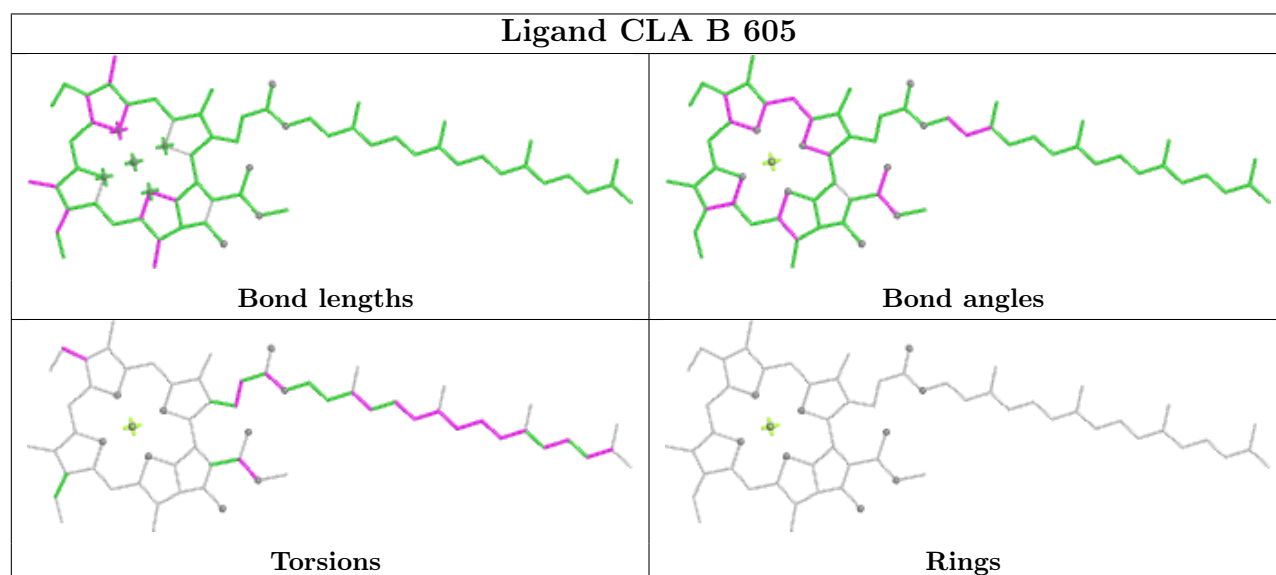
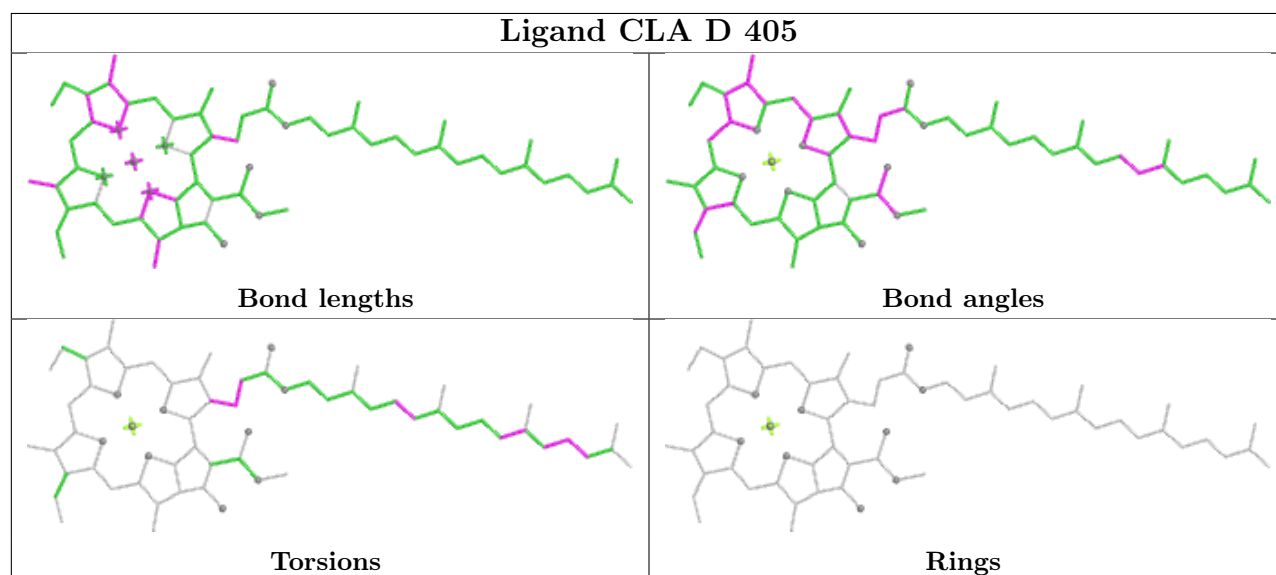
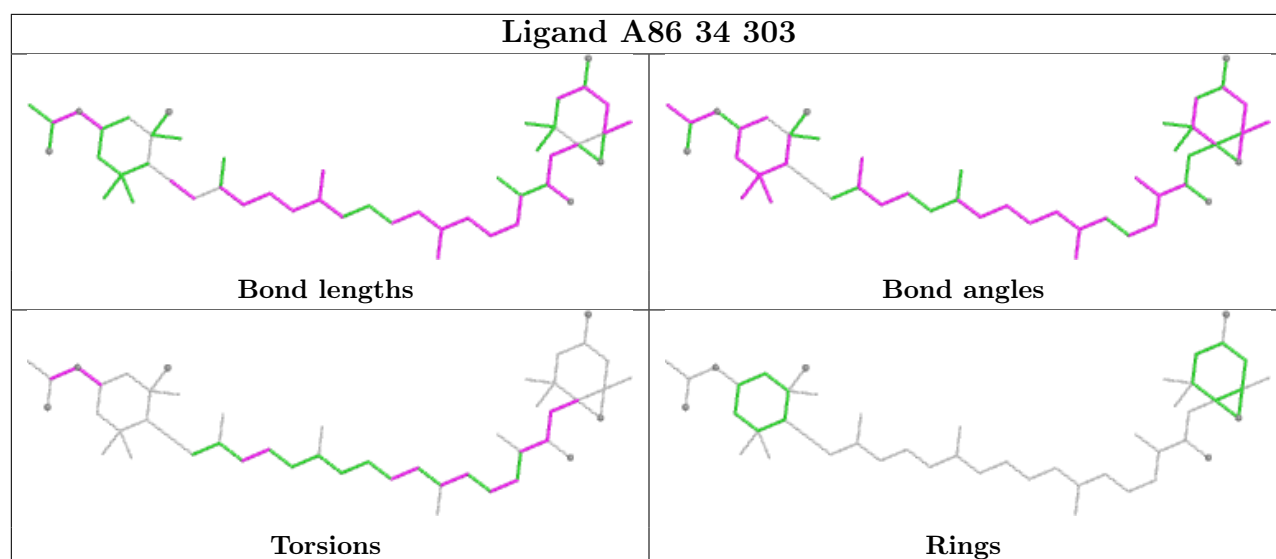


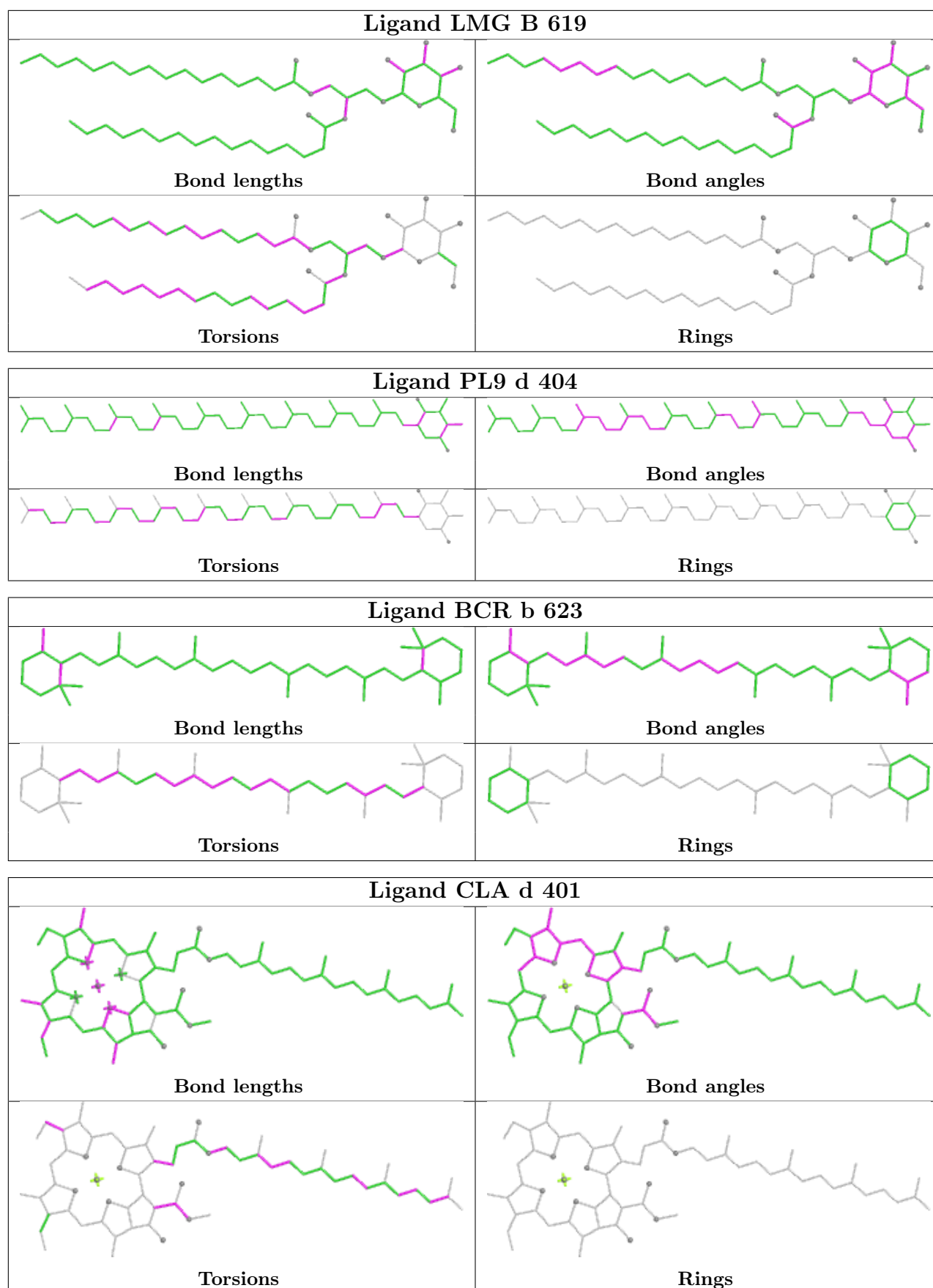
Torsions

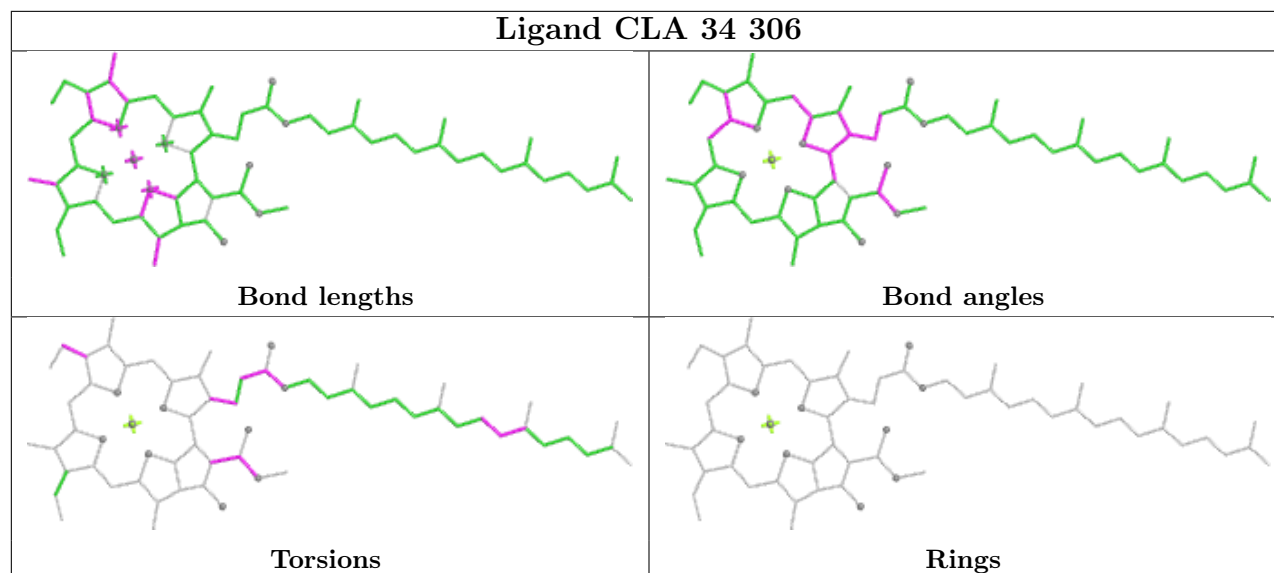
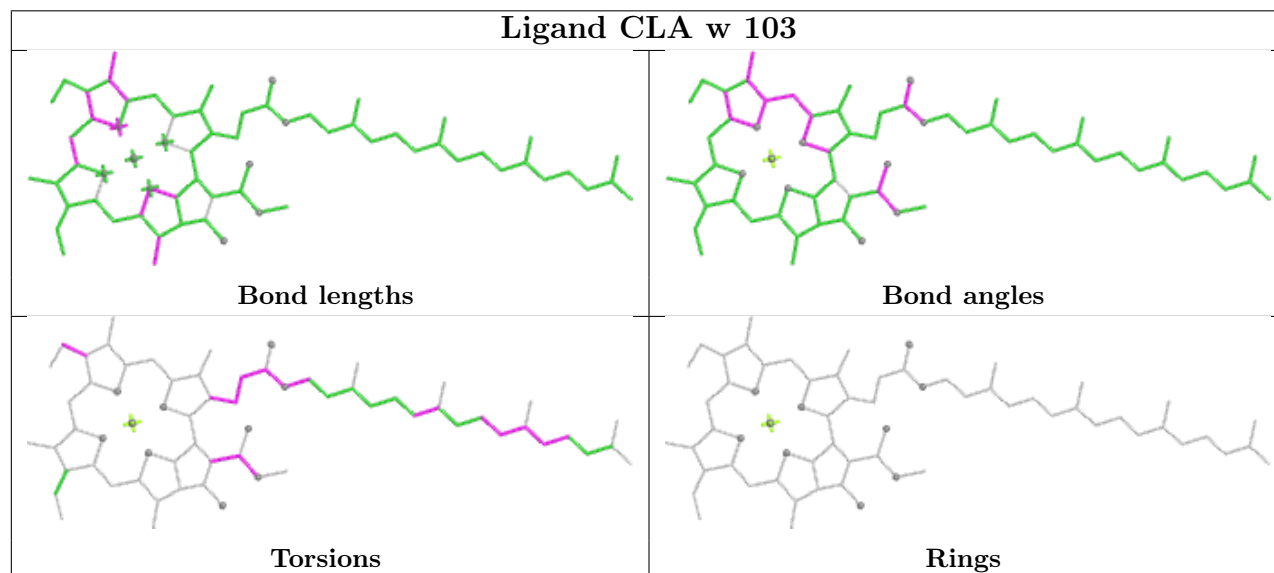
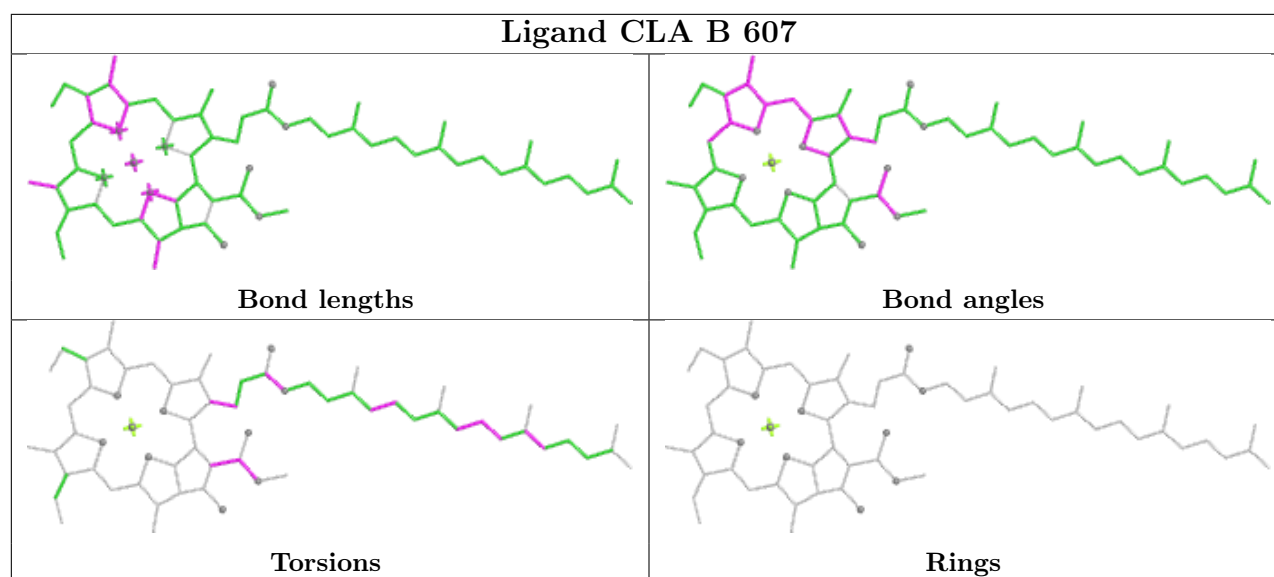


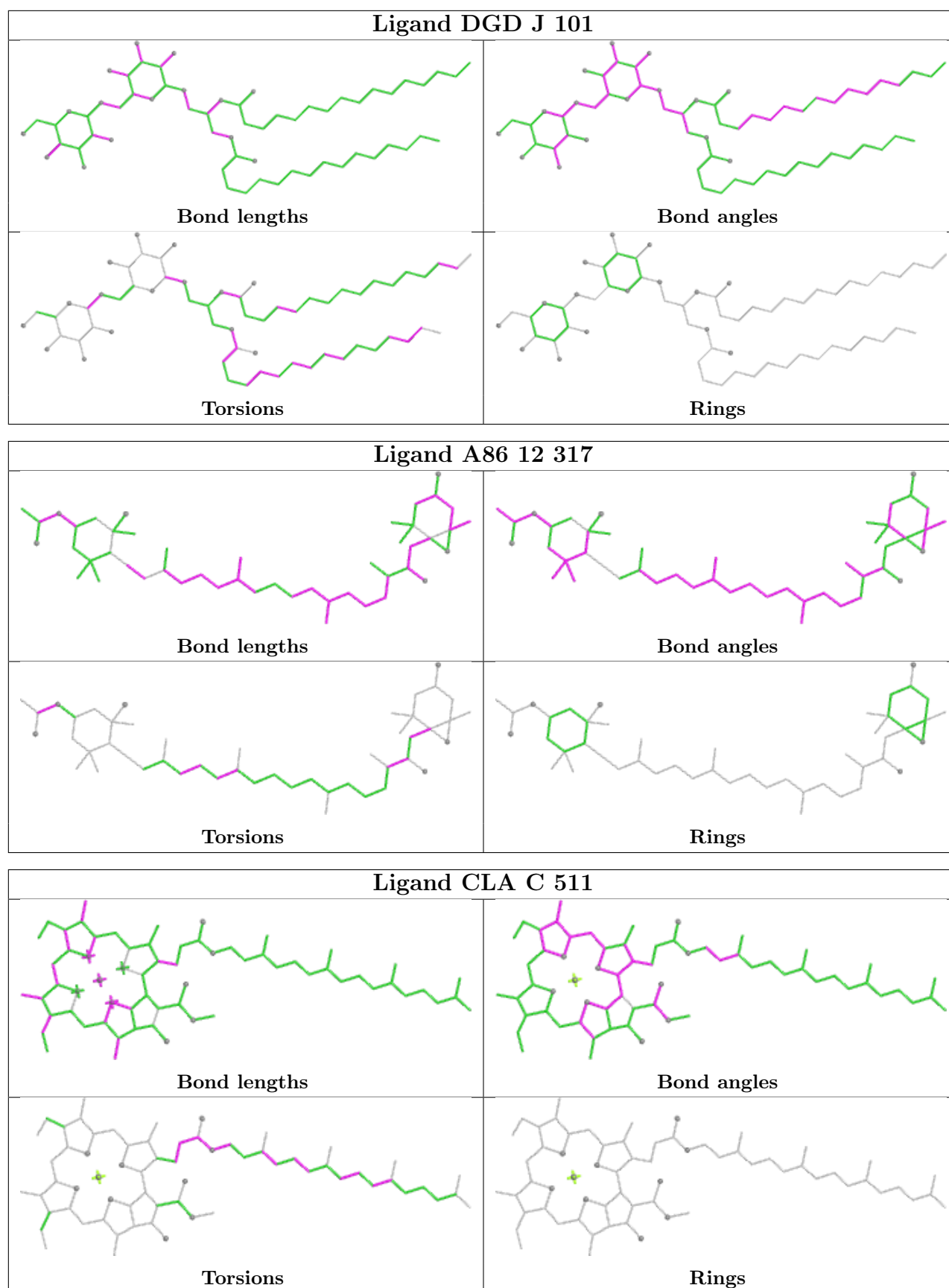
Rings

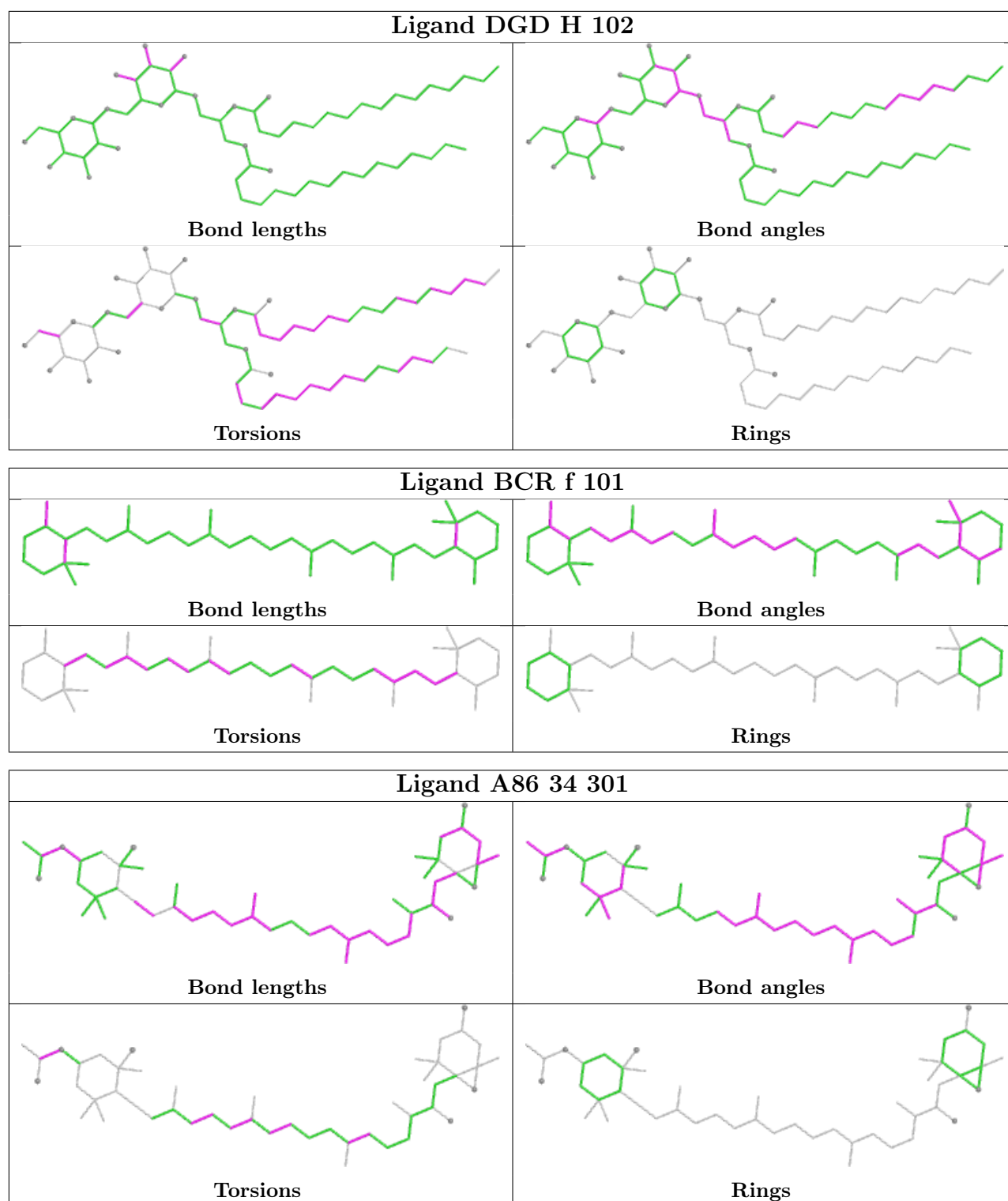


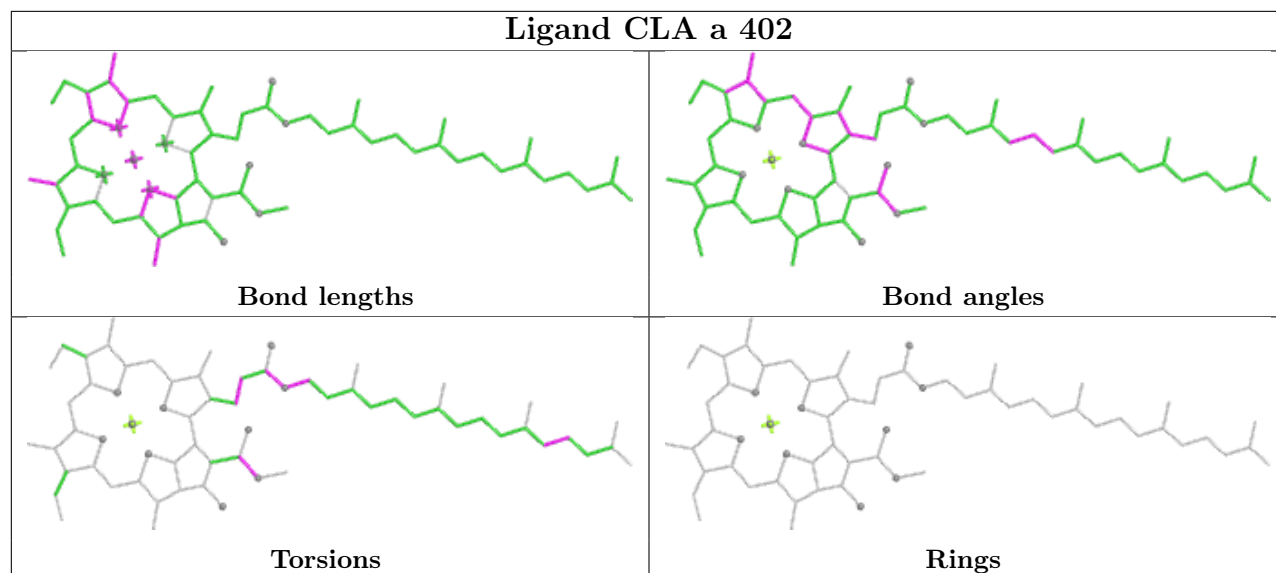
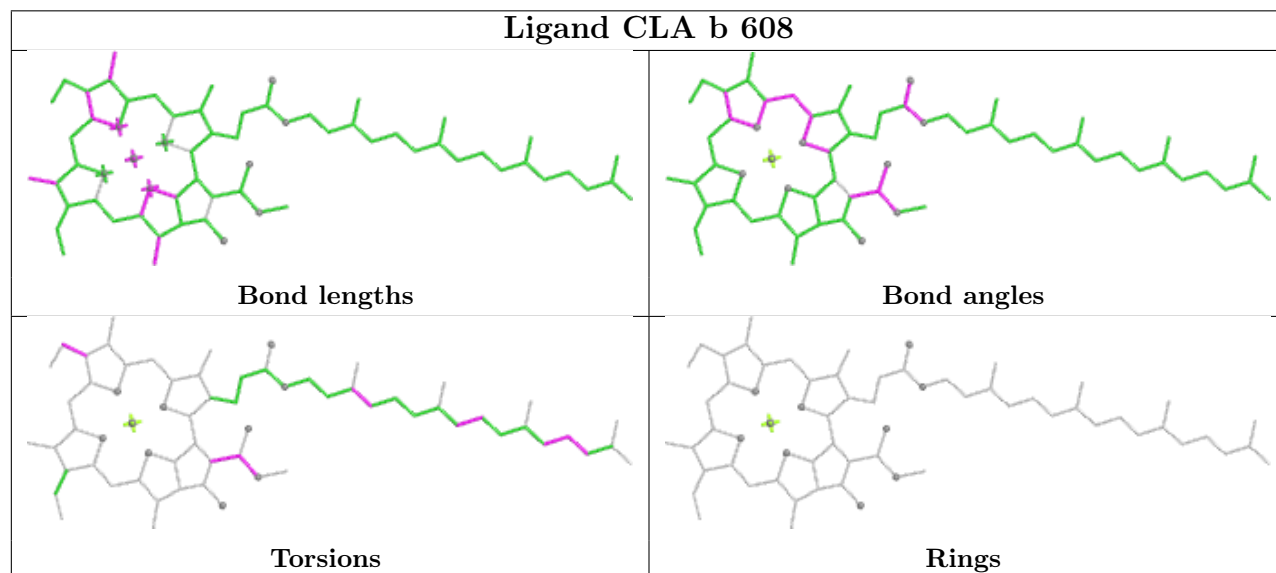
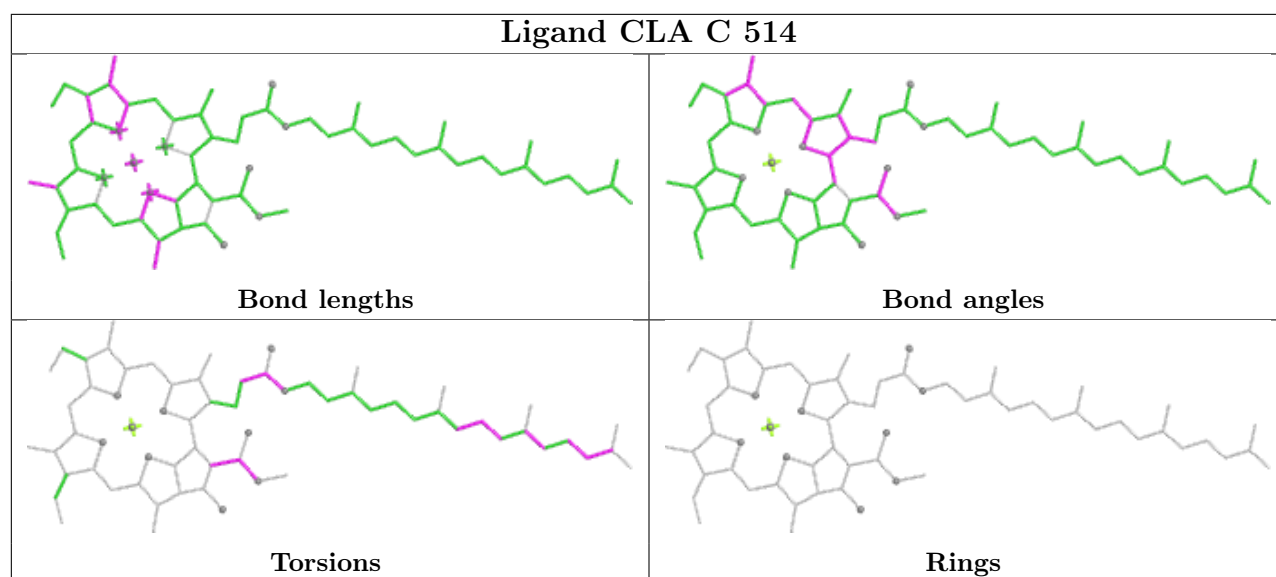


