



Full wwPDB EM Validation Report ⓘ

Mar 31, 2025 – 07:29 PM JST

PDB ID : 7CZL / pdb_00007czl
EMDB ID : EMD-30511
Title : Structural insights into a dimeric Psb27-photosystem II complex from a cyanobacterium *Thermosynechococcus vulcanus*
Authors : Pi, X.; Huang, G.; Xiao, Y.
Deposited on : 2020-09-09
Resolution : 3.78 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

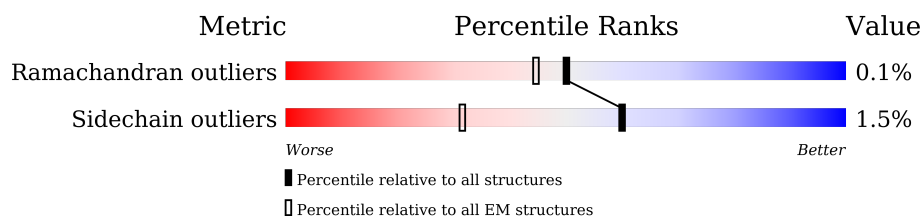
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.78 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	324	99%
1	a	324	98%
2	B	505	95%
2	b	505	96%
3	C	446	8% 100%
3	c	446	7% 100%
4	D	339	100%
4	d	339	100%
5	E	65	12% 100%

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Mol	Chain	Length	Quality of chain
5	e	65	
6	F	31	
6	f	31	
7	H	62	
7	h	62	
8	I	34	
8	i	34	
9	K	37	
9	k	37	
10	L	37	
10	l	37	
11	M	33	
11	m	33	
12	T	30	
12	t	30	
13	Z	62	
13	z	62	
14	Y	30	
14	y	30	
15	N	108	
15	n	108	
16	X	40	
16	x	40	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	A	401	X	-	-	-
17	CLA	A	402	X	-	-	-
17	CLA	A	403	X	-	-	-
17	CLA	A	405	X	-	-	-
17	CLA	B	601	X	-	-	-
17	CLA	B	602	X	-	-	-
17	CLA	B	603	X	-	-	-
17	CLA	B	604	X	-	-	-
17	CLA	B	605	X	-	-	-
17	CLA	B	606	X	-	-	-
17	CLA	B	607	X	-	-	-
17	CLA	B	608	X	-	-	-
17	CLA	B	609	X	-	-	-
17	CLA	B	610	X	-	-	-
17	CLA	B	611	X	-	-	-
17	CLA	B	612	X	-	-	-
17	CLA	B	613	X	-	-	-
17	CLA	B	614	X	-	-	-
17	CLA	B	615	X	-	-	-
17	CLA	B	616	X	-	-	-
17	CLA	C	501	X	-	-	-
17	CLA	C	502	X	-	-	-
17	CLA	C	503	X	-	-	-
17	CLA	C	504	X	-	-	-
17	CLA	C	505	X	-	-	-
17	CLA	C	506	X	-	-	-
17	CLA	C	507	X	-	-	-
17	CLA	C	508	X	-	-	-
17	CLA	C	509	X	-	-	-
17	CLA	C	510	X	-	-	-
17	CLA	C	511	X	-	-	-
17	CLA	C	512	X	-	-	-
17	CLA	C	513	X	-	-	-
17	CLA	D	404	X	-	-	-
17	CLA	D	405	X	-	-	-
17	CLA	a	5402	X	-	-	-
17	CLA	a	5403	X	-	-	-
17	CLA	a	5404	X	-	-	-
17	CLA	a	5406	X	-	-	-
17	CLA	b	5601	X	-	-	-
17	CLA	b	5602	X	-	-	-
17	CLA	b	5603	X	-	-	-
17	CLA	b	5604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	b	5605	X	-	-	-
17	CLA	b	5606	X	-	-	-
17	CLA	b	5607	X	-	-	-
17	CLA	b	5608	X	-	-	-
17	CLA	b	5609	X	-	-	-
17	CLA	b	5610	X	-	-	-
17	CLA	b	5611	X	-	-	-
17	CLA	b	5612	X	-	-	-
17	CLA	b	5613	X	-	-	-
17	CLA	b	5614	X	-	-	-
17	CLA	b	5615	X	-	-	-
17	CLA	b	5616	X	-	-	-
17	CLA	c	5501	X	-	-	-
17	CLA	c	5502	X	-	-	-
17	CLA	c	5503	X	-	-	-
17	CLA	c	5504	X	-	-	-
17	CLA	c	5505	X	-	-	-
17	CLA	c	5506	X	-	-	-
17	CLA	c	5507	X	-	-	-
17	CLA	c	5508	X	-	-	-
17	CLA	c	5509	X	-	-	-
17	CLA	c	5510	X	-	-	-
17	CLA	c	5511	X	-	-	-
17	CLA	c	5512	X	-	-	-
17	CLA	d	5403	X	-	-	-
17	CLA	d	5404	X	-	-	-
17	CLA	k	5501	X	-	-	-

2 Entry composition [i](#)

There are 30 unique types of molecules in this entry. The entry contains 40859 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 protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	324	Total	C	N	O	S	0	0
			2533	1662	414	442	15		
1	a	322	Total	C	N	O	S	0	0
			2523	1656	412	440	15		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	conflict	UNP P51765
A	286	THR	ALA	conflict	UNP P51765
a	5279	PRO	ARG	conflict	UNP P51765
a	5286	THR	ALA	conflict	UNP P51765

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	484	Total	C	N	O	S	0	0
			3784	2488	628	655	13		
2	b	484	Total	C	N	O	S	0	0
			3780	2486	628	653	13		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	506	ARG	LYS	conflict	UNP D0VWR1
b	5506	ARG	LYS	conflict	UNP D0VWR1

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	446	Total	C	N	O	S	0	0
			3412	2240	570	589	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	446	Total	C	N	O	S	0	0
			3412	2240	570	589	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	339	Total	C	N	O	S	0	0
			2693	1786	438	457	12		
4	d	339	Total	C	N	O	S	0	0
			2687	1783	435	457	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	65	Total	C	N	O	0	0
			522	345	81	96		
5	e	65	Total	C	N	O	0	0
			522	345	81	96		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	31	Total	C	N	O	S	0	0
			242	166	39	36	1		
6	f	28	Total	C	N	O	S	0	0
			219	149	36	33	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	62	Total	C	N	O	S	0	0
			482	324	75	81	2		
7	h	62	Total	C	N	O	S	0	0
			482	324	75	81	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	34	Total	C	N	O	S	0	0
			277	189	43	44	1		
8	i	34	Total	C	N	O	S	0	0
			277	189	43	44	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	K	37	Total	C	N	O	0	0
			289	201	42	46		
9	k	34	Total	C	N	O	0	0
			264	186	36	42		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	conflict	UNP P19054
K	39	TRP	VAL	conflict	UNP P19054
k	5033	LEU	PHE	conflict	UNP P19054
k	5039	TRP	VAL	conflict	UNP P19054

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	37	Total	C	N	O	0	0
			301	200	48	53		
10	l	37	Total	C	N	O	0	0
			301	200	48	53		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	33	Total	C	N	O	S	0	0
			258	172	38	47	1		
11	m	33	Total	C	N	O	S	0	0
			258	172	38	47	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	conflict	UNP P12312
m	5008	LEU	PHE	conflict	UNP P12312

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	30	Total	C	N	O	S	0	0
			254	179	36	37	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	t	30	Total	C	N	O	S	0	0
			254	179	36	37	2		

- Molecule 13 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Z	62	Total	C	N	O	S	0	0
			442	306	65	69	2		
13	z	62	Total	C	N	O	S	0	0
			442	306	65	69	2		

- Molecule 14 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Y	29	Total	C	N	O	S	0	0
			215	142	37	33	3		
14	y	29	Total	C	N	O	S	0	0
			215	142	37	33	3		

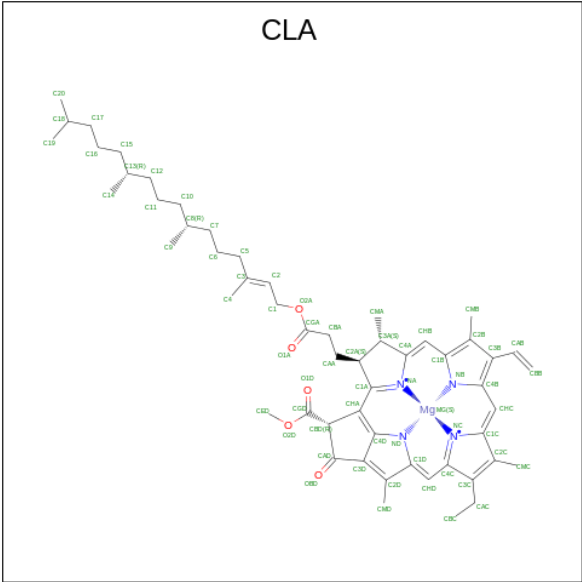
- Molecule 15 is a protein called Psb27.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	n	108	Total	C	N	O	S	0	0
			860	536	155	167	2		
15	N	108	Total	C	N	O	S	0	0
			860	536	155	167	2		

- Molecule 16 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	X	35	Total	C	N	O	0	0
			254	173	38	43		
16	x	35	Total	C	N	O	0	0
			254	173	38	43		

- Molecule 17 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	C	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	C	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	C	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
17	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	C	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	C	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	D	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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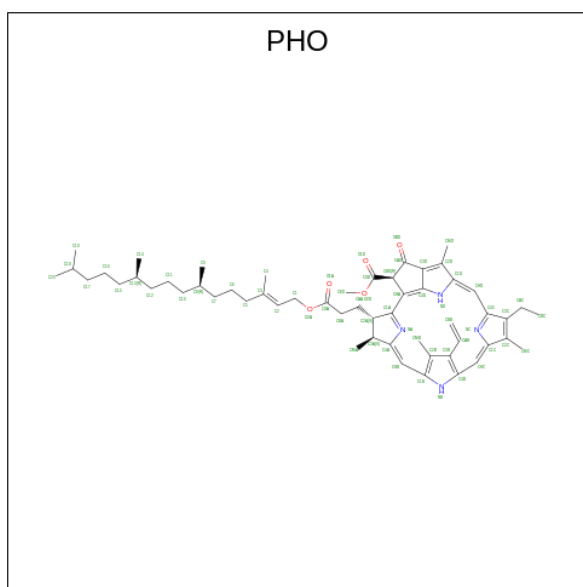
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17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	b	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 43	C 35	Mg 1	N 4	O 3	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 56	C 46	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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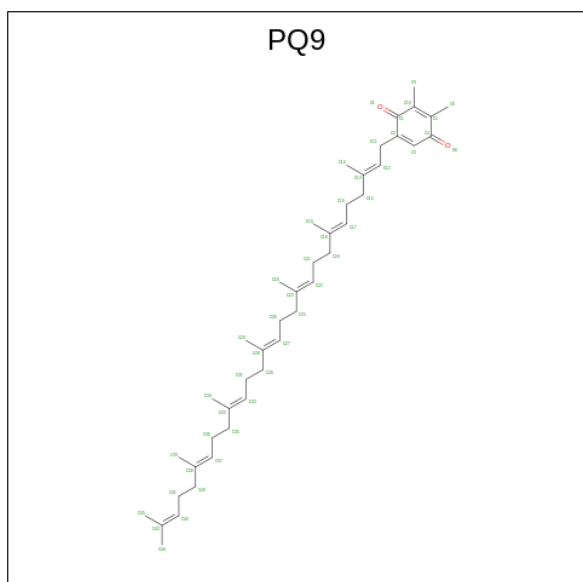
Mol	Chain	Residues	Atoms					AltConf
17	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	d	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	k	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 18 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



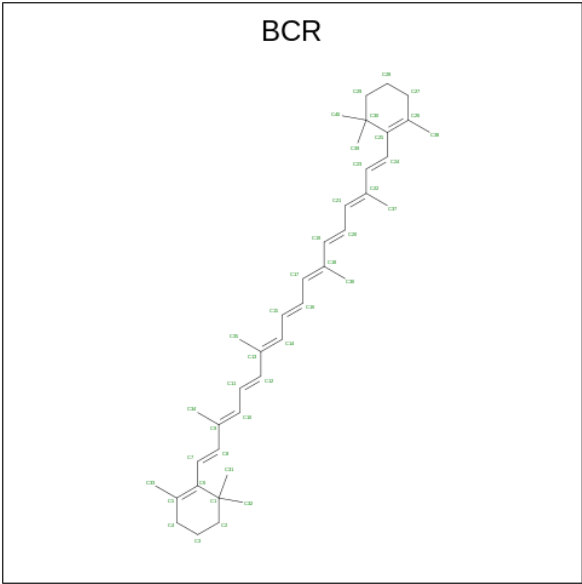
Mol	Chain	Residues	Atoms				AltConf
18	A	1	Total	C	N	O	0
			64	55	4	5	
18	D	1	Total	C	N	O	0
			64	55	4	5	
18	a	1	Total	C	N	O	0
			64	55	4	5	
18	d	1	Total	C	N	O	0
			64	55	4	5	

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



Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total	C	O	0
			45	43	2	
19	D	1	Total	C	O	0
			45	43	2	
19	a	1	Total	C	O	0
			30	28	2	
19	d	1	Total	C	O	0
			45	43	2	

- Molecule 20 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



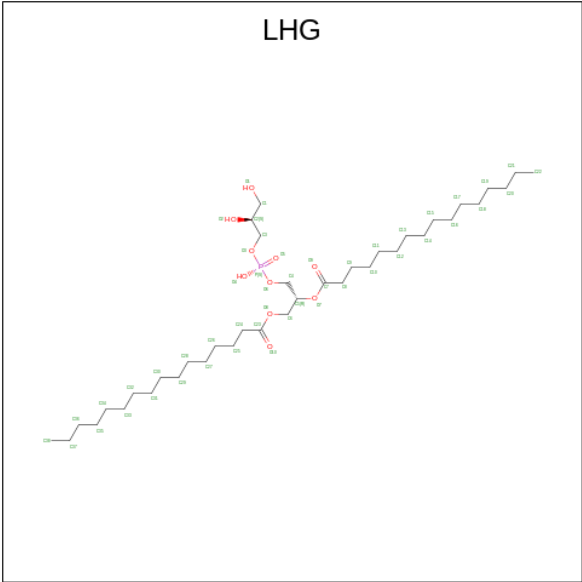
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	C	1	Total	C	0
			40	40	
20	C	1	Total	C	0
			40	40	
20	C	1	Total	C	0
			40	40	
20	D	1	Total	C	0
			40	40	
20	H	1	Total	C	0
			40	40	

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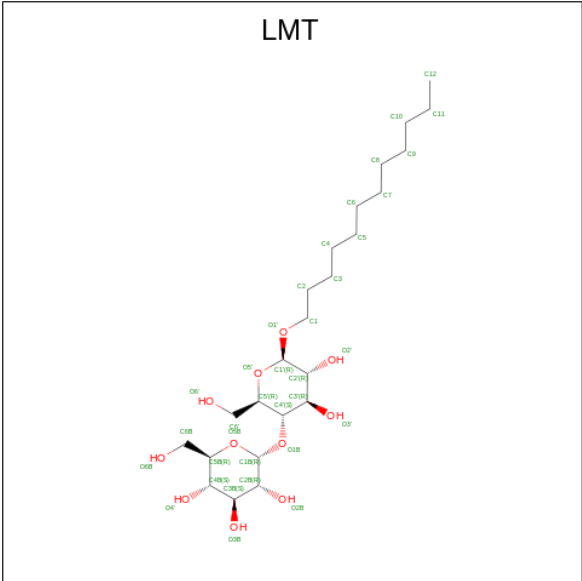
Mol	Chain	Residues	Atoms	AltConf
20	T	1	Total C 40 40	0
20	a	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	c	1	Total C 40 40	0
20	c	1	Total C 40 40	0
20	d	1	Total C 40 40	0
20	h	1	Total C 40 40	0
20	k	1	Total C 40 40	0
20	t	1	Total C 40 40	0
20	t	1	Total C 40 40	0
20	z	1	Total C 40 40	0
20	Y	1	Total C 40 40	0

- Molecule 21 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
21	A	1	Total	C	O	P	0
			39	28	10	1	
21	a	1	Total	C	O	P	0
			39	28	10	1	

- Molecule 22 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁) (labeled as "Ligand of Interest" by depositor).



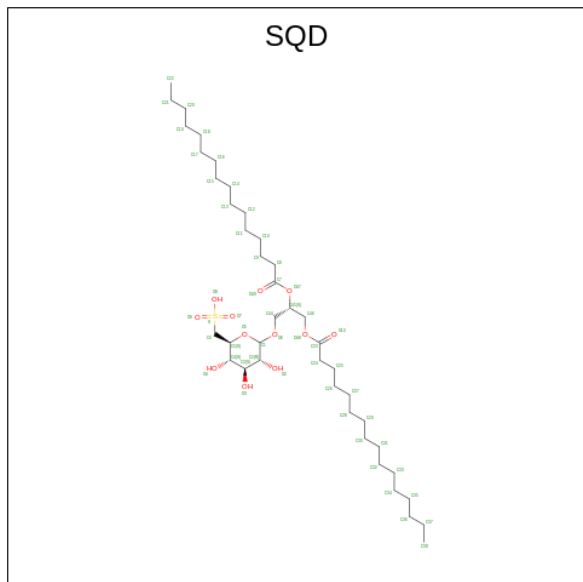
Mol	Chain	Residues	Atoms			AltConf
22	A	1	Total	C	O	0
			35	24	11	

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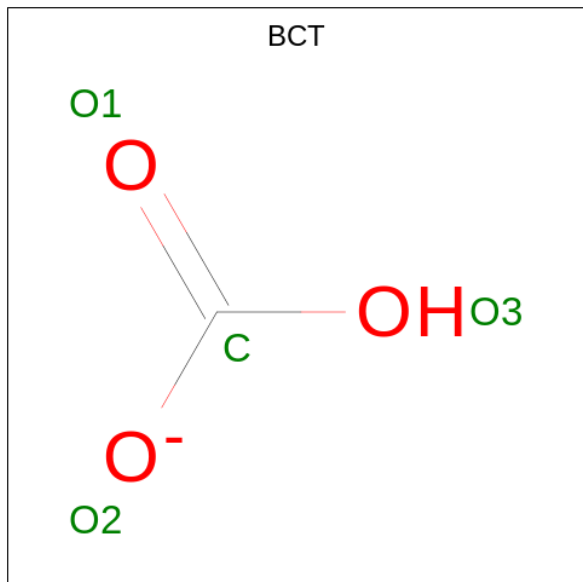
Mol	Chain	Residues	Atoms			AltConf
22	B	1	Total	C	O	0
			35	24	11	
22	M	1	Total	C	O	0
			35	24	11	
22	T	1	Total	C	O	0
			35	24	11	
22	a	1	Total	C	O	0
			35	24	11	
22	m	1	Total	C	O	0
			35	24	11	

- Molecule 23 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



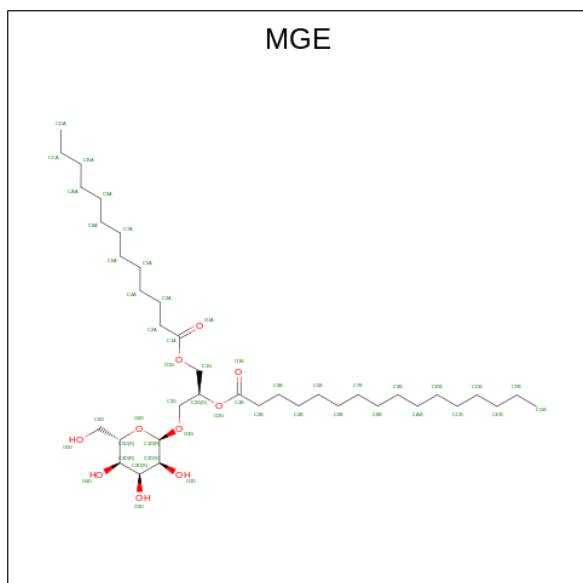
Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	S	0
			26	13	12	1	
23	D	1	Total	C	O	S	0
			54	41	12	1	
23	L	1	Total	C	O	S	0
			47	34	12	1	
23	a	1	Total	C	O	S	0
			26	13	12	1	
23	d	1	Total	C	O	S	0
			54	41	12	1	
23	l	1	Total	C	O	S	0
			47	34	12	1	

- Molecule 24 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



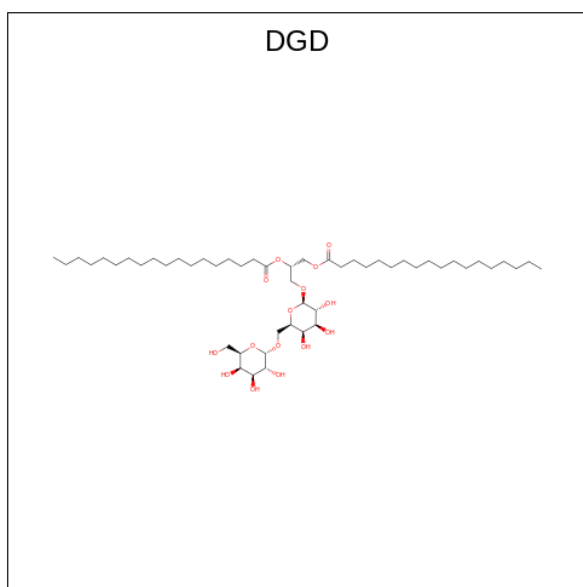
Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			4	1	3	
24	a	1	Total	C	O	0
			4	1	3	

- Molecule 25 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (CCD ID: MGE) (formula: $\text{C}_{38}\text{H}_{72}\text{O}_{10}$).



Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			48	38	10	
25	B	1	Total	C	O	0
			48	38	10	
25	C	1	Total	C	O	0
			48	38	10	
25	D	1	Total	C	O	0
			47	37	10	
25	D	1	Total	C	O	0
			41	31	10	
25	D	1	Total	C	O	0
			48	38	10	
25	b	1	Total	C	O	0
			48	38	10	
25	c	1	Total	C	O	0
			48	38	10	
25	d	1	Total	C	O	0
			47	37	10	
25	d	1	Total	C	O	0
			41	31	10	
25	d	1	Total	C	O	0
			48	38	10	
25	l	1	Total	C	O	0
			48	38	10	
25	m	1	Total	C	O	0
			48	38	10	
25	m	1	Total	C	O	0
			48	38	10	

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
26	C	1	Total	C	O	0
			53	38	15	
26	C	1	Total	C	O	0
			47	32	15	
26	C	1	Total	C	O	0
			57	42	15	
26	H	1	Total	C	O	0
			54	39	15	
26	a	1	Total	C	O	0
			57	42	15	
26	c	1	Total	C	O	0
			53	38	15	
26	c	1	Total	C	O	0
			47	32	15	
26	h	1	Total	C	O	0
			54	39	15	

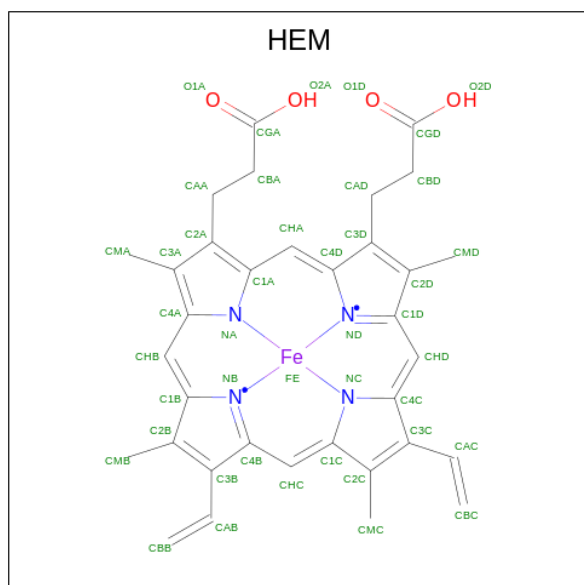
- Molecule 27 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
27	C	1	Total	Ca	0
			1	1	
27	c	1	Total	Ca	0
			1	1	

- Molecule 28 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
28	D	1	Total Fe 1 1	0
28	d	1	Total Fe 1 1	0

- Molecule 29 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
29	F	1	Total 43	C 34	Fe 1	N 4	O 4	0
29	f	1	Total 43	C 34	Fe 1	N 4	O 4	0

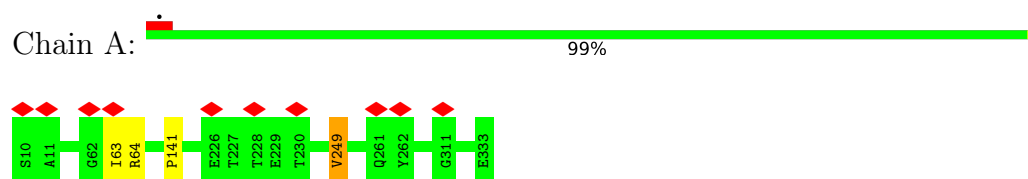
- Molecule 30 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
30	n	1	Total 1	Cl 1	0
30	N	1	Total 1	Cl 1	0

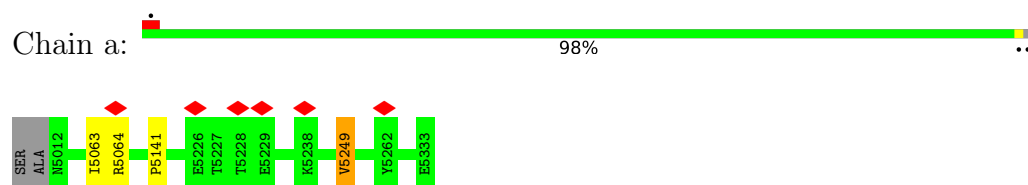
3 Residue-property plots [i](#)

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

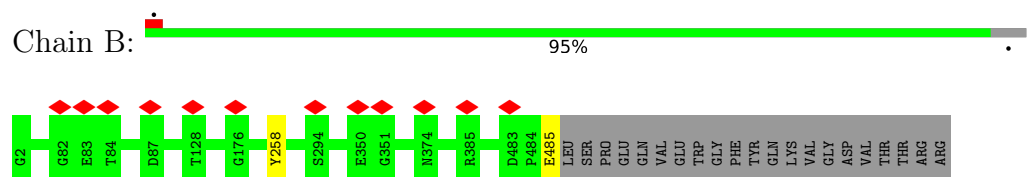
- Molecule 1: Photosystem II protein D1



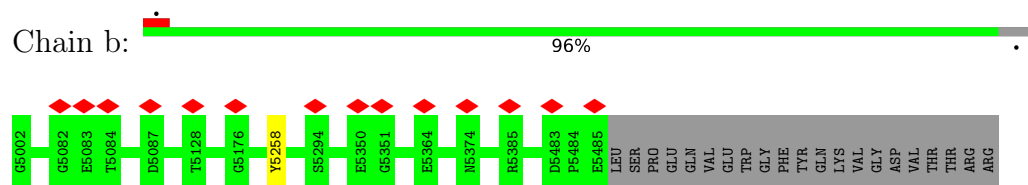
- Molecule 1: Photosystem II protein D1



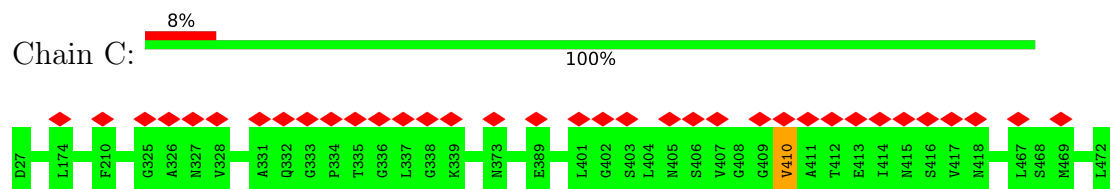
- Molecule 2: Photosystem II CP47 reaction center protein



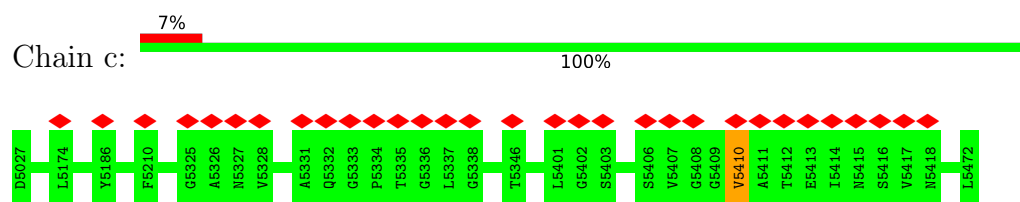
- Molecule 2: Photosystem II CP47 reaction center protein



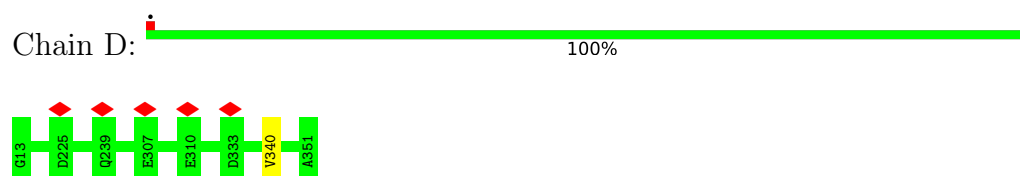
- Molecule 3: Photosystem II CP43 reaction center protein



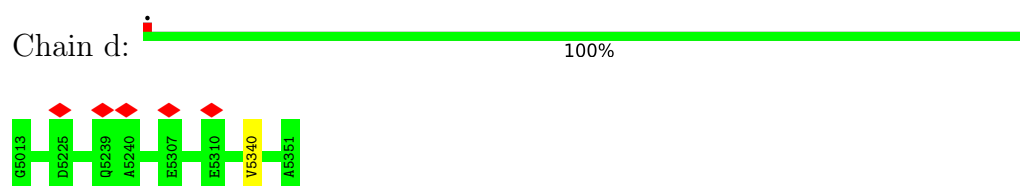
- Molecule 3: Photosystem II CP43 reaction center protein



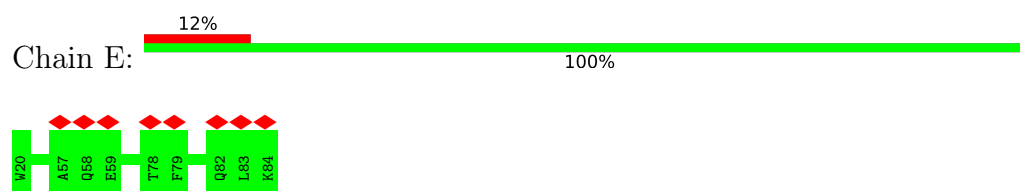
- Molecule 4: Photosystem II D2 protein



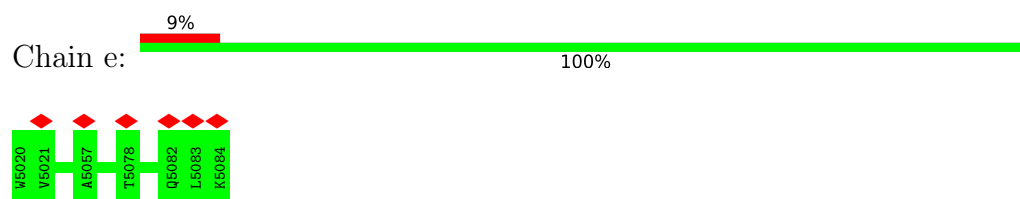
- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha

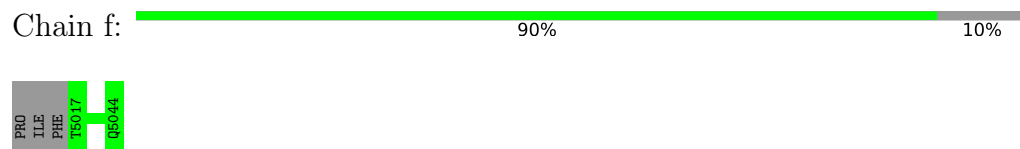


- Molecule 6: Cytochrome b559 subunit beta



There are no outlier residues recorded for this chain.

- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H

Chain H:  100%



- Molecule 7: Photosystem II reaction center protein H

Chain h:  100%



- Molecule 8: Photosystem II reaction center protein I

Chain I:  100%

There are no outlier residues recorded for this chain.

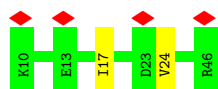
- Molecule 8: Photosystem II reaction center protein I

Chain i:  100%


There are no outlier residues recorded for this chain.

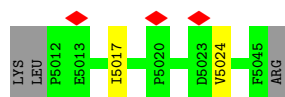
- Molecule 9: Photosystem II reaction center protein K

Chain K:  11% 95% 5%



- Molecule 9: Photosystem II reaction center protein K

Chain k:  8% 86% 5% 8%



- Molecule 10: Photosystem II reaction center protein L

Chain L:  5% 100%



- Molecule 10: Photosystem II reaction center protein L



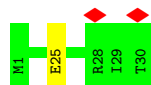
- Molecule 11: Photosystem II reaction center protein M



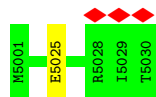
- Molecule 11: Photosystem II reaction center protein M



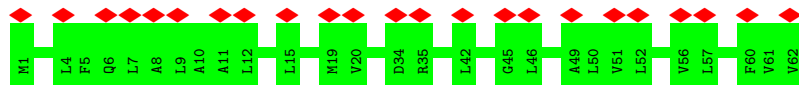
- Molecule 12: Photosystem II reaction center protein T



- Molecule 12: Photosystem II reaction center protein T

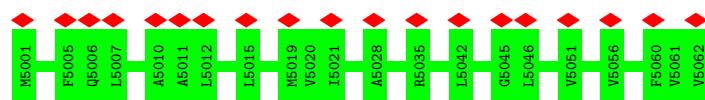


- Molecule 13: Photosystem II reaction center protein Z



- Molecule 13: Photosystem II reaction center protein Z

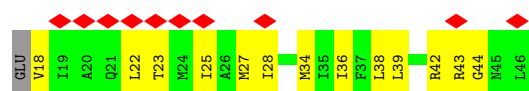




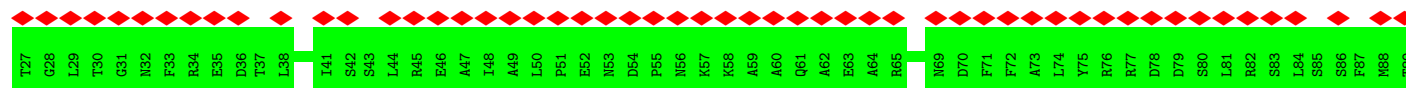
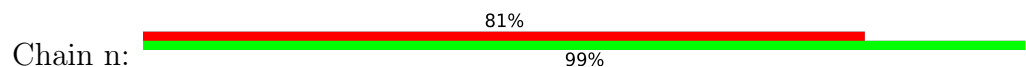
- Molecule 14: Photosystem II reaction center protein Ycf12



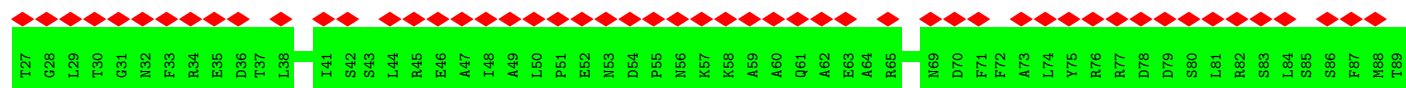
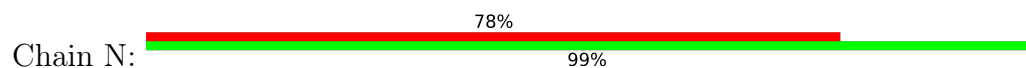
- Molecule 14: Photosystem II reaction center protein Ycf12



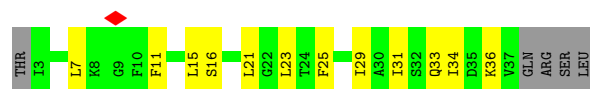
- Molecule 15: Psb27



- Molecule 15: Psb27



- Molecule 16: Photosystem II reaction center protein X



- Molecule 16: Photosystem II reaction center protein X



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87473	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.227	Depositor
Minimum map value	-0.125	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.038	Depositor
Map size (\AA)	313.5696, 313.5696, 313.5696	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.30654, 1.30654, 1.30654	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BCT, FE2, HEM, CL, CLA, MGE, PQ9, DGD, BCR, LMT, PHO, LHG, SQD

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	1/2615 (0.0%)	0.56	1/3568 (0.0%)
1	a	0.52	1/2605 (0.0%)	0.54	1/3554 (0.0%)
2	B	0.54	1/3919 (0.0%)	0.54	0/5343
2	b	0.53	0/3915	0.54	1/5338 (0.0%)
3	C	0.47	0/3524	0.54	1/4804 (0.0%)
3	c	0.47	0/3524	0.54	1/4804 (0.0%)
4	D	0.56	1/2788 (0.0%)	0.55	0/3802
4	d	0.56	1/2782 (0.0%)	0.54	0/3795
5	E	0.42	0/538	0.51	0/737
5	e	0.42	0/538	0.51	0/737
6	F	0.37	0/250	0.47	0/342
6	f	0.37	0/225	0.46	0/308
7	H	0.44	0/495	0.52	0/678
7	h	0.44	0/495	0.52	0/678
8	I	0.49	0/284	0.48	0/384
8	i	0.48	0/284	0.48	0/384
9	K	0.43	0/299	0.52	0/412
9	k	0.44	0/274	0.52	0/379
10	L	0.49	0/308	0.53	0/419
10	l	0.50	0/308	0.53	0/419
11	M	0.46	0/261	0.55	0/356
11	m	0.46	0/261	0.53	0/356
12	T	0.57	0/263	0.51	0/356
12	t	0.57	0/263	0.51	0/356
13	Z	0.30	0/451	0.38	0/620
13	z	0.30	0/451	0.38	0/620
14	Y	0.21	0/216	0.40	0/289
14	y	0.30	0/216	0.87	1/289 (0.3%)
15	N	0.31	0/873	0.46	0/1172
15	n	0.30	0/873	0.44	0/1172
16	X	0.28	0/257	0.46	0/348
16	x	0.25	0/257	0.40	0/348

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.49	5/34612 (0.0%)	0.53	6/47167 (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	2
1	a	0	2
9	K	0	2
9	k	0	2
14	y	0	1
All	All	0	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	249	VAL	CB-CG1	-6.56	1.39	1.52
2	B	258	TYR	CD2-CE2	-5.75	1.30	1.39
1	a	5249	VAL	CB-CG1	5.60	1.64	1.52
4	D	340	VAL	C-N	-5.60	1.21	1.34
4	d	5340	VAL	C-N	-5.58	1.21	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	VAL	CG1-CB-CG2	-9.95	94.98	110.90
14	y	28	ILE	C-N-CA	-8.60	104.23	122.30
3	c	5410	VAL	CG1-CB-CG2	-8.48	97.33	110.90
1	a	5249	VAL	CG1-CB-CG2	7.65	123.14	110.90
2	b	5258	TYR	CZ-CE2-CD2	-6.36	114.08	119.80
3	C	410	VAL	CG1-CB-CG2	5.79	120.17	110.90

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	63	ILE	Mainchain
1	A	64	ARG	Peptide
9	K	17	ILE	Peptide

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Mol	Chain	Res	Type	Group
9	K	24	VAL	Peptide
1	a	5063	ILE	Mainchain
1	a	5064	ARG	Peptide
9	k	5017	ILE	Peptide
9	k	5024	VAL	Peptide
14	y	18	VAL	Mainchain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	322/324 (99%)	300 (93%)	21 (6%)	1 (0%)	37	68
1	a	320/324 (99%)	299 (93%)	20 (6%)	1 (0%)	37	68
2	B	482/505 (95%)	453 (94%)	29 (6%)	0	100	100
2	b	482/505 (95%)	452 (94%)	30 (6%)	0	100	100
3	C	444/446 (100%)	408 (92%)	36 (8%)	0	100	100
3	c	444/446 (100%)	408 (92%)	36 (8%)	0	100	100
4	D	337/339 (99%)	292 (87%)	45 (13%)	0	100	100
4	d	337/339 (99%)	293 (87%)	44 (13%)	0	100	100
5	E	63/65 (97%)	50 (79%)	13 (21%)	0	100	100
5	e	63/65 (97%)	51 (81%)	12 (19%)	0	100	100
6	F	29/31 (94%)	23 (79%)	6 (21%)	0	100	100
6	f	26/31 (84%)	22 (85%)	4 (15%)	0	100	100
7	H	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
7	h	60/62 (97%)	57 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	I	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
8	i	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
9	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
9	k	32/37 (86%)	31 (97%)	1 (3%)	0	100	100
10	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
10	l	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	M	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
11	m	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
12	T	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
12	t	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
13	Z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
13	z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
14	Y	27/30 (90%)	23 (85%)	3 (11%)	1 (4%)	2	23
14	y	27/30 (90%)	24 (89%)	2 (7%)	1 (4%)	2	23
15	N	106/108 (98%)	92 (87%)	13 (12%)	1 (1%)	14	47
15	n	106/108 (98%)	94 (89%)	11 (10%)	1 (1%)	14	47
16	X	33/40 (82%)	31 (94%)	2 (6%)	0	100	100
16	x	33/40 (82%)	31 (94%)	2 (6%)	0	100	100
All	All	4240/4366 (97%)	3875 (91%)	359 (8%)	6 (0%)	50	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	Y	45	ASN
14	y	44	GLY
1	A	141	PRO
1	a	5141	PRO
15	n	124	VAL
15	N	124	VAL

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	260/262 (99%)	259 (100%)	1 (0%)	89	93
1	a	260/262 (99%)	259 (100%)	1 (0%)	89	93
2	B	379/403 (94%)	378 (100%)	1 (0%)	91	94
2	b	378/403 (94%)	378 (100%)	0	100	100
3	C	340/348 (98%)	339 (100%)	1 (0%)	91	94
3	c	340/348 (98%)	339 (100%)	1 (0%)	91	94
4	D	273/274 (100%)	273 (100%)	0	100	100
4	d	272/274 (99%)	272 (100%)	0	100	100
5	E	55/57 (96%)	55 (100%)	0	100	100
5	e	55/57 (96%)	55 (100%)	0	100	100
6	F	24/25 (96%)	24 (100%)	0	100	100
6	f	22/25 (88%)	22 (100%)	0	100	100
7	H	50/53 (94%)	50 (100%)	0	100	100
7	h	50/53 (94%)	50 (100%)	0	100	100
8	I	31/31 (100%)	31 (100%)	0	100	100
8	i	31/31 (100%)	31 (100%)	0	100	100
9	K	29/30 (97%)	29 (100%)	0	100	100
9	k	27/30 (90%)	27 (100%)	0	100	100
10	L	34/35 (97%)	34 (100%)	0	100	100
10	l	34/35 (97%)	34 (100%)	0	100	100
11	M	30/30 (100%)	30 (100%)	0	100	100
11	m	30/30 (100%)	30 (100%)	0	100	100
12	T	26/27 (96%)	25 (96%)	1 (4%)	28	53
12	t	26/27 (96%)	25 (96%)	1 (4%)	28	53
13	Z	43/52 (83%)	43 (100%)	0	100	100
13	z	43/52 (83%)	43 (100%)	0	100	100
14	Y	22/23 (96%)	11 (50%)	11 (50%)	0	0
14	y	22/23 (96%)	12 (54%)	10 (46%)	0	0
15	N	92/92 (100%)	92 (100%)	0	100	100
15	n	92/92 (100%)	92 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	X	28/33 (85%)	16 (57%)	12 (43%)	0	0
16	x	28/33 (85%)	16 (57%)	12 (43%)	0	0
All	All	3426/3550 (96%)	3374 (98%)	52 (2%)	60	75

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	249	VAL
2	B	485	GLU
3	C	410	VAL
12	T	25	GLU
1	a	5249	VAL
3	c	5410	VAL
12	t	5025	GLU
14	Y	19	ILE
14	Y	22	LEU
14	Y	25	ILE
14	Y	28	ILE
14	Y	30	ILE
14	Y	34	MET
14	Y	36	ILE
14	Y	39	LEU
14	Y	42	ARG
14	Y	43	ARG
14	Y	46	LEU
14	y	22	LEU
14	y	23	THR
14	y	25	ILE
14	y	27	MET
14	y	34	MET
14	y	36	ILE
14	y	38	LEU
14	y	39	LEU
14	y	42	ARG
14	y	43	ARG
16	X	7	LEU
16	X	11	PHE
16	X	15	LEU
16	X	16	SER
16	X	21	LEU
16	X	23	LEU

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Mol	Chain	Res	Type
16	X	25	PHE
16	X	29	ILE
16	X	31	ILE
16	X	33	GLN
16	X	34	ILE
16	X	36	LYS
16	x	8	LYS
16	x	11	PHE
16	x	12	ILE
16	x	15	LEU
16	x	16	SER
16	x	23	LEU
16	x	25	PHE
16	x	29	ILE
16	x	31	ILE
16	x	34	ILE
16	x	36	LYS
16	x	37	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	130	GLN
1	A	181	ASN
1	A	304	HIS
1	A	312	ASN
1	A	322	ASN
1	A	325	ASN
2	B	9	HIS
2	B	58	GLN
2	B	274	GLN
2	B	281	GLN
2	B	331	ASN
2	B	338	GLN
2	B	343	HIS
3	C	84	GLN
3	C	118	HIS
3	C	311	GLN
3	C	322	GLN
4	D	61	HIS
4	D	83	ASN

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Mol	Chain	Res	Type
4	D	129	GLN
4	D	189	HIS
4	D	224	GLN
4	D	292	ASN
5	E	23	HIS
7	H	59	ASN
9	K	40	GLN
10	L	8	GLN
13	Z	58	ASN
1	a	5087	ASN
1	a	5130	GLN
1	a	5312	ASN
1	a	5322	ASN
1	a	5325	ASN
2	b	5009	HIS
2	b	5058	GLN
2	b	5274	GLN
2	b	5281	GLN
2	b	5331	ASN
2	b	5338	GLN
2	b	5343	HIS
3	c	5084	GLN
3	c	5118	HIS
3	c	5311	GLN
3	c	5322	GLN
3	c	5382	ASN
4	d	5061	HIS
4	d	5083	ASN
4	d	5129	GLN
4	d	5189	HIS
4	d	5197	HIS
4	d	5220	ASN
4	d	5292	ASN
5	e	5023	HIS
5	e	5074	GLN
6	f	5024	HIS
7	h	5059	ASN
9	k	5040	GLN
10	l	5004	ASN
10	l	5008	GLN
11	m	5028	GLN
11	m	5032	GLN