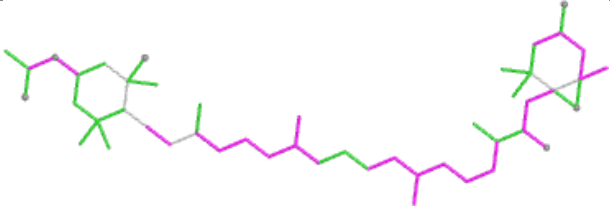
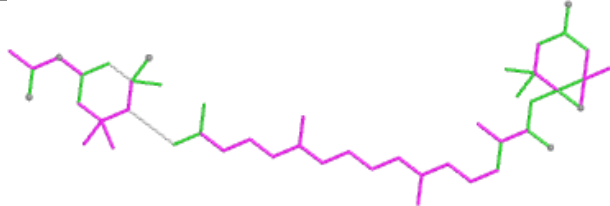
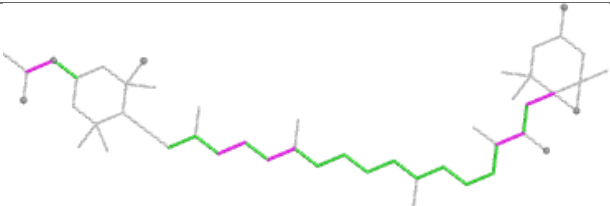
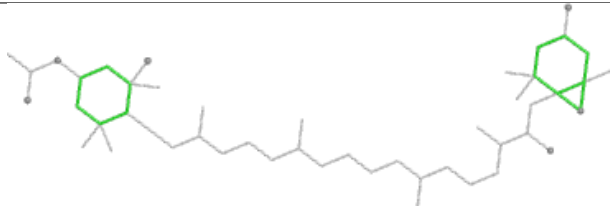
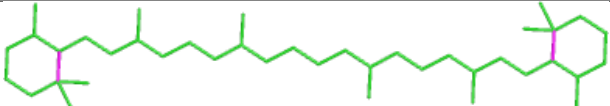
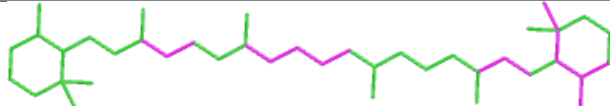
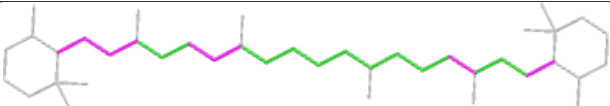
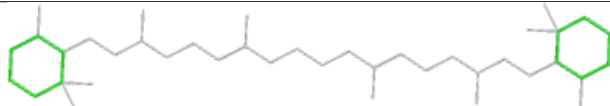
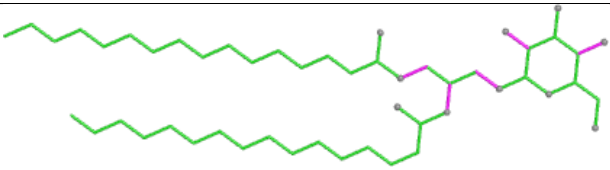
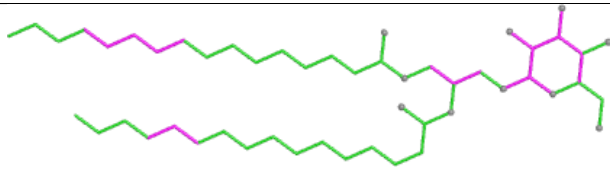
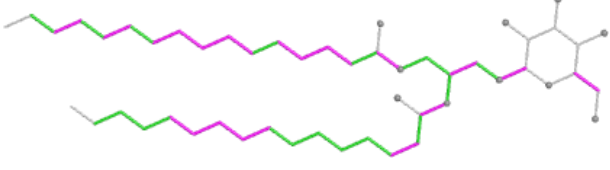
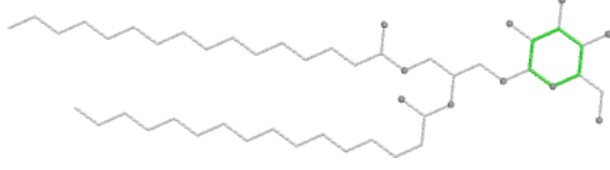


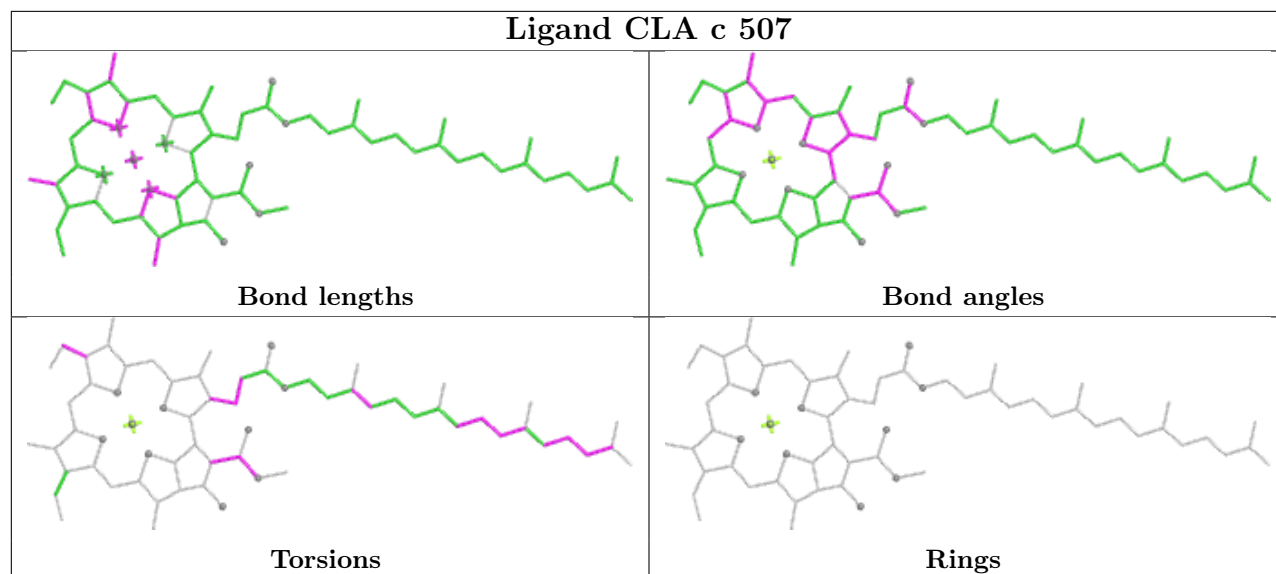
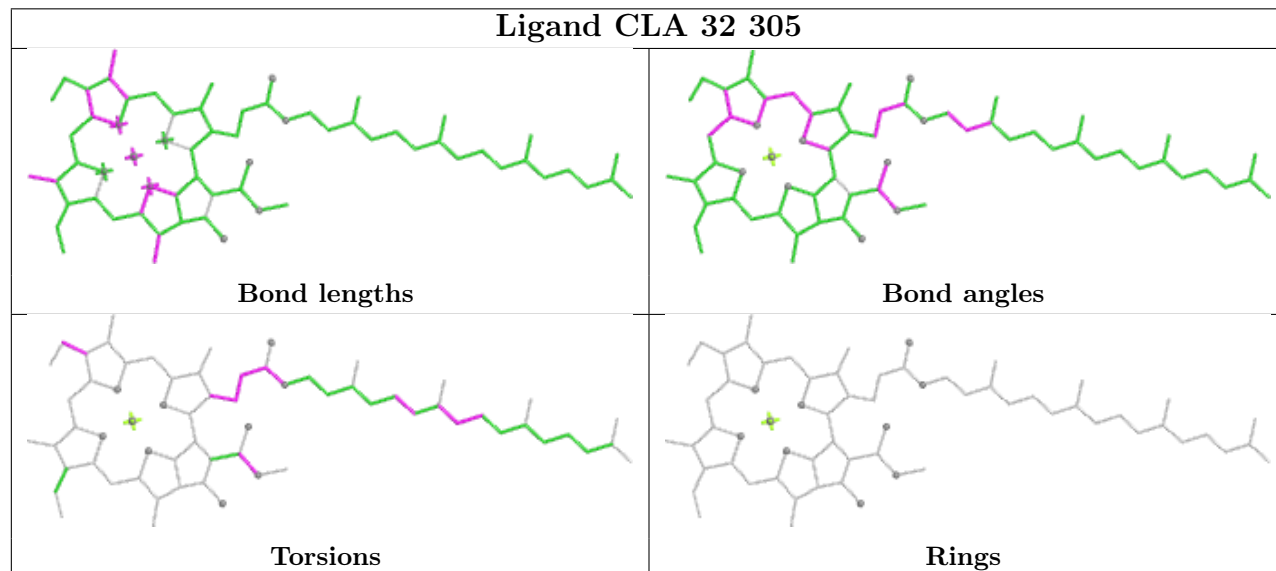


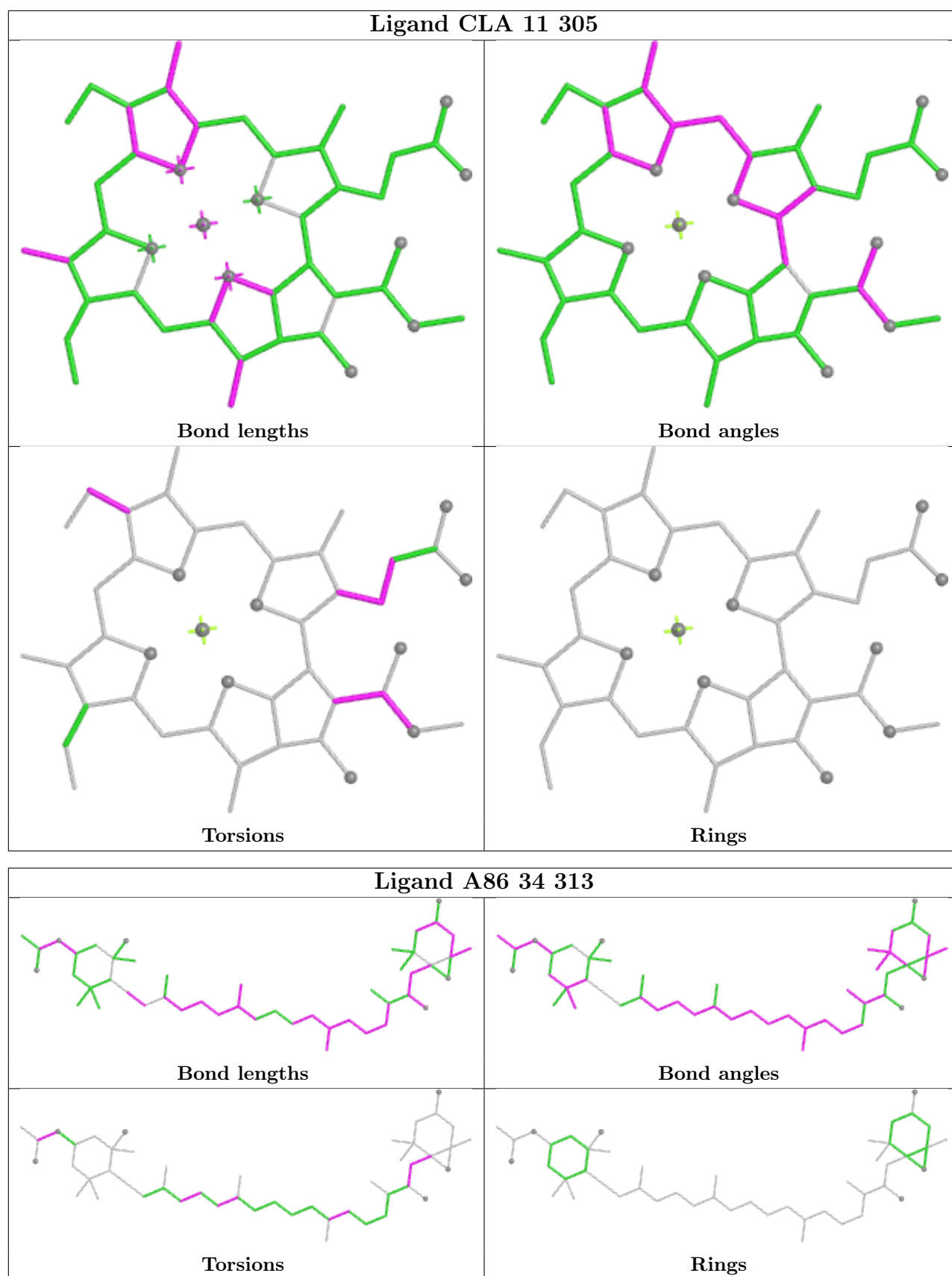


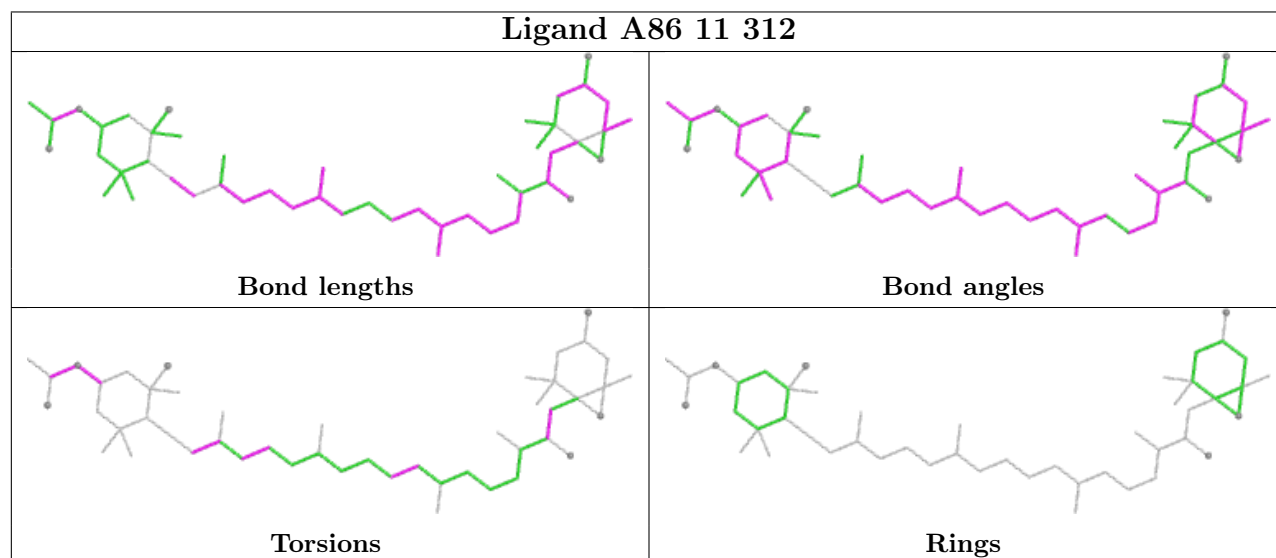
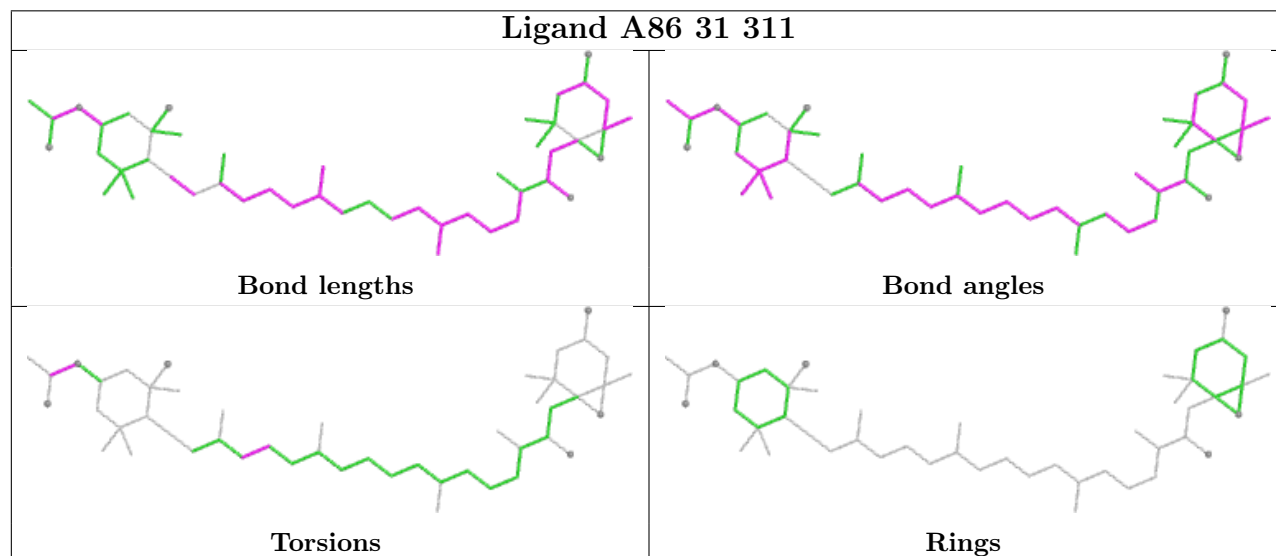
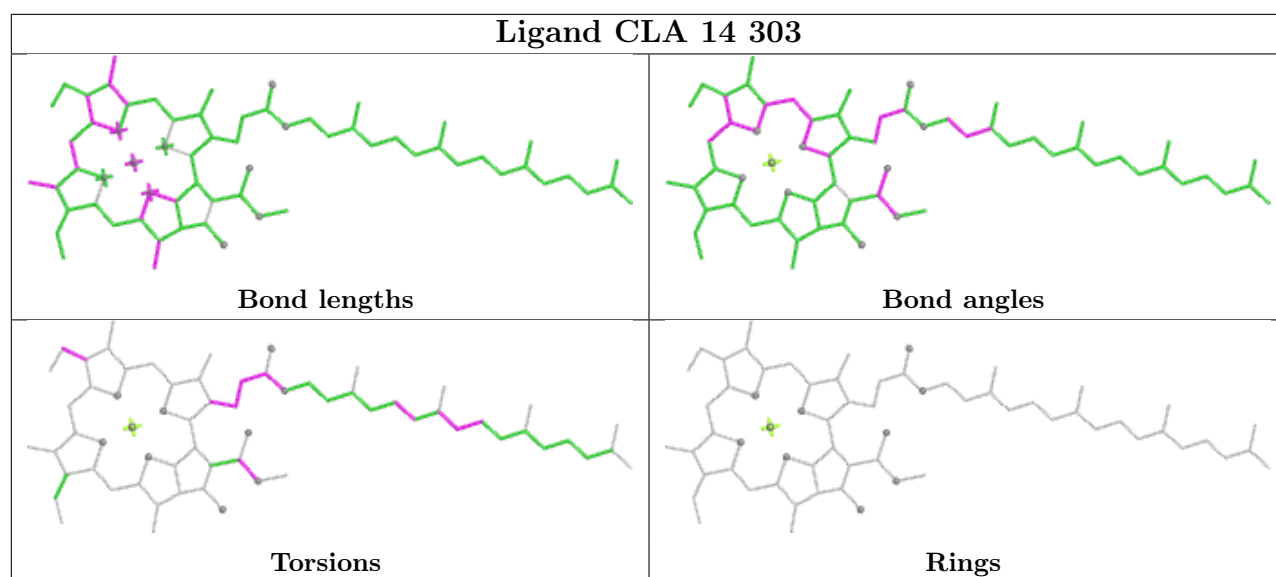


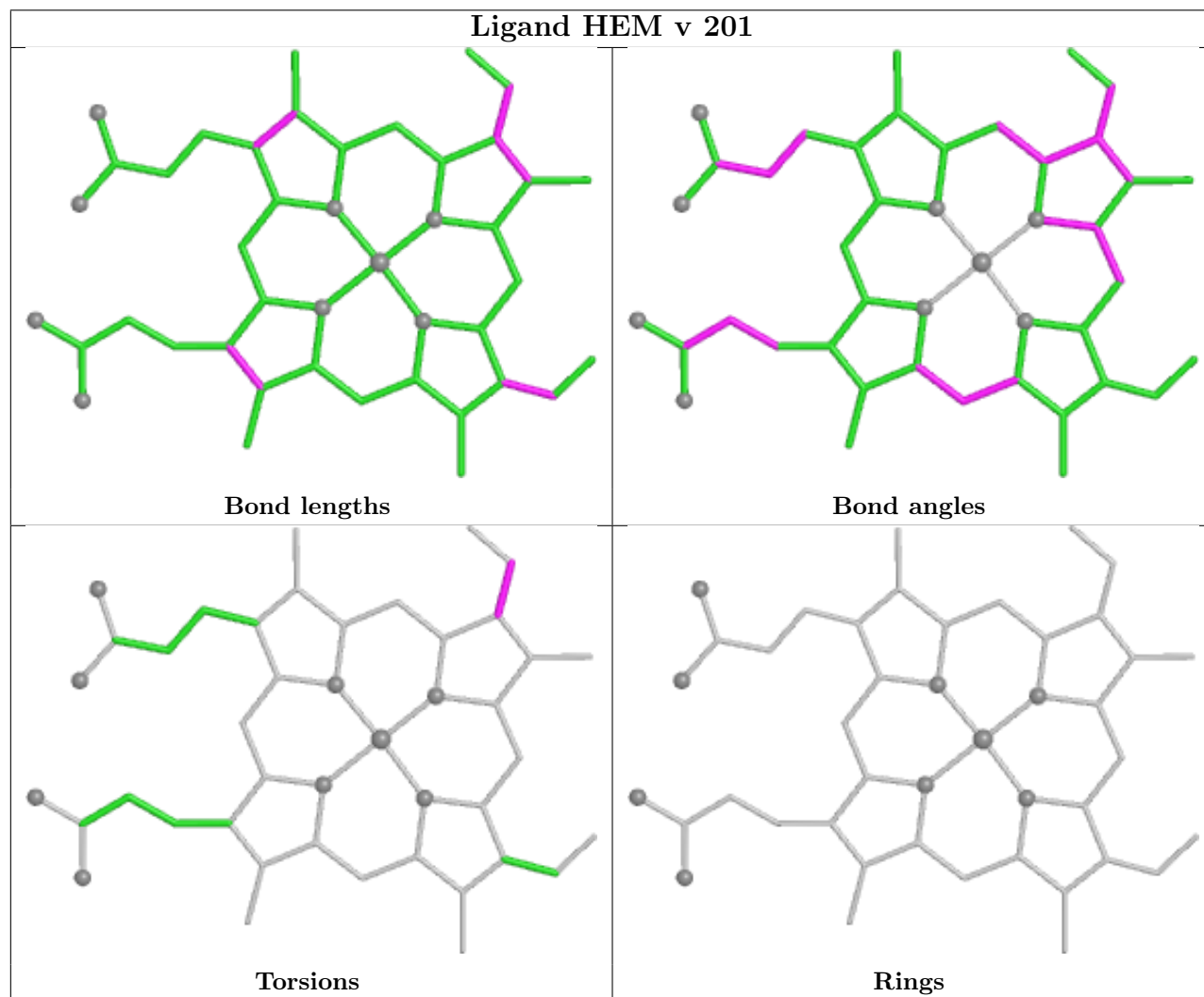
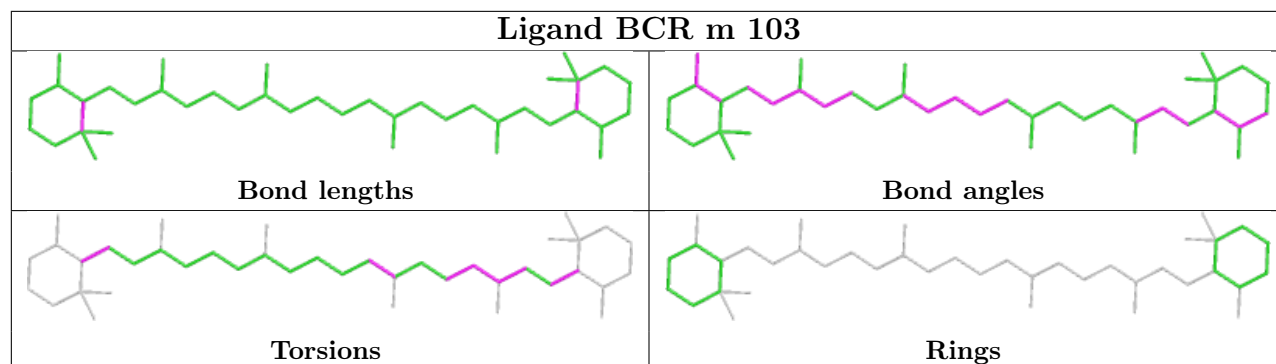


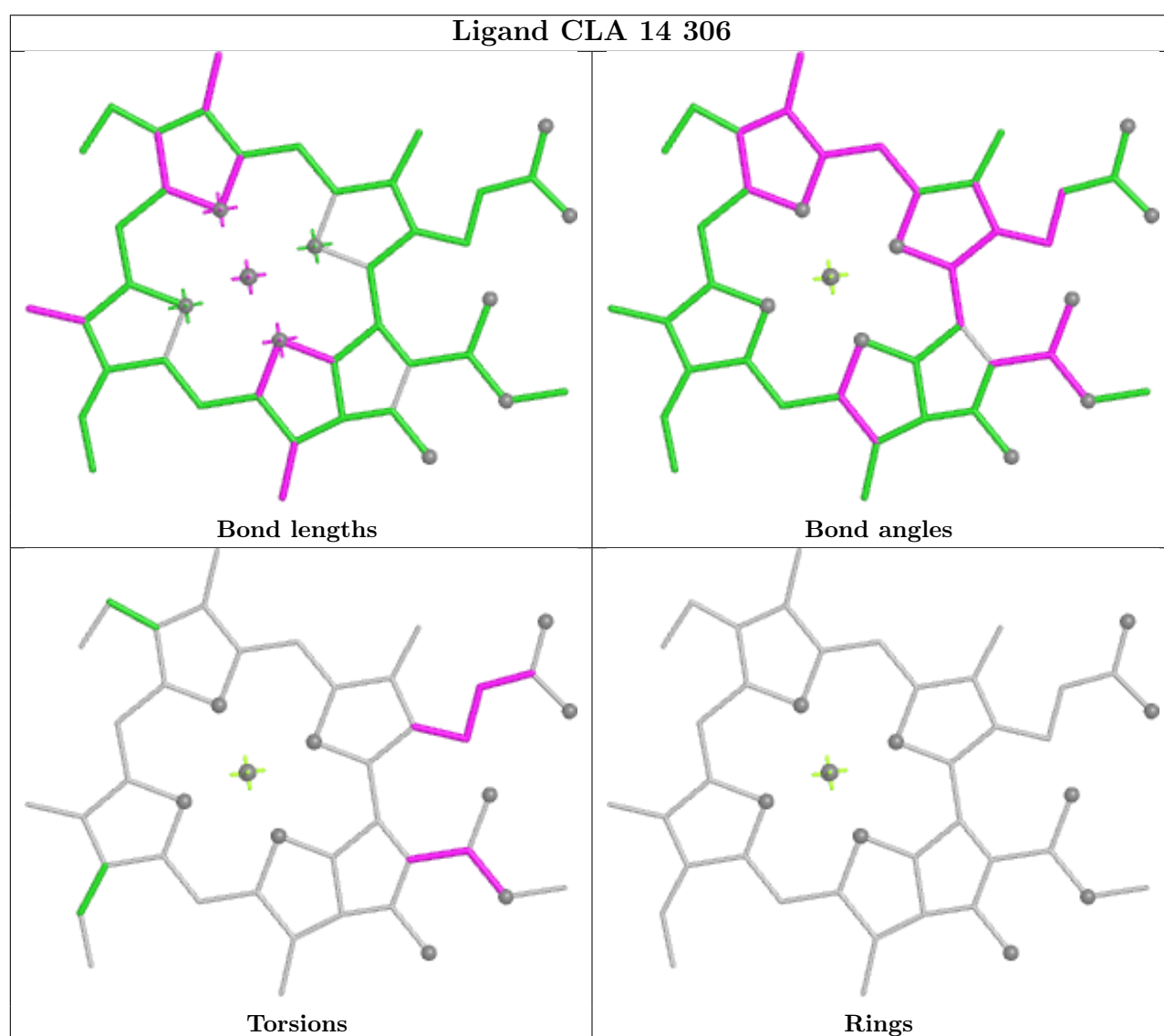
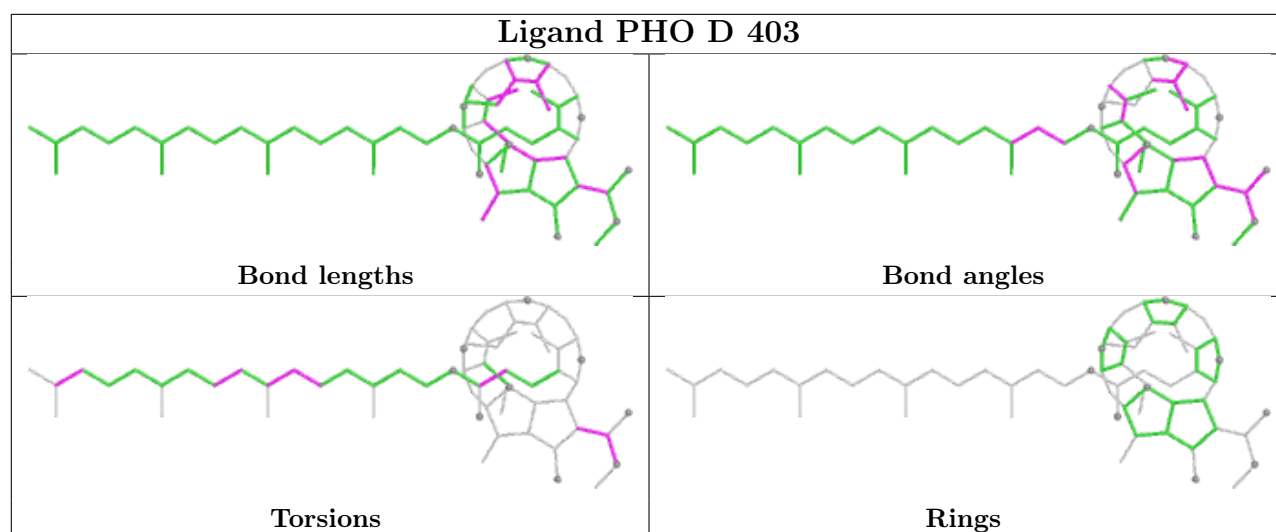
Ligand A86 34 316	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 616	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG C 519	
 Bond lengths	 Bond angles
 Torsions	 Rings

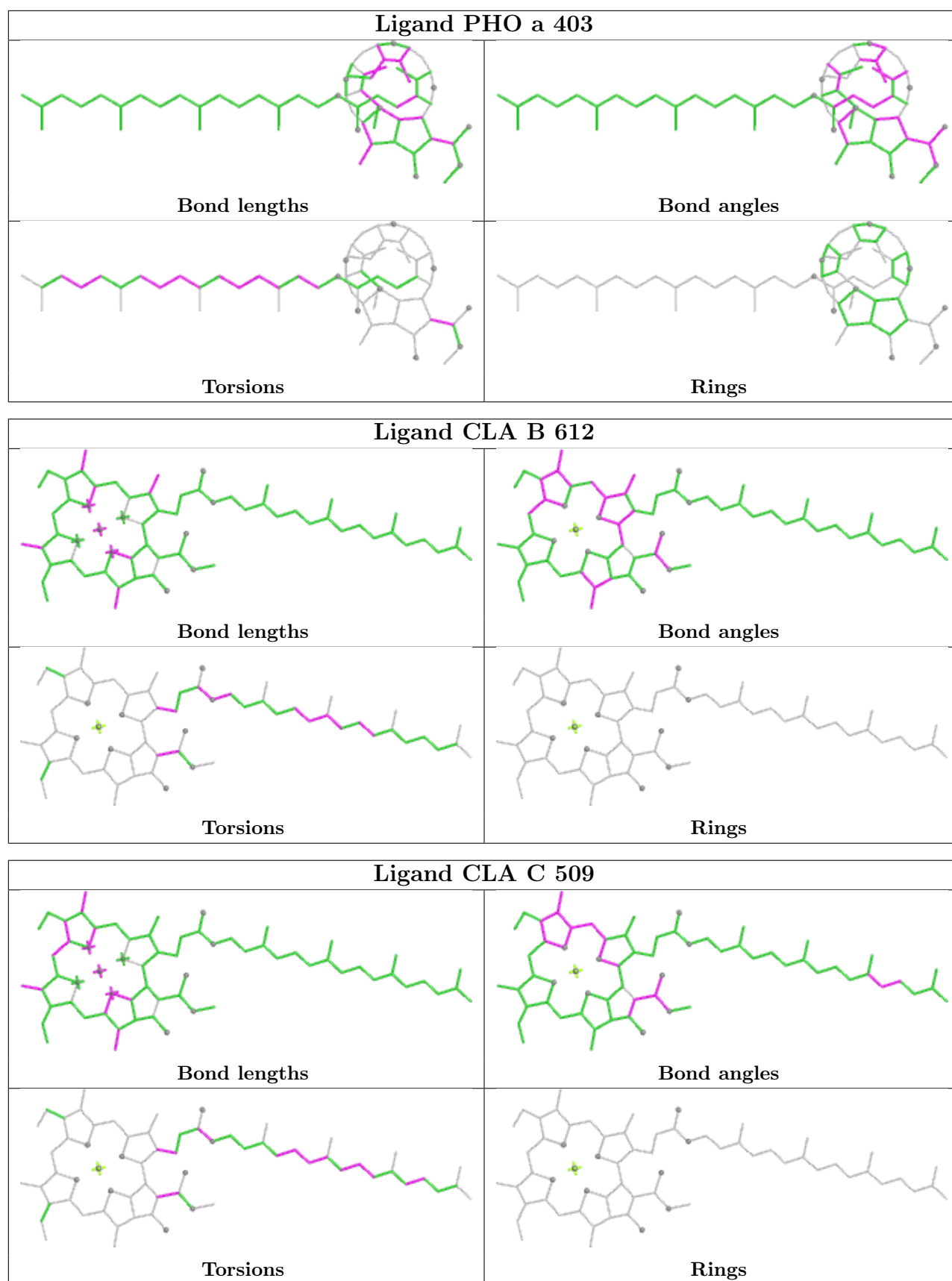
Ligand CLA c 507**Ligand CLA 32 305**

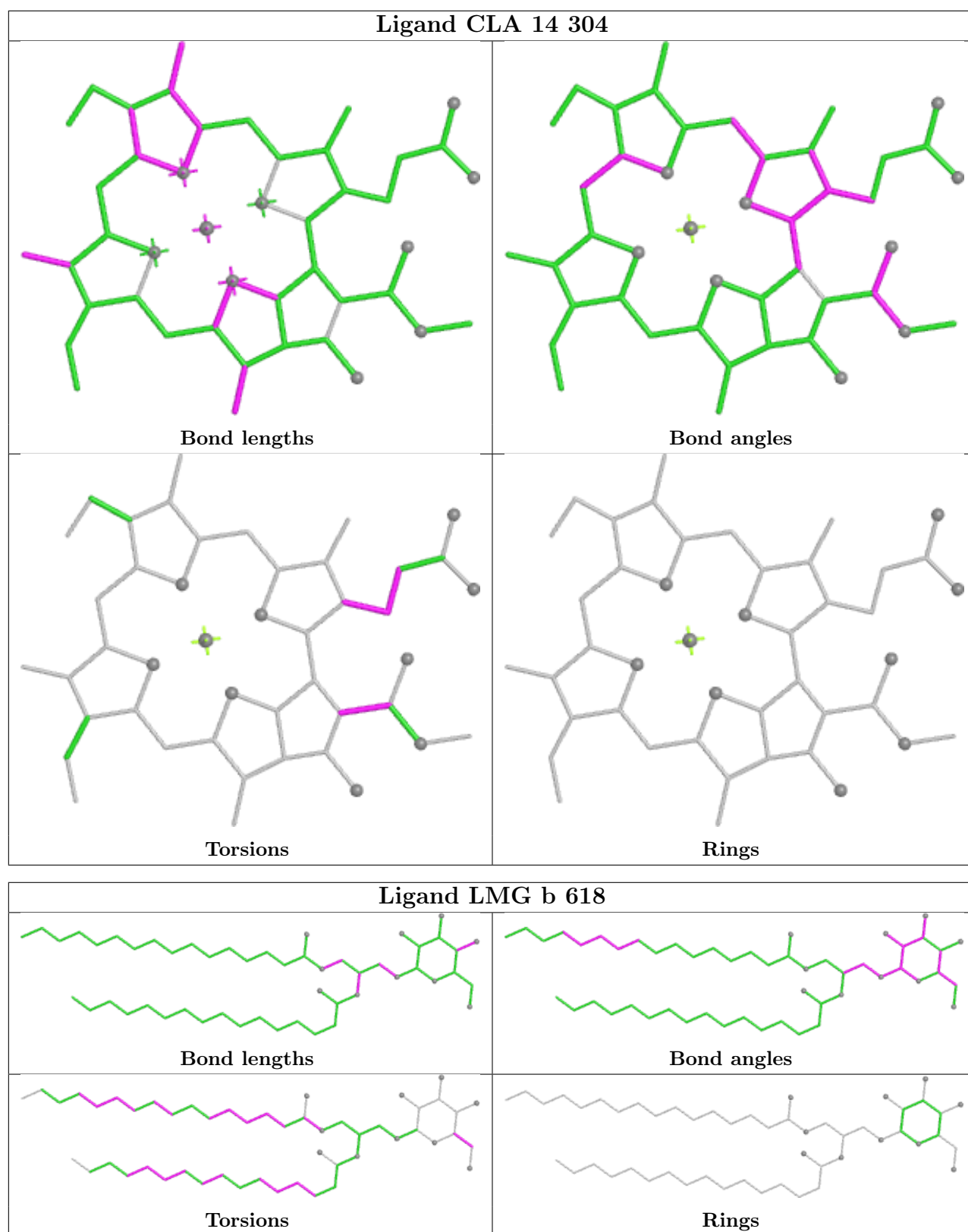


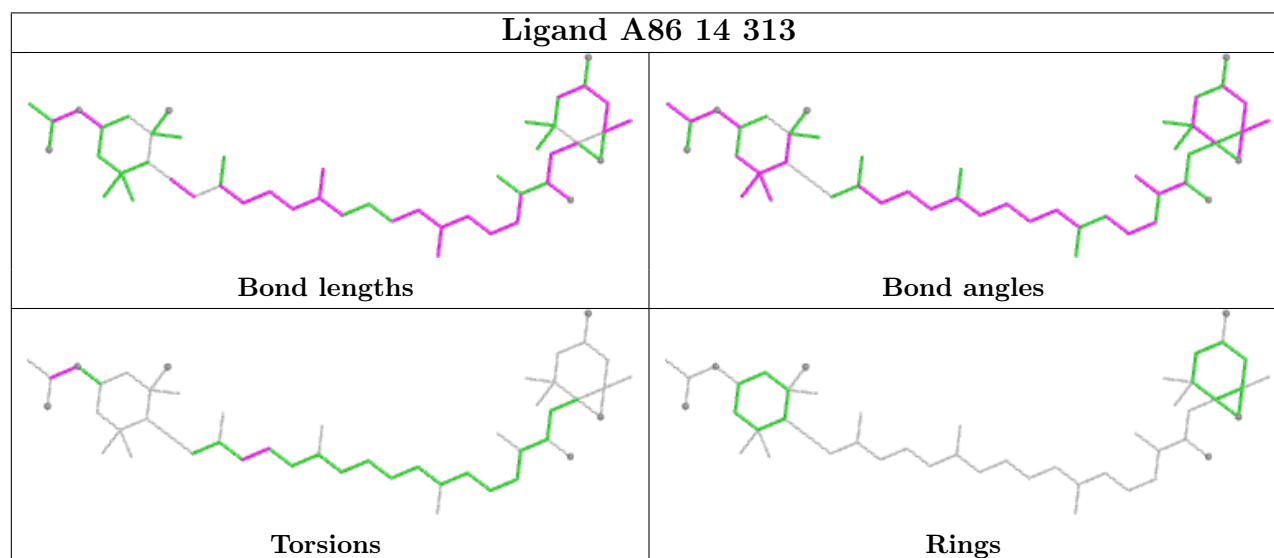
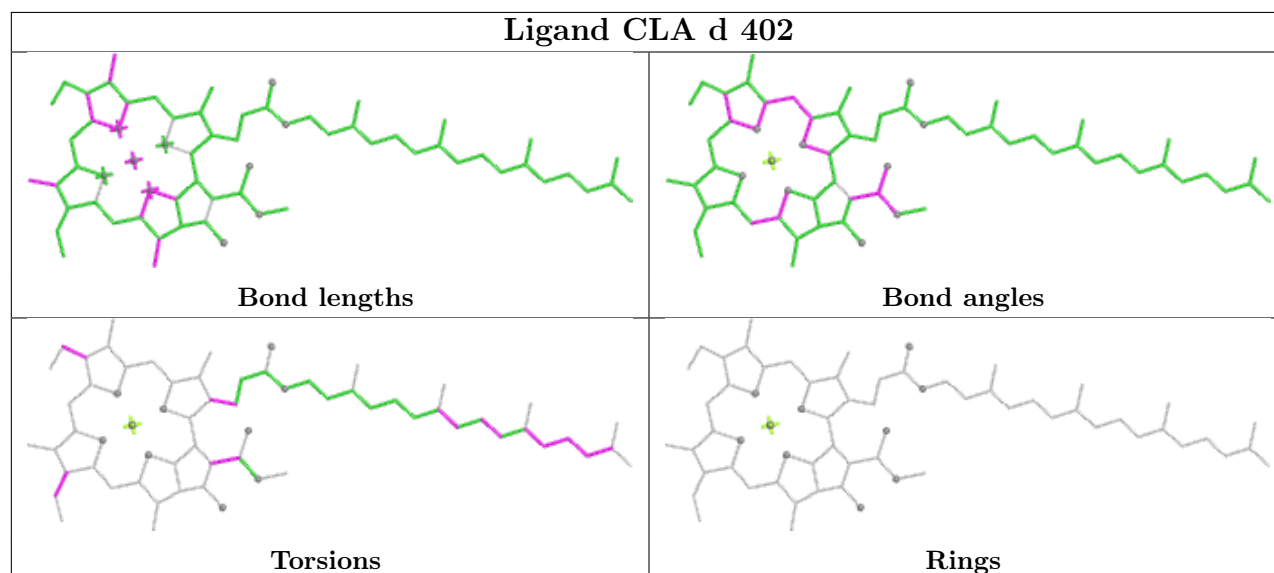
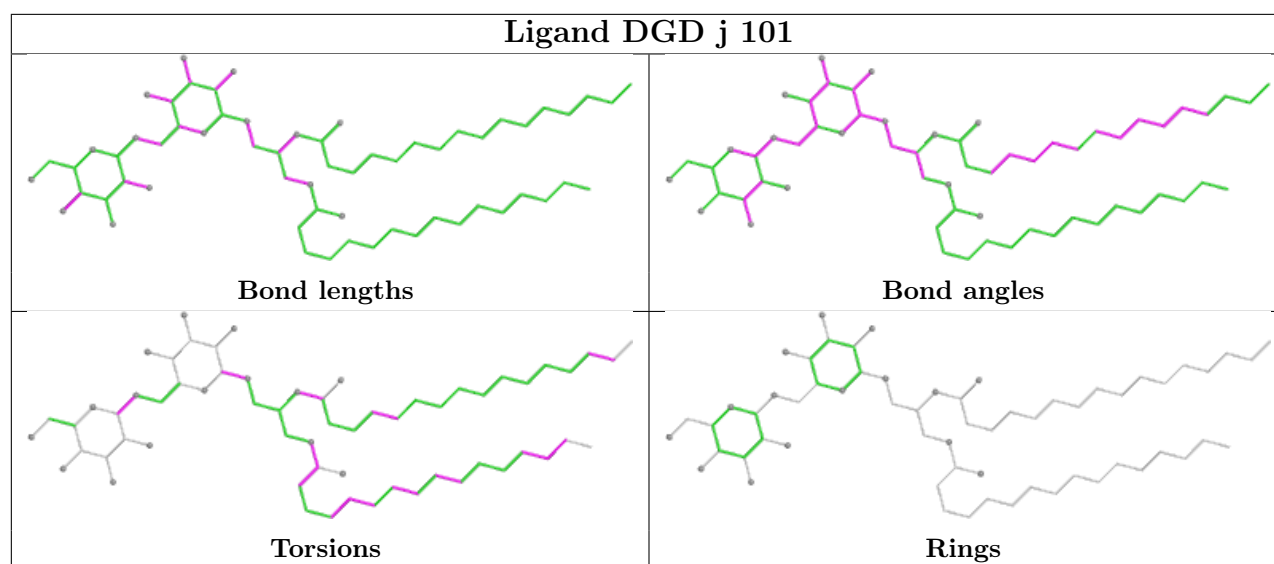


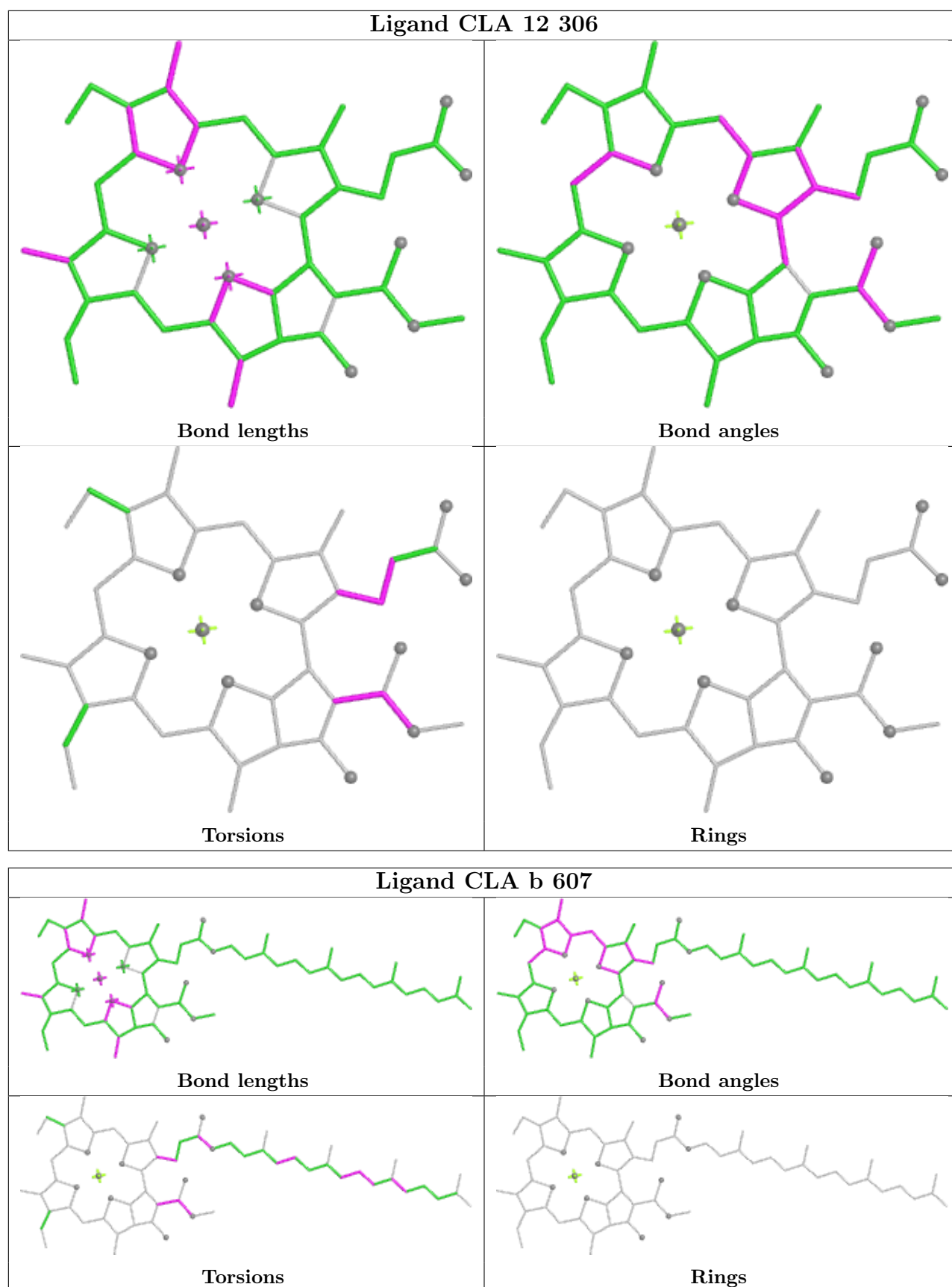




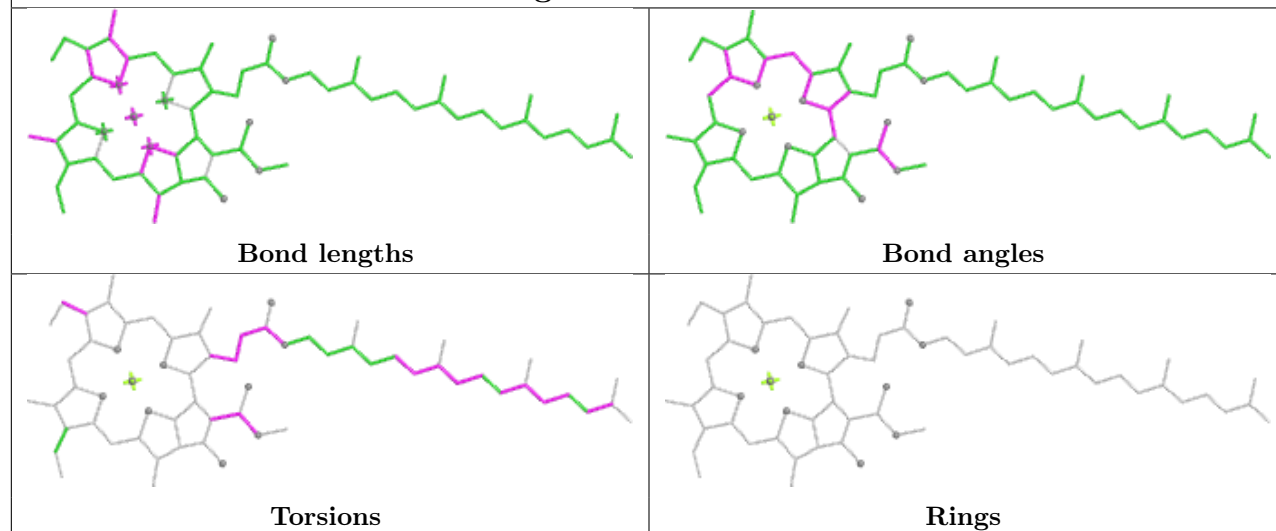




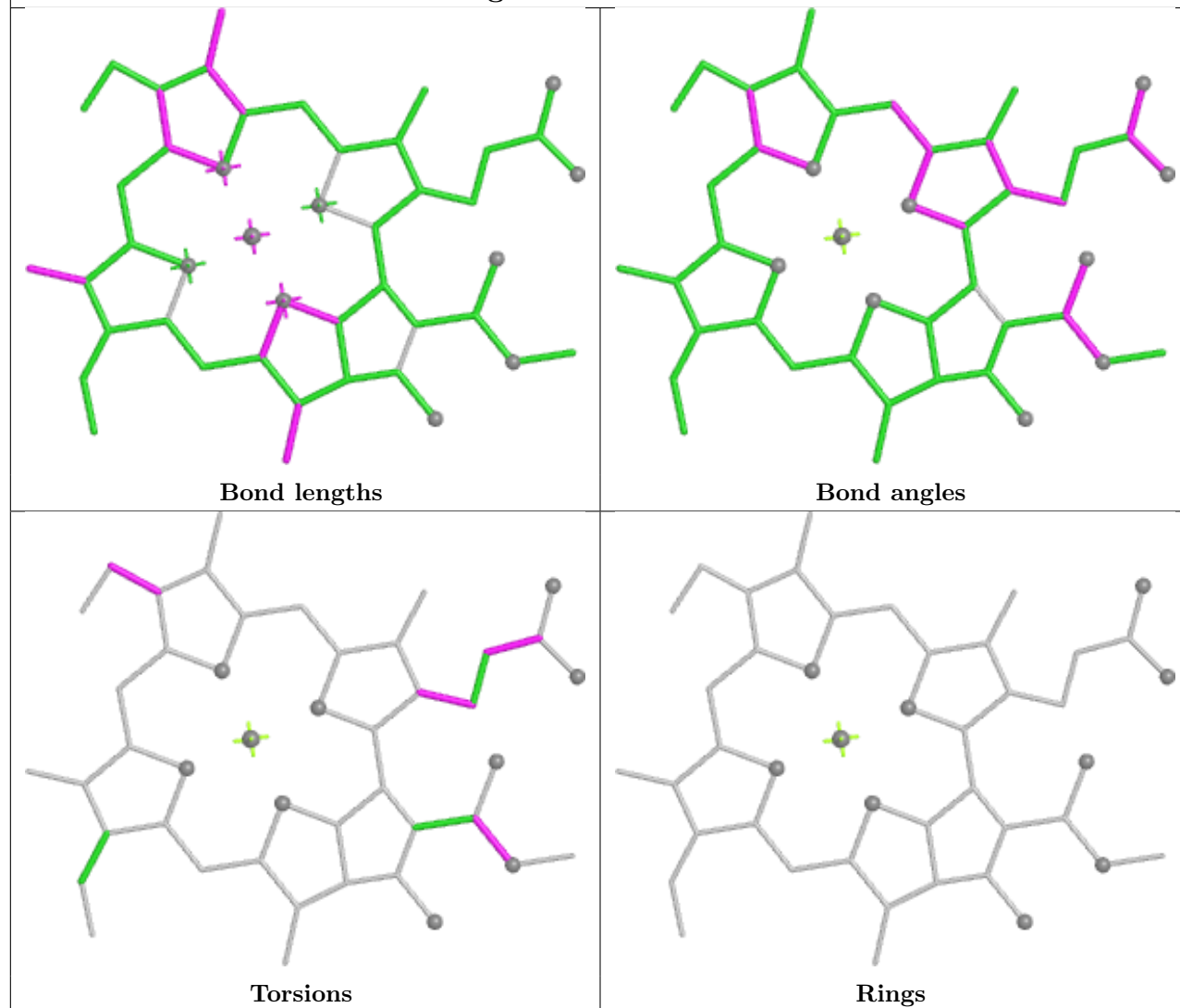


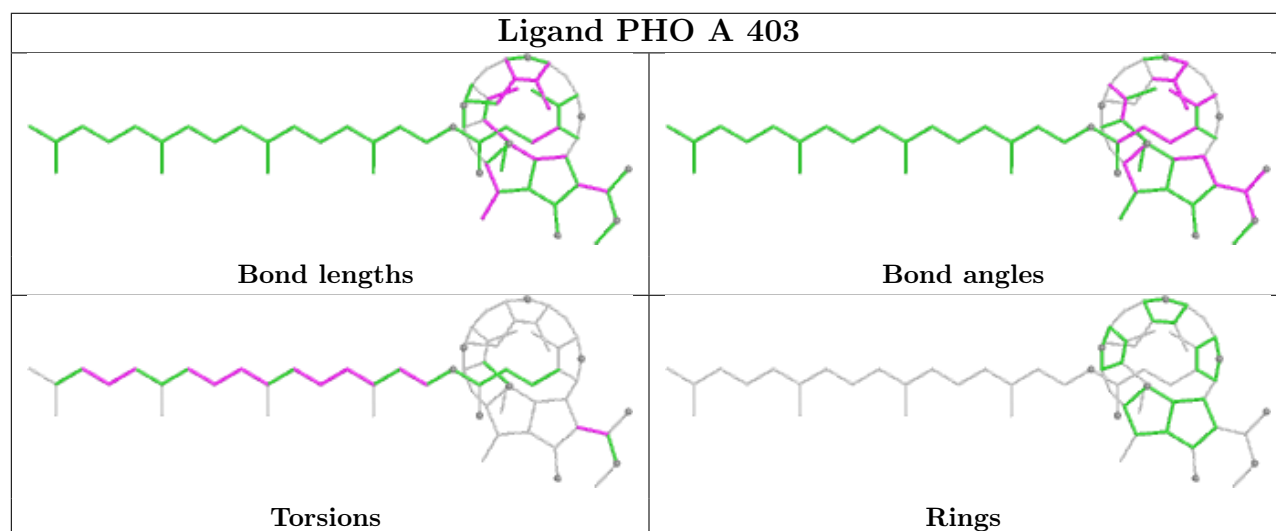
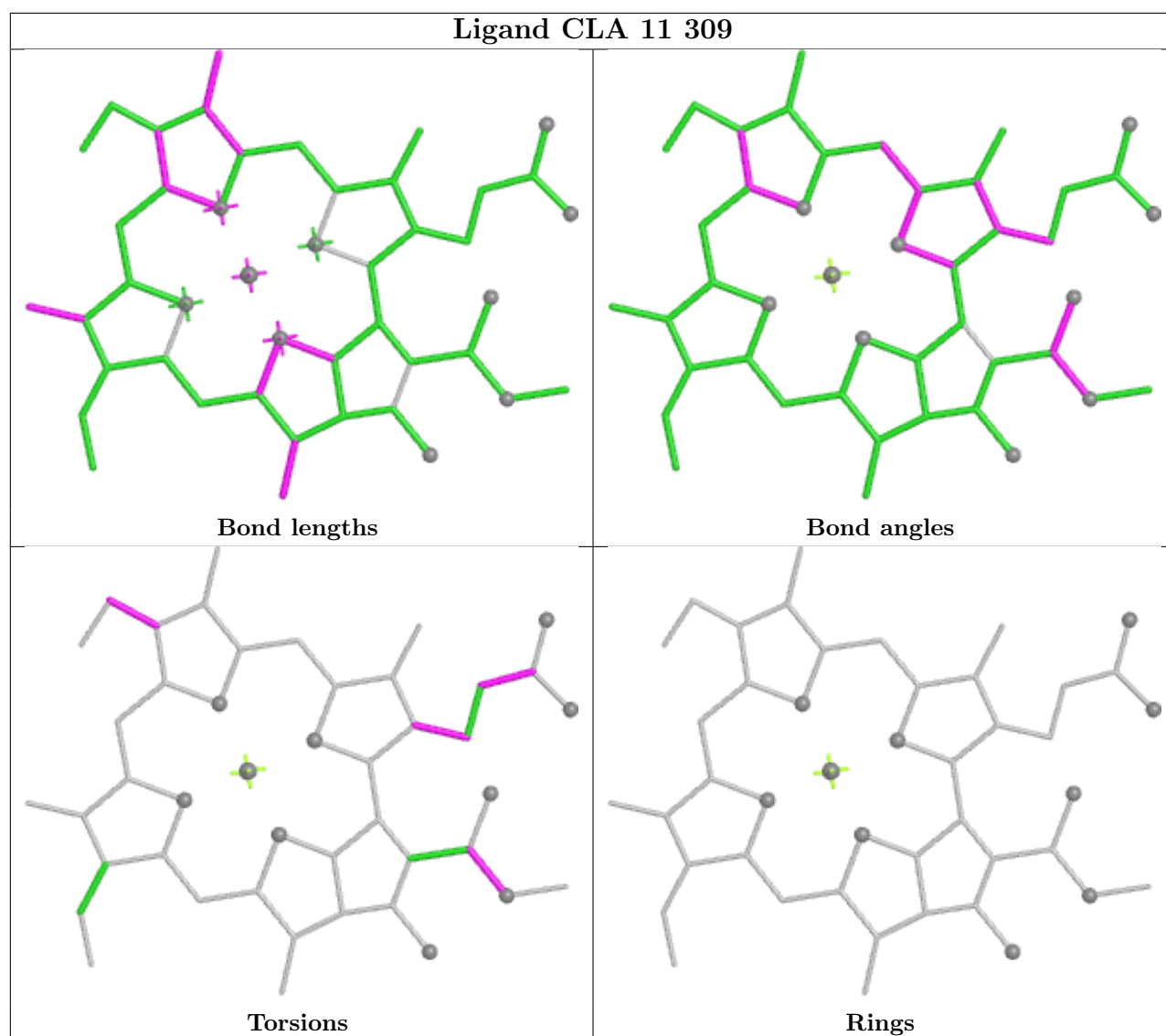