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Mol	Chain	Res	Type
13	z	5058	ASN
14	Y	21	GLN
15	n	61	GLN
15	n	91	GLN
15	n	95	ASN
15	n	100	HIS
15	N	61	GLN
15	N	100	HIS
14	y	21	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 146 ligands modelled in this entry, 6 are monoatomic - leaving 140 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	$\# Z > 2$
20	BCR	C	514	-	41,41,41	1.29	3 (7%)	56,56,56	1.39	9 (16%)
23	SQD	D	403	-	53,54,54	1.00	5 (9%)	62,65,65	1.54	11 (17%)
20	BCR	c	5514	-	41,41,41	1.35	3 (7%)	56,56,56	1.40	9 (16%)
19	PQ9	A	406	-	45,45,45	0.68	1 (2%)	56,57,57	1.60	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	C	506	-	65,73,73	1.43	10 (15%)	76,113,113	1.38	8 (10%)
23	SQD	a	5401	-	25,26,54	1.35	4 (16%)	34,37,65	1.89	7 (20%)
17	CLA	B	608	-	65,73,73	1.47	11 (16%)	76,113,113	1.51	7 (9%)
26	DGD	C	517	3,1	54,54,67	1.20	7 (12%)	68,68,81	1.42	8 (11%)
17	CLA	B	601	20	41,49,73	1.72	8 (19%)	47,84,113	1.66	7 (14%)
26	DGD	c	5515	3	54,54,67	1.20	7 (12%)	68,68,81	1.43	8 (11%)
26	DGD	h	5102	7,2	55,55,67	1.00	3 (5%)	69,69,81	1.49	7 (10%)
29	HEM	F	101	6	41,50,50	1.54	3 (7%)	45,82,82	1.12	2 (4%)
17	CLA	B	609	-	65,73,73	1.47	10 (15%)	76,113,113	1.40	9 (11%)
20	BCR	d	5406	-	41,41,41	1.27	3 (7%)	56,56,56	1.28	7 (12%)
24	BCT	a	5412	28	2,3,3	1.38	0	2,3,3	4.05	2 (100%)
23	SQD	l	5102	-	46,47,54	1.02	5 (10%)	55,58,65	1.72	13 (23%)
22	LMT	m	5102	-	36,36,36	1.18	5 (13%)	47,47,47	1.10	2 (4%)
17	CLA	B	612	-	65,73,73	1.44	11 (16%)	76,113,113	1.54	8 (10%)
21	LHG	a	5409	-	38,38,48	0.76	1 (2%)	41,44,54	1.24	5 (12%)
17	CLA	c	5509	-	47,55,73	1.69	10 (21%)	54,91,113	1.50	9 (16%)
26	DGD	H	102	7,4	55,55,67	1.00	3 (5%)	69,69,81	1.50	7 (10%)
17	CLA	b	5616	-	65,73,73	1.47	12 (18%)	76,113,113	1.46	8 (10%)
20	BCR	A	407	-	41,41,41	1.36	3 (7%)	56,56,56	1.37	9 (16%)
17	CLA	b	5613	-	65,73,73	1.47	13 (20%)	76,113,113	1.52	9 (11%)
17	CLA	c	5505	-	65,73,73	1.44	10 (15%)	76,113,113	1.49	9 (11%)
17	CLA	A	403	-	65,73,73	1.46	11 (16%)	76,113,113	1.46	9 (11%)
21	LHG	A	408	-	38,38,48	0.76	1 (2%)	41,44,54	1.25	5 (12%)
25	MGE	m	5101	-	48,48,48	0.94	2 (4%)	56,56,56	1.13	4 (7%)
17	CLA	a	5402	-	65,73,73	1.48	11 (16%)	76,113,113	1.39	8 (10%)
23	SQD	L	101	-	46,47,54	1.03	6 (13%)	55,58,65	1.63	11 (20%)
17	CLA	D	405	-	50,58,73	1.63	10 (20%)	58,95,113	1.51	8 (13%)
17	CLA	b	5615	-	65,73,73	1.46	11 (16%)	76,113,113	1.46	7 (9%)
17	CLA	C	503	17	65,73,73	1.44	10 (15%)	76,113,113	1.48	10 (13%)
18	PHO	d	5402	-	51,69,69	1.21	7 (13%)	47,99,99	1.20	6 (12%)
17	CLA	C	513	-	50,58,73	1.60	9 (18%)	58,95,113	1.54	9 (15%)
17	CLA	A	401	-	65,73,73	1.48	11 (16%)	76,113,113	1.39	9 (11%)
17	CLA	c	5510	-	65,73,73	1.48	10 (15%)	76,113,113	1.39	8 (10%)
22	LMT	B	620	-	36,36,36	1.20	5 (13%)	47,47,47	0.95	1 (2%)
17	CLA	c	5503	17	65,73,73	1.43	10 (15%)	76,113,113	1.47	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LMT	T	101	12,2	36,36,36	1.10	4 (11%)	47,47,47	1.00	1 (2%)
17	CLA	B	607	-	65,73,73	1.43	10 (15%)	76,113,113	1.51	7 (9%)
23	SQD	d	5407	-	53,54,54	0.99	5 (9%)	62,65,65	1.64	11 (17%)
25	MGE	B	619	-	48,48,48	0.94	2 (4%)	56,56,56	1.14	4 (7%)
25	MGE	d	5408	-	47,47,48	0.97	2 (4%)	55,55,56	1.13	3 (5%)
17	CLA	a	5404	-	65,73,73	1.46	11 (16%)	76,113,113	1.45	9 (11%)
20	BCR	t	5102	-	41,41,41	1.29	3 (7%)	56,56,56	1.22	7 (12%)
25	MGE	A	412	25	48,48,48	0.91	2 (4%)	56,56,56	1.23	5 (8%)
17	CLA	c	5507	-	65,73,73	1.46	11 (16%)	76,113,113	1.44	9 (11%)
25	MGE	D	409	-	41,41,48	1.01	2 (4%)	49,49,56	1.44	8 (16%)
17	CLA	B	606	-	65,73,73	1.43	11 (16%)	76,113,113	1.48	8 (10%)
17	CLA	c	5506	-	65,73,73	1.44	10 (15%)	76,113,113	1.38	8 (10%)
25	MGE	l	5101	-	48,48,48	0.92	2 (4%)	56,56,56	1.23	5 (8%)
17	CLA	b	5606	-	42,50,73	1.75	11 (26%)	48,85,113	1.78	9 (18%)
17	CLA	b	5601	20	41,49,73	1.72	7 (17%)	47,84,113	1.66	7 (14%)
22	LMT	M	101	-	36,36,36	1.26	7 (19%)	47,47,47	1.09	1 (2%)
17	CLA	a	5403	-	65,73,73	1.49	11 (16%)	76,113,113	1.54	8 (10%)
17	CLA	c	5504	-	46,54,73	1.70	10 (21%)	53,90,113	1.56	7 (13%)
20	BCR	T	102	-	41,41,41	1.17	3 (7%)	56,56,56	1.31	7 (12%)
20	BCR	Y	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.26	5 (8%)
26	DGD	a	5411	-	58,58,67	0.96	3 (5%)	72,72,81	1.53	12 (16%)
17	CLA	d	5403	-	65,73,73	1.46	10 (15%)	76,113,113	1.42	8 (10%)
20	BCR	z	5101	-	41,41,41	1.27	2 (4%)	56,56,56	1.29	8 (14%)
17	CLA	B	602	-	65,73,73	1.46	11 (16%)	76,113,113	1.37	8 (10%)
17	CLA	C	510	-	65,73,73	1.49	10 (15%)	76,113,113	1.40	7 (9%)
17	CLA	b	5611	-	65,73,73	1.54	12 (18%)	76,113,113	1.61	9 (11%)
18	PHO	a	5405	-	51,69,69	1.22	7 (13%)	47,99,99	1.17	5 (10%)
25	MGE	D	410	25	48,48,48	0.92	2 (4%)	56,56,56	1.25	4 (7%)
19	PQ9	D	406	-	45,45,45	0.66	2 (4%)	56,57,57	1.84	16 (28%)
19	PQ9	d	5405	-	45,45,45	0.66	2 (4%)	56,57,57	1.84	16 (28%)
17	CLA	B	614	25	56,64,73	1.55	10 (17%)	65,102,113	1.56	7 (10%)
17	CLA	C	509	-	47,55,73	1.70	10 (21%)	54,91,113	1.50	8 (14%)
17	CLA	B	616	-	65,73,73	1.47	12 (18%)	76,113,113	1.46	8 (10%)
25	MGE	m	5103	17	48,48,48	0.91	2 (4%)	56,56,56	1.03	3 (5%)
25	MGE	c	5517	-	48,48,48	0.92	2 (4%)	56,56,56	1.11	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCT	A	411	28	2,3,3	1.37	0	2,3,3	4.05	2 (100%)
17	CLA	A	405	-	55,63,73	1.59	10 (18%)	64,101,113	1.50	7 (10%)
20	BCR	B	618	-	41,41,41	1.31	3 (7%)	56,56,56	1.46	9 (16%)
17	CLA	C	502	17	60,68,73	1.53	11 (18%)	70,107,113	1.56	9 (12%)
17	CLA	b	5603	-	65,73,73	1.45	12 (18%)	76,113,113	1.49	7 (9%)
17	CLA	d	5404	-	50,58,73	1.63	10 (20%)	58,95,113	1.51	8 (13%)
17	CLA	B	613	-	65,73,73	1.48	13 (20%)	76,113,113	1.54	10 (13%)
17	CLA	D	404	-	65,73,73	1.46	10 (15%)	76,113,113	1.41	8 (10%)
17	CLA	b	5614	-	56,64,73	1.54	10 (17%)	65,102,113	1.56	7 (10%)
20	BCR	C	516	-	41,41,41	1.35	4 (9%)	56,56,56	1.40	9 (16%)
20	BCR	b	5619	-	41,41,41	1.39	3 (7%)	56,56,56	1.36	9 (16%)
20	BCR	t	5101	-	41,41,41	1.39	3 (7%)	56,56,56	1.36	10 (17%)
18	PHO	D	402	-	51,69,69	1.21	7 (13%)	47,99,99	1.20	6 (12%)
17	CLA	c	5511	-	51,59,73	1.61	9 (17%)	59,96,113	1.53	7 (11%)
17	CLA	c	5508	-	65,73,73	1.51	12 (18%)	76,113,113	1.53	8 (10%)
17	CLA	C	508	-	65,73,73	1.52	12 (18%)	76,113,113	1.53	8 (10%)
17	CLA	b	5604	-	65,73,73	1.49	12 (18%)	76,113,113	1.48	8 (10%)
17	CLA	b	5608	-	65,73,73	1.44	10 (15%)	76,113,113	1.51	7 (9%)
20	BCR	b	5617	-	41,41,41	1.41	3 (7%)	56,56,56	1.47	10 (17%)
26	DGD	C	519	-	58,58,67	0.96	2 (3%)	72,72,81	1.53	12 (16%)
17	CLA	B	604	-	65,73,73	1.50	12 (18%)	76,113,113	1.48	8 (10%)
20	BCR	H	101	17	41,41,41	1.34	3 (7%)	56,56,56	1.26	6 (10%)
20	BCR	B	617	-	41,41,41	1.41	3 (7%)	56,56,56	1.47	10 (17%)
29	HEM	f	5101	-	41,50,50	1.54	3 (7%)	45,82,82	1.12	2 (4%)
17	CLA	C	511	3	65,73,73	1.44	11 (16%)	76,113,113	1.49	7 (9%)
20	BCR	C	515	-	41,41,41	1.27	2 (4%)	56,56,56	1.29	8 (14%)
17	CLA	C	512	-	51,59,73	1.61	9 (17%)	59,96,113	1.52	7 (11%)
17	CLA	B	605	-	65,73,73	1.48	12 (18%)	76,113,113	1.48	11 (14%)
20	BCR	c	5513	-	41,41,41	1.30	2 (4%)	56,56,56	1.39	8 (14%)
25	MGE	d	5410	-	48,48,48	0.93	2 (4%)	56,56,56	1.25	5 (8%)
17	CLA	A	402	-	65,73,73	1.48	11 (16%)	76,113,113	1.54	8 (10%)
20	BCR	k	5502	-	41,41,41	1.20	3 (7%)	56,56,56	1.30	6 (10%)
17	CLA	b	5609	-	65,73,73	1.48	10 (15%)	76,113,113	1.40	9 (11%)
17	CLA	B	615	-	65,73,73	1.45	11 (16%)	76,113,113	1.45	7 (9%)
17	CLA	c	5502	17	60,68,73	1.52	11 (18%)	70,107,113	1.55	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	c	5512	-	50,58,73	1.61	9 (18%)	58,95,113	1.53	9 (15%)
17	CLA	B	610	-	65,73,73	1.45	10 (15%)	76,113,113	1.49	8 (10%)
17	CLA	b	5607	-	65,73,73	1.43	11 (16%)	76,113,113	1.51	7 (9%)
18	PHO	A	404	-	51,69,69	1.23	7 (13%)	47,99,99	1.17	5 (10%)
17	CLA	b	5605	-	65,73,73	1.48	12 (18%)	76,113,113	1.48	11 (14%)
26	DGD	c	5516	-	48,48,67	1.02	2 (4%)	62,62,81	1.45	7 (11%)
25	MGE	d	5409	-	41,41,48	1.00	2 (4%)	49,49,56	1.44	8 (16%)
26	DGD	C	518	-	48,48,67	1.03	2 (4%)	62,62,81	1.44	7 (11%)
17	CLA	B	611	-	65,73,73	1.54	12 (18%)	76,113,113	1.60	9 (11%)
20	BCR	a	5408	-	41,41,41	1.36	4 (9%)	56,56,56	1.36	9 (16%)
17	CLA	C	501	-	65,73,73	1.46	11 (16%)	76,113,113	1.47	9 (11%)
20	BCR	h	5101	17	41,41,41	1.35	3 (7%)	56,56,56	1.26	6 (10%)
17	CLA	C	507	-	65,73,73	1.46	11 (16%)	76,113,113	1.44	9 (11%)
22	LMT	A	409	-	36,36,36	1.16	6 (16%)	47,47,47	1.11	3 (6%)
22	LMT	a	5410	-	36,36,36	1.19	6 (16%)	47,47,47	1.01	1 (2%)
17	CLA	b	5612	-	65,73,73	1.45	11 (16%)	76,113,113	1.55	8 (10%)
17	CLA	B	603	-	65,73,73	1.45	12 (18%)	76,113,113	1.49	7 (9%)
20	BCR	D	407	-	41,41,41	1.27	3 (7%)	56,56,56	1.27	7 (12%)
20	BCR	b	5618	-	41,41,41	1.30	3 (7%)	56,56,56	1.46	9 (16%)
19	PQ9	a	5407	-	30,30,45	0.79	1 (3%)	38,39,57	1.56	10 (26%)
17	CLA	C	505	-	65,73,73	1.44	10 (15%)	76,113,113	1.48	9 (11%)
17	CLA	a	5406	-	55,63,73	1.59	10 (18%)	64,101,113	1.50	7 (10%)
23	SQD	A	410	-	25,26,54	1.34	4 (16%)	34,37,65	1.83	8 (23%)
25	MGE	D	408	-	47,47,48	0.95	2 (4%)	55,55,56	1.05	3 (5%)
17	CLA	b	5602	-	65,73,73	1.46	11 (16%)	76,113,113	1.37	8 (10%)
17	CLA	C	504	-	46,54,73	1.71	10 (21%)	53,90,113	1.56	7 (13%)
17	CLA	k	5501	3	65,73,73	1.44	11 (16%)	76,113,113	1.48	7 (9%)
25	MGE	C	520	-	48,48,48	0.92	2 (4%)	56,56,56	1.11	5 (8%)
25	MGE	b	5620	-	48,48,48	0.94	2 (4%)	56,56,56	1.14	4 (7%)
17	CLA	c	5501	-	65,73,73	1.47	11 (16%)	76,113,113	1.45	9 (11%)
17	CLA	b	5610	-	65,73,73	1.45	10 (15%)	76,113,113	1.48	8 (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
20	BCR	C	514	-	-	12/29/63/63	0/2/2/2
23	SQD	D	403	-	-	22/49/69/69	0/1/1/1
20	BCR	c	5514	-	-	19/29/63/63	0/2/2/2
19	PQ9	A	406	-	-	12/41/61/61	0/1/1/1
17	CLA	C	506	-	1/1/15/20	20/37/115/115	-
23	SQD	a	5401	-	-	10/19/39/69	0/1/1/1
17	CLA	B	608	-	1/1/15/20	11/37/115/115	-
26	DGD	C	517	3,1	-	19/42/82/95	0/2/2/2
17	CLA	B	601	20	1/1/10/20	2/8/86/115	-
26	DGD	c	5515	3	-	19/42/82/95	0/2/2/2
26	DGD	h	5102	7,2	-	21/43/83/95	0/2/2/2
29	HEM	F	101	6	-	1/12/54/54	-
17	CLA	B	609	-	1/1/15/20	21/37/115/115	-
20	BCR	d	5406	-	-	15/29/63/63	0/2/2/2
23	SQD	l	5102	-	-	15/42/62/69	0/1/1/1
22	LMT	m	5102	-	-	9/21/61/61	0/2/2/2
17	CLA	B	612	-	1/1/15/20	19/37/115/115	-
21	LHG	a	5409	-	-	22/43/43/53	-
17	CLA	c	5509	-	1/1/11/20	6/16/94/115	-
26	DGD	H	102	7,4	-	21/43/83/95	0/2/2/2
17	CLA	b	5616	-	1/1/15/20	8/37/115/115	-
20	BCR	A	407	-	-	14/29/63/63	0/2/2/2
17	CLA	b	5613	-	1/1/15/20	18/37/115/115	-
17	CLA	c	5505	-	1/1/15/20	21/37/115/115	-
17	CLA	A	403	-	1/1/15/20	13/37/115/115	-
21	LHG	A	408	-	-	22/43/43/53	-
25	MGE	m	5101	-	-	8/43/63/63	0/1/1/1
17	CLA	a	5402	-	1/1/15/20	12/37/115/115	-
23	SQD	L	101	-	-	23/42/62/69	0/1/1/1
17	CLA	D	405	-	1/1/12/20	9/19/97/115	-
17	CLA	b	5615	-	1/1/15/20	18/37/115/115	-
17	CLA	C	503	17	1/1/15/20	20/37/115/115	-
18	PHO	d	5402	-	-	12/37/103/103	0/5/6/6
17	CLA	C	513	-	1/1/12/20	5/19/97/115	-
17	CLA	A	401	-	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	c	5510	-	1/1/15/20	8/37/115/115	-
22	LMT	B	620	-	-	7/21/61/61	0/2/2/2
17	CLA	c	5503	17	1/1/15/20	20/37/115/115	-
22	LMT	T	101	12,2	-	10/21/61/61	0/2/2/2
17	CLA	B	607	-	1/1/15/20	18/37/115/115	-
23	SQD	d	5407	-	-	14/49/69/69	0/1/1/1
25	MGE	B	619	-	-	12/43/63/63	0/1/1/1
25	MGE	d	5408	-	-	15/42/62/63	0/1/1/1
17	CLA	a	5404	-	1/1/15/20	13/37/115/115	-
20	BCR	t	5102	-	-	12/29/63/63	0/2/2/2
25	MGE	A	412	25	-	12/43/63/63	0/1/1/1
17	CLA	c	5507	-	1/1/15/20	16/37/115/115	-
25	MGE	D	409	-	-	16/36/56/63	0/1/1/1
17	CLA	B	606	-	1/1/15/20	17/37/115/115	-
17	CLA	c	5506	-	1/1/15/20	20/37/115/115	-
25	MGE	l	5101	-	-	12/43/63/63	0/1/1/1
17	CLA	b	5606	-	1/1/10/20	6/10/88/115	-
17	CLA	b	5601	20	1/1/10/20	2/8/86/115	-
22	LMT	M	101	-	-	8/21/61/61	0/2/2/2
17	CLA	a	5403	-	1/1/15/20	15/37/115/115	-
17	CLA	c	5504	-	1/1/11/20	9/15/93/115	-
20	BCR	T	102	-	-	12/29/63/63	0/2/2/2
20	BCR	Y	101	-	-	11/29/63/63	0/2/2/2
26	DGD	a	5411	-	-	18/46/86/95	0/2/2/2
17	CLA	d	5403	-	1/1/15/20	22/37/115/115	-
20	BCR	z	5101	-	-	21/29/63/63	0/2/2/2
17	CLA	B	602	-	1/1/15/20	20/37/115/115	-
17	CLA	C	510	-	1/1/15/20	8/37/115/115	-
17	CLA	b	5611	-	1/1/15/20	12/37/115/115	-
18	PHO	a	5405	-	-	15/37/103/103	0/5/6/6
25	MGE	D	410	25	-	17/43/63/63	0/1/1/1
19	PQ9	D	406	-	-	9/41/61/61	0/1/1/1
19	PQ9	d	5405	-	-	9/41/61/61	0/1/1/1
17	CLA	B	614	25	1/1/13/20	12/27/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	C	509	-	1/1/11/20	6/16/94/115	-
17	CLA	B	616	-	1/1/15/20	8/37/115/115	-
25	MGE	m	5103	17	-	21/43/63/63	0/1/1/1
25	MGE	c	5517	-	-	11/43/63/63	0/1/1/1
17	CLA	A	405	-	1/1/13/20	8/25/103/115	-
20	BCR	B	618	-	-	16/29/63/63	0/2/2/2
17	CLA	C	502	17	1/1/14/20	10/31/109/115	-
17	CLA	b	5603	-	1/1/15/20	12/37/115/115	-
17	CLA	d	5404	-	1/1/12/20	9/19/97/115	-
17	CLA	B	613	-	1/1/15/20	17/37/115/115	-
17	CLA	D	404	-	1/1/15/20	22/37/115/115	-
17	CLA	b	5614	-	1/1/13/20	12/27/105/115	-
20	BCR	C	516	-	-	19/29/63/63	0/2/2/2
20	BCR	b	5619	-	-	10/29/63/63	0/2/2/2
20	BCR	t	5101	-	-	10/29/63/63	0/2/2/2
18	PHO	D	402	-	-	12/37/103/103	0/5/6/6
17	CLA	c	5511	-	1/1/12/20	10/21/99/115	-
17	CLA	c	5508	-	1/1/15/20	13/37/115/115	-
17	CLA	C	508	-	1/1/15/20	13/37/115/115	-
17	CLA	b	5604	-	1/1/15/20	14/37/115/115	-
17	CLA	b	5608	-	1/1/15/20	11/37/115/115	-
20	BCR	b	5617	-	-	14/29/63/63	0/2/2/2
26	DGD	C	519	-	-	18/46/86/95	0/2/2/2
17	CLA	B	604	-	1/1/15/20	14/37/115/115	-
20	BCR	H	101	17	-	10/29/63/63	0/2/2/2
20	BCR	B	617	-	-	14/29/63/63	0/2/2/2
29	HEM	f	5101	-	-	1/12/54/54	-
17	CLA	C	511	3	1/1/15/20	14/37/115/115	-
20	BCR	C	515	-	-	21/29/63/63	0/2/2/2
17	CLA	C	512	-	1/1/12/20	10/21/99/115	-
17	CLA	B	605	-	1/1/15/20	18/37/115/115	-
20	BCR	c	5513	-	-	13/29/63/63	0/2/2/2
25	MGE	d	5410	-	-	14/43/63/63	0/1/1/1
17	CLA	A	402	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	BCR	k	5502	-	-	15/29/63/63	0/2/2/2
17	CLA	b	5609	-	1/1/15/20	21/37/115/115	-
17	CLA	B	615	-	1/1/15/20	18/37/115/115	-
17	CLA	c	5502	17	1/1/14/20	10/31/109/115	-
17	CLA	c	5512	-	1/1/12/20	5/19/97/115	-
17	CLA	B	610	-	1/1/15/20	15/37/115/115	-
17	CLA	b	5607	-	1/1/15/20	18/37/115/115	-
18	PHO	A	404	-	-	15/37/103/103	0/5/6/6
17	CLA	b	5605	-	1/1/15/20	18/37/115/115	-
26	DGD	c	5516	-	-	17/36/76/95	0/2/2/2
25	MGE	d	5409	-	-	12/36/56/63	0/1/1/1
26	DGD	C	518	-	-	17/36/76/95	0/2/2/2
17	CLA	B	611	-	1/1/15/20	12/37/115/115	-
20	BCR	a	5408	-	-	14/29/63/63	0/2/2/2
17	CLA	C	501	-	1/1/15/20	15/37/115/115	-
20	BCR	h	5101	17	-	10/29/63/63	0/2/2/2
17	CLA	C	507	-	1/1/15/20	16/37/115/115	-
22	LMT	A	409	-	-	10/21/61/61	0/2/2/2
22	LMT	a	5410	-	-	9/21/61/61	0/2/2/2
17	CLA	b	5612	-	1/1/15/20	19/37/115/115	-
17	CLA	B	603	-	1/1/15/20	12/37/115/115	-
20	BCR	D	407	-	-	15/29/63/63	0/2/2/2
20	BCR	b	5618	-	-	16/29/63/63	0/2/2/2
19	PQ9	a	5407	-	-	7/23/43/61	0/1/1/1
17	CLA	C	505	-	1/1/15/20	21/37/115/115	-
17	CLA	a	5406	-	1/1/13/20	8/25/103/115	-
23	SQD	A	410	-	-	8/19/39/69	0/1/1/1
25	MGE	D	408	-	-	9/42/62/63	0/1/1/1
17	CLA	b	5602	-	1/1/15/20	20/37/115/115	-
17	CLA	C	504	-	1/1/11/20	9/15/93/115	-
17	CLA	k	5501	3	1/1/15/20	14/37/115/115	-
25	MGE	C	520	-	-	11/43/63/63	0/1/1/1
25	MGE	b	5620	-	-	12/43/63/63	0/1/1/1
17	CLA	c	5501	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	b	5610	-	1/1/15/20	15/37/115/115	-

All (970) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	5609	CLA	C4B-NB	6.60	1.41	1.35
17	B	609	CLA	C4B-NB	6.44	1.41	1.35
17	b	5601	CLA	C4B-NB	6.34	1.40	1.35
17	c	5504	CLA	C4B-NB	6.30	1.40	1.35
17	C	504	CLA	C4B-NB	6.30	1.40	1.35
17	B	601	CLA	C4B-NB	6.29	1.40	1.35
17	a	5406	CLA	C4B-NB	6.24	1.40	1.35
17	B	605	CLA	C4B-NB	6.20	1.40	1.35
17	c	5505	CLA	C4B-NB	6.19	1.40	1.35
17	A	405	CLA	C4B-NB	6.17	1.40	1.35
17	C	512	CLA	C4B-NB	6.16	1.40	1.35
17	c	5506	CLA	C4B-NB	6.16	1.40	1.35
17	c	5512	CLA	C4B-NB	6.16	1.40	1.35
17	C	505	CLA	C4B-NB	6.16	1.40	1.35
17	b	5605	CLA	C4B-NB	6.13	1.40	1.35
17	c	5511	CLA	C4B-NB	6.13	1.40	1.35
17	B	608	CLA	C4B-NB	6.11	1.40	1.35
17	C	513	CLA	C4B-NB	6.08	1.40	1.35
17	C	510	CLA	C4B-NB	6.06	1.40	1.35
17	k	5501	CLA	C4B-NB	6.06	1.40	1.35
17	C	506	CLA	C4B-NB	6.06	1.40	1.35
17	c	5501	CLA	C4B-NB	6.03	1.40	1.35
17	c	5510	CLA	C4B-NB	6.02	1.40	1.35
17	C	511	CLA	C4B-NB	6.00	1.40	1.35
17	b	5606	CLA	C4B-NB	5.99	1.40	1.35
17	C	508	CLA	C4B-NB	5.98	1.40	1.35
17	b	5607	CLA	C4B-NB	5.98	1.40	1.35
17	B	606	CLA	C4B-NB	5.97	1.40	1.35
17	B	607	CLA	C4B-NB	5.97	1.40	1.35
17	B	616	CLA	C4B-NB	5.96	1.40	1.35
17	C	509	CLA	C4B-NB	5.96	1.40	1.35
17	c	5503	CLA	C4B-NB	5.94	1.40	1.35
17	c	5509	CLA	C4B-NB	5.94	1.40	1.35
17	A	402	CLA	C4B-NB	5.94	1.40	1.35
17	a	5403	CLA	C4B-NB	5.93	1.40	1.35
17	b	5616	CLA	C4B-NB	5.93	1.40	1.35
17	c	5508	CLA	C4B-NB	5.92	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	610	CLA	C4B-NB	5.90	1.40	1.35
17	C	501	CLA	C4B-NB	5.89	1.40	1.35
17	b	5610	CLA	C4B-NB	5.89	1.40	1.35
17	a	5404	CLA	C4B-NB	5.88	1.40	1.35
17	b	5608	CLA	C4B-NB	5.87	1.40	1.35
17	C	503	CLA	C4B-NB	5.87	1.40	1.35
17	B	614	CLA	C4B-NB	5.83	1.40	1.35
17	A	403	CLA	C4B-NB	5.82	1.40	1.35
17	b	5614	CLA	C4B-NB	5.79	1.40	1.35
17	C	502	CLA	C4B-NB	5.78	1.40	1.35
17	b	5602	CLA	C4B-NB	5.78	1.40	1.35
17	B	604	CLA	C4B-NB	5.76	1.40	1.35
17	B	611	CLA	C4B-NB	5.75	1.40	1.35
17	d	5404	CLA	C4B-NB	5.75	1.40	1.35
17	b	5611	CLA	C4B-NB	5.74	1.40	1.35
17	B	602	CLA	C4B-NB	5.72	1.40	1.35
17	b	5604	CLA	C4B-NB	5.72	1.40	1.35
17	D	405	CLA	C4B-NB	5.71	1.40	1.35
17	c	5502	CLA	C4B-NB	5.71	1.40	1.35
17	b	5615	CLA	C4B-NB	5.67	1.40	1.35
17	B	615	CLA	C4B-NB	5.62	1.40	1.35
17	c	5507	CLA	C4B-NB	5.62	1.40	1.35
17	C	507	CLA	C4B-NB	5.61	1.40	1.35
17	A	401	CLA	C4B-NB	5.39	1.40	1.35
17	b	5603	CLA	C4B-NB	5.39	1.40	1.35
17	B	603	CLA	C4B-NB	5.35	1.40	1.35
17	a	5402	CLA	C4B-NB	5.35	1.40	1.35
17	D	404	CLA	C4B-NB	5.21	1.39	1.35
17	d	5403	CLA	C4B-NB	5.18	1.39	1.35
17	b	5612	CLA	C4B-NB	5.14	1.39	1.35
17	B	612	CLA	C4B-NB	5.08	1.39	1.35
17	B	613	CLA	C4B-NB	5.04	1.39	1.35
17	b	5613	CLA	C4B-NB	5.03	1.39	1.35
29	F	101	HEM	C3C-C2C	-4.95	1.33	1.40
29	f	5101	HEM	C3C-C2C	-4.91	1.33	1.40
20	B	617	BCR	C30-C25	-4.68	1.47	1.53
20	b	5617	BCR	C30-C25	-4.68	1.47	1.53
20	t	5101	BCR	C30-C25	-4.51	1.47	1.53
20	h	5101	BCR	C1-C6	-4.50	1.47	1.53
20	b	5619	BCR	C30-C25	-4.49	1.47	1.53
20	H	101	BCR	C1-C6	-4.43	1.47	1.53
17	b	5611	CLA	C4D-ND	-4.37	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	611	CLA	C4D-ND	-4.34	1.31	1.37
20	D	407	BCR	C1-C6	-4.28	1.47	1.53
20	A	407	BCR	C30-C25	-4.26	1.47	1.53
20	a	5408	BCR	C30-C25	-4.24	1.47	1.53
20	d	5406	BCR	C1-C6	-4.24	1.47	1.53
17	C	508	CLA	C4D-ND	-4.22	1.31	1.37
17	b	5604	CLA	C4D-ND	-4.21	1.31	1.37
20	t	5102	BCR	C30-C25	-4.21	1.48	1.53
17	B	604	CLA	C4D-ND	-4.21	1.31	1.37
25	D	409	MGE	O1G-C1A	4.20	1.45	1.33
17	b	5605	CLA	C4D-ND	-4.20	1.31	1.37
25	b	5620	MGE	O1G-C1A	4.20	1.45	1.33
17	C	510	CLA	C4D-ND	-4.19	1.31	1.37
25	d	5408	MGE	O1G-C1A	4.19	1.45	1.33
17	c	5510	CLA	C4D-ND	-4.18	1.32	1.37
25	d	5409	MGE	O1G-C1A	4.18	1.45	1.33
25	B	619	MGE	O1G-C1A	4.18	1.45	1.33
20	c	5514	BCR	C1-C6	-4.17	1.48	1.53
17	b	5615	CLA	C4D-ND	-4.17	1.32	1.37
20	C	516	BCR	C1-C6	-4.17	1.48	1.53
20	t	5101	BCR	C1-C6	-4.16	1.48	1.53
17	c	5508	CLA	C4D-ND	-4.15	1.32	1.37
25	D	408	MGE	O1G-C1A	4.15	1.45	1.33
17	A	403	CLA	C4D-ND	-4.15	1.32	1.37
20	b	5619	BCR	C1-C6	-4.14	1.48	1.53
17	b	5612	CLA	C4D-ND	-4.14	1.32	1.37
17	b	5616	CLA	C4D-ND	-4.13	1.32	1.37
25	C	520	MGE	O2G-C1B	4.13	1.45	1.34
17	B	603	CLA	C4D-ND	-4.12	1.32	1.37
25	m	5101	MGE	O1G-C1A	4.12	1.45	1.33
17	B	605	CLA	C4D-ND	-4.11	1.32	1.37
17	B	615	CLA	C4D-ND	-4.11	1.32	1.37
25	d	5408	MGE	O2G-C1B	4.11	1.45	1.34
17	b	5609	CLA	C4D-ND	-4.11	1.32	1.37
17	c	5502	CLA	C4D-ND	-4.11	1.32	1.37
25	m	5103	MGE	O1G-C1A	4.10	1.45	1.33
17	b	5603	CLA	C4D-ND	-4.10	1.32	1.37
25	C	520	MGE	O1G-C1A	4.10	1.45	1.33
17	d	5404	CLA	C4D-ND	-4.10	1.32	1.37
25	c	5517	MGE	O1G-C1A	4.10	1.45	1.33
25	c	5517	MGE	O2G-C1B	4.10	1.45	1.34
17	B	610	CLA	C4D-ND	-4.10	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	616	CLA	C4D-ND	-4.10	1.32	1.37
17	B	609	CLA	C4D-ND	-4.09	1.32	1.37
17	B	613	CLA	C4D-ND	-4.08	1.32	1.37
17	D	405	CLA	C4D-ND	-4.08	1.32	1.37
17	a	5404	CLA	C4D-ND	-4.08	1.32	1.37
25	l	5101	MGE	O2G-C1B	4.08	1.45	1.34
17	B	612	CLA	C4D-ND	-4.07	1.32	1.37
17	C	502	CLA	C4D-ND	-4.07	1.32	1.37
17	b	5610	CLA	C4D-ND	-4.07	1.32	1.37
17	A	401	CLA	C4D-ND	-4.06	1.32	1.37
17	C	501	CLA	C4D-ND	-4.06	1.32	1.37
25	d	5410	MGE	O1G-C1A	4.05	1.45	1.33
17	b	5602	CLA	C4D-ND	-4.05	1.32	1.37
17	C	507	CLA	C4D-ND	-4.05	1.32	1.37
17	c	5512	CLA	C4D-ND	-4.05	1.32	1.37
17	c	5507	CLA	C4D-ND	-4.05	1.32	1.37
17	B	608	CLA	C4D-ND	-4.05	1.32	1.37
17	a	5402	CLA	C4D-ND	-4.04	1.32	1.37
25	A	412	MGE	O2G-C1B	4.04	1.45	1.34
17	C	513	CLA	C4D-ND	-4.03	1.32	1.37
17	c	5501	CLA	C4D-ND	-4.03	1.32	1.37
25	D	410	MGE	O1G-C1A	4.03	1.45	1.33
17	a	5403	CLA	C4D-ND	-4.03	1.32	1.37
17	B	602	CLA	C4D-ND	-4.02	1.32	1.37
17	A	402	CLA	C4D-ND	-4.02	1.32	1.37
20	h	5101	BCR	C30-C25	-4.02	1.48	1.53
17	C	504	CLA	C4D-ND	-4.01	1.32	1.37
17	C	509	CLA	C4D-ND	-4.01	1.32	1.37
17	b	5613	CLA	C4D-ND	-4.01	1.32	1.37
17	c	5506	CLA	C4D-ND	-4.01	1.32	1.37
25	B	619	MGE	O2G-C1B	4.00	1.45	1.34
25	b	5620	MGE	O2G-C1B	3.99	1.45	1.34
17	C	506	CLA	C4D-ND	-3.98	1.32	1.37
17	c	5504	CLA	C4D-ND	-3.98	1.32	1.37
17	A	405	CLA	C4D-ND	-3.97	1.32	1.37
20	H	101	BCR	C30-C25	-3.96	1.48	1.53
25	l	5101	MGE	O1G-C1A	3.95	1.44	1.33
20	c	5513	BCR	C1-C6	-3.95	1.48	1.53
17	c	5509	CLA	C4D-ND	-3.95	1.32	1.37
17	b	5608	CLA	C4D-ND	-3.95	1.32	1.37
17	b	5607	CLA	C4D-ND	-3.94	1.32	1.37
25	D	408	MGE	O2G-C1B	3.93	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	z	5101	BCR	C1-C6	-3.93	1.48	1.53
17	d	5403	CLA	C4D-ND	-3.93	1.32	1.37
17	a	5406	CLA	C4D-ND	-3.92	1.32	1.37
20	A	407	BCR	C1-C6	-3.92	1.48	1.53
25	A	412	MGE	O1G-C1A	3.92	1.44	1.33
17	b	5606	CLA	C4D-ND	-3.91	1.32	1.37
20	C	515	BCR	C1-C6	-3.91	1.48	1.53
25	d	5409	MGE	O2G-C1B	3.91	1.45	1.34
17	C	505	CLA	C4D-ND	-3.90	1.32	1.37
17	c	5505	CLA	C4D-ND	-3.90	1.32	1.37
20	a	5408	BCR	C1-C6	-3.90	1.48	1.53
17	B	614	CLA	C4D-ND	-3.89	1.32	1.37
20	C	514	BCR	C1-C6	-3.89	1.48	1.53
20	z	5101	BCR	C30-C25	-3.89	1.48	1.53
25	m	5103	MGE	O2G-C1B	3.88	1.45	1.34
25	m	5101	MGE	O2G-C1B	3.87	1.45	1.34
17	D	404	CLA	C4D-ND	-3.87	1.32	1.37
17	B	607	CLA	C4D-ND	-3.86	1.32	1.37
20	C	515	BCR	C30-C25	-3.86	1.48	1.53
17	B	606	CLA	C4D-ND	-3.84	1.32	1.37
17	c	5511	CLA	C4D-ND	-3.83	1.32	1.37
25	D	409	MGE	O2G-C1B	3.82	1.45	1.34
17	b	5614	CLA	C4D-ND	-3.81	1.32	1.37
17	C	512	CLA	C4D-ND	-3.79	1.32	1.37
25	d	5410	MGE	O2G-C1B	3.79	1.45	1.34
17	C	511	CLA	C4D-ND	-3.78	1.32	1.37
20	b	5618	BCR	C30-C25	-3.77	1.48	1.53
20	b	5617	BCR	C1-C6	-3.76	1.48	1.53
20	B	618	BCR	C30-C25	-3.74	1.48	1.53
20	t	5102	BCR	C1-C6	-3.74	1.48	1.53
17	k	5501	CLA	C4D-ND	-3.74	1.32	1.37
20	B	617	BCR	C1-C6	-3.72	1.48	1.53
17	C	503	CLA	C4D-ND	-3.72	1.32	1.37
20	C	514	BCR	C30-C25	-3.71	1.48	1.53
25	D	410	MGE	O2G-C1B	3.71	1.44	1.34
29	f	5101	HEM	C3C-CAC	3.70	1.55	1.47
20	c	5513	BCR	C30-C25	-3.70	1.48	1.53
29	F	101	HEM	C3C-CAC	3.70	1.55	1.47
20	c	5514	BCR	C30-C25	-3.69	1.48	1.53
20	C	516	BCR	C30-C25	-3.68	1.48	1.53
17	c	5503	CLA	C4D-ND	-3.67	1.32	1.37
20	k	5502	BCR	C1-C6	-3.66	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	d	5402	PHO	CAC-C3C	-3.60	1.45	1.52
18	D	402	PHO	CAC-C3C	-3.59	1.45	1.52
20	B	618	BCR	C1-C6	-3.52	1.48	1.53
20	b	5618	BCR	C1-C6	-3.47	1.49	1.53
18	A	404	PHO	CAC-C3C	-3.46	1.46	1.52
18	a	5405	PHO	CAC-C3C	-3.43	1.46	1.52
20	T	102	BCR	C1-C6	-3.40	1.49	1.53
17	B	604	CLA	C3B-C2B	-3.38	1.35	1.40
18	a	5405	PHO	C3B-C2B	-3.36	1.35	1.40
18	A	404	PHO	C3B-C2B	-3.36	1.35	1.40
20	Y	101	BCR	C1-C6	-3.34	1.49	1.53
17	b	5604	CLA	C3B-C2B	-3.33	1.35	1.40
17	B	601	CLA	C4D-ND	-3.32	1.33	1.37
17	b	5601	CLA	C4D-ND	-3.30	1.33	1.37
20	d	5406	BCR	C30-C25	-3.26	1.49	1.53
20	D	407	BCR	C30-C25	-3.25	1.49	1.53
17	b	5601	CLA	C1D-ND	3.24	1.41	1.37
17	b	5611	CLA	C3B-C2B	-3.23	1.35	1.40
17	B	611	CLA	C3B-C2B	-3.23	1.35	1.40
20	Y	101	BCR	C30-C25	-3.22	1.49	1.53
17	B	601	CLA	C1D-ND	3.22	1.41	1.37
17	b	5611	CLA	CMC-C2C	-3.20	1.44	1.50
23	a	5401	SQD	O47-C7	3.20	1.42	1.35
20	k	5502	BCR	C30-C25	-3.19	1.49	1.53
17	B	611	CLA	CMC-C2C	-3.18	1.44	1.50
17	c	5508	CLA	C3B-C2B	-3.17	1.36	1.40
17	d	5403	CLA	C3B-C2B	-3.17	1.36	1.40
17	A	402	CLA	C3B-C2B	-3.16	1.36	1.40
17	b	5613	CLA	C3B-C2B	-3.15	1.36	1.40
17	B	611	CLA	CMB-C2B	-3.15	1.45	1.51
23	A	410	SQD	O47-C7	3.14	1.42	1.35
17	D	404	CLA	C3B-C2B	-3.13	1.36	1.40
17	b	5611	CLA	CMB-C2B	-3.13	1.45	1.51
17	B	604	CLA	CMB-C2B	-3.12	1.45	1.51
17	b	5604	CLA	CMB-C2B	-3.12	1.45	1.51
17	D	404	CLA	CMB-C2B	-3.12	1.45	1.51
17	B	608	CLA	CMB-C2B	-3.11	1.45	1.51
17	b	5608	CLA	CMB-C2B	-3.11	1.45	1.51
17	B	613	CLA	C3B-C2B	-3.11	1.36	1.40
17	C	508	CLA	C3B-C2B	-3.11	1.36	1.40
17	a	5402	CLA	C3B-C2B	-3.10	1.36	1.40
23	D	403	SQD	O48-C23	3.09	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	d	5403	CLA	CMB-C2B	-3.09	1.45	1.51
17	a	5403	CLA	C3B-C2B	-3.08	1.36	1.40
17	a	5403	CLA	CMB-C2B	-3.07	1.45	1.51
17	C	507	CLA	C3B-C2B	-3.07	1.36	1.40
26	H	102	DGD	O1G-C1G	-3.06	1.38	1.45
17	C	508	CLA	CMC-C2C	-3.06	1.44	1.50
23	d	5407	SQD	O48-C23	3.05	1.42	1.33
20	T	102	BCR	C30-C25	-3.05	1.49	1.53
17	A	401	CLA	C3B-C2B	-3.04	1.36	1.40
17	C	502	CLA	C1D-ND	3.03	1.41	1.37
26	h	5102	DGD	O1G-C1G	-3.03	1.38	1.45
17	c	5508	CLA	CMC-C2C	-3.03	1.44	1.50
17	B	603	CLA	C3B-C2B	-3.03	1.36	1.40
17	B	613	CLA	CMB-C2B	-3.02	1.45	1.51
17	A	402	CLA	CMB-C2B	-3.01	1.45	1.51
17	a	5406	CLA	CMB-C2B	-3.01	1.45	1.51
17	A	401	CLA	CMB-C2B	-3.01	1.45	1.51
17	c	5502	CLA	C1D-ND	3.01	1.41	1.37
17	b	5613	CLA	CMB-C2B	-3.00	1.45	1.51
26	c	5515	DGD	O1G-C1G	-2.99	1.38	1.45
17	b	5603	CLA	C3B-C2B	-2.99	1.36	1.40
17	C	502	CLA	CMB-C2B	-2.99	1.45	1.51
17	a	5402	CLA	CMB-C2B	-2.98	1.45	1.51
17	B	603	CLA	CMB-C2B	-2.98	1.45	1.51
22	B	620	LMT	O3'-C3'	-2.98	1.36	1.43
17	c	5507	CLA	C3B-C2B	-2.97	1.36	1.40
17	b	5615	CLA	CMB-C2B	-2.97	1.45	1.51
26	C	517	DGD	O1G-C1G	-2.97	1.38	1.45
17	c	5502	CLA	CMB-C2B	-2.97	1.45	1.51
17	B	615	CLA	CMB-C2B	-2.97	1.45	1.51
17	D	404	CLA	CMD-C2D	-2.97	1.44	1.50
17	A	405	CLA	CMB-C2B	-2.97	1.45	1.51
18	D	402	PHO	C3B-C2B	-2.96	1.36	1.40
17	d	5403	CLA	CMD-C2D	-2.96	1.44	1.50
18	d	5402	PHO	C3B-C2B	-2.96	1.36	1.40
17	b	5603	CLA	CMB-C2B	-2.95	1.45	1.51
23	L	101	SQD	O48-C23	2.95	1.42	1.33
17	b	5602	CLA	C3B-C2B	-2.95	1.36	1.40
23	l	5102	SQD	O48-C23	2.94	1.41	1.33
17	C	512	CLA	C1D-ND	2.94	1.41	1.37
17	B	602	CLA	C3B-C2B	-2.93	1.36	1.40
17	c	5509	CLA	CMB-C2B	-2.93	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	c	5507	CLA	CMB-C2B	-2.93	1.45	1.51
17	c	5506	CLA	CMB-C2B	-2.92	1.45	1.51
17	C	506	CLA	CMB-C2B	-2.92	1.45	1.51
17	B	610	CLA	CMB-C2B	-2.91	1.45	1.51
17	b	5614	CLA	CMB-C2B	-2.91	1.45	1.51
17	b	5601	CLA	CHC-C1C	2.91	1.42	1.35
17	B	611	CLA	C3B-CAB	-2.91	1.42	1.47
17	b	5616	CLA	CMB-C2B	-2.91	1.45	1.51
17	b	5611	CLA	C3B-CAB	-2.91	1.42	1.47
17	C	502	CLA	C3B-C2B	-2.90	1.36	1.40
17	b	5610	CLA	CMB-C2B	-2.90	1.45	1.51
17	C	507	CLA	CMB-C2B	-2.90	1.45	1.51
17	C	508	CLA	CMB-C2B	-2.90	1.45	1.51
17	C	511	CLA	C1D-ND	2.90	1.41	1.37
17	c	5502	CLA	C3B-C2B	-2.89	1.36	1.40
17	C	509	CLA	CMB-C2B	-2.89	1.45	1.51
17	B	605	CLA	CMB-C2B	-2.89	1.45	1.51
17	B	614	CLA	CMB-C2B	-2.89	1.45	1.51
17	b	5605	CLA	CMB-C2B	-2.89	1.45	1.51
17	B	612	CLA	CMB-C2B	-2.88	1.45	1.51
17	k	5501	CLA	C1D-ND	2.88	1.41	1.37
17	C	510	CLA	CHC-C1C	2.87	1.42	1.35
17	B	601	CLA	CHC-C1C	2.87	1.42	1.35
17	c	5508	CLA	CMB-C2B	-2.87	1.45	1.51
17	c	5511	CLA	C1D-ND	2.87	1.41	1.37
17	b	5613	CLA	C3B-CAB	-2.87	1.42	1.47
17	c	5510	CLA	CHC-C1C	2.87	1.42	1.35
17	b	5612	CLA	CMB-C2B	-2.87	1.45	1.51
17	c	5501	CLA	C1D-ND	2.87	1.41	1.37
17	B	616	CLA	CMB-C2B	-2.86	1.45	1.51
17	b	5602	CLA	CMB-C2B	-2.86	1.45	1.51
17	d	5404	CLA	CMB-C2B	-2.85	1.45	1.51
17	a	5406	CLA	C1D-ND	2.85	1.41	1.37
17	b	5609	CLA	CMB-C2B	-2.85	1.45	1.51
17	B	609	CLA	CMB-C2B	-2.85	1.45	1.51
17	c	5503	CLA	CHC-C1C	2.84	1.42	1.35