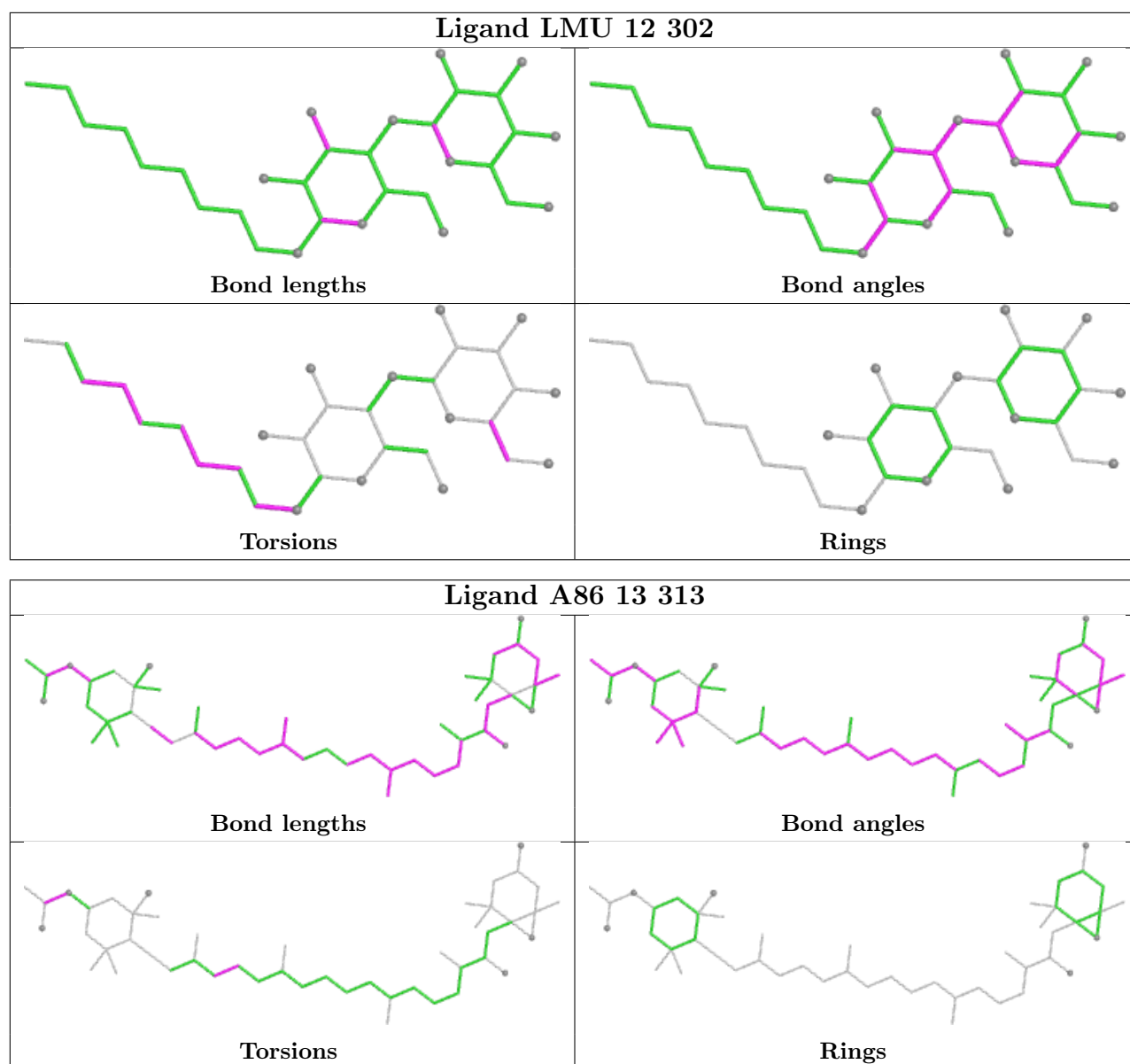
Ligand CLA Z 102

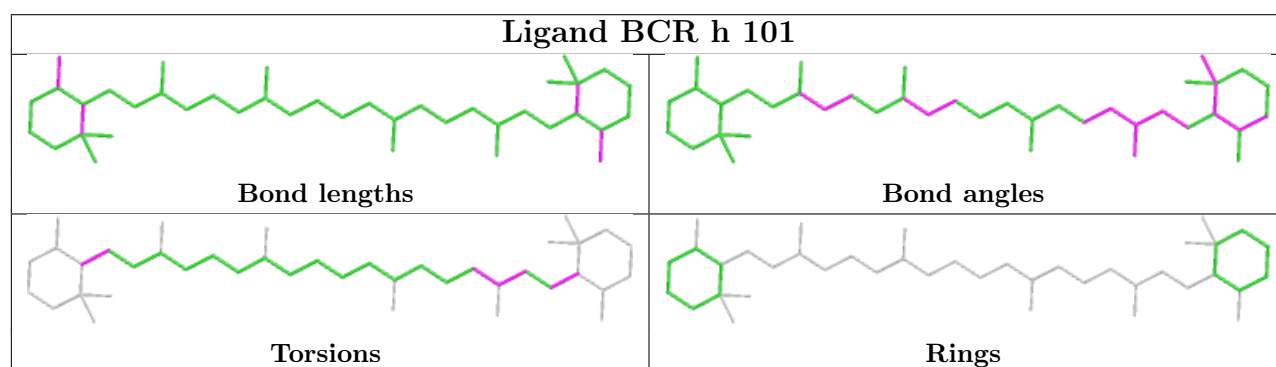
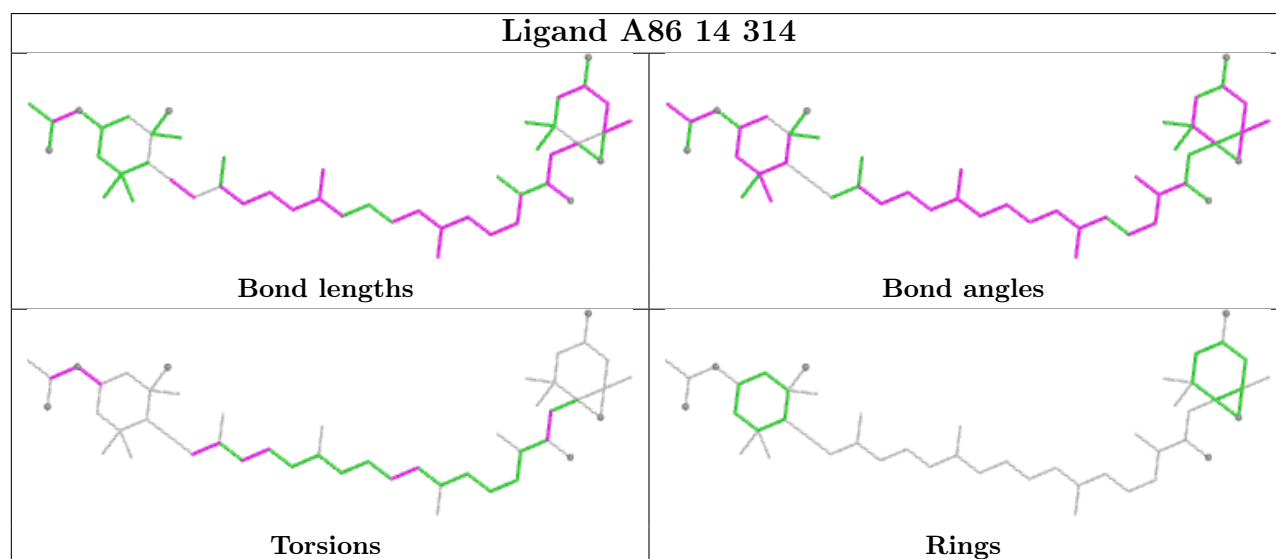
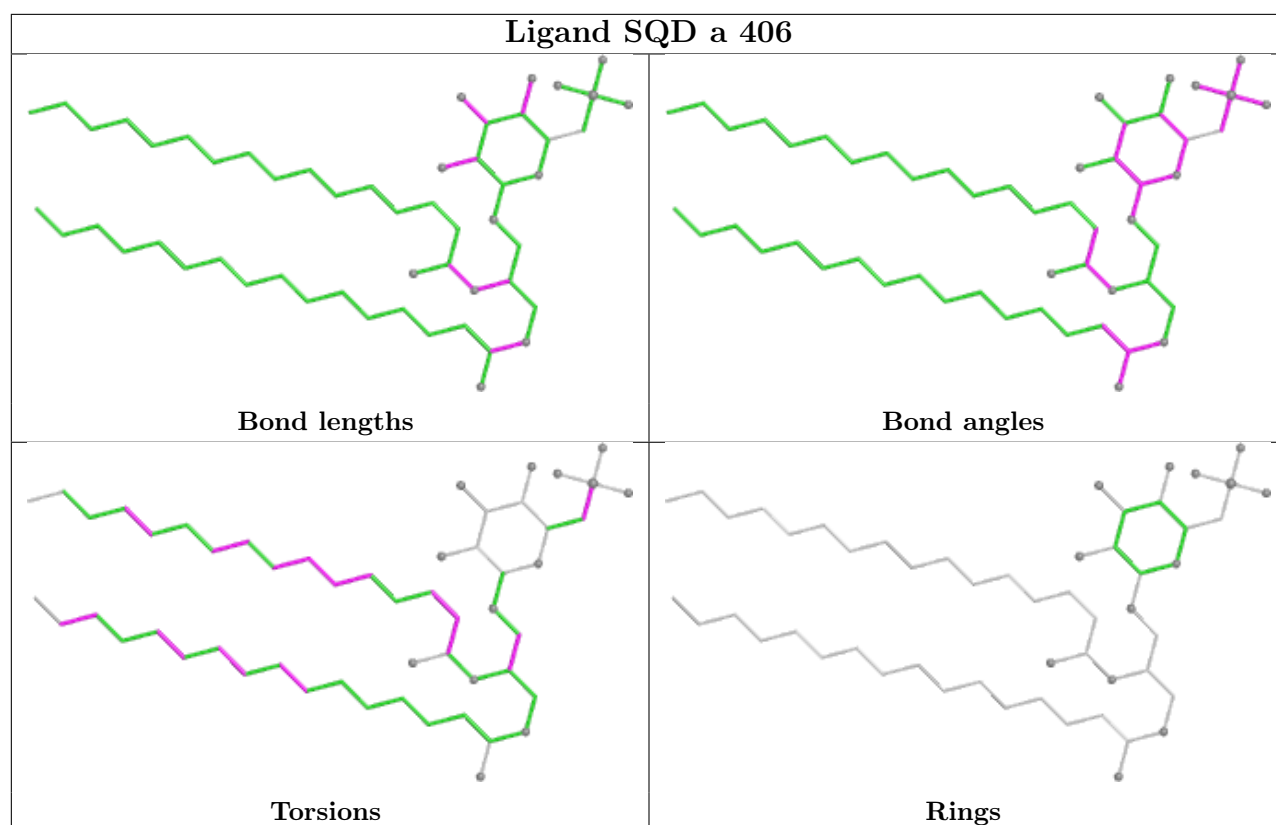


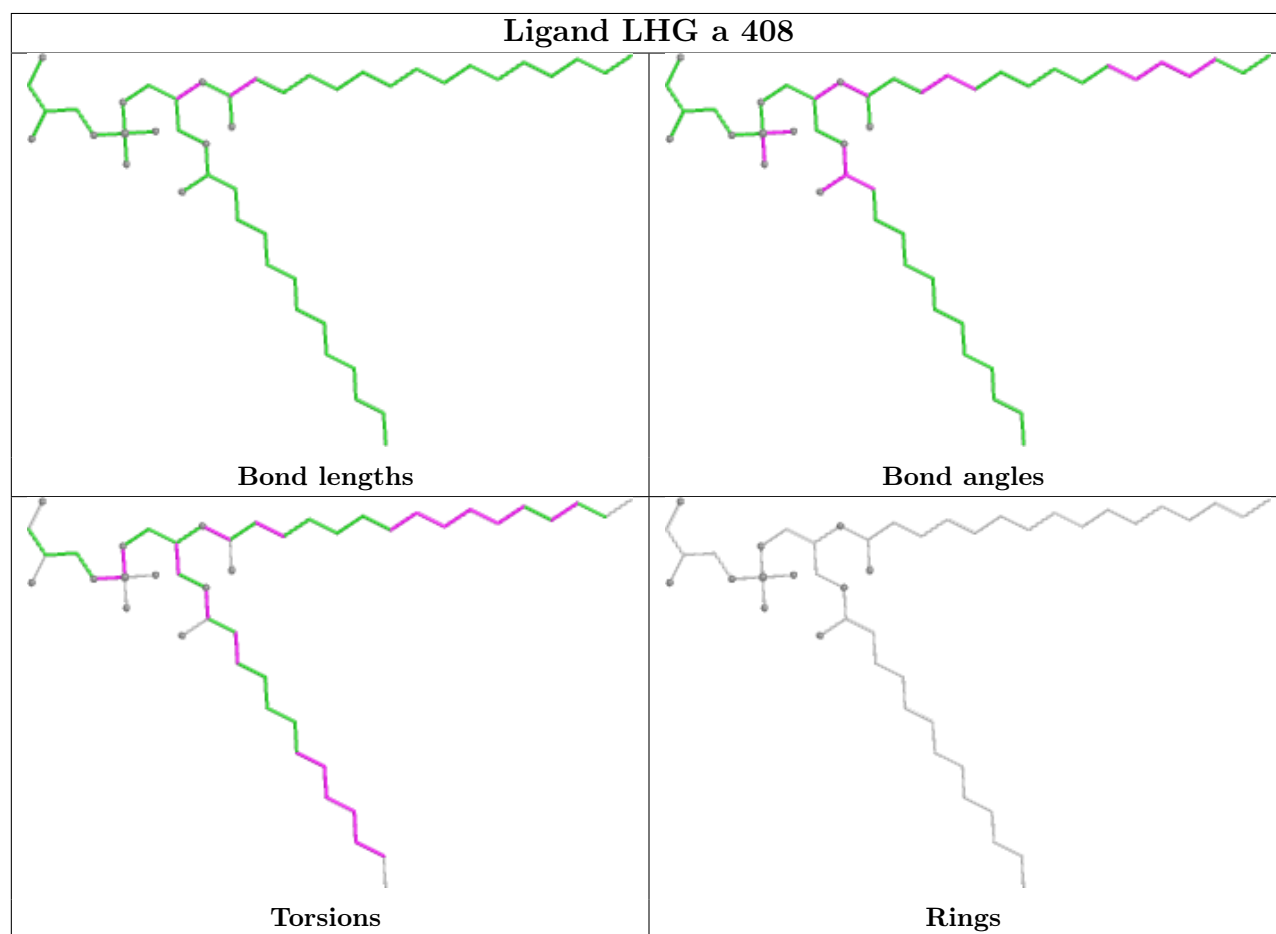
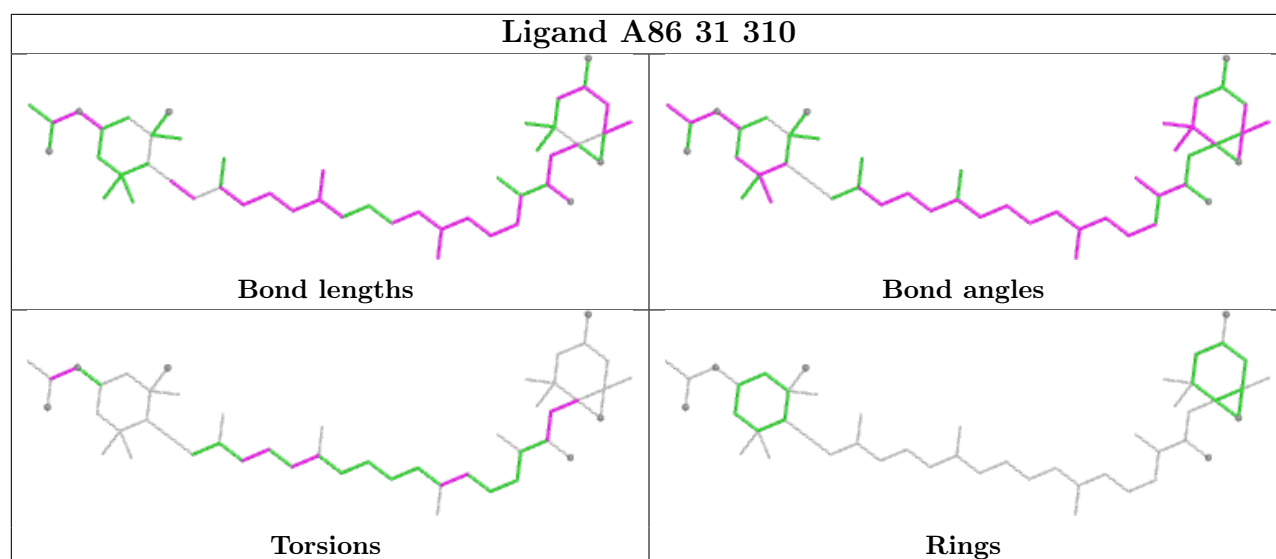
Ligand CLA 32 313

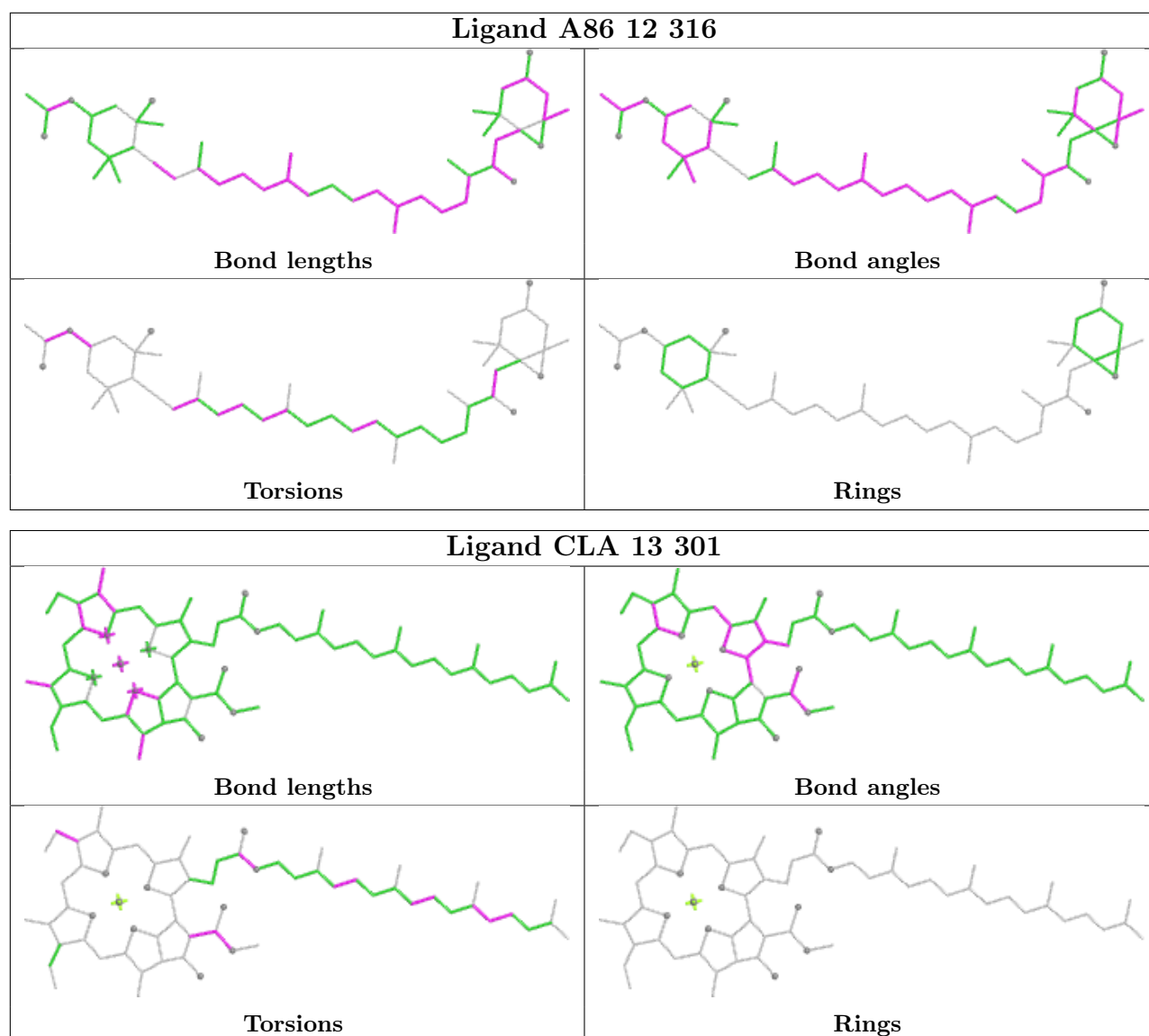


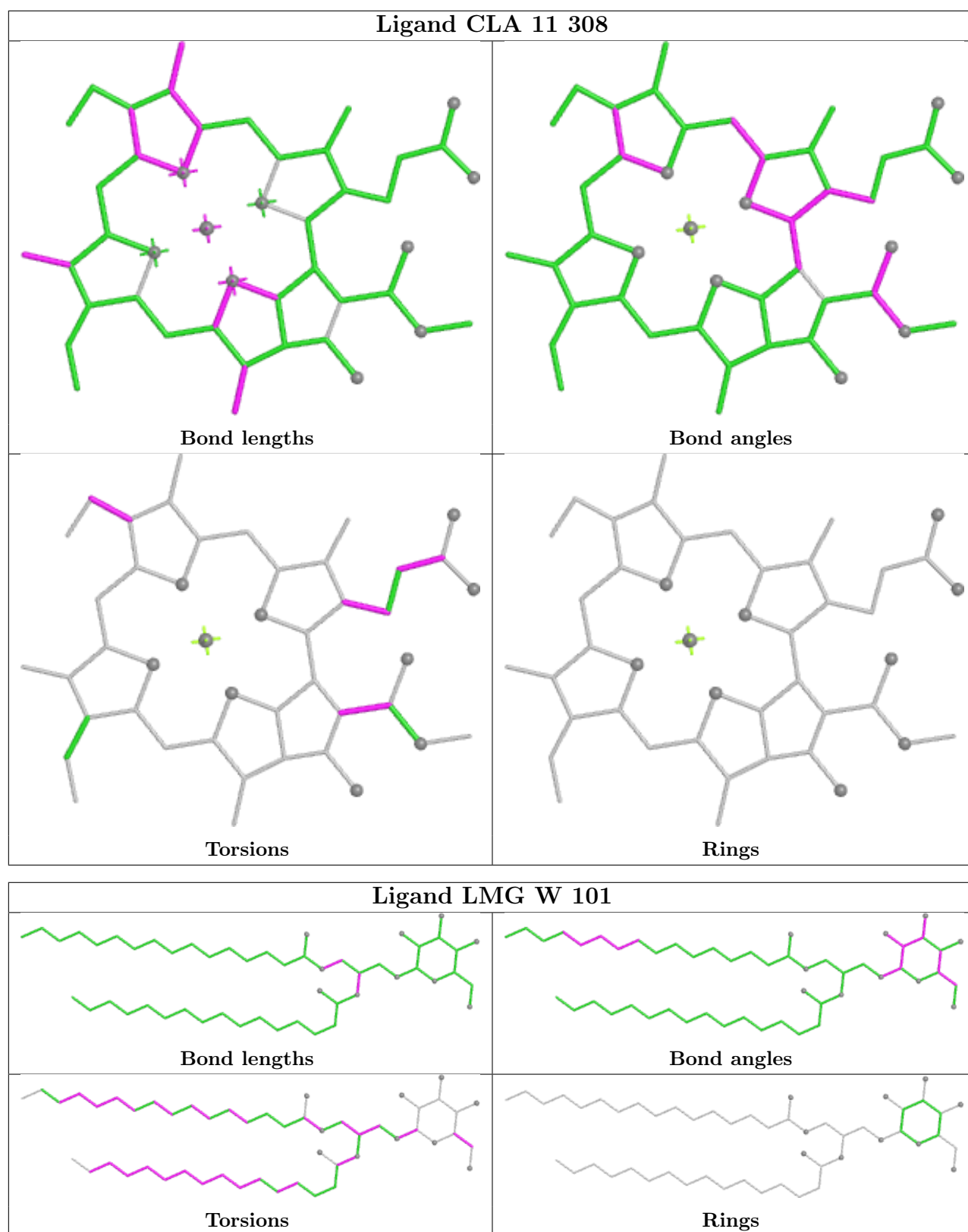


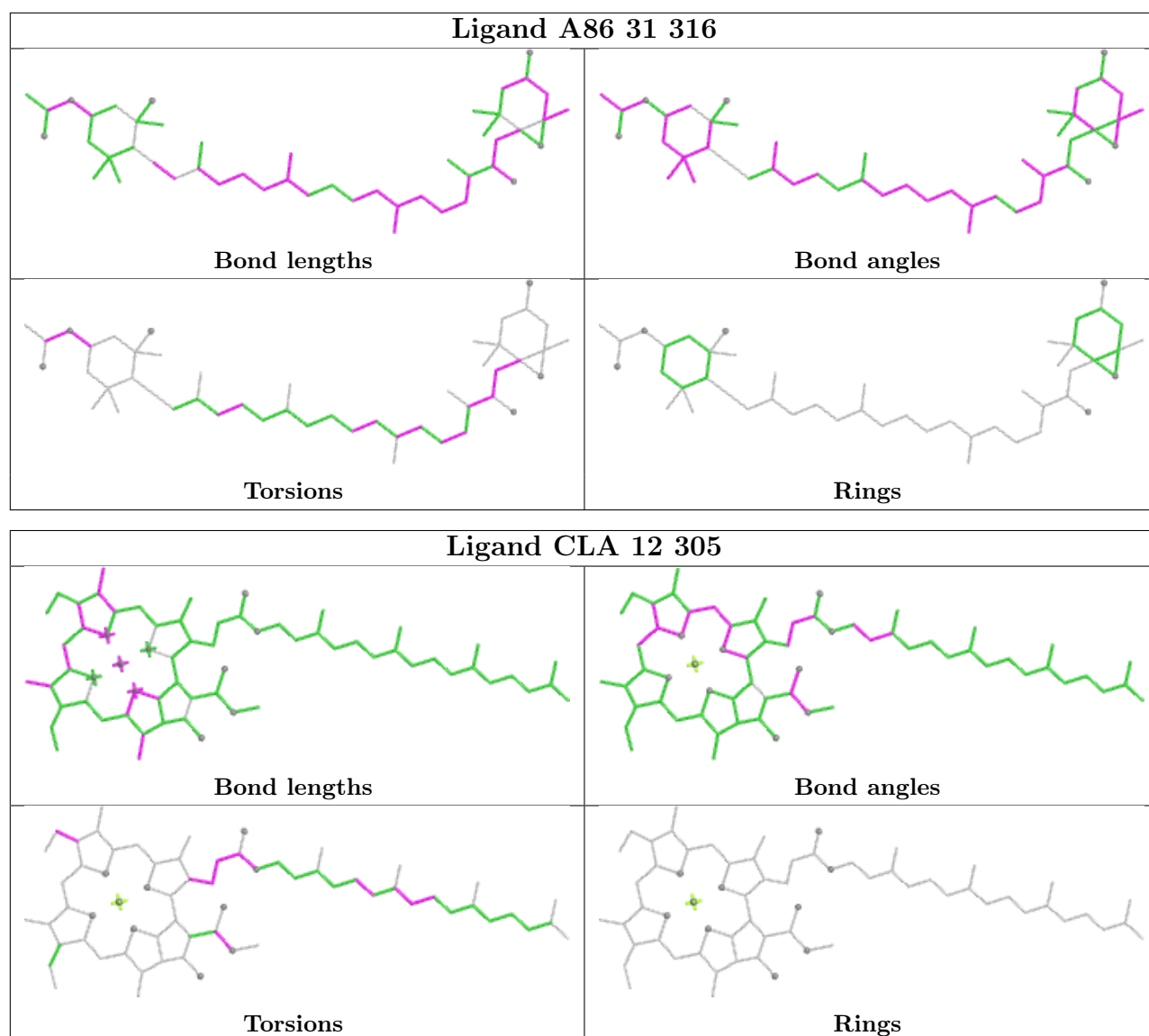


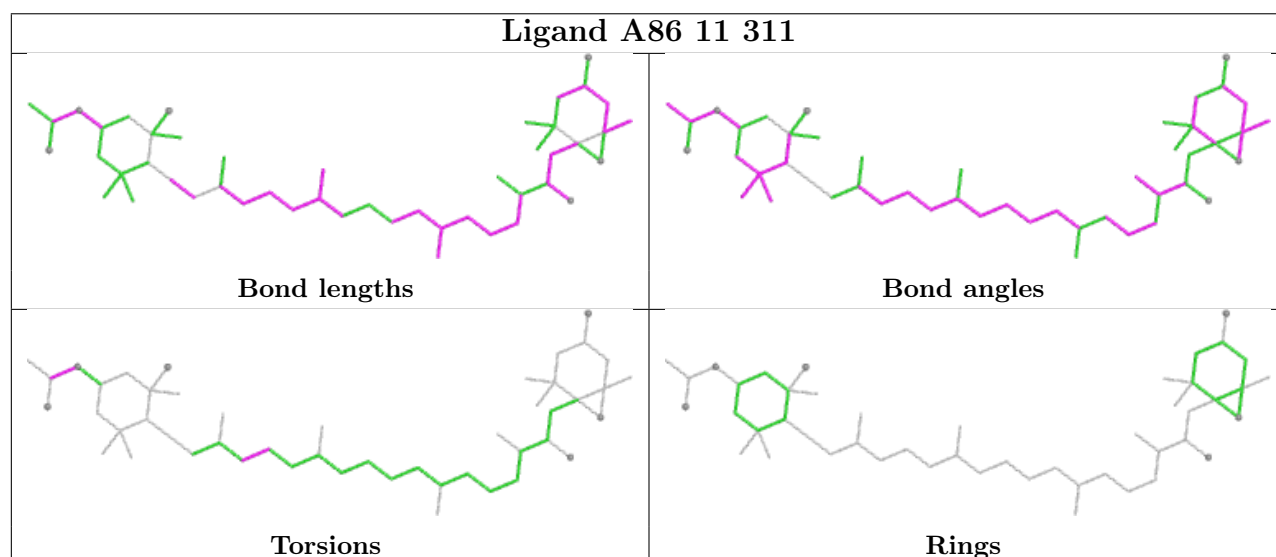
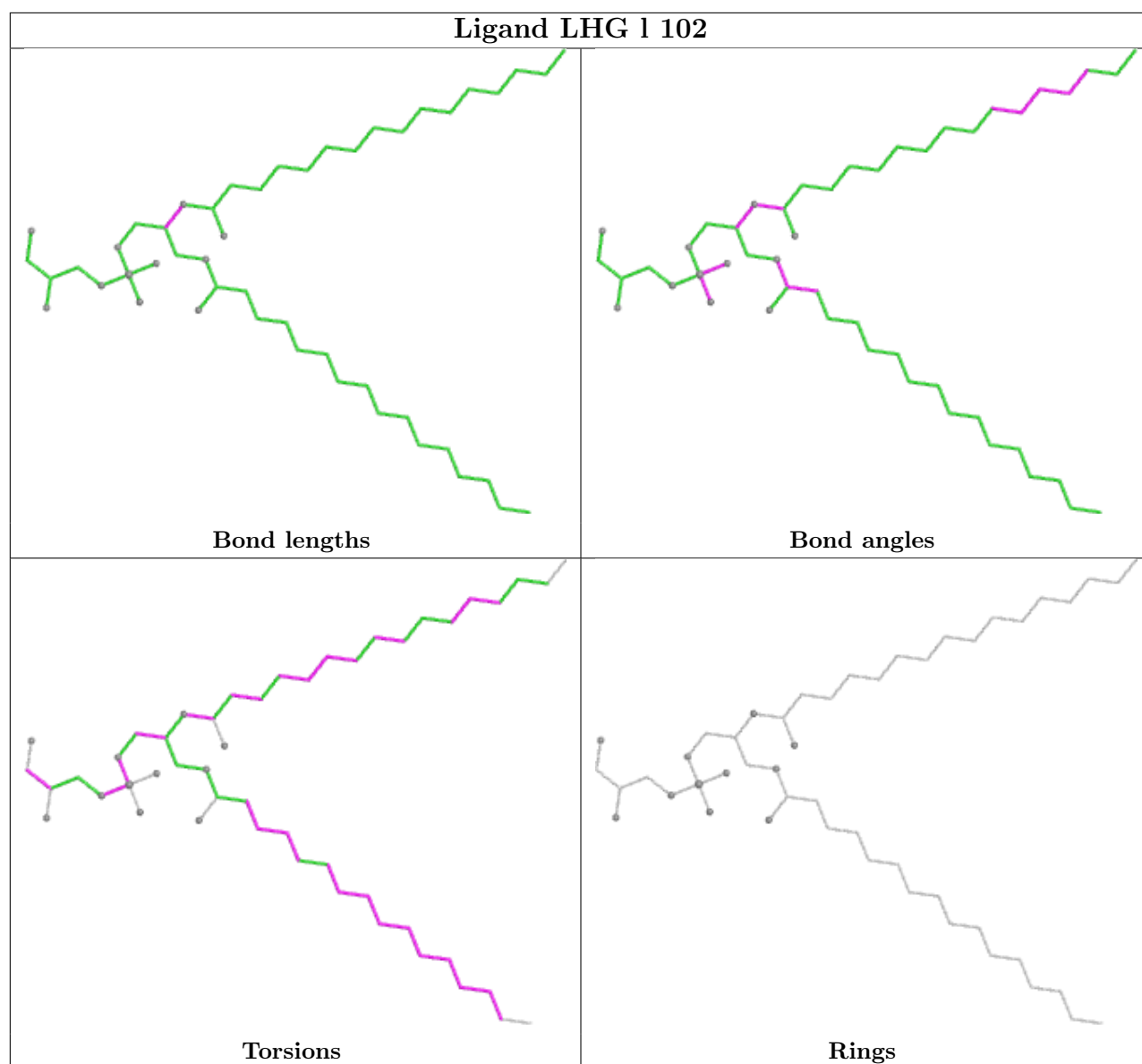