17	k	5501	CLA	CMB-C2B	-2.84	1.45	1.51
17	C	501	CLA	C1D-ND	2.84	1.41	1.37
17	D	405	CLA	CMB-C2B	-2.84	1.45	1.51
29	F	101	HEM	CAB-C3B	2.83	1.55	1.47
17	b	5606	CLA	CMB-C2B	-2.83	1.45	1.51
17	B	606	CLA	CMB-C2B	-2.83	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	l	5102	SQD	O47-C7	2.83	1.42	1.34
17	C	503	CLA	CHC-C1C	2.83	1.42	1.35
17	D	405	CLA	CHC-C1C	2.83	1.42	1.35
29	f	5101	HEM	CAB-C3B	2.83	1.55	1.47
17	d	5404	CLA	CHC-C1C	2.83	1.42	1.35
17	a	5402	CLA	CHC-C1C	2.82	1.42	1.35
17	C	510	CLA	CMB-C2B	-2.82	1.45	1.51
17	B	613	CLA	C3B-CAB	-2.82	1.42	1.47
17	B	602	CLA	CMB-C2B	-2.82	1.45	1.51
17	A	405	CLA	C3B-C2B	-2.82	1.36	1.40
17	C	509	CLA	C1D-ND	2.82	1.41	1.37
17	A	401	CLA	CHC-C1C	2.82	1.42	1.35
17	A	405	CLA	C1D-ND	2.82	1.41	1.37
17	a	5406	CLA	C3B-C2B	-2.81	1.36	1.40
17	a	5403	CLA	C1D-ND	2.81	1.41	1.37
17	C	503	CLA	C1D-ND	2.81	1.41	1.37
17	B	602	CLA	C1D-ND	2.81	1.41	1.37
17	c	5512	CLA	C1D-ND	2.80	1.41	1.37
17	C	501	CLA	C3B-C2B	-2.80	1.36	1.40
17	B	609	CLA	CHC-C1C	2.80	1.42	1.35
17	C	511	CLA	CMB-C2B	-2.79	1.45	1.51
17	A	403	CLA	C1D-ND	2.79	1.41	1.37
17	a	5404	CLA	CMB-C2B	-2.79	1.45	1.51
17	B	614	CLA	CHC-C1C	2.79	1.42	1.35
17	b	5615	CLA	C3B-C2B	-2.79	1.36	1.40
17	b	5602	CLA	CHC-C1C	2.79	1.42	1.35
17	b	5612	CLA	C3B-C2B	-2.79	1.36	1.40
17	c	5510	CLA	CMB-C2B	-2.79	1.45	1.51
22	B	620	LMT	O2'-C2'	-2.78	1.36	1.43
17	c	5503	CLA	C1D-ND	2.78	1.41	1.37
17	B	602	CLA	CHC-C1C	2.78	1.42	1.35
17	A	403	CLA	CMB-C2B	-2.77	1.45	1.51
17	C	506	CLA	CHC-C1C	2.77	1.42	1.35
17	c	5501	CLA	C3B-C2B	-2.77	1.36	1.40
17	c	5509	CLA	C1D-ND	2.77	1.41	1.37
17	a	5402	CLA	MG-ND	-2.77	2.00	2.05
17	C	505	CLA	CMB-C2B	-2.77	1.45	1.51
22	M	101	LMT	O2B-C2B	-2.77	1.36	1.43
17	d	5403	CLA	CHC-C1C	2.77	1.42	1.35
17	a	5404	CLA	C1D-ND	2.77	1.41	1.37
17	b	5609	CLA	CHC-C1C	2.77	1.42	1.35
17	C	504	CLA	CMB-C2B	-2.77	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	c	5512	CLA	CHC-C1C	2.77	1.42	1.35
17	b	5607	CLA	C1D-ND	2.77	1.41	1.37
17	c	5504	CLA	C1D-ND	2.76	1.41	1.37
17	b	5614	CLA	CHC-C1C	2.76	1.42	1.35
17	A	402	CLA	C1D-ND	2.76	1.41	1.37
23	d	5407	SQD	O47-C7	2.76	1.42	1.34
23	D	403	SQD	O47-C7	2.76	1.42	1.34
17	C	504	CLA	C1D-ND	2.76	1.41	1.37
17	C	513	CLA	CHC-C1C	2.76	1.42	1.35
22	B	620	LMT	O2B-C2B	-2.75	1.36	1.43
18	A	404	PHO	CBD-CGD	-2.75	1.48	1.52
17	C	513	CLA	C1D-ND	2.75	1.41	1.37
17	c	5501	CLA	CMB-C2B	-2.75	1.45	1.51
17	c	5506	CLA	CHC-C1C	2.75	1.42	1.35
17	c	5504	CLA	CMB-C2B	-2.75	1.45	1.51
17	c	5505	CLA	CMB-C2B	-2.75	1.45	1.51
21	A	408	LHG	O7-C5	-2.75	1.39	1.46
22	T	101	LMT	O3'-C3'	-2.75	1.36	1.43
17	C	508	CLA	C3B-CAB	-2.75	1.42	1.47
17	A	403	CLA	C3B-C2B	-2.75	1.36	1.40
17	B	607	CLA	C1D-ND	2.75	1.41	1.37
17	C	510	CLA	C1D-ND	2.75	1.41	1.37
17	B	612	CLA	C3B-C2B	-2.74	1.36	1.40
21	a	5409	LHG	O7-C5	-2.74	1.39	1.46
18	d	5402	PHO	CBD-CGD	-2.74	1.48	1.52
17	b	5602	CLA	C1D-ND	2.74	1.41	1.37
17	A	401	CLA	MG-ND	-2.74	2.00	2.05
18	D	402	PHO	CBD-CGD	-2.74	1.48	1.52
17	c	5510	CLA	C1D-ND	2.74	1.41	1.37
17	C	501	CLA	CMB-C2B	-2.74	1.45	1.51
17	C	504	CLA	CHC-C1C	2.74	1.42	1.35
17	B	616	CLA	C1D-ND	2.73	1.41	1.37
17	D	404	CLA	CHC-C1C	2.73	1.42	1.35
17	D	404	CLA	MG-ND	-2.73	2.00	2.05
17	c	5511	CLA	CMB-C2B	-2.73	1.46	1.51
17	c	5508	CLA	C3B-CAB	-2.73	1.42	1.47
17	B	615	CLA	C3B-C2B	-2.72	1.36	1.40
17	B	611	CLA	CHC-C1C	2.72	1.41	1.35
17	b	5611	CLA	CHC-C1C	2.72	1.41	1.35
17	b	5606	CLA	C1D-ND	2.72	1.41	1.37
17	B	604	CLA	MG-ND	-2.72	2.00	2.05
17	D	405	CLA	C1D-ND	2.72	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	5404	CLA	C3B-C2B	-2.71	1.36	1.40
17	c	5504	CLA	CHC-C1C	2.71	1.41	1.35
17	d	5404	CLA	C1D-ND	2.71	1.41	1.37
17	d	5403	CLA	C3B-CAB	-2.71	1.42	1.47
18	a	5405	PHO	CBD-CGD	-2.71	1.48	1.52
17	c	5509	CLA	C3B-C2B	-2.71	1.36	1.40
17	B	608	CLA	MG-ND	-2.71	2.00	2.05
17	d	5403	CLA	MG-ND	-2.71	2.00	2.05
17	B	602	CLA	MG-ND	-2.71	2.00	2.05
17	C	509	CLA	CHC-C1C	2.71	1.41	1.35
17	b	5604	CLA	C3B-CAB	-2.70	1.42	1.47
17	A	401	CLA	C3B-CAB	-2.70	1.42	1.47
17	b	5604	CLA	MG-ND	-2.70	2.00	2.05
17	a	5402	CLA	C3B-CAB	-2.69	1.42	1.47
17	C	507	CLA	C1D-ND	2.69	1.41	1.37
22	M	101	LMT	O3'-C3'	-2.69	1.36	1.43
17	B	613	CLA	CHC-C1C	2.69	1.41	1.35
17	b	5608	CLA	MG-ND	-2.69	2.00	2.05
17	c	5510	CLA	C3B-C2B	-2.69	1.36	1.40
17	c	5503	CLA	CMB-C2B	-2.69	1.46	1.51
17	C	505	CLA	CHC-C1C	2.69	1.41	1.35
17	D	404	CLA	C3B-CAB	-2.68	1.42	1.47
17	C	512	CLA	CMB-C2B	-2.68	1.46	1.51
17	B	607	CLA	CMB-C2B	-2.68	1.46	1.51
17	C	512	CLA	CHC-C1C	2.68	1.41	1.35
17	B	604	CLA	CHC-C1C	2.68	1.41	1.35
17	C	510	CLA	C3B-C2B	-2.68	1.36	1.40
17	b	5605	CLA	C3B-C2B	-2.68	1.36	1.40
17	c	5509	CLA	CHC-C1C	2.68	1.41	1.35
17	b	5607	CLA	CMB-C2B	-2.68	1.46	1.51
17	b	5616	CLA	C1D-ND	2.68	1.41	1.37
17	C	505	CLA	C3B-C2B	-2.68	1.36	1.40
17	B	606	CLA	C1D-ND	2.68	1.41	1.37
17	B	608	CLA	CHC-C1C	2.68	1.41	1.35
17	b	5613	CLA	MG-ND	-2.68	2.00	2.05
17	c	5507	CLA	C1D-ND	2.68	1.41	1.37
17	A	405	CLA	CHC-C1C	2.67	1.41	1.35
17	C	503	CLA	CMB-C2B	-2.67	1.46	1.51
17	B	604	CLA	C3B-CAB	-2.67	1.42	1.47
17	b	5602	CLA	MG-ND	-2.67	2.00	2.05
17	B	613	CLA	MG-ND	-2.67	2.00	2.05
17	b	5612	CLA	CHC-C1C	2.67	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	605	CLA	C3B-C2B	-2.67	1.36	1.40
17	b	5613	CLA	CHC-C1C	2.66	1.41	1.35
17	B	612	CLA	CMD-C2D	-2.66	1.45	1.50
17	C	507	CLA	MG-ND	-2.66	2.00	2.05
17	C	503	CLA	CMD-C2D	-2.66	1.45	1.50
17	b	5604	CLA	CHC-C1C	2.66	1.41	1.35
17	b	5608	CLA	CHC-C1C	2.66	1.41	1.35
17	c	5502	CLA	CHC-C1C	2.66	1.41	1.35
17	c	5508	CLA	CHC-C1C	2.66	1.41	1.35
17	C	510	CLA	C3B-CAB	-2.65	1.42	1.47
17	c	5507	CLA	MG-ND	-2.65	2.00	2.05
17	B	612	CLA	CHC-C1C	2.65	1.41	1.35
17	b	5609	CLA	C1D-ND	2.65	1.41	1.37
17	a	5406	CLA	CHC-C1C	2.65	1.41	1.35
17	b	5610	CLA	CHC-C1C	2.64	1.41	1.35
17	c	5505	CLA	CHC-C1C	2.64	1.41	1.35
17	C	509	CLA	C3B-C2B	-2.64	1.36	1.40
17	c	5510	CLA	C3B-CAB	-2.64	1.42	1.47
17	d	5404	CLA	C3B-C2B	-2.64	1.36	1.40
17	k	5501	CLA	C3B-C2B	-2.64	1.36	1.40
17	c	5505	CLA	C3B-C2B	-2.64	1.36	1.40
17	C	508	CLA	MG-ND	-2.64	2.00	2.05
17	C	508	CLA	CHC-C1C	2.64	1.41	1.35
17	C	502	CLA	CHC-C1C	2.64	1.41	1.35
17	B	610	CLA	MG-ND	-2.63	2.00	2.05
17	B	613	CLA	CMD-C2D	-2.63	1.45	1.50
17	k	5501	CLA	CHC-C1C	2.63	1.41	1.35
17	b	5610	CLA	MG-ND	-2.63	2.00	2.05
17	B	610	CLA	CHC-C1C	2.63	1.41	1.35
17	c	5511	CLA	CHC-C1C	2.63	1.41	1.35
17	b	5605	CLA	CHC-C1C	2.63	1.41	1.35
17	B	605	CLA	CHC-C1C	2.63	1.41	1.35
17	B	616	CLA	CHC-C1C	2.63	1.41	1.35
22	A	409	LMT	O3'-C3'	-2.62	1.36	1.43
17	B	612	CLA	MG-ND	-2.62	2.00	2.05
17	b	5612	CLA	C1D-ND	2.62	1.41	1.37
17	b	5611	CLA	CMD-C2D	-2.62	1.45	1.50
17	B	615	CLA	CHC-C1C	2.62	1.41	1.35
17	b	5607	CLA	CHC-C1C	2.62	1.41	1.35
17	b	5616	CLA	CHC-C1C	2.62	1.41	1.35
17	C	511	CLA	CHC-C1C	2.62	1.41	1.35
17	c	5508	CLA	MG-ND	-2.62	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	c	5509	CLA	CMD-C2D	-2.62	1.45	1.50
17	C	513	CLA	CMB-C2B	-2.61	1.46	1.51
17	A	403	CLA	CHC-C1C	2.61	1.41	1.35
22	a	5410	LMT	O3'-C3'	-2.61	1.36	1.43
22	m	5102	LMT	O3'-C3'	-2.61	1.36	1.43
17	c	5512	CLA	CMB-C2B	-2.61	1.46	1.51
17	B	611	CLA	CMD-C2D	-2.61	1.45	1.50
17	C	511	CLA	C3B-C2B	-2.61	1.36	1.40
22	a	5410	LMT	O2'-C2'	-2.61	1.36	1.43
17	c	5507	CLA	C3B-CAB	-2.60	1.42	1.47
17	c	5503	CLA	CMD-C2D	-2.60	1.45	1.50
17	b	5612	CLA	CMD-C2D	-2.60	1.45	1.50
17	b	5616	CLA	CMC-C2C	-2.60	1.45	1.50
17	a	5404	CLA	MG-ND	-2.60	2.00	2.05
17	b	5615	CLA	CHC-C1C	2.60	1.41	1.35
17	B	614	CLA	C1D-ND	2.60	1.41	1.37
17	c	5501	CLA	CHC-C1C	2.60	1.41	1.35
17	a	5404	CLA	CHC-C1C	2.59	1.41	1.35
17	b	5612	CLA	MG-ND	-2.59	2.00	2.05
17	C	508	CLA	C1D-ND	2.59	1.41	1.37
17	b	5613	CLA	CMD-C2D	-2.59	1.45	1.50
17	B	603	CLA	CHC-C1C	2.59	1.41	1.35
17	b	5603	CLA	CHC-C1C	2.59	1.41	1.35
17	A	403	CLA	MG-ND	-2.59	2.00	2.05
17	C	507	CLA	C3B-CAB	-2.59	1.42	1.47
17	C	509	CLA	CMD-C2D	-2.59	1.45	1.50
17	B	607	CLA	CHC-C1C	2.59	1.41	1.35
17	C	501	CLA	CHC-C1C	2.59	1.41	1.35
17	C	506	CLA	C1D-ND	2.59	1.41	1.37
17	B	606	CLA	CHC-C1C	2.59	1.41	1.35
17	b	5606	CLA	CHC-C1C	2.59	1.41	1.35
17	c	5507	CLA	CHC-C1C	2.58	1.41	1.35
17	B	609	CLA	C3B-C2B	-2.58	1.36	1.40
17	c	5506	CLA	C3B-C2B	-2.58	1.36	1.40
17	B	616	CLA	C3B-C2B	-2.58	1.36	1.40
17	c	5505	CLA	MG-ND	-2.58	2.00	2.05
17	B	609	CLA	C1D-ND	2.58	1.41	1.37
17	b	5603	CLA	C3B-CAB	-2.58	1.42	1.47
17	b	5614	CLA	C1D-ND	2.58	1.41	1.37
22	m	5102	LMT	O2B-C2B	-2.58	1.36	1.43
17	b	5610	CLA	CMD-C2D	-2.57	1.45	1.50
17	A	401	CLA	CMD-C2D	-2.57	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	5402	CLA	C1D-ND	2.57	1.40	1.37
17	B	612	CLA	C1D-ND	2.57	1.40	1.37
17	B	616	CLA	CMC-C2C	-2.57	1.45	1.50
17	c	5506	CLA	C1D-ND	2.57	1.40	1.37
17	C	507	CLA	CHC-C1C	2.57	1.41	1.35
17	b	5603	CLA	C1D-ND	2.57	1.40	1.37
17	B	603	CLA	C3B-CAB	-2.57	1.42	1.47
17	C	505	CLA	MG-ND	-2.56	2.00	2.05
22	M	101	LMT	O2'-C2'	-2.56	1.36	1.43
17	b	5616	CLA	C3B-C2B	-2.56	1.36	1.40
18	A	404	PHO	C3B-CAB	-2.55	1.42	1.47
17	B	605	CLA	C1D-ND	2.55	1.40	1.37
17	C	509	CLA	MG-ND	-2.55	2.00	2.05
17	a	5402	CLA	CMD-C2D	-2.55	1.45	1.50
26	c	5515	DGD	O6D-C5D	-2.55	1.38	1.44
17	C	506	CLA	C3B-C2B	-2.55	1.36	1.40
17	D	405	CLA	C3B-C2B	-2.55	1.36	1.40
17	B	603	CLA	C1D-ND	2.55	1.40	1.37
17	B	607	CLA	CMC-C2C	-2.55	1.45	1.50
26	C	517	DGD	O6D-C5D	-2.54	1.38	1.44
17	a	5403	CLA	C3B-CAB	-2.54	1.42	1.47
17	b	5614	CLA	CMD-C2D	-2.54	1.45	1.50
17	b	5603	CLA	MG-ND	-2.54	2.00	2.05
17	B	610	CLA	CMD-C2D	-2.54	1.45	1.50
17	c	5508	CLA	C1D-ND	2.54	1.40	1.37
17	a	5403	CLA	CHC-C1C	2.54	1.41	1.35
17	b	5607	CLA	CMC-C2C	-2.54	1.45	1.50
17	A	402	CLA	C3B-CAB	-2.54	1.42	1.47
17	B	614	CLA	CMD-C2D	-2.53	1.45	1.50
17	b	5610	CLA	C1D-ND	2.53	1.40	1.37
17	c	5502	CLA	C3B-CAB	-2.53	1.42	1.47
17	B	608	CLA	C3B-C2B	-2.53	1.36	1.40
17	c	5501	CLA	C3B-CAB	-2.53	1.42	1.47
17	A	402	CLA	CHC-C1C	2.53	1.41	1.35
17	A	403	CLA	C3B-CAB	-2.53	1.42	1.47
17	A	403	CLA	CMD-C2D	-2.53	1.45	1.50
17	b	5606	CLA	CMD-C2D	-2.52	1.45	1.50
17	a	5404	CLA	C3B-CAB	-2.52	1.42	1.47
17	C	502	CLA	C3B-CAB	-2.52	1.42	1.47
18	a	5405	PHO	C3B-CAB	-2.52	1.42	1.47
17	c	5507	CLA	CMD-C2D	-2.52	1.45	1.50
17	a	5403	CLA	MG-ND	-2.52	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	5609	CLA	C3B-C2B	-2.52	1.36	1.40
17	b	5614	CLA	C3B-CAB	-2.52	1.42	1.47
17	b	5604	CLA	CMD-C2D	-2.52	1.45	1.50
19	A	406	PQ9	C10-C5	2.51	1.48	1.35
17	B	603	CLA	MG-ND	-2.51	2.00	2.05
17	b	5608	CLA	C3B-C2B	-2.51	1.36	1.40
17	B	614	CLA	C3B-C2B	-2.51	1.36	1.40
19	a	5407	PQ9	C10-C5	2.51	1.48	1.35
17	C	501	CLA	C3B-CAB	-2.51	1.42	1.47
17	B	604	CLA	CMD-C2D	-2.50	1.45	1.50
17	B	610	CLA	C1D-ND	2.50	1.40	1.37
18	a	5405	PHO	CMD-C2D	-2.50	1.45	1.51
17	B	614	CLA	C3B-CAB	-2.50	1.42	1.47
22	m	5102	LMT	O3B-C3B	-2.50	1.37	1.43
17	c	5509	CLA	MG-ND	-2.50	2.00	2.05
17	B	612	CLA	C3B-CAB	-2.50	1.42	1.47
17	b	5605	CLA	C1D-ND	2.50	1.40	1.37
17	b	5608	CLA	C1D-ND	2.49	1.40	1.37
17	B	607	CLA	CMD-C2D	-2.49	1.45	1.50
17	A	405	CLA	CMD-C2D	-2.49	1.45	1.50
17	a	5404	CLA	CMD-C2D	-2.49	1.45	1.50
17	a	5406	CLA	CMD-C2D	-2.49	1.45	1.50
17	B	615	CLA	MG-ND	-2.49	2.00	2.05
17	b	5616	CLA	C3B-CAB	-2.49	1.42	1.47
22	M	101	LMT	O3B-C3B	-2.49	1.37	1.43
17	A	401	CLA	C1D-ND	2.49	1.40	1.37
17	B	614	CLA	MG-ND	-2.49	2.00	2.05
17	b	5615	CLA	MG-ND	-2.49	2.00	2.05
17	B	606	CLA	CMD-C2D	-2.49	1.45	1.50
17	B	608	CLA	CMD-C2D	-2.49	1.45	1.50
17	D	404	CLA	CMC-C2C	-2.49	1.45	1.50
22	A	409	LMT	O2'-C2'	-2.48	1.37	1.43
18	A	404	PHO	CMD-C2D	-2.48	1.45	1.51
17	b	5614	CLA	C3B-C2B	-2.48	1.36	1.40
17	b	5614	CLA	MG-ND	-2.48	2.00	2.05
17	c	5505	CLA	CMD-C2D	-2.48	1.45	1.50
17	C	511	CLA	C3B-CAB	-2.48	1.42	1.47
17	c	5502	CLA	CMC-C2C	-2.48	1.45	1.50
17	B	610	CLA	CMC-C2C	-2.48	1.45	1.50
17	B	608	CLA	C1D-ND	2.48	1.40	1.37
17	k	5501	CLA	C3B-CAB	-2.47	1.42	1.47
17	b	5608	CLA	CMD-C2D	-2.47	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	5616	CLA	MG-ND	-2.47	2.00	2.05
17	C	507	CLA	CMD-C2D	-2.47	1.45	1.50
17	A	402	CLA	MG-ND	-2.47	2.00	2.05
17	B	616	CLA	C3B-CAB	-2.47	1.42	1.47
17	B	615	CLA	C1D-ND	2.47	1.40	1.37
17	b	5612	CLA	C3B-CAB	-2.47	1.42	1.47
17	C	504	CLA	C3B-C2B	-2.46	1.36	1.40
17	C	503	CLA	C3B-C2B	-2.46	1.36	1.40
17	a	5402	CLA	CMC-C2C	-2.46	1.45	1.50
17	b	5603	CLA	CMD-C2D	-2.46	1.45	1.50
17	B	616	CLA	MG-ND	-2.46	2.00	2.05
18	a	5405	PHO	CMB-C2B	-2.46	1.45	1.51
17	b	5607	CLA	CMD-C2D	-2.46	1.45	1.50
17	b	5610	CLA	CMC-C2C	-2.46	1.45	1.50
17	b	5613	CLA	CMC-C2C	-2.46	1.45	1.50
17	k	5501	CLA	MG-ND	-2.46	2.00	2.05
17	b	5602	CLA	CMD-C2D	-2.46	1.45	1.50
17	d	5404	CLA	MG-ND	-2.45	2.00	2.05
17	c	5504	CLA	C3B-C2B	-2.45	1.37	1.40
17	C	510	CLA	MG-ND	-2.45	2.00	2.05
17	C	511	CLA	MG-ND	-2.45	2.00	2.05
17	B	611	CLA	MG-ND	-2.45	2.00	2.05
17	A	401	CLA	CMC-C2C	-2.45	1.45	1.50
17	B	603	CLA	CMD-C2D	-2.45	1.45	1.50