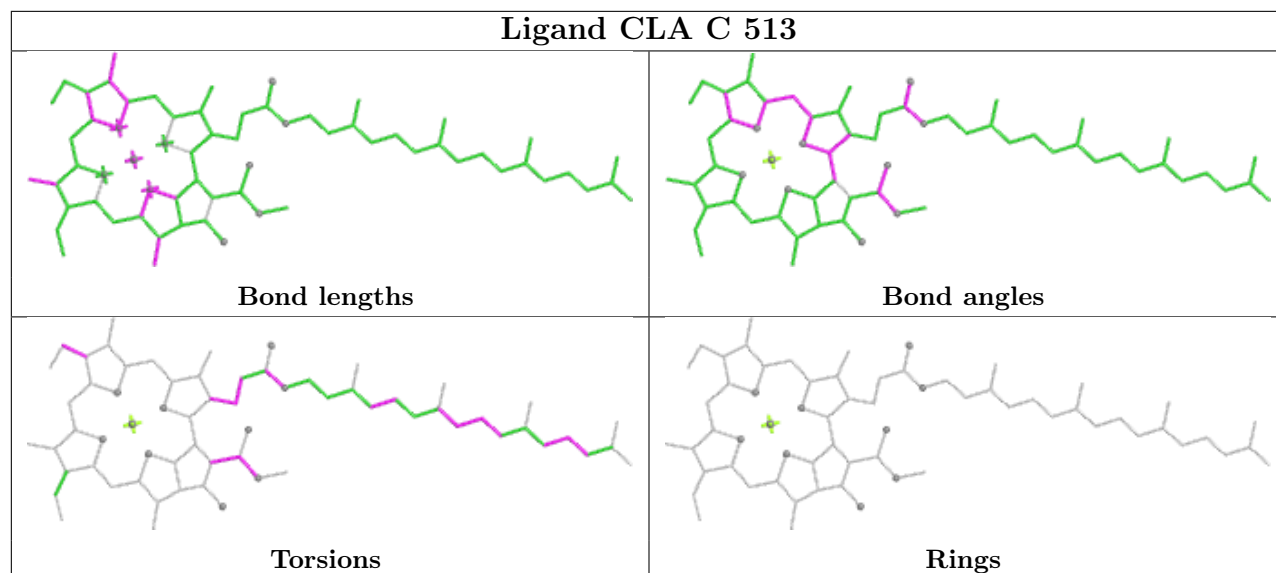
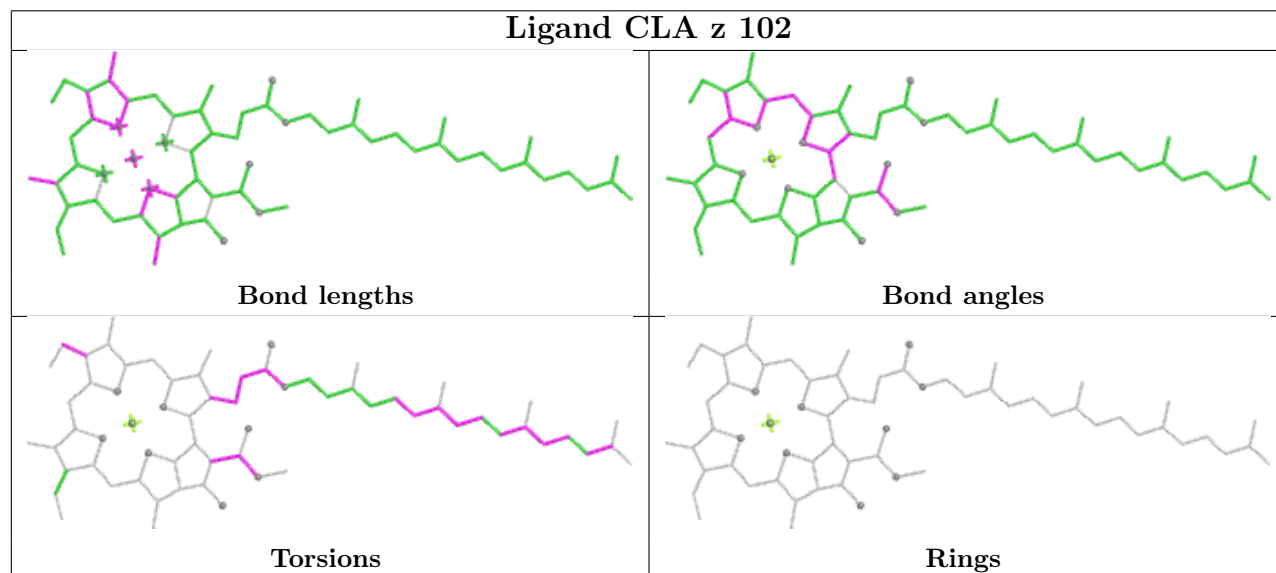
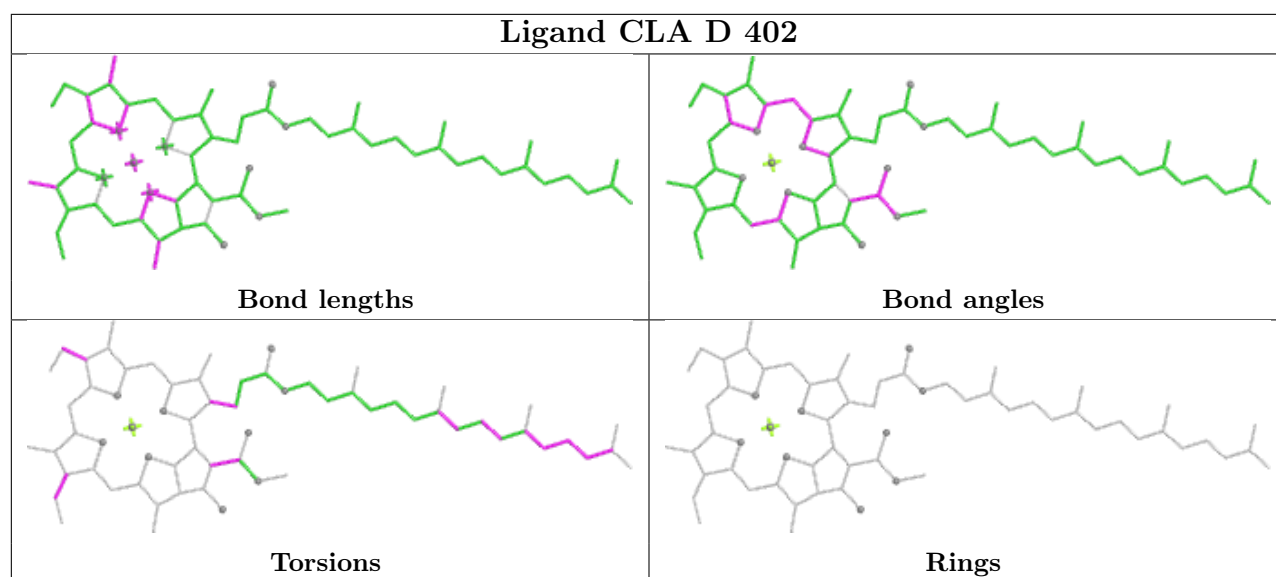


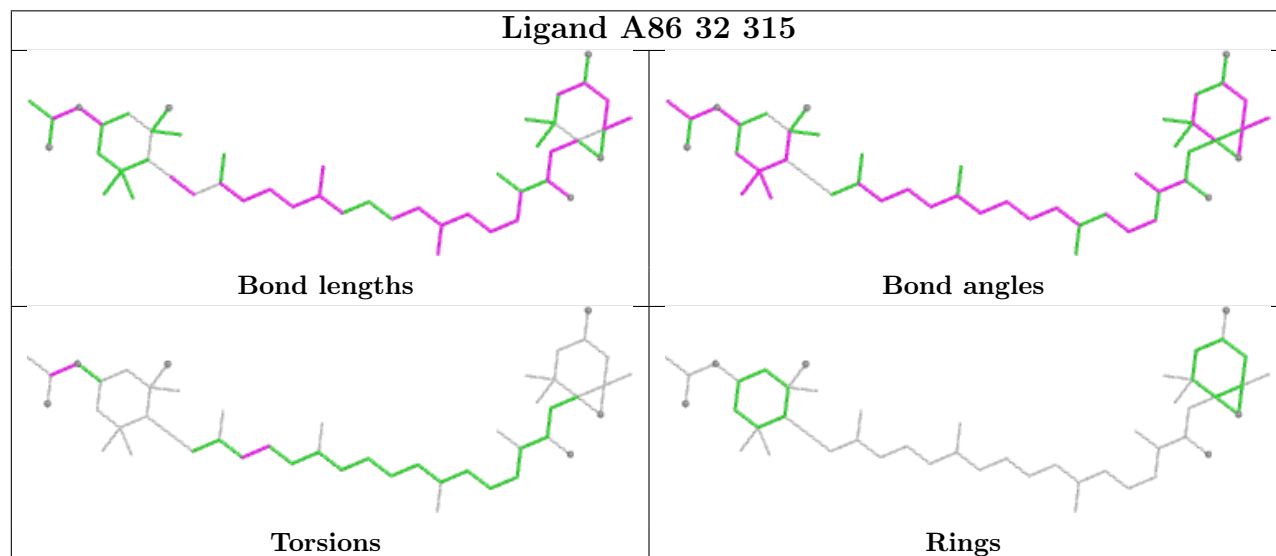
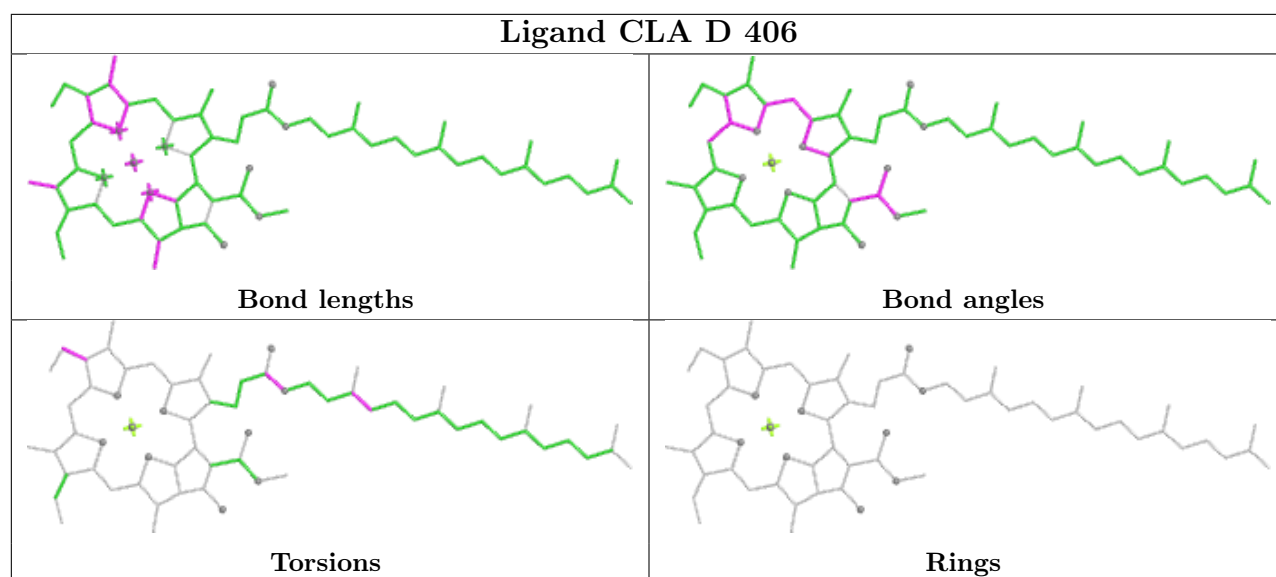


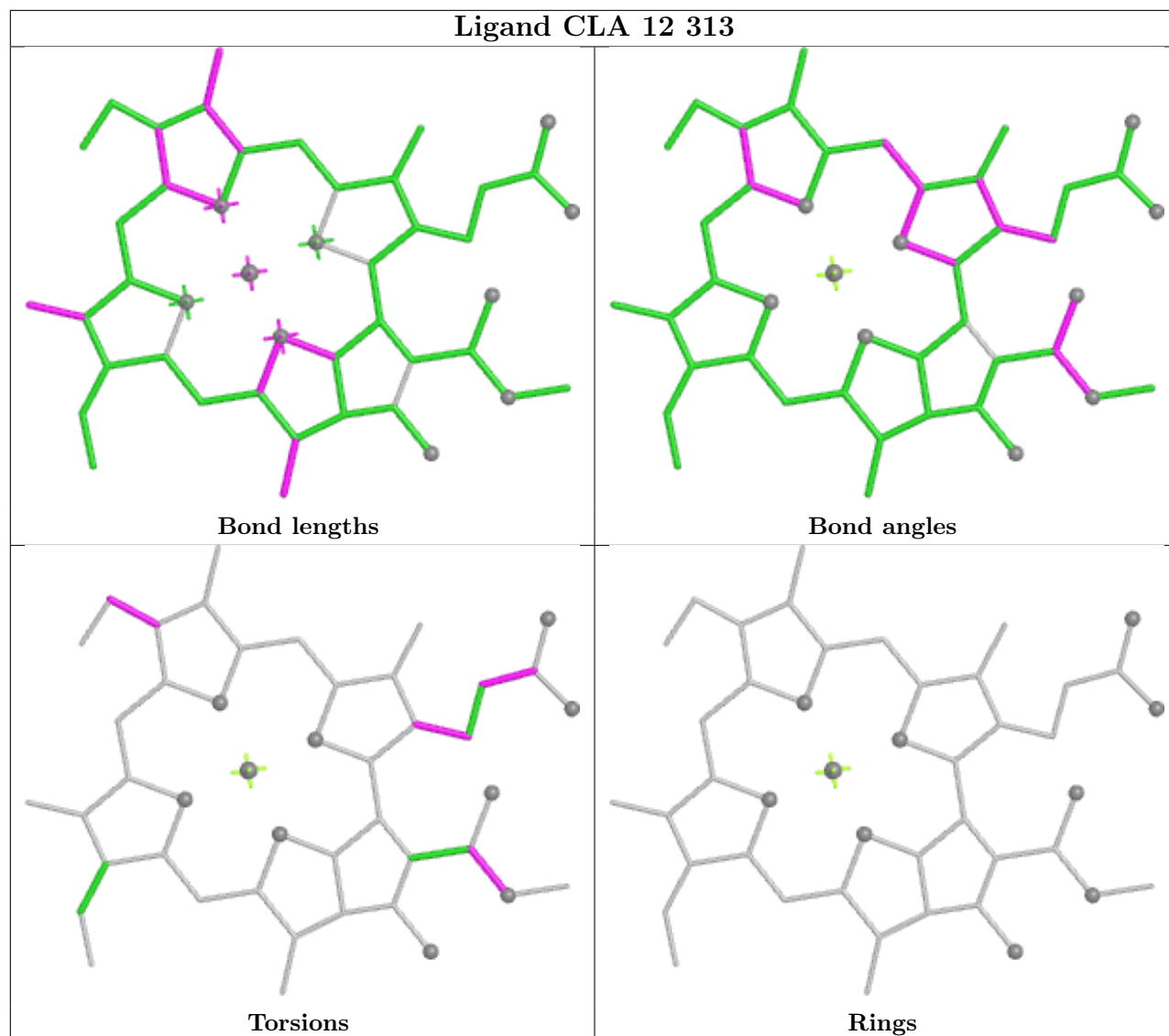


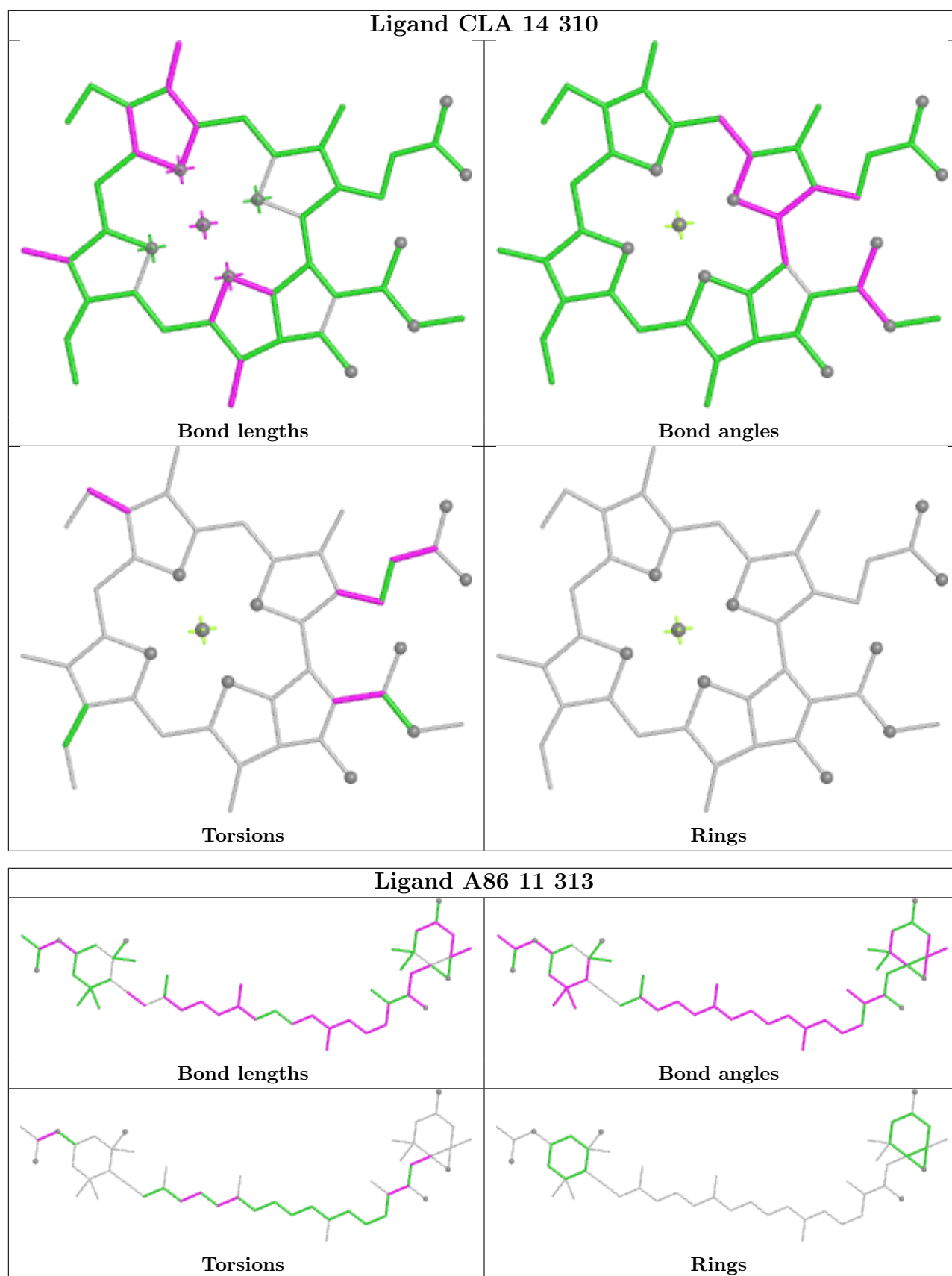


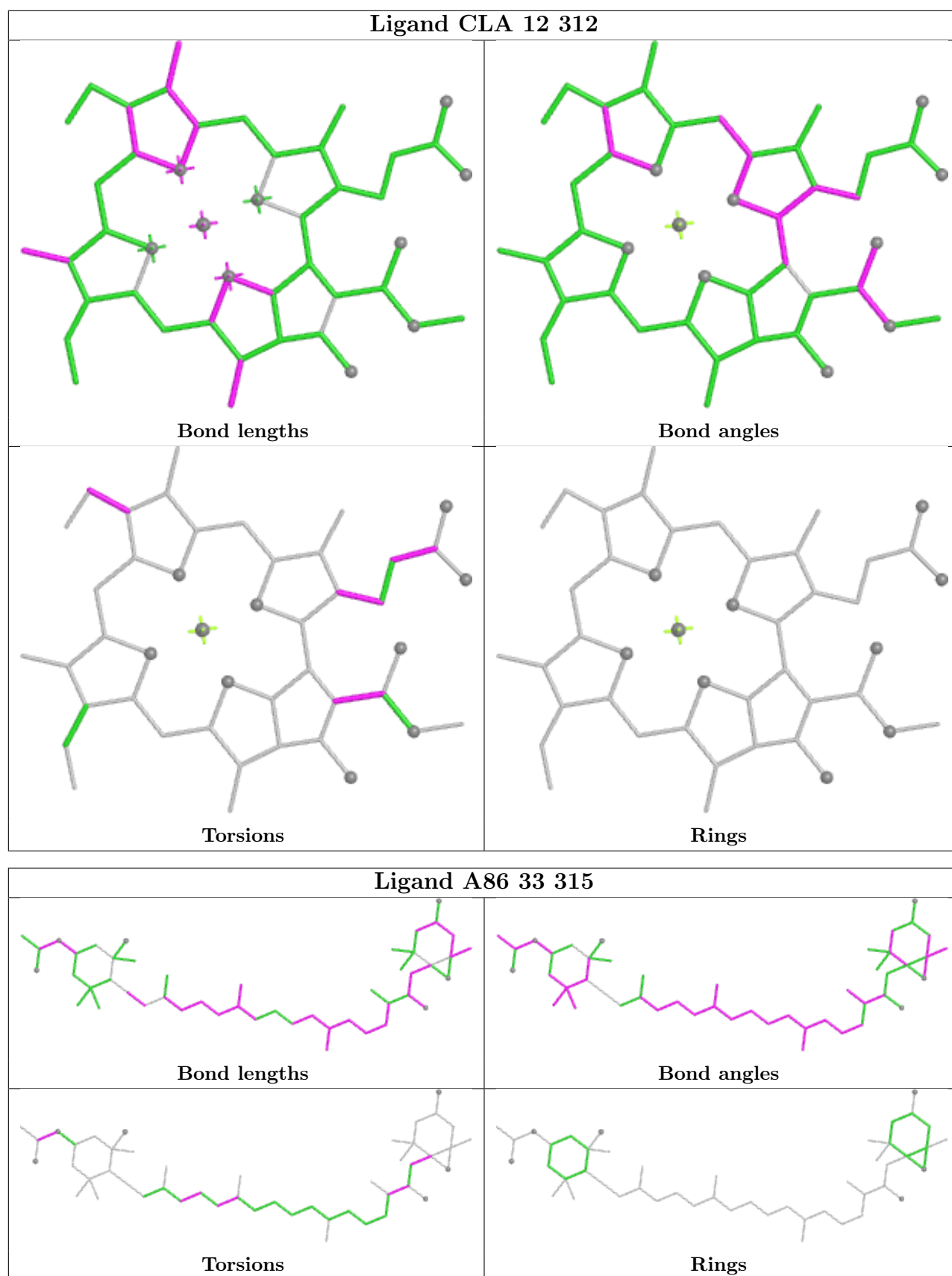


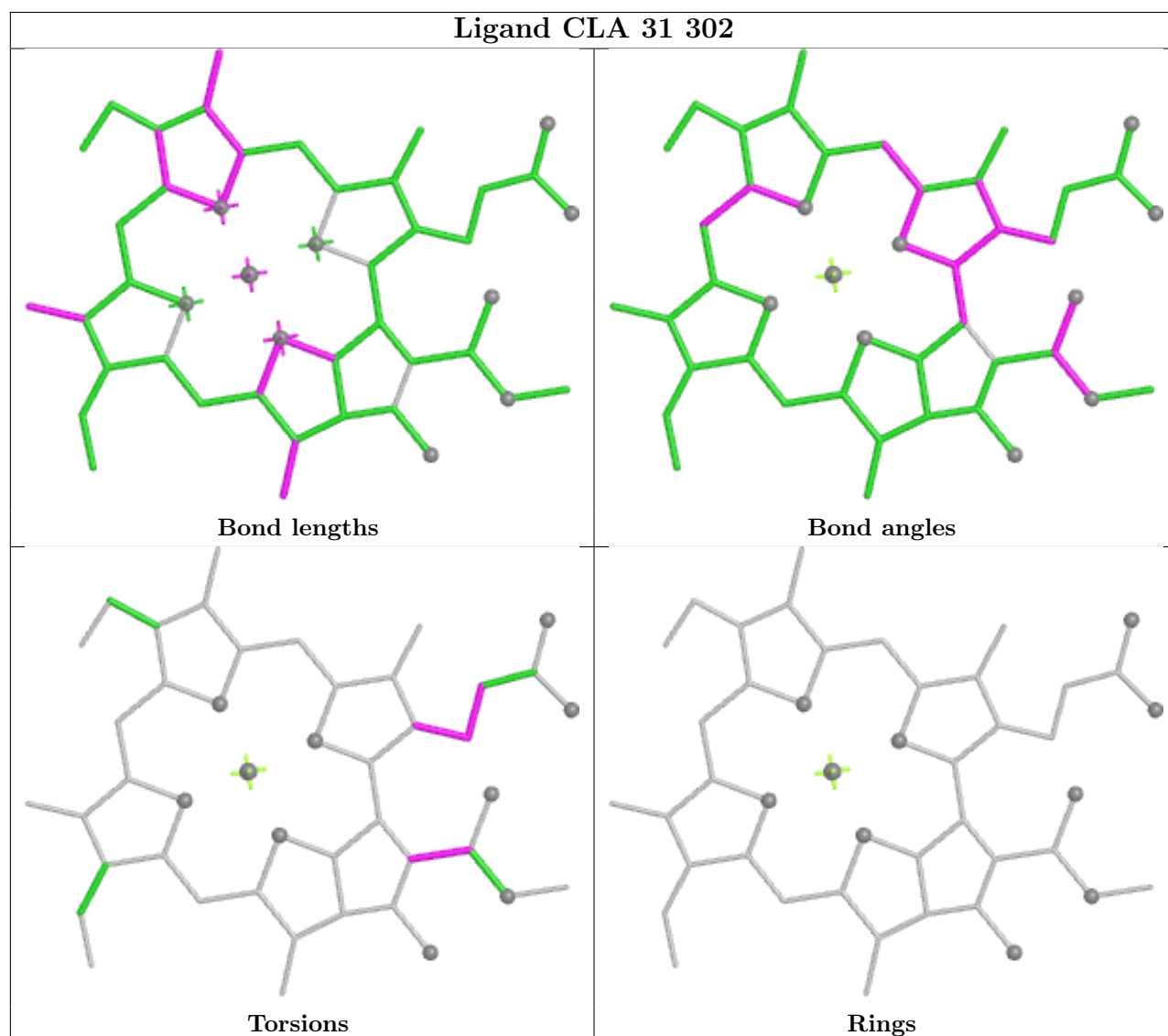
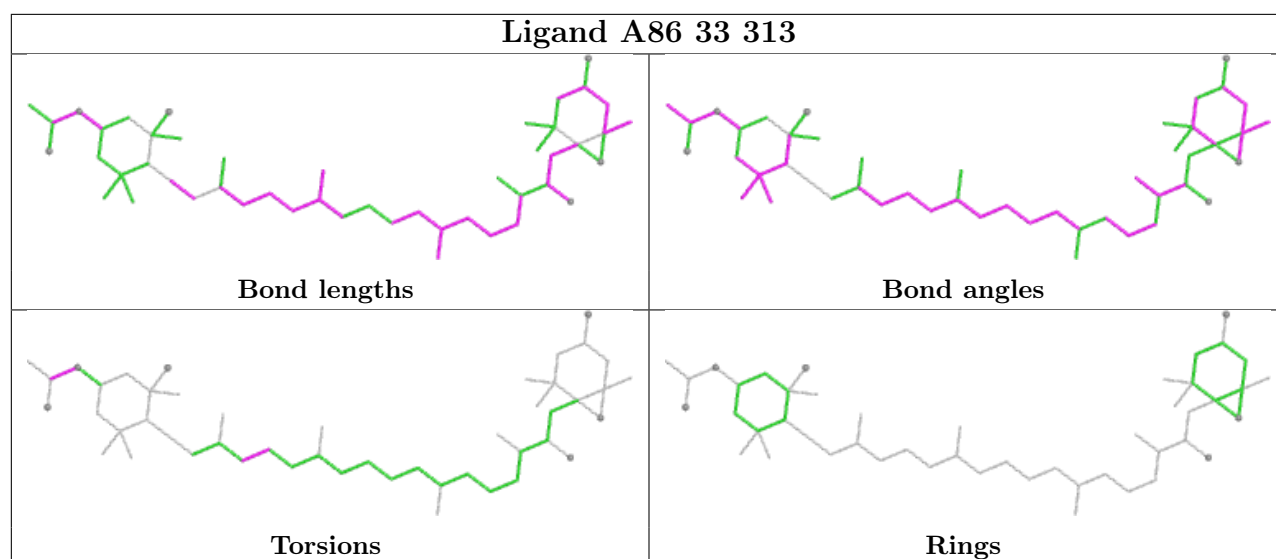