17	A	402	CLA	CMD-C2D	-2.45	1.45	1.50
17	C	506	CLA	MG-ND	-2.45	2.00	2.05
17	B	615	CLA	C3B-CAB	-2.44	1.43	1.47
17	D	405	CLA	MG-ND	-2.44	2.00	2.05
18	A	404	PHO	CMC-C2C	-2.44	1.45	1.51
22	m	5102	LMT	O2'-C2'	-2.44	1.37	1.43
17	B	605	CLA	MG-ND	-2.44	2.00	2.05
17	B	612	CLA	CMC-C2C	-2.44	1.45	1.50
17	B	608	CLA	CMC-C2C	-2.44	1.45	1.50
17	B	607	CLA	MG-ND	-2.44	2.01	2.05
23	L	101	SQD	O47-C7	2.44	1.41	1.34
17	B	608	CLA	C3B-CAB	-2.44	1.43	1.47
17	b	5615	CLA	C1D-ND	2.44	1.40	1.37
17	a	5403	CLA	CMD-C2D	-2.44	1.45	1.50
17	A	405	CLA	CMC-C2C	-2.44	1.45	1.50
18	D	402	PHO	CMB-C2B	-2.44	1.45	1.51
17	C	505	CLA	CMD-C2D	-2.44	1.45	1.50
22	T	101	LMT	O3B-C3B	-2.44	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	5405	PHO	CMC-C2C	-2.44	1.45	1.51
17	B	613	CLA	CMC-C2C	-2.43	1.45	1.50
17	B	605	CLA	CMD-C2D	-2.43	1.45	1.50
17	d	5403	CLA	CMC-C2C	-2.43	1.45	1.50
17	c	5510	CLA	MG-ND	-2.43	2.01	2.05
17	B	604	CLA	C1D-ND	2.43	1.40	1.37
17	C	502	CLA	CMC-C2C	-2.43	1.45	1.50
18	A	404	PHO	CMB-C2B	-2.43	1.45	1.51
17	b	5604	CLA	C1D-ND	2.43	1.40	1.37
17	a	5406	CLA	CMC-C2C	-2.43	1.45	1.50
17	b	5608	CLA	C3B-CAB	-2.43	1.43	1.47
17	c	5508	CLA	CMD-C2D	-2.43	1.45	1.50
17	C	508	CLA	CMD-C2D	-2.43	1.45	1.50
17	b	5615	CLA	C3B-CAB	-2.43	1.43	1.47
17	c	5511	CLA	MG-ND	-2.43	2.01	2.05
17	b	5612	CLA	CMC-C2C	-2.42	1.45	1.50
17	b	5605	CLA	CMD-C2D	-2.42	1.45	1.50
18	d	5402	PHO	CMB-C2B	-2.42	1.45	1.51
17	c	5503	CLA	C3B-C2B	-2.42	1.37	1.40
23	d	5407	SQD	O2-C2	-2.42	1.37	1.43
17	D	405	CLA	C3B-CAB	-2.42	1.43	1.47
17	B	611	CLA	C1D-ND	2.42	1.40	1.37
17	b	5605	CLA	MG-ND	-2.41	2.01	2.05
22	B	620	LMT	O3B-C3B	-2.41	1.37	1.43
17	B	615	CLA	CMC-C2C	-2.41	1.45	1.50
17	b	5615	CLA	CMC-C2C	-2.41	1.45	1.50
18	D	402	PHO	CMC-C2C	-2.41	1.45	1.51
17	b	5607	CLA	MG-ND	-2.41	2.01	2.05
17	B	602	CLA	CMD-C2D	-2.41	1.45	1.50
17	C	505	CLA	C1D-ND	2.41	1.40	1.37
17	c	5506	CLA	MG-ND	-2.41	2.01	2.05
17	C	512	CLA	MG-ND	-2.41	2.01	2.05
17	B	610	CLA	C3B-CAB	-2.41	1.43	1.47
17	b	5605	CLA	C3B-CAB	-2.40	1.43	1.47
17	B	606	CLA	C3B-C2B	-2.40	1.37	1.40
17	d	5404	CLA	C3B-CAB	-2.40	1.43	1.47
17	B	605	CLA	C3B-CAB	-2.40	1.43	1.47
17	c	5507	CLA	CMC-C2C	-2.40	1.45	1.50
26	c	5515	DGD	O6E-C5E	-2.40	1.38	1.44
17	b	5606	CLA	C3B-C2B	-2.40	1.37	1.40
26	C	517	DGD	O6E-C5E	-2.39	1.38	1.44
17	C	512	CLA	C3B-C2B	-2.39	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	c	5509	CLA	CMC-C2C	-2.39	1.45	1.50
17	C	507	CLA	CMC-C2C	-2.39	1.45	1.50
17	C	511	CLA	CMC-C2C	-2.39	1.45	1.50
18	d	5402	PHO	CMC-C2C	-2.39	1.45	1.51
17	C	509	CLA	CMC-C2C	-2.39	1.45	1.50
17	B	606	CLA	MG-ND	-2.39	2.01	2.05
17	c	5501	CLA	MG-ND	-2.39	2.01	2.05
17	c	5510	CLA	CMD-C2D	-2.38	1.45	1.50
17	c	5505	CLA	C1D-ND	2.38	1.40	1.37
17	d	5404	CLA	CMD-C2D	-2.38	1.45	1.50
17	C	513	CLA	MG-ND	-2.38	2.01	2.05
17	C	509	CLA	C3B-CAB	-2.38	1.43	1.47
17	D	405	CLA	CMD-C2D	-2.38	1.45	1.50
17	c	5501	CLA	CMC-C2C	-2.38	1.45	1.50
17	c	5506	CLA	CMD-C2D	-2.38	1.45	1.50
17	b	5615	CLA	CMD-C2D	-2.38	1.45	1.50
26	C	517	DGD	O2G-C2G	-2.38	1.40	1.46
17	B	615	CLA	CMD-C2D	-2.38	1.45	1.50
22	a	5410	LMT	O3B-C3B	-2.37	1.37	1.43
17	k	5501	CLA	CMC-C2C	-2.37	1.45	1.50
17	c	5512	CLA	MG-ND	-2.37	2.01	2.05
17	C	501	CLA	MG-ND	-2.37	2.01	2.05
17	k	5501	CLA	CMD-C2D	-2.37	1.45	1.50
18	D	402	PHO	CMD-C2D	-2.37	1.45	1.51
17	b	5603	CLA	CMC-C2C	-2.37	1.45	1.50
17	c	5511	CLA	CMD-C2D	-2.37	1.45	1.50
17	b	5610	CLA	C3B-C2B	-2.36	1.37	1.40
17	C	511	CLA	CMD-C2D	-2.36	1.45	1.50
17	c	5505	CLA	C3B-CAB	-2.36	1.43	1.47
17	b	5606	CLA	MG-ND	-2.36	2.01	2.05
17	C	506	CLA	CMD-C2D	-2.36	1.45	1.50
17	b	5610	CLA	C3B-CAB	-2.36	1.43	1.47
17	C	512	CLA	CMD-C2D	-2.36	1.45	1.50
17	C	510	CLA	CMD-C2D	-2.36	1.45	1.50
18	d	5402	PHO	CMD-C2D	-2.36	1.46	1.51
17	b	5611	CLA	MG-ND	-2.36	2.01	2.05
17	b	5608	CLA	CMC-C2C	-2.36	1.45	1.50
17	c	5511	CLA	C3B-C2B	-2.35	1.37	1.40
17	b	5606	CLA	C3B-CAB	-2.35	1.43	1.47
17	B	603	CLA	CMC-C2C	-2.35	1.45	1.50
17	B	610	CLA	C3B-C2B	-2.35	1.37	1.40
26	c	5515	DGD	O2G-C2G	-2.35	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	606	CLA	C3B-CAB	-2.35	1.43	1.47
22	A	409	LMT	O3B-C3B	-2.35	1.37	1.43
17	B	607	CLA	C3B-C2B	-2.34	1.37	1.40
17	C	501	CLA	CMC-C2C	-2.34	1.45	1.50
17	B	602	CLA	CMC-C2C	-2.34	1.45	1.50
17	B	601	CLA	CMB-C2B	-2.34	1.46	1.51
17	b	5604	CLA	CMC-C2C	-2.34	1.45	1.50
17	c	5509	CLA	C3B-CAB	-2.34	1.43	1.47
17	b	5616	CLA	CMD-C2D	-2.34	1.45	1.50
17	c	5504	CLA	CMD-C2D	-2.34	1.45	1.50
17	C	504	CLA	CMD-C2D	-2.33	1.45	1.50
17	b	5607	CLA	C3B-C2B	-2.33	1.37	1.40
17	B	609	CLA	MG-ND	-2.33	2.01	2.05
17	b	5609	CLA	MG-ND	-2.33	2.01	2.05
17	b	5602	CLA	CMC-C2C	-2.33	1.45	1.50
17	B	602	CLA	C3B-CAB	-2.33	1.43	1.47
17	B	616	CLA	CMD-C2D	-2.33	1.45	1.50
17	A	405	CLA	MG-ND	-2.33	2.01	2.05
17	c	5502	CLA	MG-ND	-2.33	2.01	2.05
17	b	5611	CLA	C1D-ND	2.33	1.40	1.37
17	a	5406	CLA	MG-ND	-2.32	2.01	2.05
17	c	5504	CLA	CMC-C2C	-2.32	1.45	1.50
23	D	403	SQD	O2-C2	-2.31	1.37	1.43
17	C	505	CLA	C3B-CAB	-2.31	1.43	1.47
17	b	5601	CLA	CMB-C2B	-2.31	1.46	1.51
17	C	504	CLA	MG-ND	-2.31	2.01	2.05
17	b	5602	CLA	C3B-CAB	-2.31	1.43	1.47
17	B	605	CLA	CMC-C2C	-2.31	1.45	1.50
17	C	504	CLA	CMC-C2C	-2.30	1.45	1.50
17	C	506	CLA	C3B-CAB	-2.30	1.43	1.47
17	C	505	CLA	CMC-C2C	-2.30	1.45	1.50
17	B	604	CLA	CMC-C2C	-2.30	1.45	1.50
17	D	404	CLA	C1D-ND	2.30	1.40	1.37
17	C	502	CLA	CMD-C2D	-2.30	1.45	1.50
17	C	503	CLA	C3B-CAB	-2.30	1.43	1.47
17	B	609	CLA	CMC-C2C	-2.30	1.45	1.50
17	c	5502	CLA	CMD-C2D	-2.30	1.45	1.50
26	C	518	DGD	O1G-C1G	-2.30	1.39	1.45
17	c	5505	CLA	CMC-C2C	-2.30	1.45	1.50
17	C	502	CLA	MG-ND	-2.29	2.01	2.05
17	b	5606	CLA	CMC-C2C	-2.29	1.45	1.50
17	b	5613	CLA	C1D-ND	2.29	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	c	5504	CLA	C3B-CAB	-2.29	1.43	1.47
17	b	5609	CLA	CMC-C2C	-2.29	1.45	1.50
22	M	101	LMT	O1'-C1'	-2.29	1.36	1.40
22	a	5410	LMT	O2B-C2B	-2.28	1.37	1.43
17	c	5506	CLA	C3B-CAB	-2.28	1.43	1.47
17	c	5504	CLA	MG-ND	-2.28	2.01	2.05
17	c	5510	CLA	CMC-C2C	-2.28	1.46	1.50
17	B	609	CLA	CMD-C2D	-2.28	1.46	1.50
17	B	613	CLA	CAA-C2A	-2.27	1.49	1.54
18	d	5402	PHO	C3B-CAB	-2.27	1.43	1.47
17	c	5503	CLA	C3B-CAB	-2.27	1.43	1.47
17	b	5601	CLA	CMD-C2D	-2.27	1.46	1.50
26	C	518	DGD	O2G-C2G	-2.27	1.40	1.46
17	C	510	CLA	CMC-C2C	-2.26	1.46	1.50
22	M	101	LMT	O4'-C4B	-2.26	1.37	1.43
17	D	405	CLA	CMC-C2C	-2.26	1.46	1.50
17	d	5403	CLA	C1D-ND	2.26	1.40	1.37
26	c	5516	DGD	O1G-C1G	-2.26	1.40	1.45
17	B	613	CLA	C1D-ND	2.26	1.40	1.37
26	c	5516	DGD	O2G-C2G	-2.26	1.41	1.46
17	c	5501	CLA	CMD-C2D	-2.26	1.46	1.50
17	b	5613	CLA	CAA-C2A	-2.25	1.49	1.54
23	D	403	SQD	O3-C3	-2.25	1.37	1.43
17	b	5605	CLA	CMC-C2C	-2.25	1.46	1.50
17	b	5614	CLA	CMC-C2C	-2.25	1.46	1.50
17	C	504	CLA	C3B-CAB	-2.24	1.43	1.47
17	A	403	CLA	CMC-C2C	-2.24	1.46	1.50
17	B	601	CLA	CMD-C2D	-2.24	1.46	1.50
17	B	606	CLA	CMC-C2C	-2.23	1.46	1.50
17	C	503	CLA	MG-ND	-2.23	2.01	2.05
18	D	402	PHO	C3B-CAB	-2.23	1.43	1.47
17	B	614	CLA	CMC-C2C	-2.23	1.46	1.50
17	c	5506	CLA	CMC-C2C	-2.23	1.46	1.50
19	D	406	PQ9	C10-C5	2.23	1.47	1.35
17	c	5503	CLA	MG-ND	-2.23	2.01	2.05
19	d	5405	PQ9	C3-C4	-2.23	1.38	1.44
20	A	407	BCR	C33-C5	-2.23	1.47	1.50
17	b	5609	CLA	CMD-C2D	-2.23	1.46	1.50
17	C	513	CLA	CMC-C2C	-2.23	1.46	1.50
19	D	406	PQ9	C3-C4	-2.22	1.38	1.44
17	a	5404	CLA	CMC-C2C	-2.22	1.46	1.50
17	d	5404	CLA	CMC-C2C	-2.22	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	501	CLA	CMD-C2D	-2.22	1.46	1.50
17	C	506	CLA	CMC-C2C	-2.22	1.46	1.50
23	A	410	SQD	O3-C3	-2.21	1.37	1.43
19	d	5405	PQ9	C10-C5	2.21	1.46	1.35
17	a	5403	CLA	C4B-CHC	-2.21	1.34	1.41
26	c	5515	DGD	O3E-C3E	-2.21	1.37	1.43
17	A	402	CLA	C4B-CHC	-2.21	1.34	1.41
17	c	5512	CLA	CMC-C2C	-2.20	1.46	1.50
26	C	517	DGD	O3E-C3E	-2.20	1.37	1.43
20	h	5101	BCR	C33-C5	-2.20	1.47	1.50
17	B	613	CLA	CAC-C3C	-2.20	1.45	1.51
17	C	507	CLA	C4B-CHC	-2.20	1.34	1.41
23	d	5407	SQD	O3-C3	-2.19	1.37	1.43
20	H	101	BCR	C33-C5	-2.19	1.47	1.50
17	b	5605	CLA	CAC-C3C	-2.19	1.45	1.51
17	b	5613	CLA	CAC-C3C	-2.19	1.45	1.51
20	a	5408	BCR	C33-C5	-2.18	1.47	1.50
17	b	5604	CLA	CAC-C3C	-2.18	1.45	1.51
23	A	410	SQD	O2-C2	-2.18	1.37	1.43
23	a	5401	SQD	O3-C3	-2.18	1.37	1.43
17	B	604	CLA	CAC-C3C	-2.18	1.45	1.51
17	c	5507	CLA	C4B-CHC	-2.18	1.34	1.41
17	B	605	CLA	CAC-C3C	-2.18	1.45	1.51
17	B	611	CLA	CAC-C3C	-2.18	1.45	1.51
26	a	5411	DGD	O5D-C6D	-2.18	1.39	1.43
26	H	102	DGD	O2G-C2G	-2.18	1.41	1.46
26	H	102	DGD	O6D-C5D	-2.17	1.39	1.44
17	C	503	CLA	CMC-C2C	-2.17	1.46	1.50
23	a	5401	SQD	O4-C4	-2.17	1.37	1.43
17	A	401	CLA	CAA-C2A	-2.17	1.50	1.54
23	a	5401	SQD	O2-C2	-2.17	1.37	1.43
22	A	409	LMT	O4'-C4B	-2.16	1.37	1.43
17	c	5501	CLA	C4B-CHC	-2.16	1.35	1.41
17	A	402	CLA	CMC-C2C	-2.16	1.46	1.50
26	h	5102	DGD	O2G-C2G	-2.16	1.41	1.46
22	T	101	LMT	O4'-C4B	-2.15	1.37	1.43
17	C	501	CLA	C4B-CHC	-2.15	1.35	1.41
17	b	5611	CLA	CAC-C3C	-2.15	1.45	1.51
26	C	519	DGD	O5D-C6D	-2.15	1.39	1.43
17	a	5403	CLA	CMC-C2C	-2.15	1.46	1.50
26	h	5102	DGD	O6D-C5D	-2.15	1.39	1.44
17	C	512	CLA	CMC-C2C	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	c	5503	CLA	CMC-C2C	-2.14	1.46	1.50
23	A	410	SQD	O4-C4	-2.14	1.37	1.43
23	L	101	SQD	O2-C2	-2.14	1.37	1.43
17	A	403	CLA	C4B-CHC	-2.14	1.35	1.41
17	c	5511	CLA	CMC-C2C	-2.14	1.46	1.50
20	t	5102	BCR	C33-C5	-2.13	1.47	1.50
23	L	101	SQD	O47-C45	-2.13	1.41	1.46
17	B	604	CLA	C4B-CHC	-2.13	1.35	1.41
17	b	5604	CLA	C4B-CHC	-2.13	1.35	1.41
17	c	5502	CLA	C4B-CHC	-2.13	1.35	1.41
17	C	513	CLA	C3B-C2B	-2.13	1.37	1.40
23	D	403	SQD	O4-C4	-2.12	1.38	1.43
17	B	609	CLA	C3B-CAB	-2.12	1.43	1.47
23	d	5407	SQD	O4-C4	-2.12	1.38	1.43
23	L	101	SQD	O4-C4	-2.12	1.38	1.43
17	b	5601	CLA	MG-ND	-2.12	2.01	2.05
17	c	5512	CLA	C3B-C2B	-2.12	1.37	1.40
23	l	5102	SQD	O4-C4	-2.12	1.38	1.43
17	a	5404	CLA	C4B-CHC	-2.11	1.35	1.41
17	b	5609	CLA	C3B-CAB	-2.11	1.43	1.47
17	b	5613	CLA	C4B-CHC	-2.11	1.35	1.41
26	C	517	DGD	O4D-C4D	-2.11	1.38	1.43
17	B	607	CLA	C3B-CAB	-2.11	1.43	1.47
17	C	502	CLA	C4B-CHC	-2.11	1.35	1.41
17	B	601	CLA	MG-ND	-2.11	2.01	2.05
17	B	616	CLA	C4B-CHC	-2.11	1.35	1.41
26	C	519	DGD	O2G-C2G	-2.11	1.41	1.46
17	a	5402	CLA	CAA-C2A	-2.11	1.50	1.54
23	L	101	SQD	O3-C3	-2.11	1.38	1.43
23	l	5102	SQD	O3-C3	-2.10	1.38	1.43
17	B	605	CLA	C4B-CHC	-2.10	1.35	1.41
17	B	613	CLA	C4B-CHC	-2.10	1.35	1.41
22	B	620	LMT	O4'-C4B	-2.10	1.38	1.43
20	b	5618	BCR	C38-C26	-2.10	1.47	1.50
26	a	5411	DGD	O2G-C2G	-2.10	1.41	1.46
17	b	5607	CLA	C3B-CAB	-2.10	1.43	1.47
17	C	513	CLA	CMD-C2D	-2.10	1.46	1.50
17	c	5508	CLA	CAC-C3C	-2.09	1.45	1.51
17	C	508	CLA	CAC-C3C	-2.09	1.45	1.51
22	a	5410	LMT	O4'-C4B	-2.09	1.38	1.43
17	c	5512	CLA	CMD-C2D	-2.09	1.46	1.50
20	D	407	BCR	C33-C5	-2.09	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	618	BCR	C38-C26	-2.08	1.47	1.50
17	B	603	CLA	C4B-CHC	-2.08	1.35	1.41
26	c	5515	DGD	O4D-C4D	-2.08	1.38	1.43
17	b	5616	CLA	C4B-CHC	-2.08	1.35	1.41
22	a	5410	LMT	O1'-C1'	-2.07	1.36	1.40
17	b	5605	CLA	C4B-CHC	-2.07	1.35	1.41
17	B	606	CLA	C4B-CHC	-2.06	1.35	1.41
17	k	5501	CLA	C4B-CHC	-2.06	1.35	1.41
17	b	5612	CLA	C4B-CHC	-2.06	1.35	1.41
17	c	5508	CLA	C4B-CHC	-2.06	1.35	1.41
22	M	101	LMT	O5'-C5'	-2.06	1.39	1.44
20	d	5406	BCR	C33-C5	-2.05	1.47	1.50
17	b	5616	CLA	CAC-C3C	-2.05	1.45	1.51
20	t	5101	BCR	C33-C5	-2.05	1.47	1.50
17	a	5406	CLA	C3B-CAB	-2.05	1.43	1.47
17	C	511	CLA	C4B-CHC	-2.05	1.35	1.41
20	a	5408	BCR	C38-C26	-2.05	1.47	1.50
20	c	5514	BCR	C38-C26	-2.05	1.47	1.50
17	b	5603	CLA	C4B-CHC	-2.04	1.35	1.41
20	C	516	BCR	C33-C5	-2.04	1.47	1.50
22	m	5102	LMT	O5'-C5'	-2.04	1.39	1.44
23	l	5102	SQD	O2-C2	-2.04	1.38	1.43
26	a	5411	DGD	O1G-C1G	-2.04	1.40	1.45
17	C	508	CLA	C4B-CHC	-2.04	1.35	1.41
20	C	516	BCR	C38-C26	-2.04	1.47	1.50
17	B	612	CLA	C4B-CHC	-2.04	1.35	1.41
17	b	5615	CLA	C4B-CHC	-2.04	1.35	1.41
20	C	514	BCR	C33-C5	-2.04	1.47	1.50
22	T	101	LMT	O2B-C2B	-2.03	1.38	1.43
17	A	405	CLA	C3B-CAB	-2.03	1.43	1.47
17	B	615	CLA	C4B-CHC	-2.03	1.35	1.41
20	b	5619	BCR	C33-C5	-2.03	1.47	1.50
17	b	5611	CLA	CAA-C2A	-2.03	1.50	1.54
17	B	616	CLA	CAC-C3C	-2.03	1.45	1.51
17	B	611	CLA	CAA-C2A	-2.02	1.50	1.54
17	b	5606	CLA	C4B-CHC	-2.02	1.35	1.41
20	B	617	BCR	C38-C26	-2.02	1.47	1.50
17	B	601	CLA	C3B-C2B	-2.02	1.37	1.40
17	B	602	CLA	CAC-C3C	-2.02	1.45	1.51
17	B	603	CLA	CAC-C3C	-2.02	1.45	1.51
17	b	5607	CLA	C4B-CHC	-2.02	1.35	1.41
22	A	409	LMT	O2B-C2B	-2.01	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	5617	BCR	C33-C5	-2.01	1.47	1.50
20	T	102	BCR	C33-C5	-2.01	1.47	1.50
17	b	5603	CLA	CAC-C3C	-2.01	1.46	1.51
17	B	608	CLA	C4B-CHC	-2.01	1.35	1.41
20	k	5502	BCR	C33-C5	-2.01	1.47	1.50
26	C	517	DGD	O4E-C4E	-2.01	1.38	1.43
22	A	409	LMT	O1'-C1'	-2.01	1.36	1.40
17	b	5602	CLA	CAC-C3C	-2.00	1.46	1.51
26	c	5515	DGD	O4E-C4E	-2.00	1.38	1.43

All (1049) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	5403	CLA	C4A-NA-C1A	7.84	110.23	106.71
17	A	402	CLA	C4A-NA-C1A	7.73	110.18	106.71
17	C	508	CLA	C4A-NA-C1A	7.56	110.11	106.71
17	c	5508	CLA	C4A-NA-C1A	7.56	110.11	106.71
17	b	5611	CLA	C4A-NA-C1A	7.46	110.06	106.71
17	B	607	CLA	C4A-NA-C1A	7.43	110.05	106.71
17	b	5607	CLA	C4A-NA-C1A	7.38	110.02	106.71
17	B	611	CLA	C4A-NA-C1A	7.34	110.00	106.71
17	C	511	CLA	C4A-NA-C1A	7.32	110.00	106.71
17	k	5501	CLA	C4A-NA-C1A	7.25	109.96	106.71
17	b	5615	CLA	C4A-NA-C1A	7.24	109.96	106.71
17	B	615	CLA	C4A-NA-C1A	7.22	109.95	106.71
17	b	5606	CLA	C4A-NA-C1A	7.16	109.93	106.71
17	A	405	CLA	C4A-NA-C1A	7.06	109.88	106.71
17	a	5406	CLA	C4A-NA-C1A	7.06	109.88	106.71
17	b	5614	CLA	C4A-NA-C1A	7.06	109.88	106.71
17	B	606	CLA	C4A-NA-C1A	7.04	109.87	106.71
17	C	501	CLA	C4A-NA-C1A	7.04	109.87	106.71
17	B	614	CLA	C4A-NA-C1A	7.02	109.86	106.71
17	B	613	CLA	C4A-NA-C1A	6.99	109.85	106.71
17	b	5612	CLA	C4A-NA-C1A	6.96	109.83	106.71
17	C	503	CLA	C4A-NA-C1A	6.93	109.82	106.71
17	c	5501	CLA	C4A-NA-C1A	6.92	109.82	106.71
17	c	5503	CLA	C4A-NA-C1A	6.91	109.81	106.71
17	A	403	CLA	C4A-NA-C1A	6.89	109.80	106.71
17	B	612	CLA	C4A-NA-C1A	6.88	109.80	106.71
17	b	5603	CLA	C4A-NA-C1A	6.83	109.78	106.71
17	B	603	CLA	C4A-NA-C1A	6.82	109.77	106.71
17	b	5613	CLA	C4A-NA-C1A	6.79	109.76	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	604	CLA	C4A-NA-C1A	6.78	109.75	106.71
17	B	610	CLA	C4A-NA-C1A	6.73	109.73	106.71
17	b	5604	CLA	C4A-NA-C1A	6.72	109.72	106.71
17	a	5404	CLA	C4A-NA-C1A	6.71	109.72	106.71
17	C	502	CLA	C4A-NA-C1A	6.67	109.70	106.71
17	b	5610	CLA	C4A-NA-C1A	6.62	109.68	106.71
17	b	5605	CLA	C4A-NA-C1A	6.60	109.67	106.71
17	b	5609	CLA	C4A-NA-C1A	6.60	109.67	106.71
17	B	609	CLA	C4A-NA-C1A	6.59	109.67	106.71
17	c	5502	CLA	C4A-NA-C1A	6.59	109.67	106.71
17	b	5602	CLA	C4A-NA-C1A	6.54	109.65	106.71
17	B	605	CLA	C4A-NA-C1A	6.53	109.64	106.71
17	c	5511	CLA	C4A-NA-C1A	6.51	109.63	106.71
17	C	506	CLA	C4A-NA-C1A	6.50	109.63	106.71
17	B	602	CLA	C4A-NA-C1A	6.49	109.62	106.71
17	C	512	CLA	C4A-NA-C1A	6.47	109.61	106.71
17	C	504	CLA	C4A-NA-C1A	6.45	109.61	106.71
17	c	5504	CLA	C4A-NA-C1A	6.40	109.58	106.71
17	c	5506	CLA	C4A-NA-C1A	6.39	109.58	106.71
17	B	616	CLA	C4A-NA-C1A	6.37	109.57	106.71
17	B	608	CLA	C4A-NA-C1A	6.35	109.56	106.71
17	b	5608	CLA	C4A-NA-C1A	6.33	109.55	106.71
17	d	5404	CLA	C4A-NA-C1A	6.32	109.55	106.71
17	D	405	CLA	C4A-NA-C1A	6.31	109.54	106.71
17	b	5616	CLA	C4A-NA-C1A	6.25	109.52	106.71
17	C	510	CLA	C4A-NA-C1A	6.01	109.41	106.71
17	C	513	CLA	C4A-NA-C1A	5.98	109.40	106.71
17	c	5512	CLA	C4A-NA-C1A	5.98	109.40	106.71
17	c	5510	CLA	C4A-NA-C1A	5.91	109.36	106.71
17	C	507	CLA	C4A-NA-C1A	5.86	109.34	106.71
17	c	5507	CLA	C4A-NA-C1A	5.83	109.33	106.71
17	C	509	CLA	C4A-NA-C1A	5.59	109.22	106.71
17	d	5403	CLA	C4A-NA-C1A	5.54	109.20	106.71
17	c	5509	CLA	C4A-NA-C1A	5.52	109.19	106.71
17	B	601	CLA	C4A-NA-C1A	5.50	109.18	106.71
17	b	5601	CLA	C4A-NA-C1A	5.50	109.18	106.71
19	d	5405	PQ9	C11-C12-C13	-5.46	117.71	126.79
26	h	5102	DGD	O3G-C3G-C2G	-5.46	97.73	110.90
17	D	404	CLA	C4A-NA-C1A	5.45	109.16	106.71
26	H	102	DGD	O3G-C3G-C2G	-5.45	97.75	110.90
19	D	406	PQ9	C11-C12-C13	-5.42	117.77	126.79
17	c	5505	CLA	C4A-NA-C1A	5.36	109.11	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	5402	CLA	C4A-NA-C1A	5.33	109.10	106.71
17	A	401	CLA	C4A-NA-C1A	5.30	109.09	106.71
17	C	505	CLA	C4A-NA-C1A	5.25	109.07	106.71
24	A	411	BCT	O2-C-O1	5.06	132.66	119.55
24	a	5412	BCT	O2-C-O1	5.05	132.66	119.55
23	a	5401	SQD	O47-C7-C8	4.99	120.28	111.09
23	A	410	SQD	O47-C7-C8	4.90	120.10	111.09
17	B	608	CLA	CMB-C2B-C1B	-4.85	121.01	128.46
17	b	5608	CLA	CMB-C2B-C1B	-4.84	121.02	128.46
25	d	5408	MGE	O2G-C1B-C2B	4.79	121.83	111.50
17	c	5502	CLA	C6-C5-C3	-4.74	101.02	113.45
23	l	5102	SQD	O7-S-C6	4.74	112.57	106.94
17	C	502	CLA	C6-C5-C3	-4.72	101.07	113.45
23	d	5407	SQD	O5-C5-C4	4.63	118.11	109.69
26	c	5516	DGD	O3G-C3G-C2G	-4.62	99.75	110.90
26	C	518	DGD	O3G-C3G-C2G	-4.61	99.78	110.90
23	L	101	SQD	O8-S-C6	4.58	113.04	105.74
25	B	619	MGE	O2G-C1B-C2B	4.44	121.08	111.50
25	b	5620	MGE	O2G-C1B-C2B	4.44	121.08	111.50
25	d	5410	MGE	O2G-C1B-C2B	4.44	121.07	111.50
25	D	410	MGE	O2G-C1B-C2B	4.44	121.07	111.50
26	a	5411	DGD	O3G-C3G-C2G	-4.44	100.20	110.90
25	D	409	MGE	C3G-O3G-C1D	-4.42	105.10	113.74
26	C	519	DGD	O3G-C3G-C2G	-4.40	100.27	110.90
23	l	5102	SQD	O47-C7-C8	4.36	120.91	111.50
17	B	610	CLA	CMB-C2B-C1B	-4.30	121.85	128.46
17	b	5610	CLA	CMB-C2B-C1B	-4.29	121.87	128.46
21	A	408	LHG	O4-P-O5	4.29	133.45	112.24
21	a	5409	LHG	O4-P-O5	4.29	133.45	112.24
17	b	5612	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
20	b	5618	BCR	C15-C14-C13	-4.24	121.25	127.31
20	B	618	BCR	C15-C14-C13	-4.24	121.26	127.31
17	B	612	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
17	b	5616	CLA	CMB-C2B-C1B	-4.21	122.00	128.46
25	D	409	MGE	O2G-C1B-C2B	4.20	120.56	111.50
17	B	616	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
23	L	101	SQD	O47-C7-C8	4.19	120.53	111.50
20	b	5618	BCR	C15-C16-C17	-4.12	115.03	123.47
23	l	5102	SQD	O9-S-C6	4.11	111.83	106.94
20	B	618	BCR	C15-C16-C17	-4.10	115.07	123.47
25	D	408	MGE	O2G-C1B-C2B	4.08	120.29	111.50
25	A	412	MGE	O2G-C1B-C2B	4.02	120.17	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	l	5101	MGE	O2G-C1B-C2B	4.01	120.14	111.50
25	D	410	MGE	C2G-O2G-C1B	-4.00	107.94	117.79
17	c	5512	CLA	CMB-C2B-C1B	-3.94	122.40	128.46
17	b	5614	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
17	B	614	CLA	CMB-C2B-C1B	-3.93	122.43	128.46
17	C	513	CLA	CMB-C2B-C1B	-3.93	122.43	128.46
17	b	5615	CLA	CMB-C2B-C1B	-3.92	122.43	128.46
17	B	615	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
17	b	5607	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
25	d	5409	MGE	O2G-C1B-C2B	3.89	119.88	111.50
17	b	5606	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
17	b	5608	CLA	CMB-C2B-C3B	3.88	131.94	124.68
26	h	5102	DGD	O6D-C1D-O3G	-3.88	100.78	109.97
17	b	5611	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
26	H	102	DGD	O6D-C1D-O3G	-3.88	100.79	109.97
17	B	607	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
17	B	606	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
25	d	5409	MGE	C3G-O3G-C1D	-3.86	106.20	113.74
23	d	5407	SQD	O47-C7-C8	3.86	119.82	111.50
23	d	5407	SQD	O7-S-C6	3.86	111.53	106.94
17	B	611	CLA	CMB-C2B-C1B	-3.86	122.54	128.46
17	B	608	CLA	CMB-C2B-C3B	3.85	131.89	124.68
17	c	5505	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
17	C	505	CLA	CMB-C2B-C1B	-3.82	122.58	128.46
23	D	403	SQD	O7-S-C6	3.82	111.48	106.94
17	B	601	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
17	b	5601	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
25	C	520	MGE	O2G-C1B-C2B	3.80	119.69	111.50
25	d	5410	MGE	C2G-O2G-C1B	-3.80	108.44	117.79
17	b	5604	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
25	c	5517	MGE	O2G-C1B-C2B	3.80	119.68	111.50
23	A	410	SQD	O7-S-C6	3.79	111.45	106.94
25	m	5103	MGE	O2G-C1B-C2B	3.79	119.67	111.50
25	m	5101	MGE	O2G-C1B-C2B	3.79	119.67	111.50
23	l	5102	SQD	O9-S-O7	-3.78	100.85	113.95
17	C	505	CLA	CAA-C2A-C3A	-3.78	102.42	112.78
17	c	5510	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
17	B	604	CLA	CMB-C2B-C1B	-3.77	122.66	128.46
17	c	5505	CLA	CAA-C2A-C3A	-3.77	102.45	112.78
17	C	510	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
20	c	5513	BCR	C15-C16-C17	-3.77	115.75	123.47
23	a	5401	SQD	O9-S-O7	-3.77	100.91	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	t	5101	BCR	C24-C23-C22	-3.77	120.54	126.23
20	b	5619	BCR	C24-C23-C22	-3.77	120.55	126.23
20	C	514	BCR	C15-C16-C17	-3.76	115.78	123.47
17	b	5612	CLA	CMB-C2B-C3B	3.75	131.69	124.68
17	B	612	CLA	CMB-C2B-C3B	3.72	131.65	124.68
17	c	5509	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
17	C	509	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
19	A	406	PQ9	C11-C2-C1	3.69	119.87	116.88
23	L	101	SQD	O9-S-O7	-3.66	101.27	113.95
23	A	410	SQD	O9-S-O7	-3.65	101.31	113.95
17	b	5610	CLA	CMB-C2B-C3B	3.65	131.51	124.68
17	B	610	CLA	CMB-C2B-C3B	3.65	131.50	124.68
26	C	519	DGD	O6D-C1D-O3G	-3.64	101.34	109.97
26	a	5411	DGD	O6D-C1D-O3G	-3.64	101.34	109.97
17	b	5613	CLA	CMB-C2B-C1B	-3.64	122.88	128.46
17	C	507	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
17	c	5506	CLA	CMB-C2B-C1B	-3.62	122.91	128.46
17	B	613	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
23	D	403	SQD	O5-C5-C4	3.61	116.25	109.69
17	c	5507	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
17	C	506	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
23	D	403	SQD	O47-C7-C8	3.60	119.26	111.50
19	a	5407	PQ9	C11-C2-C1	3.60	119.80	116.88
20	b	5617	BCR	C15-C16-C17	-3.59	116.13	123.47
17	A	403	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
20	B	617	BCR	C15-C16-C17	-3.58	116.15	123.47
23	d	5407	SQD	C3-C4-C5	3.56	116.58	110.24
25	A	412	MGE	C3G-O3G-C1D	-3.55	106.80	113.74
25	l	5101	MGE	C3G-O3G-C1D	-3.55	106.80	113.74
17	B	603	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
17	a	5404	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
22	M	101	LMT	C1'-O5'-C5'	-3.53	106.75	113.69
17	b	5603	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
17	d	5403	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
17	C	503	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
17	k	5501	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
19	d	5405	PQ9	C19-C18-C20	3.51	121.17	115.27
17	c	5503	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
19	D	406	PQ9	C19-C18-C20	3.50	121.16	115.27
17	C	504	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
17	C	511	CLA	CMB-C2B-C1B	-3.49	123.09	128.46
26	c	5515	DGD	O6D-C1D-O3G	-3.49	101.70	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	404	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
26	C	517	DGD	O6D-C1D-O3G	-3.48	101.72	109.97
17	d	5404	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
17	c	5504	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
17	D	405	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
17	b	5601	CLA	C1B-CHB-C4A	-3.46	123.27	130.12
17	B	601	CLA	C1B-CHB-C4A	-3.45	123.28	130.12
20	C	516	BCR	C15-C16-C17	-3.44	116.42	123.47
20	c	5514	BCR	C15-C16-C17	-3.44	116.43	123.47
23	a	5401	SQD	O7-S-C6	3.43	111.02	106.94
23	d	5407	SQD	O9-S-O7	-3.43	102.06	113.95
22	A	409	LMT	C1'-O5'-C5'	-3.42	106.97	113.69
26	c	5516	DGD	O6D-C1D-O3G	-3.42	101.87	109.97
23	D	403	SQD	O9-S-O7	-3.41	102.14	113.95
17	B	601	CLA	CMB-C2B-C3B	3.41	131.06	124.68
17	b	5616	CLA	CMB-C2B-C3B	3.41	131.06	124.68
17	b	5601	CLA	CMB-C2B-C3B	3.41	131.06	124.68
17	a	5406	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
17	A	405	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
17	C	505	CLA	CMB-C2B-C3B	3.40	131.04	124.68
26	C	518	DGD	O6D-C1D-O3G	-3.40	101.93	109.97
20	b	5617	BCR	C15-C14-C13	-3.39	122.47	127.31
25	d	5409	MGE	O1G-C1A-C2A	3.39	122.56	111.91
17	c	5505	CLA	CMB-C2B-C3B	3.39	131.02	124.68
22	m	5102	LMT	C1'-O5'-C5'	-3.39	107.04	113.69
17	C	512	CLA	CMB-C2B-C1B	-3.38	123.26	128.46
26	a	5411	DGD	O5D-C6D-C5D	-3.38	102.79	109.05
17	b	5605	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
19	D	406	PQ9	C36-C37-C38	-3.38	119.52	127.66
20	B	617	BCR	C15-C14-C13	-3.38	122.49	127.31
26	C	519	DGD	O5D-C6D-C5D	-3.38	102.79	109.05
19	d	5405	PQ9	C36-C37-C38	-3.38	119.53	127.66
17	c	5511	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
17	B	616	CLA	CMB-C2B-C3B	3.37	130.98	124.68
17	B	605	CLA	CMB-C2B-C1B	-3.36	123.29	128.46
20	d	5406	BCR	C24-C23-C22	-3.36	121.16	126.23
23	L	101	SQD	O6-C1-C2	3.35	113.54	108.30
26	C	518	DGD	O5D-C6D-C5D	-3.35	102.84	109.05
26	c	5516	DGD	O5D-C6D-C5D	-3.35	102.84	109.05
17	b	5614	CLA	CMB-C2B-C3B	3.35	130.94	124.68
20	D	407	BCR	C24-C23-C22	-3.34	121.19	126.23
17	B	614	CLA	CMB-C2B-C3B	3.34	130.92	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	c	5508	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
17	C	513	CLA	CMB-C2B-C3B	3.33	130.91	124.68
17	c	5512	CLA	CMB-C2B-C3B	3.33	130.91	124.68
17	C	508	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
23	a	5401	SQD	O9-S-C6	3.33	110.89	106.94
25	D	409	MGE	O1G-C1A-C2A	3.32	122.33	111.91
23	l	5102	SQD	O5-C5-C4	3.30	115.69	109.69
17	b	5607	CLA	CMB-C2B-C3B	3.30	130.85	124.68
17	c	5508	CLA	C1-C2-C3	-3.28	120.37	126.04
17	B	607	CLA	CMB-C2B-C3B	3.27	130.80	124.68
17	a	5402	CLA	CMB-C2B-C1B	-3.27	123.43	128.46
17	C	508	CLA	C1-C2-C3	-3.27	120.40	126.04
17	b	5609	CLA	C1-C2-C3	-3.25	120.42	126.04
20	k	5502	BCR	C24-C23-C22	-3.25	121.33	126.23
17	B	609	CLA	C1-C2-C3	-3.24	120.43	126.04
17	A	401	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
17	a	5403	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
17	b	5606	CLA	CMB-C2B-C3B	3.24	130.73	124.68
20	Y	101	BCR	C24-C23-C22	-3.23	121.35	126.23
17	b	5608	CLA	C1-C2-C3	-3.22	120.47	126.04
19	D	406	PQ9	C24-C23-C25	3.22	120.69	115.27
19	d	5405	PQ9	C24-C23-C25	3.22	120.69	115.27
17	B	608	CLA	C1-C2-C3	-3.22	120.47	126.04
17	B	606	CLA	CMB-C2B-C3B	3.22	130.70	124.68
17	C	503	CLA	C1-C2-C3	-3.22	120.48	126.04
17	c	5503	CLA	C1-C2-C3	-3.21	120.49	126.04
17	A	402	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
23	l	5102	SQD	C1-O5-C5	3.21	119.99	113.69
20	A	407	BCR	C15-C16-C17	-3.21	116.91	123.47
20	a	5408	BCR	C15-C16-C17	-3.20	116.92	123.47
25	B	619	MGE	C2G-O2G-C1B	-3.20	109.92	117.79
23	d	5407	SQD	C4-C3-C2	3.19	116.39	110.82
25	b	5620	MGE	C2G-O2G-C1B	-3.18	109.95	117.79
17	b	5611	CLA	CMB-C2B-C3B	3.18	130.63	124.68
17	B	613	CLA	CMB-C2B-C3B	3.18	130.63	124.68
23	A	410	SQD	O8-S-C6	3.18	110.80	105.74
17	b	5613	CLA	CMB-C2B-C3B	3.18	130.62	124.68
23	A	410	SQD	C44-O6-C1	3.18	119.94	113.74
20	H	101	BCR	C24-C23-C22	-3.17	121.44	126.23
20	z	5101	BCR	C15-C16-C17	-3.17	116.97	123.47
17	B	611	CLA	CMB-C2B-C3B	3.17	130.61	124.68
20	C	515	BCR	C15-C16-C17	-3.16	117.00	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	L	101	SQD	O9-S-C6	3.16	110.69	106.94
20	h	5101	BCR	C24-C23-C22	-3.15	121.47	126.23
17	A	403	CLA	CMB-C2B-C3B	3.15	130.57	124.68
17	b	5615	CLA	CMB-C2B-C3B	3.15	130.57	124.68
26	C	519	DGD	CDB-CCB-CBB	-3.14	98.48	114.42
23	d	5407	SQD	O8-S-C6	3.14	110.74	105.74
26	a	5411	DGD	CDB-CCB-CBB	-3.14	98.50	114.42
17	C	510	CLA	CMB-C2B-C3B	3.13	130.54	124.68
17	a	5404	CLA	CMB-C2B-C3B	3.13	130.54	124.68
17	B	615	CLA	CMB-C2B-C3B	3.13	130.53	124.68
19	d	5405	PQ9	C31-C32-C33	-3.13	120.13	127.66
17	c	5505	CLA	C1B-CHB-C4A	-3.13	123.93	130.12
17	B	606	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
17	c	5510	CLA	CMB-C2B-C3B	3.12	130.51	124.68
19	A	406	PQ9	C34-C33-C35	3.12	120.51	115.27
23	a	5401	SQD	O8-S-C6	3.12	110.70	105.74
17	b	5606	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
17	C	501	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
17	A	401	CLA	C1B-CHB-C4A	-3.11	123.96	130.12
19	D	406	PQ9	C31-C32-C33	-3.11	120.18	127.66
17	B	609	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
17	c	5501	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
17	C	505	CLA	C1B-CHB-C4A	-3.10	123.98	130.12
20	c	5513	BCR	C15-C14-C13	-3.09	122.89	127.31
17	a	5402	CLA	C1B-CHB-C4A	-3.09	123.99	130.12
17	c	5502	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
23	a	5401	SQD	C44-O6-C1	3.08	119.75	113.74
17	c	5509	CLA	CMB-C2B-C3B	3.08	130.44	124.68
23	A	410	SQD	O9-S-C6	3.08	110.60	106.94
17	b	5609	CLA	CMB-C2B-C1B	-3.07	123.74	128.46
20	k	5502	BCR	C15-C16-C17	-3.07	117.18	123.47
17	C	502	CLA	CMB-C2B-C1B	-3.07	123.74	128.46
19	D	406	PQ9	C21-C22-C23	-3.07	120.27	127.66
20	C	514	BCR	C15-C14-C13	-3.07	122.93	127.31
17	c	5507	CLA	CMB-C2B-C3B	3.06	130.41	124.68
17	C	509	CLA	CMB-C2B-C3B	3.06	130.40	124.68
19	d	5405	PQ9	C21-C22-C23	-3.06	120.29	127.66
17	C	507	CLA	CMB-C2B-C3B	3.05	130.39	124.68
20	b	5618	BCR	C35-C13-C14	-3.04	118.66	122.92
20	B	618	BCR	C35-C13-C14	-3.03	118.68	122.92
17	d	5404	CLA	CMB-C2B-C3B	3.02	130.33	124.68
17	b	5611	CLA	C1-C2-C3	-3.02	120.82	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	405	CLA	CMB-C2B-C3B	3.01	130.32	124.68
17	B	611	CLA	C1-C2-C3	-3.00	120.85	126.04
20	a	5408	BCR	C15-C14-C13	-3.00	123.03	127.31
20	Y	101	BCR	C15-C16-C17	-2.99	117.35	123.47
26	H	102	DGD	C3D-C4D-C5D	-2.98	104.93	110.24
23	D	403	SQD	C4-C3-C2	2.97	116.02	110.82
23	D	403	SQD	O8-S-C6	2.97	110.48	105.74
17	B	613	CLA	CHB-C4A-NA	2.97	128.61	124.51
20	A	407	BCR	C15-C14-C13	-2.96	123.08	127.31
25	A	412	MGE	O1G-C1A-C2A	2.96	121.18	111.91
26	a	5411	DGD	O6E-C1E-O5D	-2.95	102.98	109.97
26	C	519	DGD	O6E-C1E-O5D	-2.95	102.98	109.97
26	h	5102	DGD	C3D-C4D-C5D	-2.95	104.98	110.24
17	c	5508	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
20	h	5101	BCR	C7-C8-C9	-2.94	121.79	126.23
17	C	508	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
25	l	5101	MGE	O1G-C1A-C2A	2.93	121.11	111.91
17	b	5612	CLA	CHB-C4A-NA	2.93	128.57	124.51
17	B	603	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
17	c	5503	CLA	CMB-C2B-C3B	2.93	130.16	124.68
20	H	101	BCR	C7-C8-C9	-2.93	121.81	126.23
17	c	5502	CLA	C4-C3-C5	2.92	120.18	115.27
17	c	5506	CLA	CMB-C2B-C3B	2.91	130.13	124.68
17	C	503	CLA	CMB-C2B-C3B	2.91	130.12	124.68
17	B	612	CLA	CHB-C4A-NA	2.91	128.53	124.51
17	b	5613	CLA	CHB-C4A-NA	2.90	128.53	124.51
17	c	5508	CLA	CMB-C2B-C3B	2.90	130.11	124.68
17	C	506	CLA	CMB-C2B-C3B	2.90	130.10	124.68
17	C	508	CLA	CMB-C2B-C3B	2.90	130.10	124.68
17	b	5603	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
19	D	406	PQ9	C6-C5-C4	2.90	120.91	114.99
25	m	5101	MGE	C2G-O2G-C1B	-2.90	110.66	117.79
17	D	404	CLA	CMB-C2B-C3B	2.90	130.10	124.68
17	C	505	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
17	c	5505	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
25	D	408	MGE	C2G-O2G-C1B	-2.89	110.67	117.79
19	d	5405	PQ9	C6-C5-C4	2.89	120.90	114.99
25	c	5517	MGE	C3G-O3G-C1D	-2.89	108.10	113.74
17	C	502	CLA	C4-C3-C5	2.88	120.12	115.27
17	B	603	CLA	CMB-C2B-C3B	2.88	130.07	124.68
17	d	5403	CLA	CMB-C2B-C3B	2.88	130.07	124.68
25	C	520	MGE	C3G-O3G-C1D	-2.88	108.12	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	c	5511	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
17	b	5603	CLA	CMB-C2B-C3B	2.87	130.05	124.68
20	T	102	BCR	C15-C16-C17	-2.87	117.59	123.47
17	c	5508	CLA	CHB-C4A-NA	2.87	128.48	124.51
17	a	5402	CLA	CMB-C2B-C3B	2.87	130.05	124.68
17	a	5404	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
17	C	508	CLA	CHB-C4A-NA	2.87	128.48	124.51
17	b	5604	CLA	CMB-C2B-C3B	2.87	130.04	124.68
20	C	514	BCR	C33-C5-C6	-2.87	121.31	124.53
17	D	404	CLA	C1B-CHB-C4A	-2.86	124.44	130.12
26	a	5411	DGD	C1D-C2D-C3D	-2.86	104.04	110.00
17	a	5403	CLA	CHB-C4A-NA	2.86	128.46	124.51
17	b	5611	CLA	CHB-C4A-NA	2.86	128.46	124.51
23	d	5407	SQD	O48-C23-C24	2.86	120.87	111.91
19	A	406	PQ9	C26-C27-C28	-2.86	120.78	127.66
17	A	403	CLA	C1B-CHB-C4A	-2.85	124.46	130.12
17	C	512	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
19	A	406	PQ9	C11-C12-C13	-2.85	122.04	126.79
26	C	519	DGD	C1D-C2D-C3D	-2.85	104.05	110.00
26	c	5515	DGD	O6D-C5D-C6D	-2.85	100.91	106.67
23	D	403	SQD	C3-C4-C5	2.85	115.33	110.24
17	A	401	CLA	CMB-C2B-C3B	2.85	130.01	124.68
17	k	5501	CLA	CMB-C2B-C3B	2.85	130.01	124.68
25	m	5101	MGE	O1G-C1A-C2A	2.85	120.85	111.91
17	d	5403	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
17	B	605	CLA	CHB-C4A-NA	2.84	128.44	124.51
17	b	5605	CLA	CHB-C4A-NA	2.84	128.44	124.51
22	B	620	LMT	C3'-C4'-C5'	-2.84	104.41	110.93
17	b	5602	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
26	C	517	DGD	O6D-C5D-C6D	-2.84	100.93	106.67
17	A	405	CLA	CHB-C4A-NA	2.84	128.44	124.51
20	B	617	BCR	C11-C10-C9	-2.84	123.26	127.31
18	A	404	PHO	O1D-CGD-CBD	2.83	129.46	124.74
17	C	511	CLA	CMB-C2B-C3B	2.83	129.97	124.68
17	C	511	CLA	CHB-C4A-NA	2.83	128.42	124.51
17	A	402	CLA	CHB-C4A-NA	2.83	128.42	124.51
19	a	5407	PQ9	C11-C12-C13	-2.83	122.08	126.79
17	B	604	CLA	CMB-C2B-C3B	2.83	129.96	124.68
17	k	5501	CLA	CHB-C4A-NA	2.82	128.42	124.51
17	B	602	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
20	b	5617	BCR	C35-C13-C14	-2.82	118.97	122.92
20	b	5617	BCR	C11-C10-C9	-2.82	123.28	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	617	BCR	C7-C8-C9	-2.82	121.98	126.23
25	C	520	MGE	O1G-C1A-C2A	2.81	120.74	111.91
17	B	607	CLA	CHB-C4A-NA	2.81	128.40	124.51
25	c	5517	MGE	O1G-C1A-C2A	2.81	120.72	111.91
17	A	402	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
17	b	5604	CLA	C1-C2-C3	-2.81	121.19	126.04
20	B	617	BCR	C35-C13-C14	-2.80	119.00	122.92
18	a	5405	PHO	O1D-CGD-CBD	2.80	129.41	124.74
20	b	5617	BCR	C7-C8-C9	-2.80	122.01	126.23
17	a	5403	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
17	B	602	CLA	CMB-C2B-C1B	-2.79	124.17	128.46
17	B	611	CLA	CHB-C4A-NA	2.79	128.38	124.51
17	c	5507	CLA	CAC-C3C-C4C	2.79	128.43	124.81
17	a	5406	CLA	CHB-C4A-NA	2.79	128.37	124.51
17	B	604	CLA	C1-C2-C3	-2.79	121.22	126.04
17	C	507	CLA	CAC-C3C-C4C	2.79	128.43	124.81
23	D	403	SQD	O6-C1-C2	2.79	112.66	108.30
17	b	5602	CLA	CMB-C2B-C1B	-2.79	124.18	128.46
20	c	5513	BCR	C33-C5-C6	-2.79	121.40	124.53
17	b	5607	CLA	CHB-C4A-NA	2.79	128.37	124.51
17	c	5511	CLA	CMB-C2B-C3B	2.78	129.88	124.68
17	B	610	CLA	CHB-C4A-NA	2.78	128.36	124.51
17	C	504	CLA	CMB-C2B-C3B	2.78	129.88	124.68
17	B	607	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