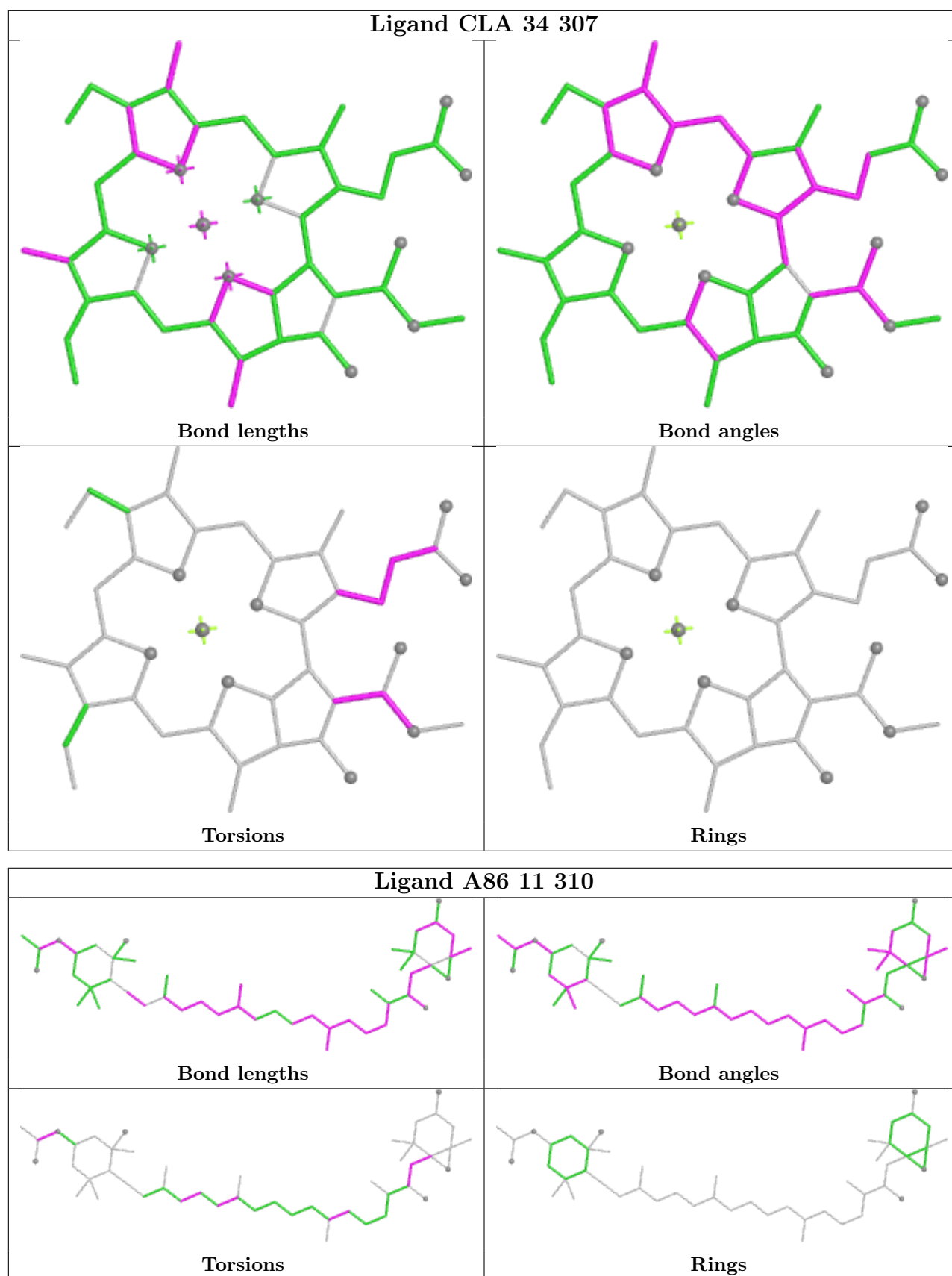


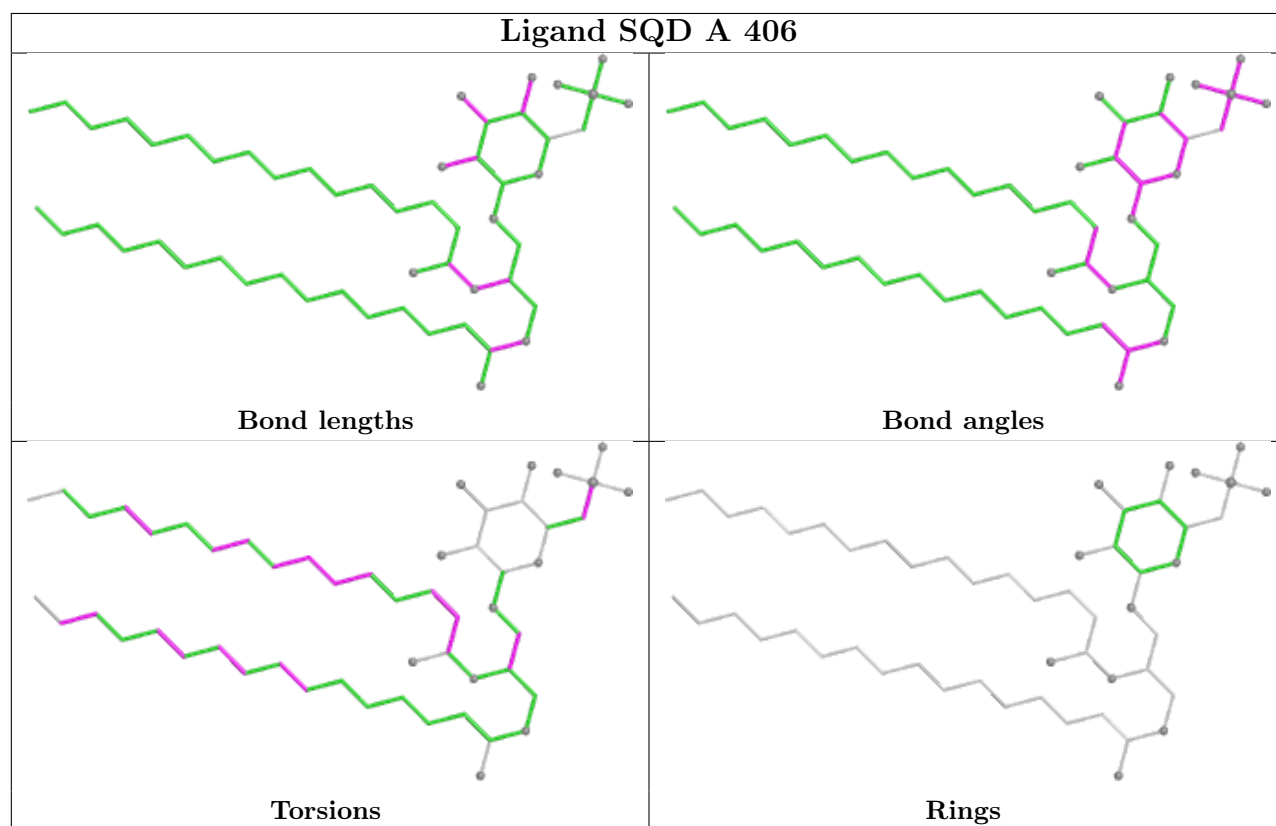
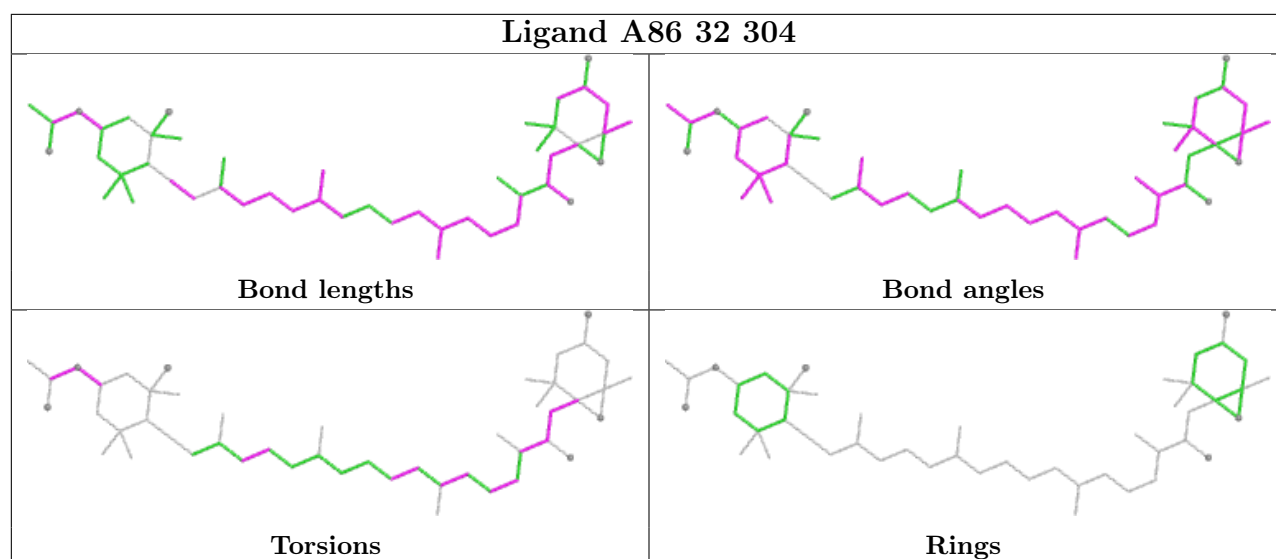


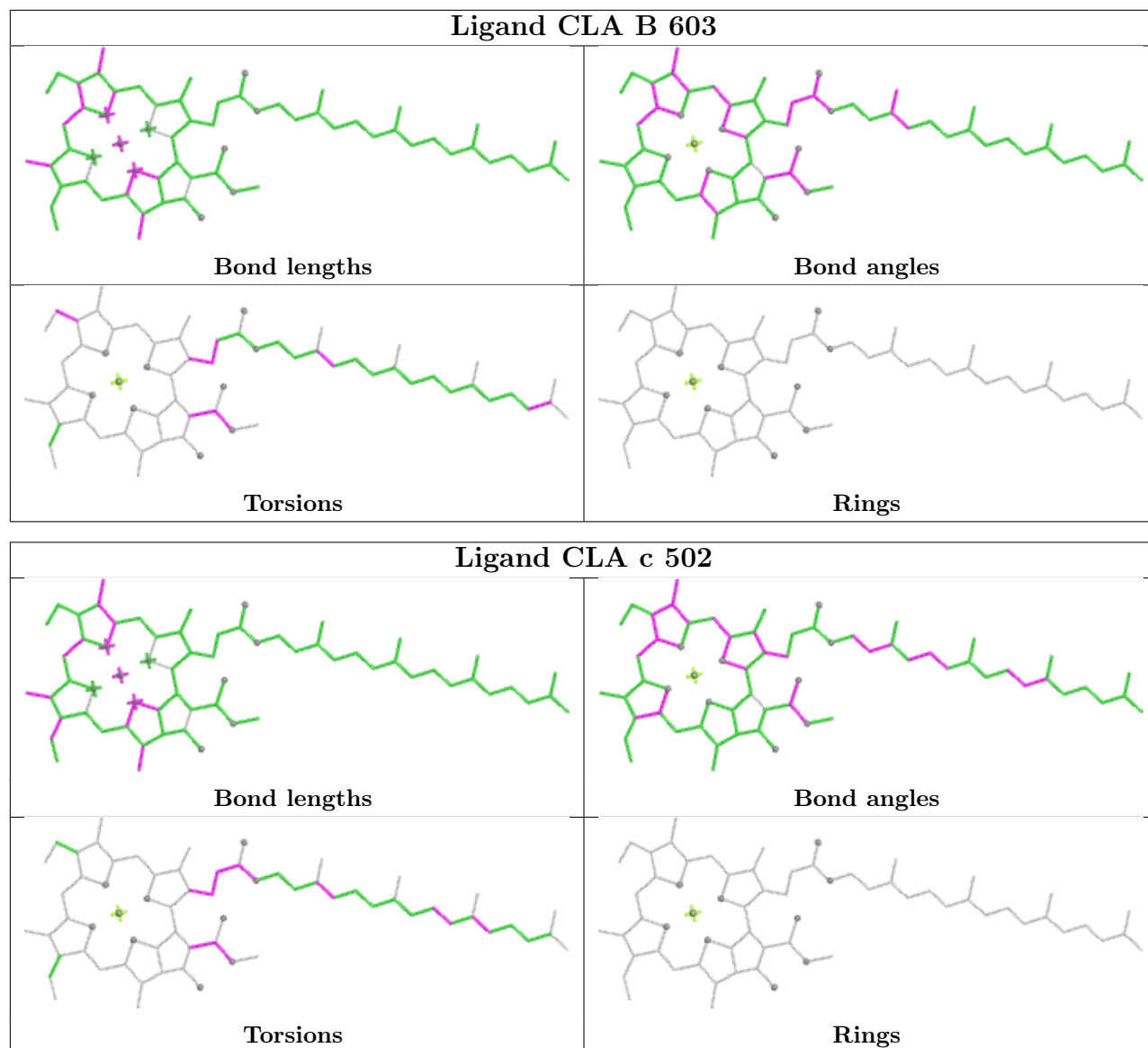


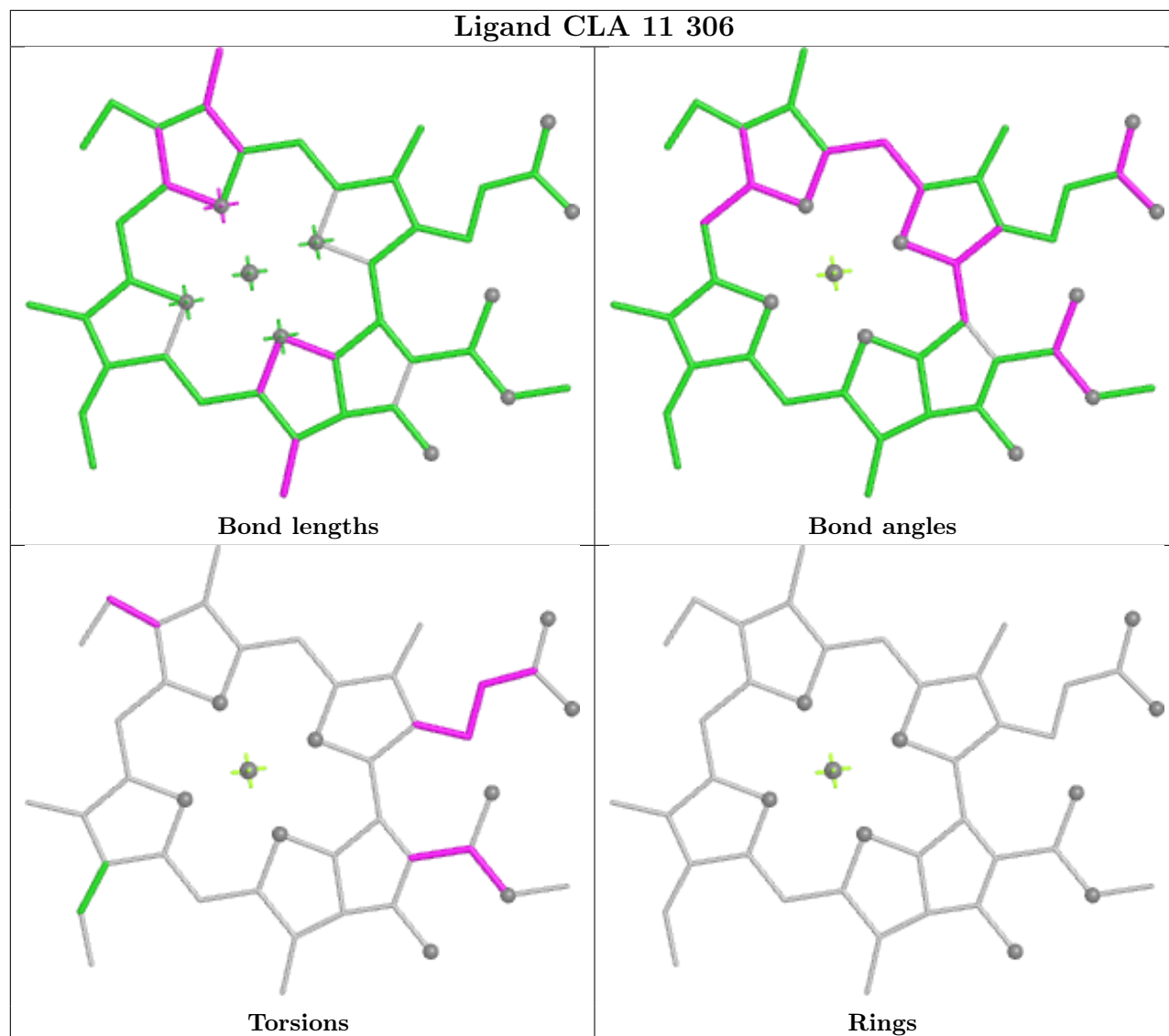


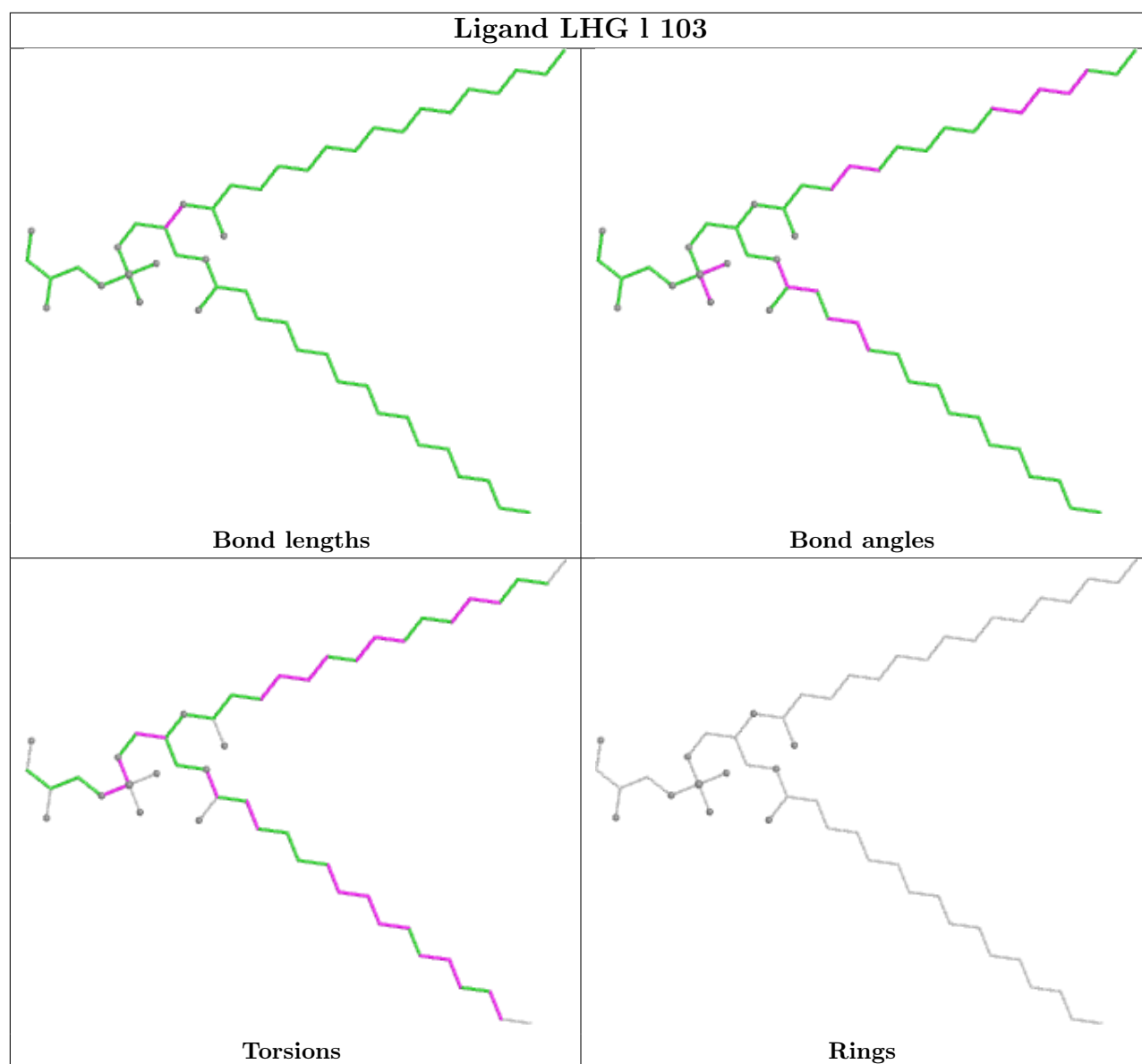


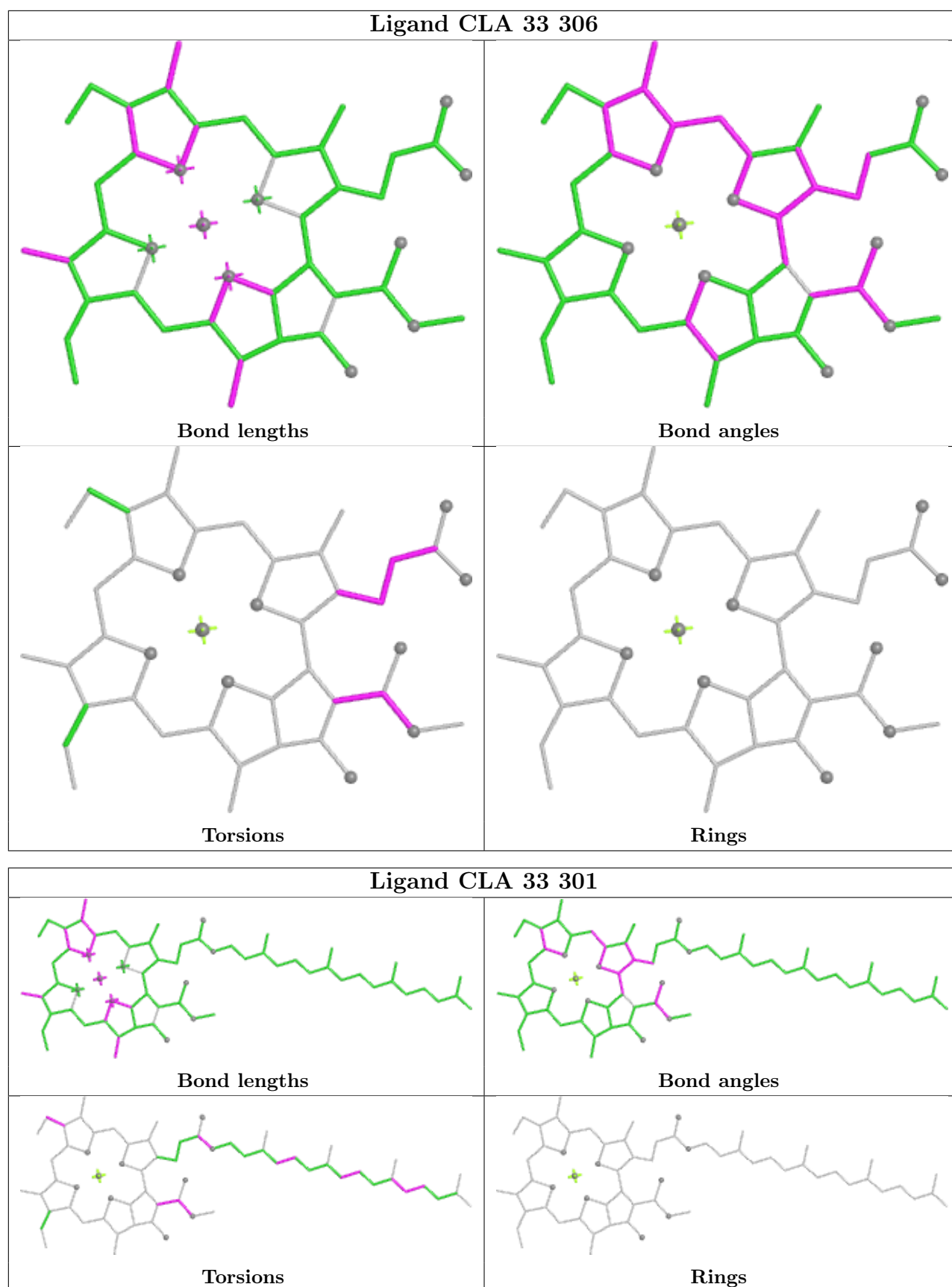


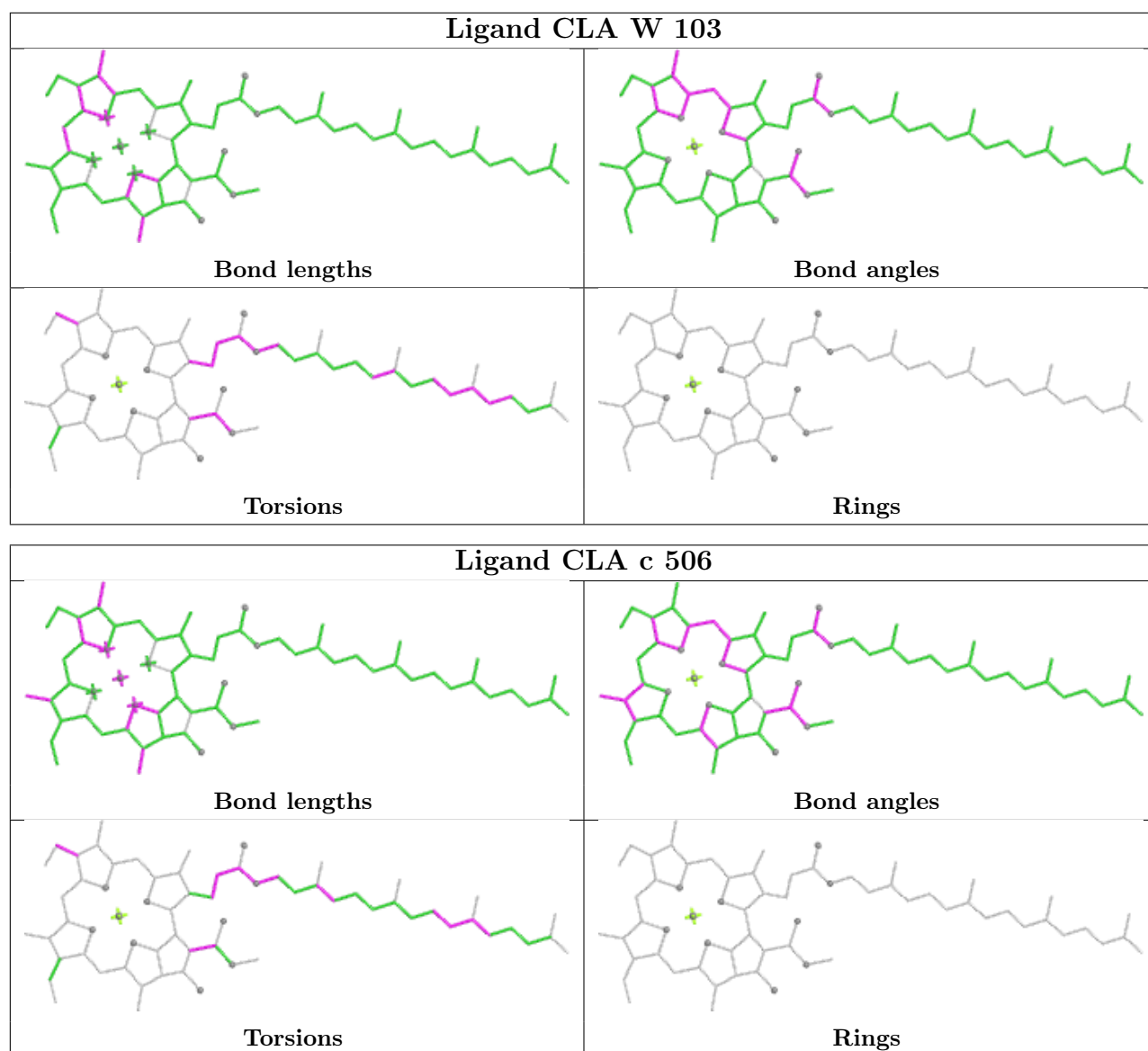


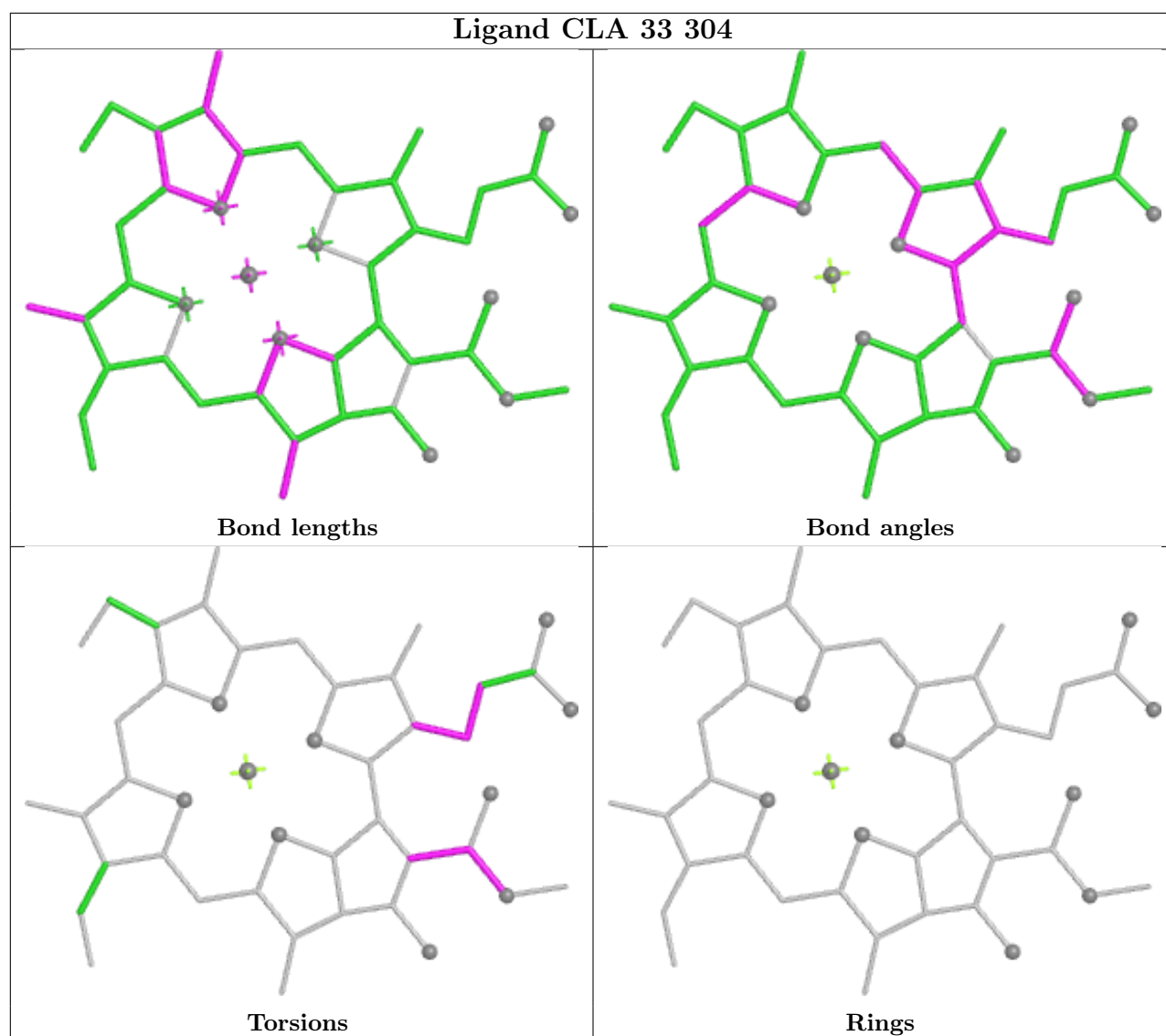


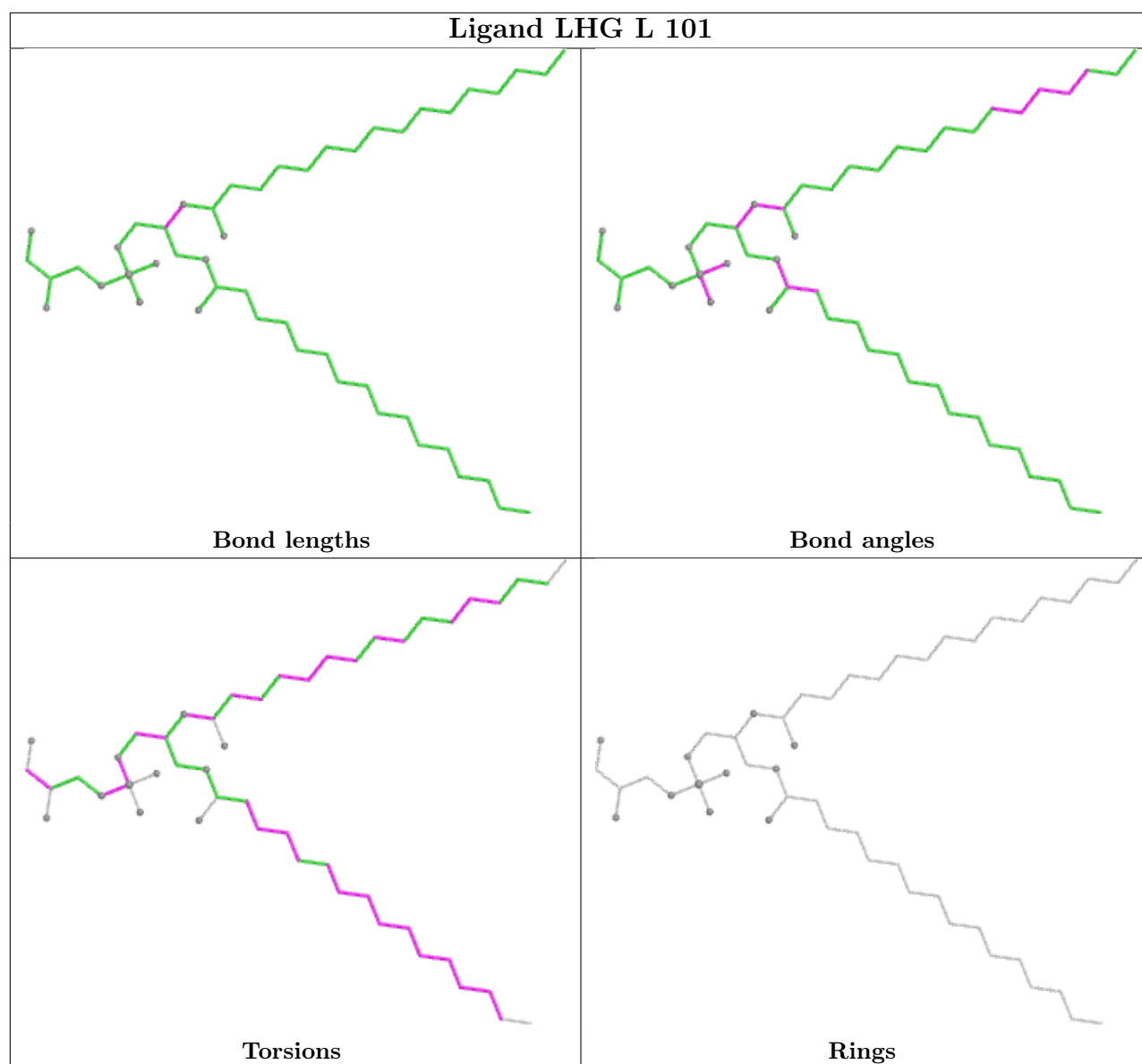


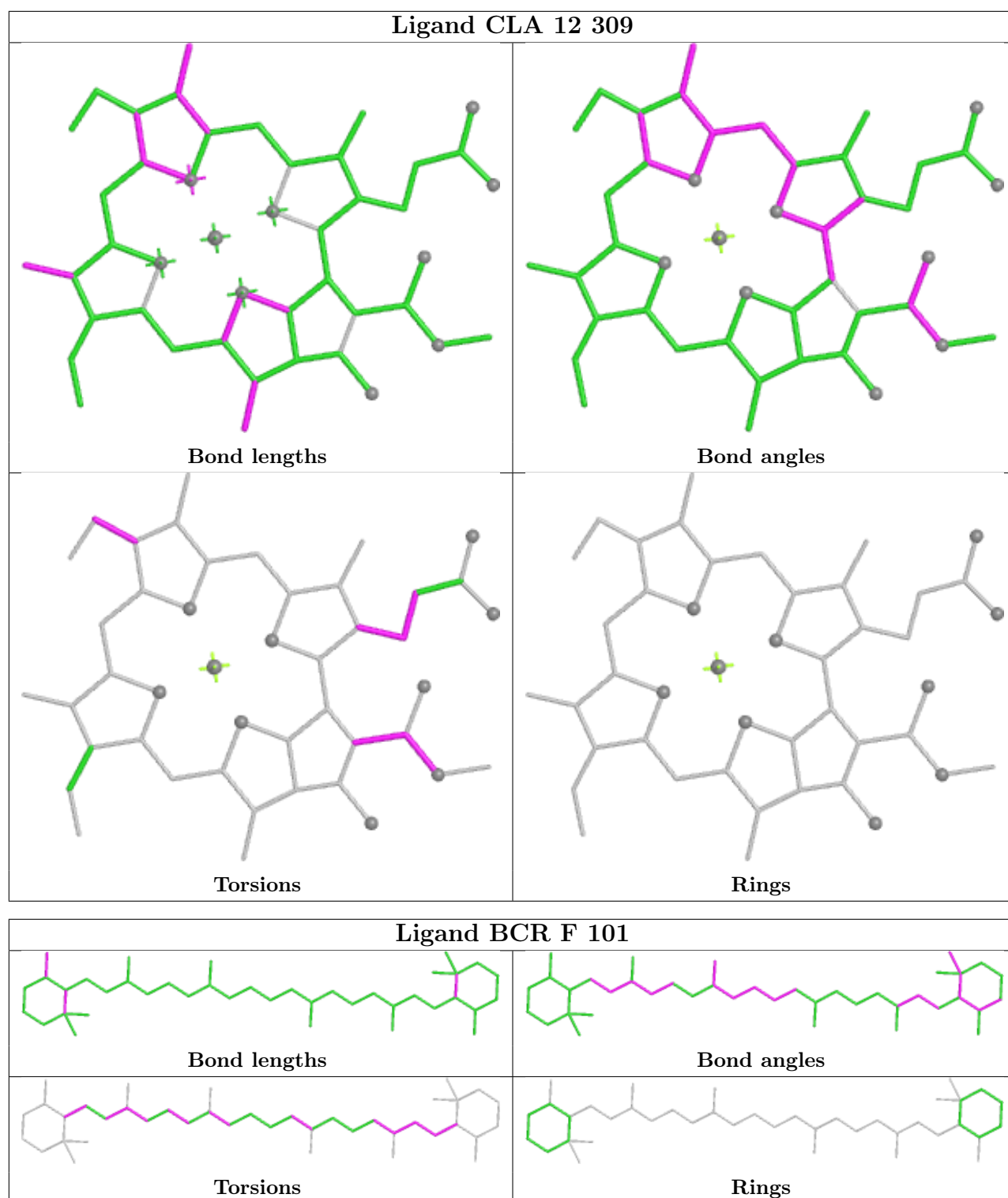




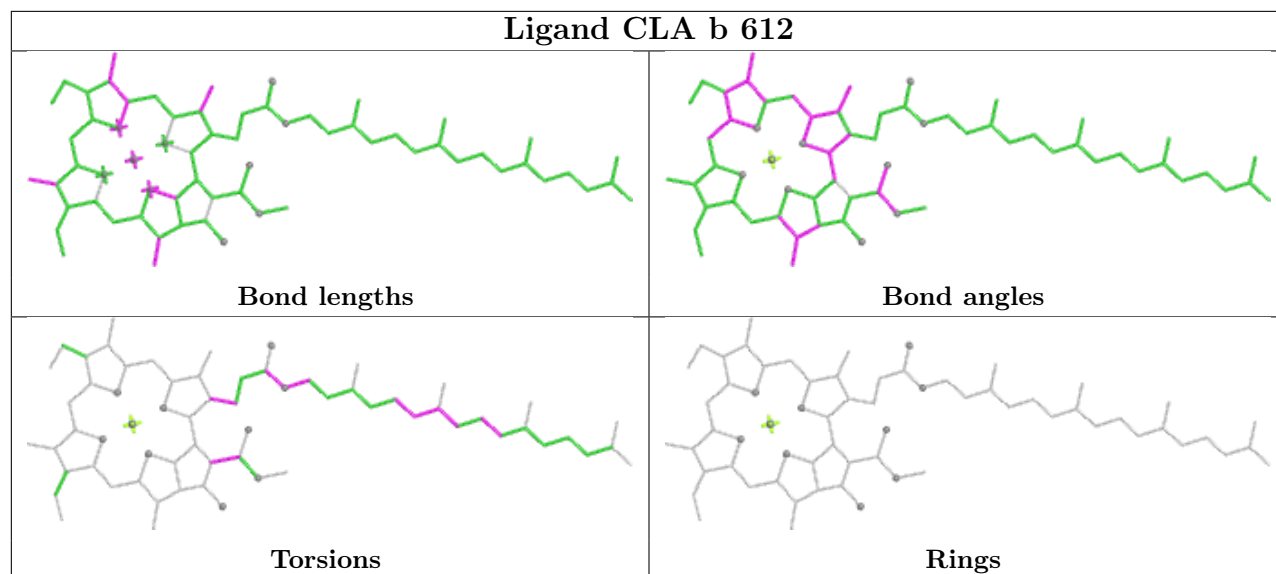




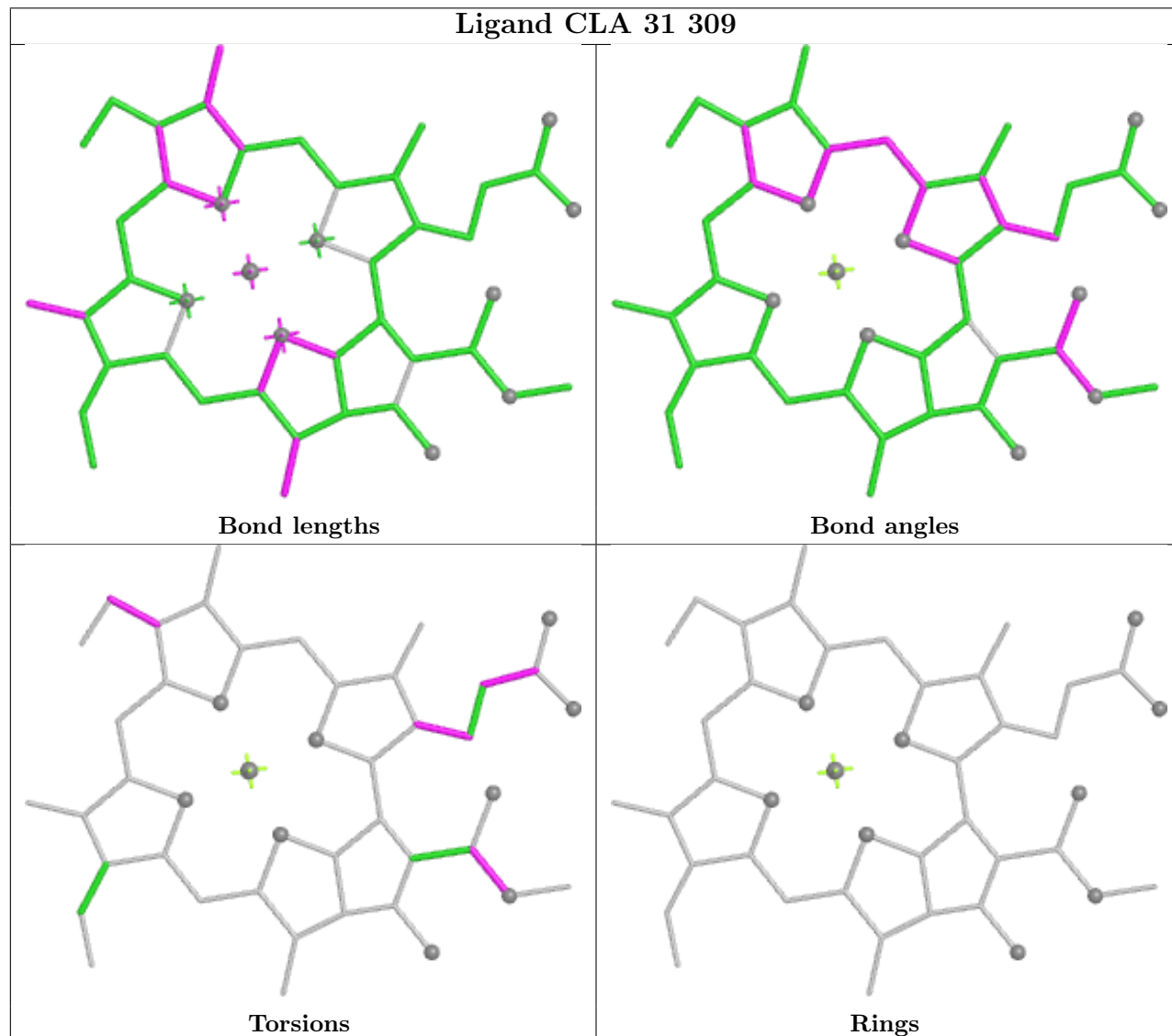


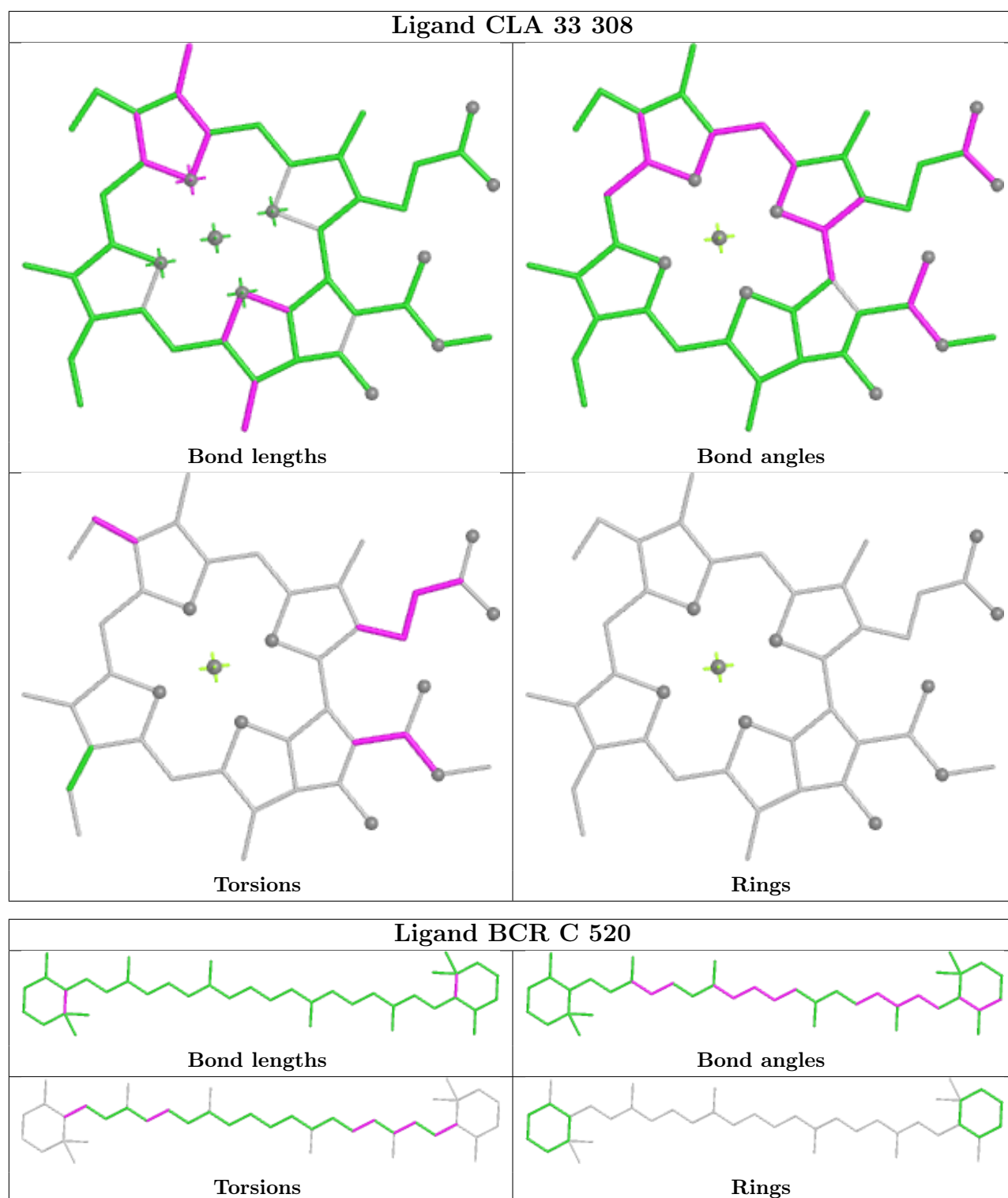


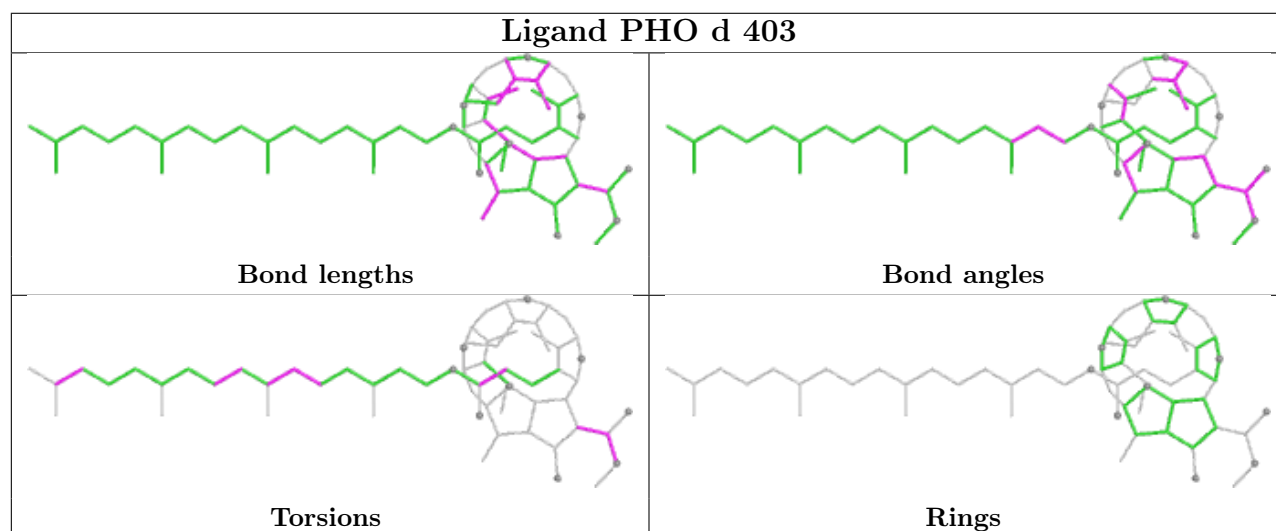
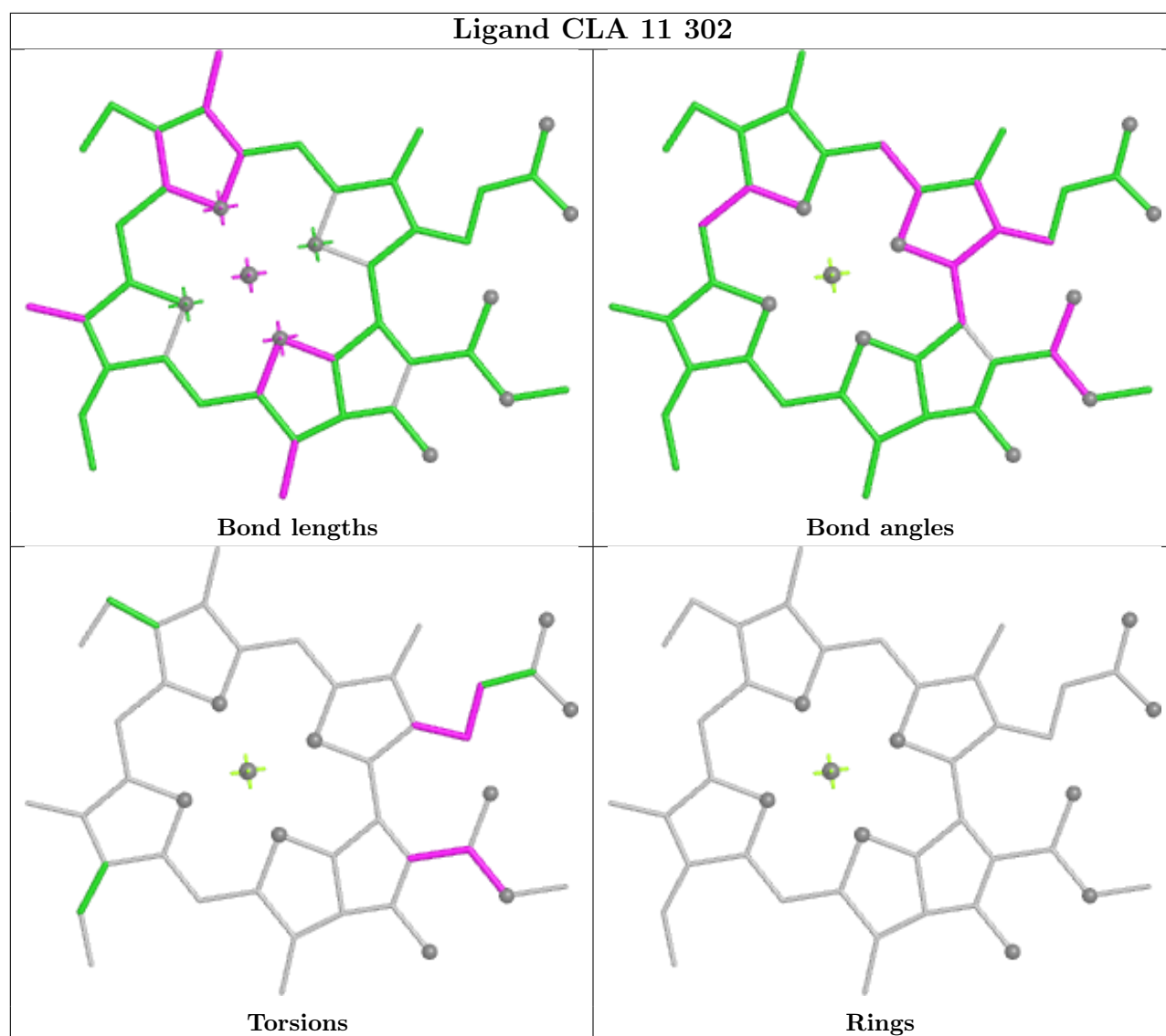
Ligand CLA b 612

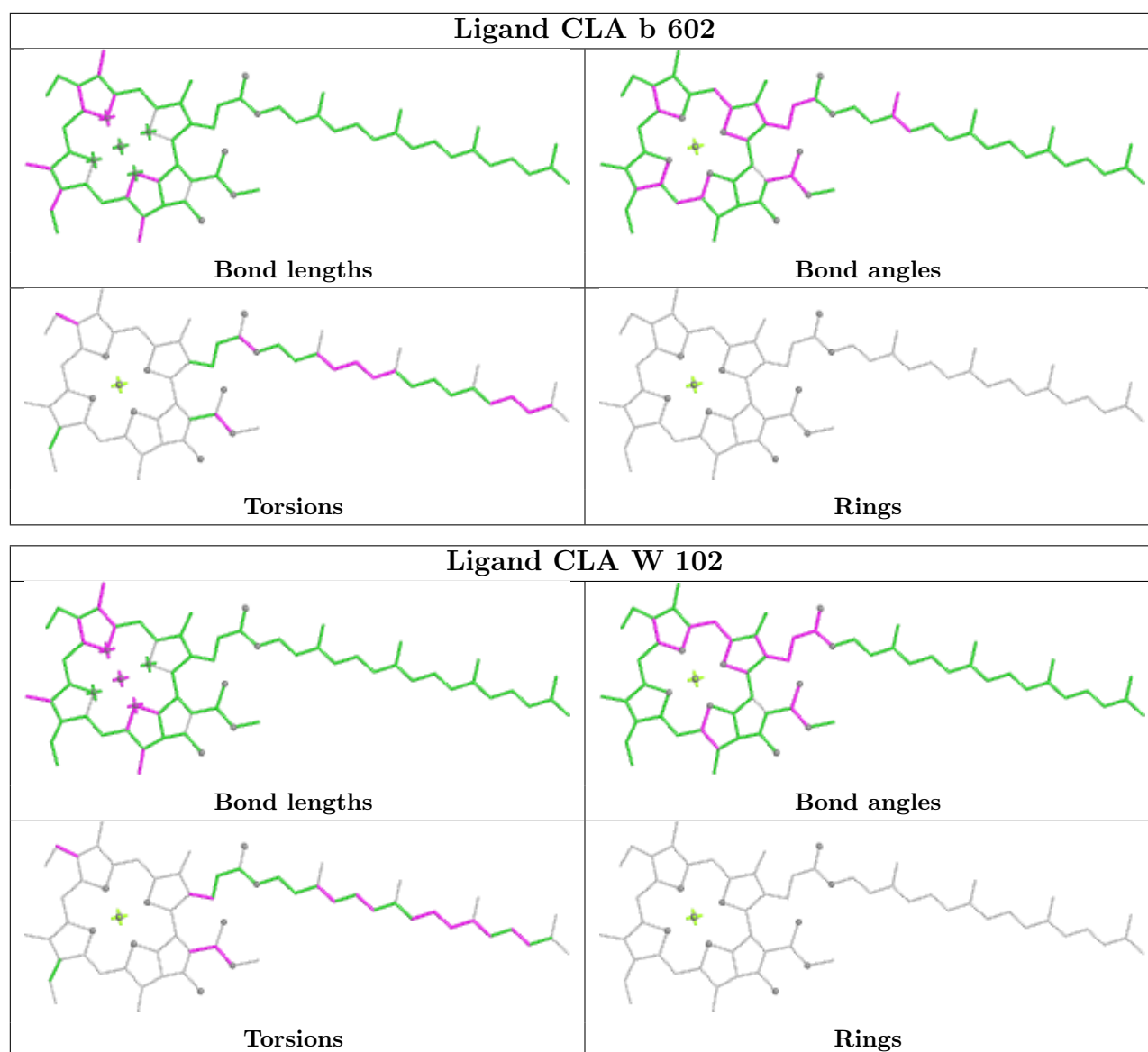


Ligand CLA 31 309









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.

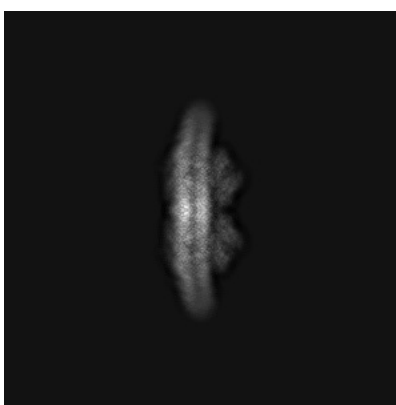
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

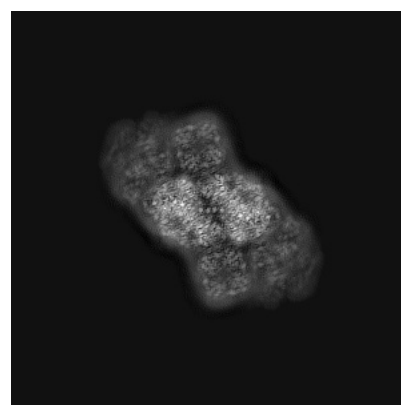
6.1.1 Primary map



X



Y



Z

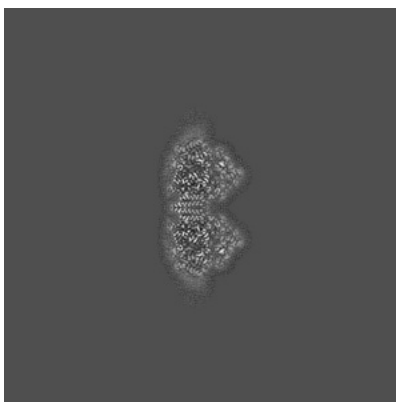
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

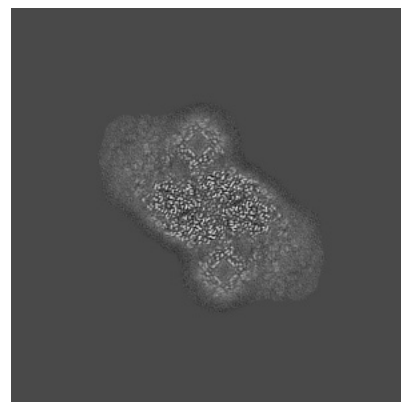
6.2.1 Primary map



X Index: 256



Y Index: 256

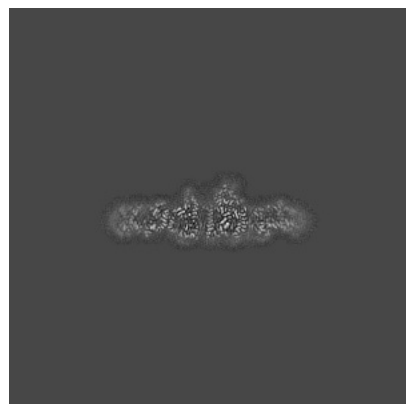


Z Index: 256

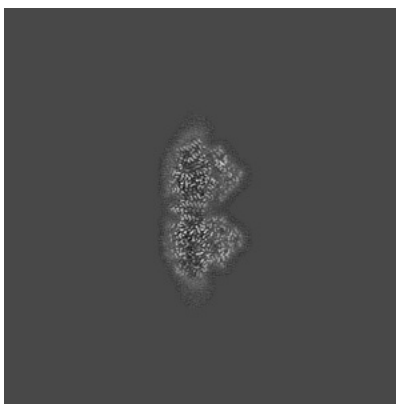
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

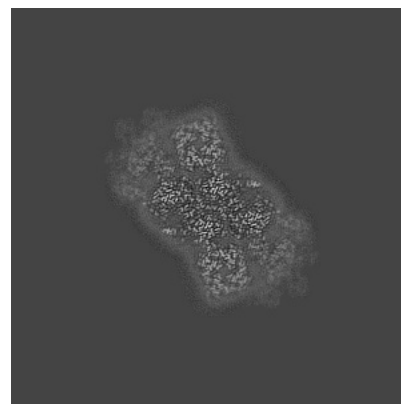
6.3.1 Primary map



X Index: 261



Y Index: 258

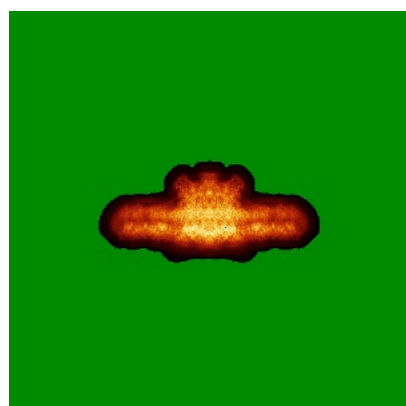


Z Index: 232

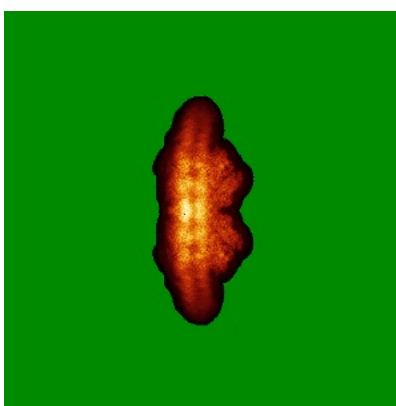
The images above show the largest variance slices of the map in three orthogonal directions.

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

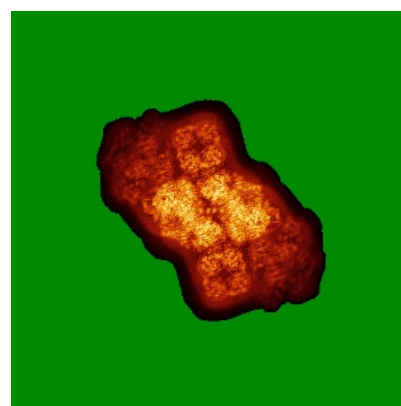
6.4.1 Primary map



X



Y

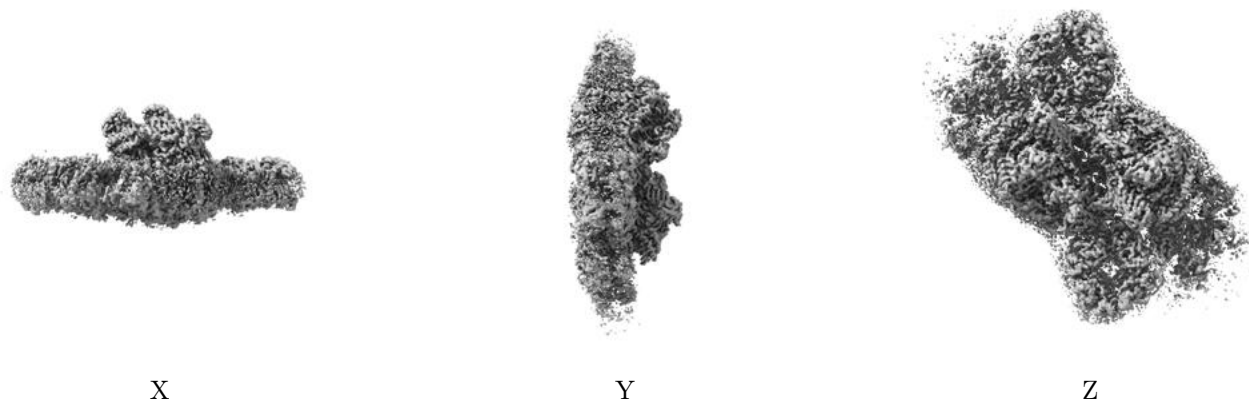


Z

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.

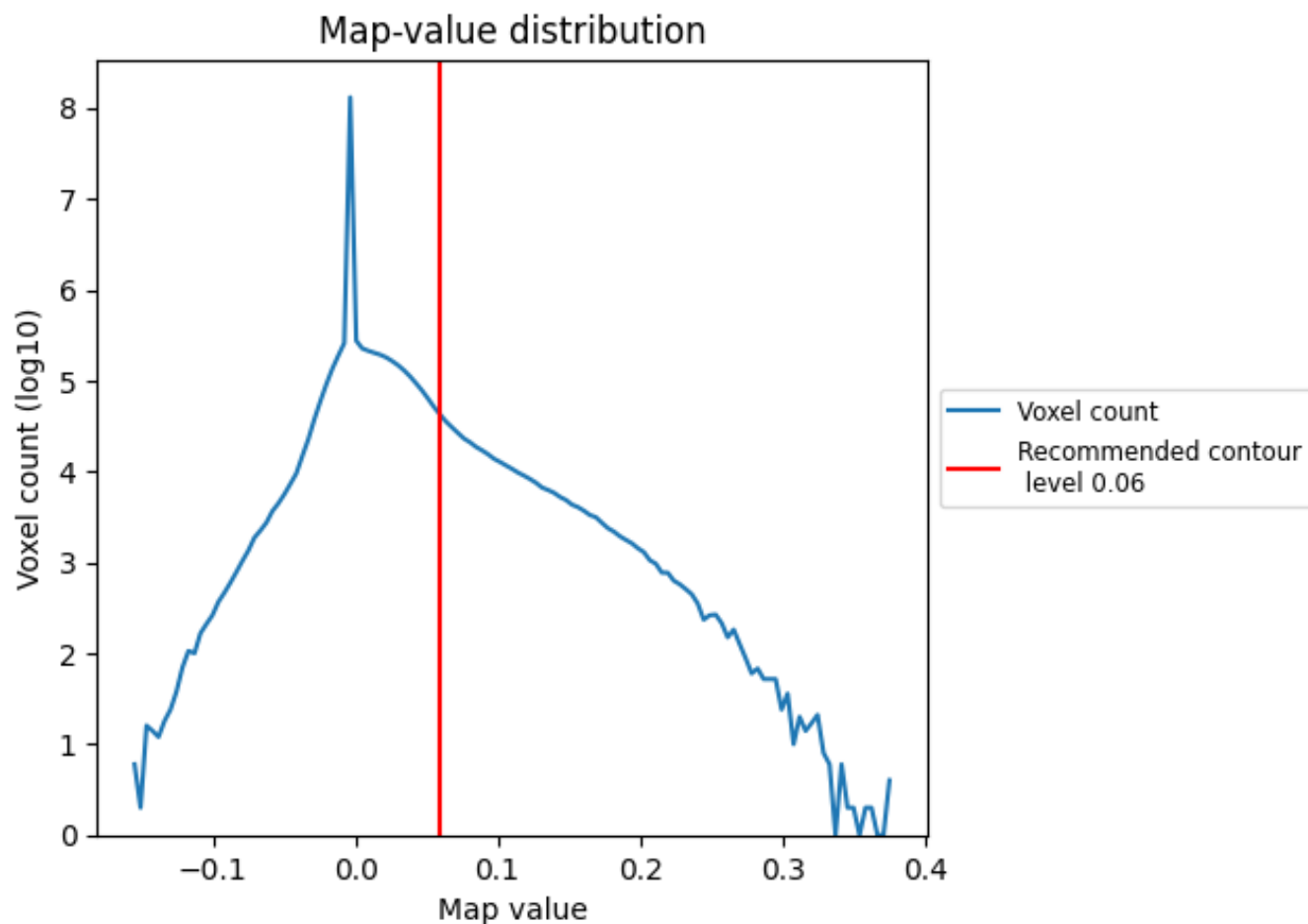
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

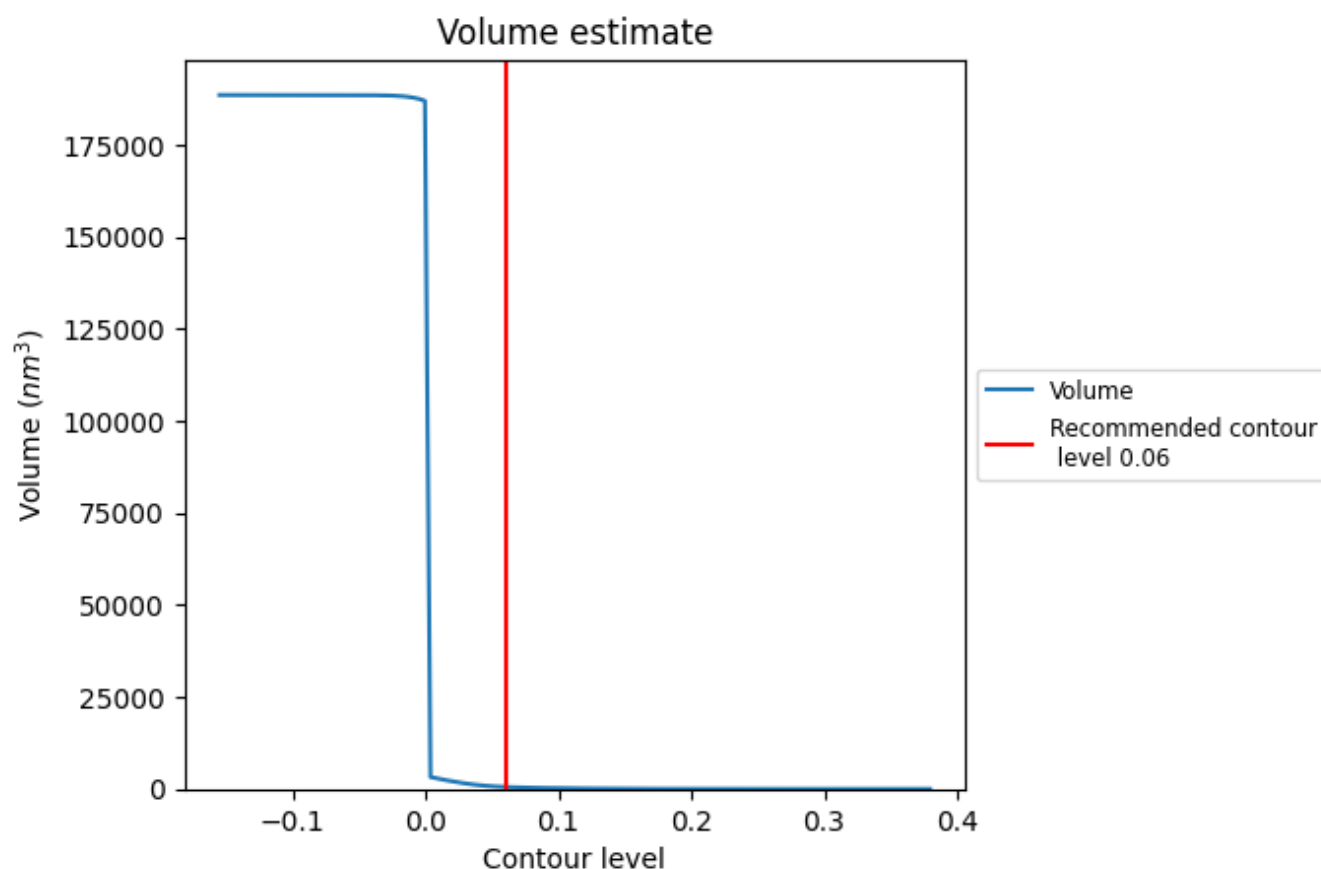
This section contains the results of statistical analysis of the map.

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.

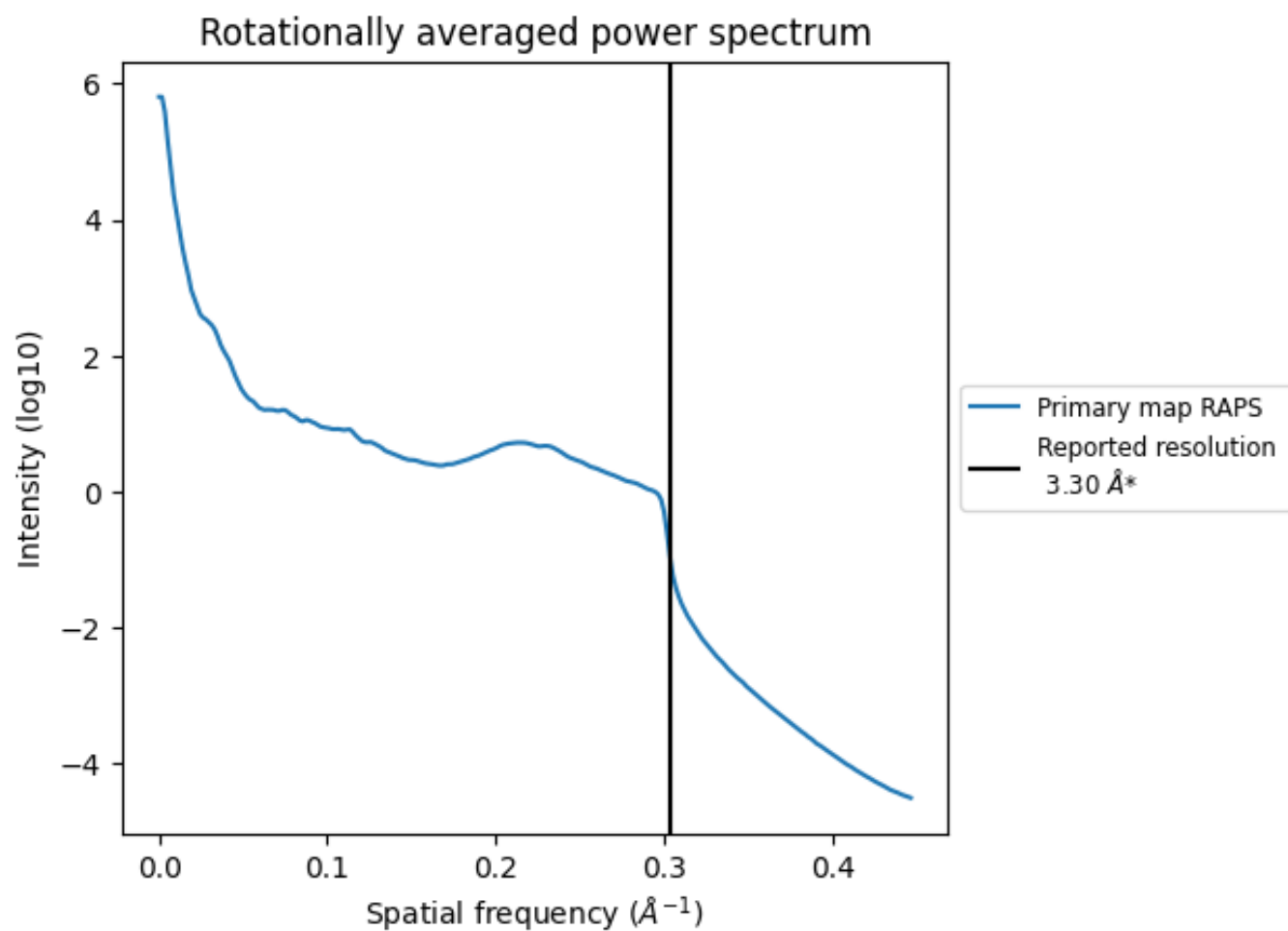
7.2 Volume estimate [i](#)



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 ⓘ

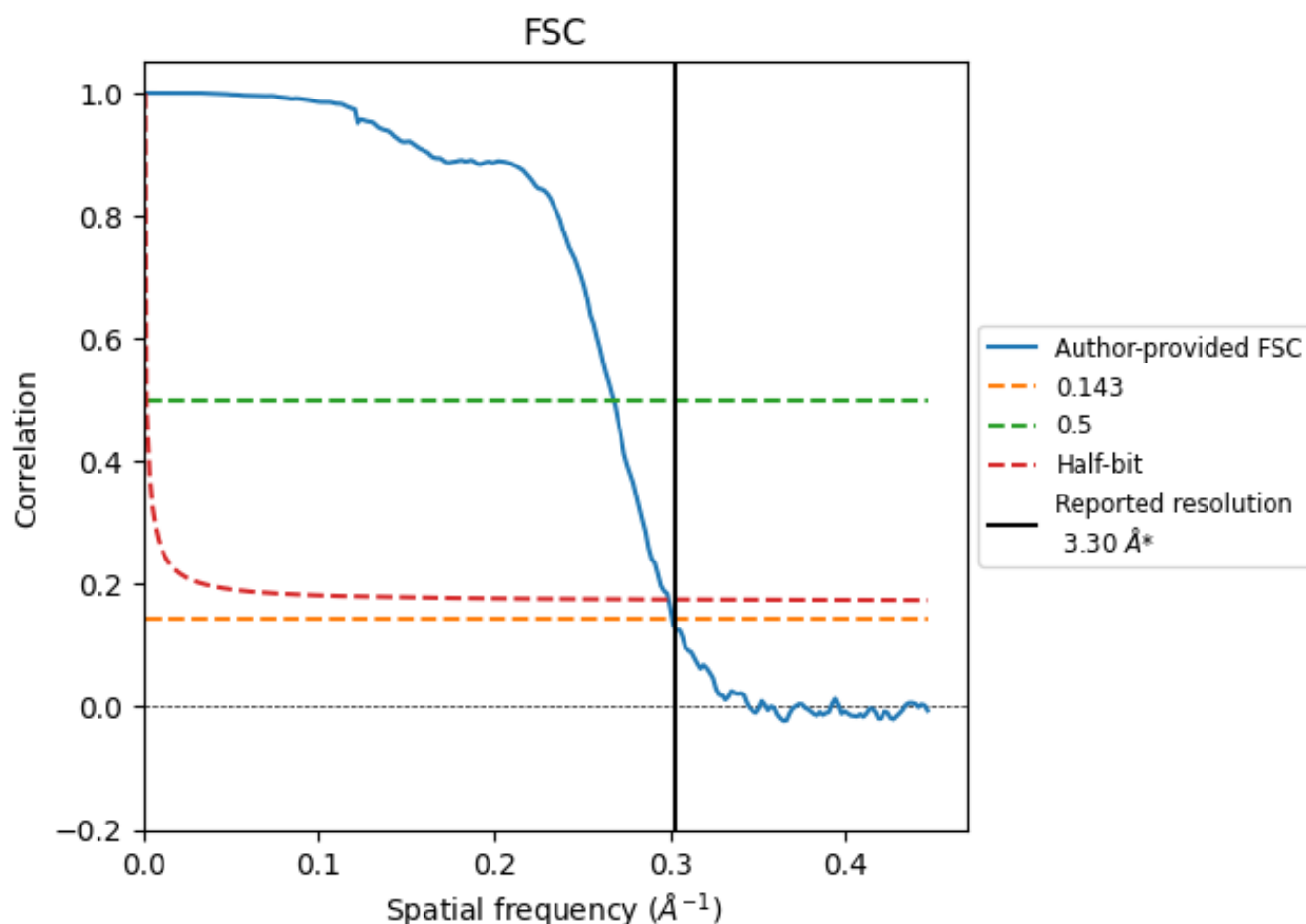


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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](#)

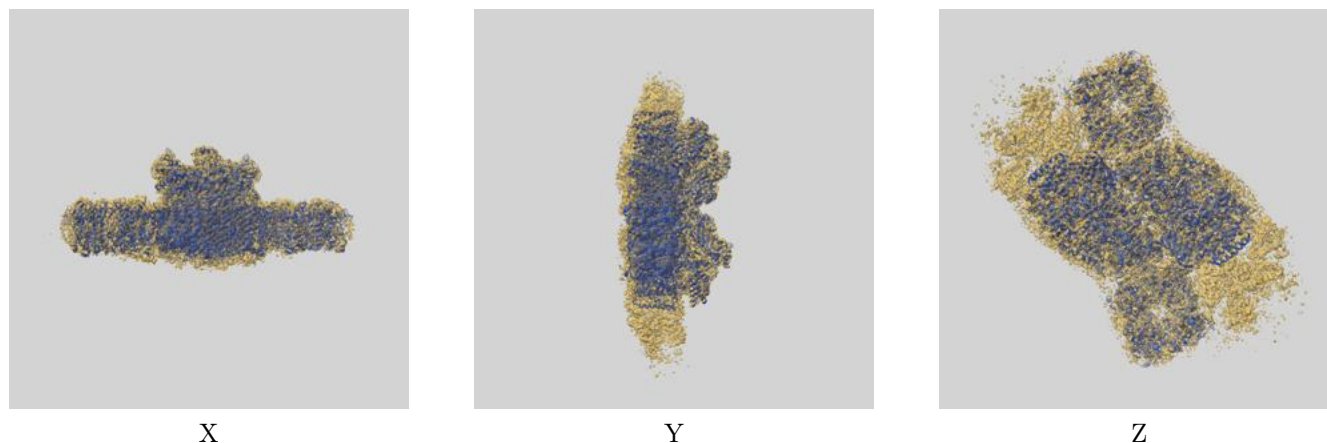
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.74	3.35
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

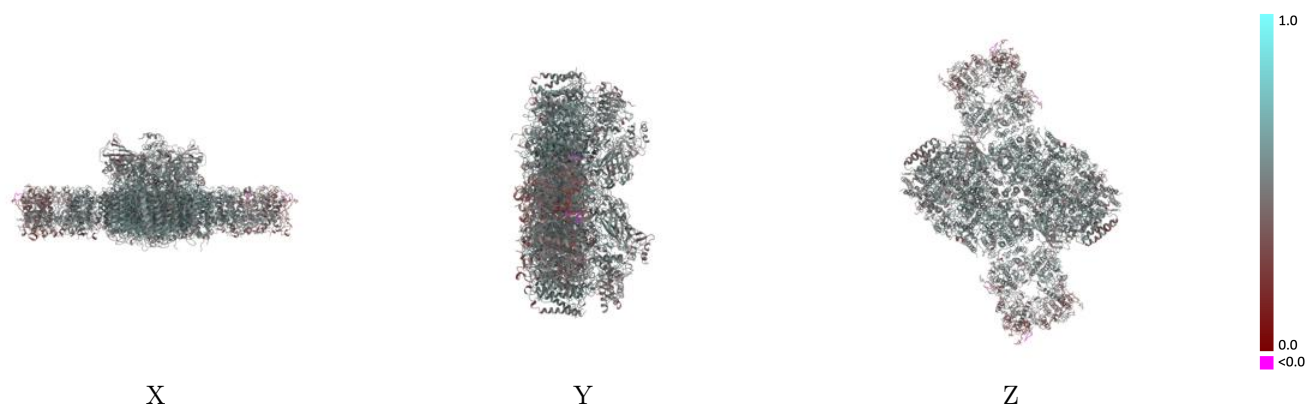
This section contains information regarding the fit between EMDB map EMD-9775 and PDB model 6J3Y. Per-residue inclusion information can be found in section [3](#) on page [32](#).

9.1 Map-model overlay [i](#)



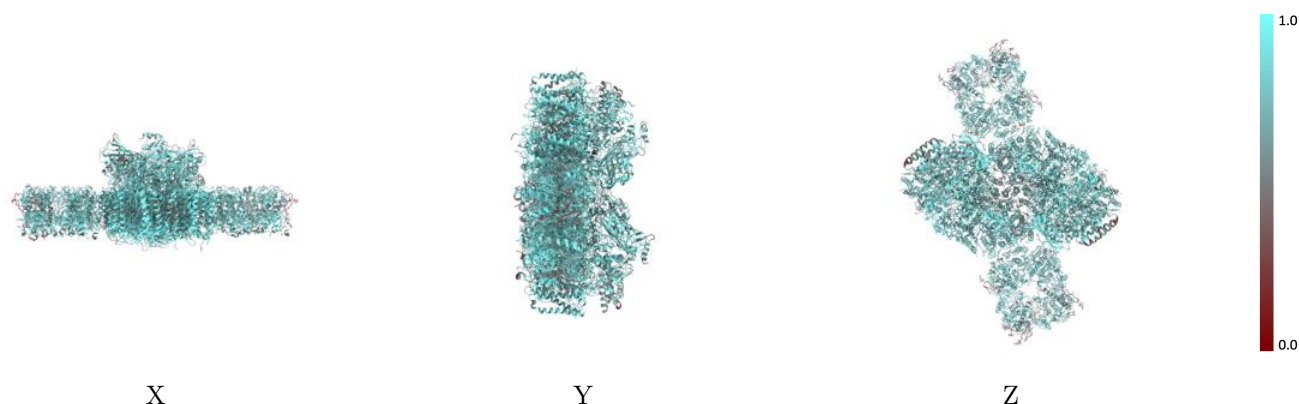
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



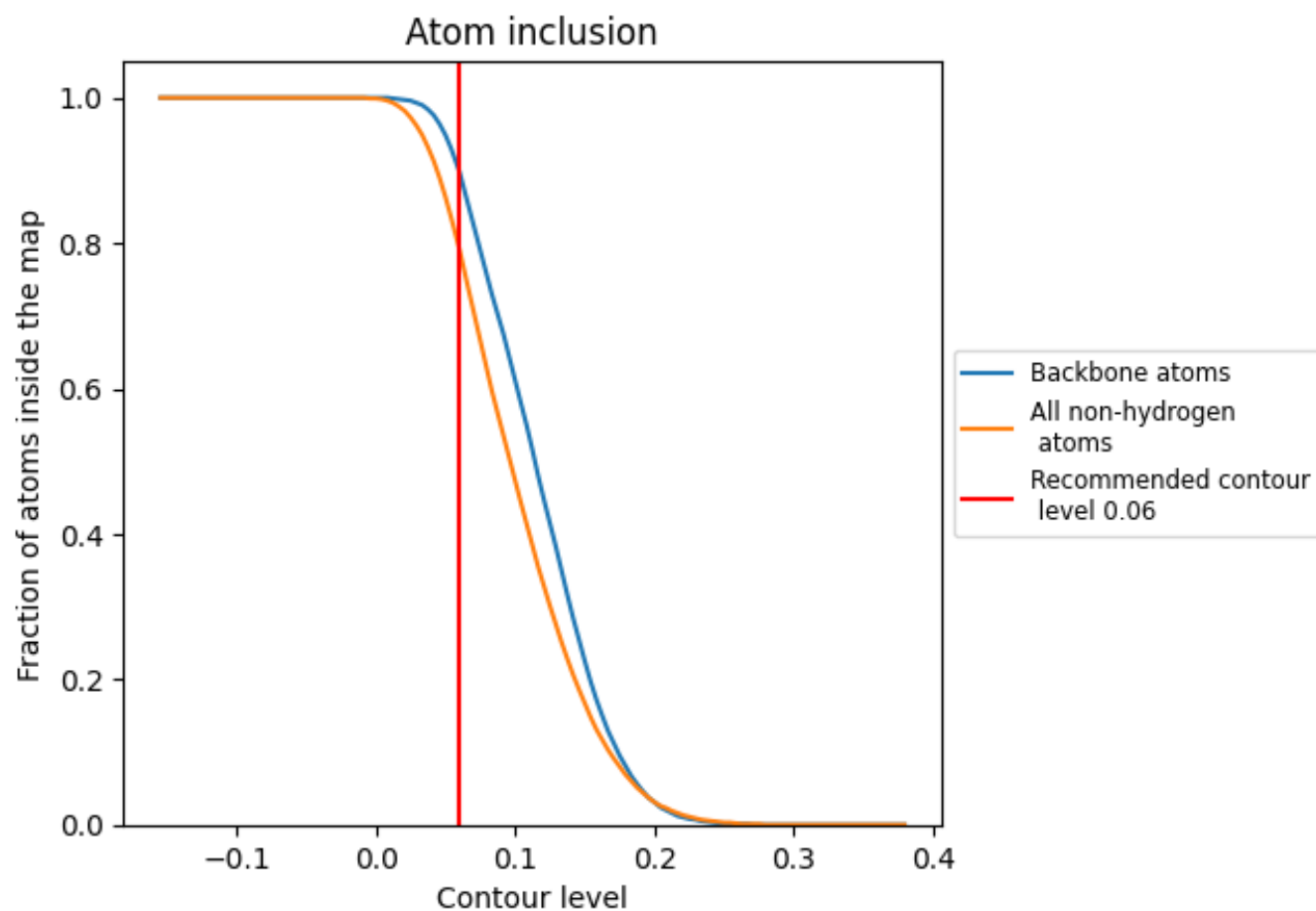
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

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



Continued on next page...

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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