17	b	5601	CLA	CAA-C2A-C3A	-2.77	109.63	116.10
25	D	409	MGE	C2G-O2G-C1B	-2.77	110.97	117.79
17	B	601	CLA	CAA-C2A-C3A	-2.77	109.64	116.10
17	C	505	CLA	O2A-CGA-O1A	-2.76	116.61	123.59
17	c	5505	CLA	O2A-CGA-O1A	-2.76	116.61	123.59
19	a	5407	PQ9	C14-C13-C15	2.76	119.92	115.27
25	D	409	MGE	O3G-C1D-C2D	2.76	112.61	108.30
19	A	406	PQ9	C39-C38-C40	2.76	119.91	115.27
26	C	517	DGD	O3G-C3G-C2G	-2.75	104.25	110.90
17	C	512	CLA	CMB-C2B-C3B	2.75	129.83	124.68
17	b	5610	CLA	CHB-C4A-NA	2.75	128.32	124.51
20	D	407	BCR	C15-C14-C13	-2.75	123.38	127.31
20	b	5618	BCR	C27-C26-C25	2.75	126.73	122.73
17	c	5504	CLA	CMB-C2B-C3B	2.75	129.83	124.68
17	B	608	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
20	B	618	BCR	C27-C26-C25	2.75	126.72	122.73
26	c	5515	DGD	O3G-C3G-C2G	-2.75	104.27	110.90
20	T	102	BCR	C27-C26-C25	2.75	126.72	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	5607	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
19	A	406	PQ9	C14-C13-C15	2.74	119.89	115.27
17	d	5403	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
20	d	5406	BCR	C33-C5-C6	-2.74	121.46	124.53
17	C	501	CLA	CMB-C2B-C3B	2.73	129.79	124.68
20	d	5406	BCR	C15-C14-C13	-2.73	123.42	127.31
22	a	5410	LMT	C1'-O5'-C5'	-2.72	108.34	113.69
17	b	5608	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
17	b	5604	CLA	O2A-CGA-O1A	-2.72	116.72	123.59
17	B	604	CLA	O2A-CGA-O1A	-2.72	116.72	123.59
17	B	612	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
17	B	610	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
19	A	406	PQ9	C11-C2-C3	-2.72	119.72	123.30
19	a	5407	PQ9	C11-C2-C3	-2.72	119.73	123.30
17	c	5501	CLA	CMB-C2B-C3B	2.72	129.76	124.68
17	C	511	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
17	b	5610	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
24	a	5412	BCT	O3-C-O1	-2.71	112.52	119.55
20	t	5101	BCR	C11-C10-C9	-2.71	123.45	127.31
20	D	407	BCR	C33-C5-C6	-2.71	121.49	124.53
17	C	501	CLA	C1B-CHB-C4A	-2.71	124.76	130.12
17	D	404	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
17	B	614	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
24	A	411	BCT	O3-C-O1	-2.70	112.54	119.55
25	B	619	MGE	O1G-C1A-C2A	2.70	120.38	111.91
17	A	402	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
23	l	5102	SQD	O48-C23-C24	2.70	120.38	111.91
17	k	5501	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
17	C	501	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
20	c	5514	BCR	C15-C14-C13	-2.70	123.46	127.31
17	B	605	CLA	CMB-C2B-C3B	2.69	129.72	124.68
17	b	5612	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
17	c	5501	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
25	d	5410	MGE	O1G-C1A-C2A	2.69	120.36	111.91
18	D	402	PHO	CMC-C2C-C3C	2.69	130.01	124.94
25	b	5620	MGE	O1G-C1A-C2A	2.69	120.34	111.91
17	a	5403	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
17	d	5404	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
26	C	518	DGD	C3D-C4D-C5D	-2.69	105.45	110.24
20	C	516	BCR	C15-C14-C13	-2.68	123.48	127.31
17	D	405	CLA	C1B-CHB-C4A	-2.68	124.80	130.12
25	d	5409	MGE	C3G-C2G-C1G	-2.68	105.44	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	D	406	PQ9	C26-C27-C28	-2.68	121.20	127.66
20	b	5619	BCR	C11-C10-C9	-2.68	123.48	127.31
19	d	5405	PQ9	C26-C27-C28	-2.68	121.20	127.66
20	A	407	BCR	C24-C23-C22	-2.68	122.19	126.23
25	d	5408	MGE	O1G-C1A-C2A	2.68	120.31	111.91
17	A	403	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
26	C	517	DGD	O3E-C3E-C2E	-2.68	104.16	110.35
17	a	5404	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
17	d	5403	CLA	C2D-C1D-ND	-2.67	108.13	110.10
17	b	5605	CLA	CMB-C2B-C3B	2.67	129.68	124.68
17	B	606	CLA	CHB-C4A-NA	2.67	128.21	124.51
17	b	5606	CLA	CHB-C4A-NA	2.67	128.21	124.51
20	h	5101	BCR	C33-C5-C6	-2.67	121.53	124.53
17	c	5501	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
17	b	5614	CLA	CHB-C4A-NA	2.67	128.21	124.51
17	b	5614	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
17	C	501	CLA	CHB-C4A-NA	2.67	128.20	124.51
19	A	406	PQ9	C19-C18-C20	2.67	119.76	115.27
26	c	5515	DGD	O3E-C3E-C2E	-2.67	104.18	110.35
17	c	5507	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
26	c	5516	DGD	C3D-C4D-C5D	-2.66	105.49	110.24
23	D	403	SQD	O48-C23-C24	2.66	120.27	111.91
17	b	5611	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
20	H	101	BCR	C33-C5-C6	-2.66	121.54	124.53
19	a	5407	PQ9	C19-C18-C20	2.66	119.75	115.27
17	C	507	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
17	c	5503	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
19	a	5407	PQ9	C6-C5-C4	2.65	120.41	114.99
17	D	404	CLA	C2D-C1D-ND	-2.65	108.15	110.10
17	B	608	CLA	CHB-C4A-NA	2.65	128.18	124.51
17	A	405	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
19	A	406	PQ9	C6-C5-C4	2.65	120.41	114.99
17	B	611	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
19	d	5405	PQ9	C39-C38-C40	2.65	119.72	115.27
17	C	503	CLA	CAA-C2A-C3A	-2.65	105.53	112.78
17	B	614	CLA	CHB-C4A-NA	2.65	128.17	124.51
19	D	406	PQ9	C39-C38-C40	2.65	119.72	115.27
17	B	613	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
18	a	5405	PHO	CMB-C2B-C3B	2.64	129.62	124.68
20	a	5408	BCR	C24-C23-C22	-2.64	122.24	126.23
20	t	5102	BCR	C27-C26-C25	2.64	126.56	122.73
17	C	509	CLA	O2A-CGA-O1A	-2.64	116.94	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	c	5509	CLA	O2A-CGA-O1A	-2.64	116.94	123.59
17	c	5501	CLA	CHB-C4A-NA	2.64	128.16	124.51
17	B	613	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
17	b	5616	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
20	h	5101	BCR	C27-C26-C25	2.63	126.55	122.73
20	C	514	BCR	C24-C23-C22	-2.63	122.26	126.23
18	d	5402	PHO	CMC-C2C-C3C	2.63	129.89	124.94
17	B	611	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
18	A	404	PHO	CMB-C2B-C3B	2.63	129.59	124.68
17	b	5613	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
17	B	616	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
20	H	101	BCR	C27-C26-C25	2.62	126.53	122.73
17	a	5406	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
20	t	5101	BCR	C33-C5-C6	-2.62	121.59	124.53
17	b	5613	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
17	a	5403	CLA	CMB-C2B-C3B	2.62	129.57	124.68
20	t	5102	BCR	C33-C5-C6	-2.62	121.59	124.53
18	d	5402	PHO	CMB-C2B-C3B	2.62	129.57	124.68
22	m	5102	LMT	C3B-C4B-C5B	-2.61	105.58	110.24
19	D	406	PQ9	C29-C28-C30	2.61	119.66	115.27
17	b	5608	CLA	CHB-C4A-NA	2.61	128.12	124.51
20	a	5408	BCR	C33-C5-C6	-2.61	121.60	124.53
17	b	5611	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
20	c	5513	BCR	C24-C23-C22	-2.61	122.30	126.23
17	b	5606	CLA	CAA-C2A-C3A	-2.60	107.76	114.26
17	a	5402	CLA	CAA-C2A-C1A	-2.60	103.46	111.97
26	c	5516	DGD	C4E-C3E-C2E	-2.60	106.29	110.82
18	D	402	PHO	CMB-C2B-C3B	2.60	129.53	124.68
17	B	605	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
17	A	401	CLA	CAA-C2A-C1A	-2.59	103.48	111.97
23	d	5407	SQD	O6-C1-C2	2.59	112.34	108.30
20	A	407	BCR	C33-C5-C6	-2.58	121.63	124.53
17	d	5404	CLA	CHB-C4A-NA	2.58	128.08	124.51
17	b	5615	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
19	d	5405	PQ9	C29-C28-C30	2.58	119.61	115.27
17	A	402	CLA	CMB-C2B-C3B	2.58	129.50	124.68
20	C	515	BCR	C33-C5-C6	-2.58	121.63	124.53
20	t	5101	BCR	C27-C26-C25	2.58	126.47	122.73
20	b	5619	BCR	C33-C5-C6	-2.57	121.64	124.53
20	k	5502	BCR	C33-C5-C6	-2.57	121.64	124.53
18	d	5402	PHO	C1-C2-C3	-2.57	121.60	126.04
17	b	5605	CLA	C1B-CHB-C4A	-2.57	125.03	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	C	504	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
26	C	518	DGD	C4E-C3E-C2E	-2.57	106.34	110.82
17	c	5504	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
17	C	503	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
17	A	403	CLA	CHB-C4A-NA	2.56	128.06	124.51
17	C	502	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
20	b	5619	BCR	C27-C26-C25	2.56	126.45	122.73
17	c	5511	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
17	a	5406	CLA	CMB-C2B-C3B	2.56	129.47	124.68
17	c	5503	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
18	d	5402	PHO	O2D-CGD-O1D	-2.55	118.85	123.84
17	D	405	CLA	CHB-C4A-NA	2.55	128.04	124.51
17	B	604	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
23	l	5102	SQD	C4-C3-C2	2.55	115.27	110.82
17	c	5502	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
20	c	5514	BCR	C7-C8-C9	-2.55	122.39	126.23
23	L	101	SQD	C4-C3-C2	2.55	115.27	110.82
17	C	512	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
17	b	5604	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
17	A	405	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
20	z	5101	BCR	C33-C5-C6	-2.54	121.67	124.53
17	B	615	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
18	D	402	PHO	O2D-CGD-O1D	-2.54	118.86	123.84
17	C	513	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
18	D	402	PHO	C1-C2-C3	-2.54	121.64	126.04
17	C	510	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
17	b	5615	CLA	CHB-C4A-NA	2.54	128.03	124.51
17	C	511	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
17	b	5609	CLA	CHB-C4A-NA	2.54	128.02	124.51
26	c	5516	DGD	C3G-C2G-C1G	-2.54	105.78	111.79
23	L	101	SQD	O48-C23-O10	-2.54	117.19	123.59
17	a	5406	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
17	k	5501	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
26	C	519	DGD	C3G-C2G-C1G	-2.53	105.80	111.79
17	c	5512	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
17	A	405	CLA	CMB-C2B-C3B	2.53	129.41	124.68
26	C	518	DGD	C3G-C2G-C1G	-2.53	105.81	111.79
26	a	5411	DGD	C3G-C2G-C1G	-2.53	105.81	111.79
17	C	507	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
17	a	5404	CLA	CHB-C4A-NA	2.52	128.00	124.51
20	C	516	BCR	C7-C8-C9	-2.52	122.43	126.23
20	C	516	BCR	C11-C10-C9	-2.52	123.72	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	609	CLA	CHB-C4A-NA	2.52	127.99	124.51
17	B	616	CLA	CHB-C4A-NA	2.51	127.99	124.51
17	b	5616	CLA	CHB-C4A-NA	2.51	127.99	124.51
20	c	5514	BCR	C11-C10-C9	-2.51	123.72	127.31
17	C	502	CLA	CHB-C4A-NA	2.51	127.99	124.51
17	c	5507	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
17	B	605	CLA	C1-C2-C3	-2.51	121.70	126.04
20	A	407	BCR	C27-C26-C25	2.51	126.37	122.73
17	c	5502	CLA	CMB-C2B-C3B	2.50	129.36	124.68
17	B	601	CLA	C2A-C1A-CHA	2.50	128.22	123.85
20	C	515	BCR	C15-C14-C13	-2.50	123.74	127.31
23	l	5102	SQD	C44-O6-C1	2.50	118.63	113.74
17	c	5504	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
17	C	506	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
17	C	501	CLA	C1-C2-C3	-2.50	121.72	126.04
20	c	5514	BCR	C33-C5-C6	-2.50	121.72	124.53
17	c	5506	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
17	b	5601	CLA	C2A-C1A-CHA	2.50	128.21	123.85
20	b	5617	BCR	C27-C26-C25	2.50	126.36	122.73
23	L	101	SQD	O7-S-C6	2.50	109.91	106.94
26	h	5102	DGD	C4E-C3E-C2E	-2.50	106.47	110.82
17	c	5510	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
17	B	615	CLA	CHB-C4A-NA	2.49	127.96	124.51
26	H	102	DGD	C4E-C3E-C2E	-2.49	106.48	110.82
17	C	504	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
17	c	5511	CLA	CHB-C4A-NA	2.49	127.95	124.51
17	b	5616	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
17	b	5612	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
17	B	609	CLA	CMB-C2B-C3B	2.49	129.33	124.68
17	c	5502	CLA	CHB-C4A-NA	2.48	127.94	124.51
17	C	502	CLA	CMB-C2B-C3B	2.48	129.32	124.68
20	z	5101	BCR	C27-C26-C25	2.48	126.33	122.73
17	C	501	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
20	z	5101	BCR	C15-C14-C13	-2.48	123.77	127.31
17	b	5605	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
17	C	506	CLA	CHB-C4A-NA	2.48	127.94	124.51
23	L	101	SQD	C44-O6-C1	2.47	118.57	113.74
17	b	5605	CLA	C1-C2-C3	-2.47	121.77	126.04
17	B	616	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
17	b	5604	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
17	b	5614	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
17	B	605	CLA	O2D-CGD-O1D	-2.47	119.01	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	c	5501	CLA	O2A-CGA-O1A	-2.47	117.36	123.59
17	B	605	CLA	CHD-C1D-ND	-2.47	122.18	124.45
17	c	5501	CLA	C1-C2-C3	-2.47	121.77	126.04
17	B	612	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
17	C	512	CLA	CHB-C4A-NA	2.47	127.92	124.51
17	a	5403	CLA	C1-C2-C3	-2.47	121.78	126.04
23	d	5407	SQD	C44-O6-C1	2.46	118.55	113.74
25	D	408	MGE	O1G-C1A-C2A	2.46	119.64	111.91
17	B	614	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
17	b	5609	CLA	CMB-C2B-C3B	2.46	129.28	124.68
17	A	402	CLA	C1-C2-C3	-2.46	121.79	126.04
19	A	406	PQ9	C31-C32-C33	-2.46	121.74	127.66
20	C	515	BCR	C11-C10-C9	-2.46	123.80	127.31
17	c	5506	CLA	CHB-C4A-NA	2.46	127.91	124.51
20	B	617	BCR	C27-C26-C25	2.45	126.29	122.73
20	a	5408	BCR	C27-C26-C25	2.45	126.29	122.73
17	B	604	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
17	d	5404	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
19	d	5405	PQ9	C16-C17-C18	-2.45	121.76	127.66
17	C	509	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
17	B	608	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
21	A	408	LHG	O8-C23-C24	2.44	119.57	111.91
20	C	516	BCR	C33-C5-C6	-2.44	121.79	124.53
17	b	5606	CLA	O2D-CGD-CBD	2.44	115.61	111.27
20	D	407	BCR	C15-C16-C17	-2.44	118.47	123.47
20	z	5101	BCR	C11-C10-C9	-2.44	123.83	127.31
19	A	406	PQ9	C29-C28-C30	2.44	119.38	115.27
17	B	609	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
26	c	5515	DGD	O2D-C2D-C1D	-2.44	104.12	110.05
18	A	404	PHO	CMC-C2C-C3C	2.44	129.54	124.94
19	D	406	PQ9	C16-C17-C18	-2.44	121.79	127.66
20	d	5406	BCR	C27-C26-C25	2.44	126.27	122.73
17	D	405	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
17	b	5609	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
26	C	517	DGD	O2D-C2D-C1D	-2.43	104.13	110.05
23	D	403	SQD	O9-S-C6	2.43	109.83	106.94
17	B	606	CLA	O2D-CGD-CBD	2.43	115.59	111.27
20	C	515	BCR	C27-C26-C25	2.43	126.26	122.73
17	C	513	CLA	C1-C2-C3	-2.43	122.82	126.75
21	a	5409	LHG	O8-C23-C24	2.43	119.54	111.91
17	C	507	CLA	CHB-C4A-NA	2.43	127.87	124.51
17	c	5509	CLA	O2D-CGD-O1D	-2.43	119.09	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	5409	MGE	O6D-C5D-C4D	2.43	114.10	109.69
17	b	5605	CLA	CHD-C1D-ND	-2.43	122.22	124.45
17	B	603	CLA	C1B-CHB-C4A	-2.42	125.31	130.12
20	T	102	BCR	C15-C14-C13	-2.42	123.85	127.31
17	c	5512	CLA	C1-C2-C3	-2.42	122.83	126.75
17	b	5615	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
20	d	5406	BCR	C15-C16-C17	-2.42	118.52	123.47
17	C	505	CLA	CAC-C3C-C4C	2.42	127.95	124.81
17	b	5603	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
17	b	5608	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
17	D	405	CLA	C1-C2-C3	-2.42	122.84	126.75
17	c	5505	CLA	CAC-C3C-C4C	2.42	127.94	124.81
17	B	615	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
17	c	5506	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
20	t	5101	BCR	C8-C7-C6	-2.41	120.43	127.20
20	b	5617	BCR	C33-C5-C6	-2.41	121.82	124.53
17	c	5507	CLA	CHB-C4A-NA	2.41	127.84	124.51
18	a	5405	PHO	CMC-C2C-C3C	2.41	129.48	124.94
17	C	506	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
23	L	101	SQD	O48-C23-C24	2.40	119.45	111.91
17	d	5404	CLA	C1-C2-C3	-2.40	122.86	126.75
17	c	5508	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
17	c	5509	CLA	CHB-C4A-NA	2.40	127.83	124.51
17	C	508	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
20	b	5619	BCR	C8-C7-C6	-2.40	120.46	127.20
17	b	5609	CLA	CHD-C1D-ND	-2.40	122.25	124.45
17	B	604	CLA	CHB-C4A-NA	2.40	127.83	124.51
17	b	5604	CLA	CHB-C4A-NA	2.40	127.83	124.51
17	B	610	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
20	D	407	BCR	C27-C26-C25	2.40	126.21	122.73
20	t	5102	BCR	C15-C14-C13	-2.39	123.89	127.31
20	B	617	BCR	C33-C5-C6	-2.39	121.84	124.53
17	c	5505	CLA	CHB-C4A-NA	2.39	127.81	124.51
17	b	5610	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
17	C	503	CLA	CHB-C4A-NA	2.38	127.81	124.51
17	C	509	CLA	CHB-C4A-NA	2.38	127.81	124.51
17	B	609	CLA	CHD-C1D-ND	-2.38	122.27	124.45
20	b	5618	BCR	C24-C23-C22	-2.38	122.64	126.23
17	d	5403	CLA	CHB-C4A-NA	2.38	127.80	124.51
20	C	514	BCR	C27-C26-C25	2.38	126.19	122.73
17	B	603	CLA	CHB-C4A-NA	2.38	127.80	124.51
17	c	5512	CLA	O2D-CGD-O1D	-2.37	119.20	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	5513	BCR	C7-C8-C9	-2.37	122.65	126.23
17	B	606	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
20	D	407	BCR	C7-C8-C9	-2.37	122.66	126.23
17	b	5603	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
17	B	603	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
25	m	5103	MGE	O1G-C1A-C2A	2.37	119.33	111.91
20	c	5513	BCR	C27-C26-C25	2.37	126.17	122.73
17	c	5503	CLA	CHB-C4A-NA	2.36	127.78	124.51
18	A	404	PHO	O2D-CGD-O1D	-2.36	119.22	123.84
17	C	513	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
17	D	404	CLA	CHB-C4A-NA	2.36	127.78	124.51
18	a	5405	PHO	O2D-CGD-O1D	-2.36	119.22	123.84
17	b	5606	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
25	D	410	MGE	O1G-C1A-C2A	2.36	119.31	111.91
20	t	5101	BCR	C38-C26-C25	-2.36	121.88	124.53
19	A	406	PQ9	C45-C43-C44	2.36	119.81	114.60
20	h	5101	BCR	C16-C15-C14	-2.36	118.64	123.47
20	b	5619	BCR	C38-C26-C25	-2.36	121.88	124.53
18	d	5402	PHO	O1D-CGD-CBD	2.36	128.66	124.74
20	H	101	BCR	C16-C15-C14	-2.35	118.65	123.47
20	C	514	BCR	C7-C8-C9	-2.35	122.68	126.23
17	C	505	CLA	CHB-C4A-NA	2.35	127.77	124.51
17	b	5603	CLA	CHB-C4A-NA	2.35	127.76	124.51
20	B	618	BCR	C24-C23-C22	-2.35	122.69	126.23
20	c	5514	BCR	C24-C23-C22	-2.34	122.69	126.23
20	d	5406	BCR	C7-C8-C9	-2.34	122.70	126.23
26	C	519	DGD	C6D-O5D-C1E	2.34	118.31	113.74
26	a	5411	DGD	C6D-O5D-C1E	2.34	118.31	113.74
25	l	5101	MGE	C2G-O2G-C1B	-2.34	112.04	117.79
25	A	412	MGE	C2G-O2G-C1B	-2.34	112.04	117.79
17	b	5601	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
17	A	403	CLA	C1-C2-C3	-2.33	122.01	126.04
20	t	5101	BCR	C15-C14-C13	-2.33	123.99	127.31
17	B	601	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
17	a	5404	CLA	C1-C2-C3	-2.32	122.02	126.04
17	C	503	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
20	C	516	BCR	C24-C23-C22	-2.32	122.72	126.23
17	B	610	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
18	D	402	PHO	O1D-CGD-CBD	2.32	128.60	124.74
17	c	5504	CLA	CHD-C1D-ND	-2.32	122.32	124.45
17	c	5503	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
17	B	611	CLA	O2A-CGA-O1A	-2.31	117.75	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	5615	CLA	C1-C2-C3	-2.31	122.04	126.04
20	b	5619	BCR	C15-C14-C13	-2.31	124.01	127.31
17	C	504	CLA	CHD-C1D-ND	-2.31	122.33	124.45
17	B	613	CLA	CAA-CBA-CGA	-2.31	106.49	113.25
23	l	5102	SQD	C3-C4-C5	2.31	114.36	110.24
21	A	408	LHG	C27-C26-C25	-2.31	102.69	114.42
17	A	401	CLA	CAA-CBA-CGA	-2.31	106.50	113.25
21	a	5409	LHG	C27-C26-C25	-2.31	102.70	114.42
22	T	101	LMT	C3'-C4'-C5'	-2.31	105.63	110.93
23	D	403	SQD	C44-O6-C1	2.31	118.25	113.74
17	C	513	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
17	C	510	CLA	CHB-C4A-NA	2.30	127.70	124.51
20	C	515	BCR	C24-C23-C22	-2.30	122.76	126.23
20	A	407	BCR	C2-C1-C6	2.30	114.02	110.48
20	Y	101	BCR	C27-C26-C25	2.30	126.07	122.73
17	B	607	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
23	L	101	SQD	O5-C5-C4	2.30	113.87	109.69
17	b	5611	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
17	b	5610	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
23	a	5401	SQD	O5-C5-C4	2.29	113.86	109.69
20	a	5408	BCR	C2-C1-C6	2.29	114.01	110.48
17	a	5402	CLA	CAA-CBA-CGA	-2.29	106.56	113.25
17	b	5613	CLA	CAA-CBA-CGA	-2.29	106.56	113.25
17	b	5613	CLA	C1-C2-C3	-2.29	122.08	126.04
26	C	519	DGD	CBB-CAB-C9B	-2.29	102.80	114.42
26	a	5411	DGD	CBB-CAB-C9B	-2.29	102.80	114.42
17	b	5607	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
20	T	102	BCR	C40-C30-C25	2.29	114.01	110.30
17	b	5613	CLA	C2D-C1D-ND	-2.29	108.42	110.10
17	C	513	CLA	CHB-C4A-NA	2.29	127.67	124.51
17	c	5512	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
17	c	5509	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
17	B	609	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
17	C	509	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
26	C	519	DGD	O6D-C5D-C6D	-2.28	102.07	106.67
29	F	101	HEM	CMA-C3A-C4A	-2.28	124.97	128.46
17	B	613	CLA	C1-C2-C3	-2.28	122.11	126.04
17	B	602	CLA	CHB-C4A-NA	2.27	127.66	124.51
19	D	406	PQ9	C41-C42-C43	-2.27	119.99	127.75
20	Y	101	BCR	C33-C5-C6	-2.27	121.98	124.53
20	z	5101	BCR	C24-C23-C22	-2.27	122.80	126.23
17	c	5512	CLA	CHB-C4A-NA	2.27	127.65	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	d	5405	PQ9	C41-C42-C43	-2.27	120.00	127.75
29	f	5101	HEM	CMA-C3A-C4A	-2.27	124.98	128.46
17	C	508	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
20	T	102	BCR	C30-C25-C26	-2.27	119.42	122.61
26	h	5102	DGD	C3G-C2G-C1G	-2.26	106.44	111.79
17	b	5602	CLA	CMB-C2B-C3B	2.26	128.91	124.68
17	b	5602	CLA	CHB-C4A-NA	2.26	127.64	124.51
17	c	5504	CLA	CHB-C4A-NA	2.26	127.64	124.51
17	B	615	CLA	C1-C2-C3	-2.26	122.14	126.04
29	f	5101	HEM	C4D-ND-C1D	2.26	107.41	105.07
25	d	5408	MGE	C2G-O2G-C1B	-2.26	112.23	117.79
25	d	5410	MGE	O2G-C1B-O1B	-2.26	118.25	123.70
17	C	511	CLA	C1-C2-C3	-2.26	122.14	126.04
20	b	5617	BCR	C20-C21-C22	-2.25	124.09	127.31
26	H	102	DGD	C3G-C2G-C1G	-2.25	106.46	111.79
17	C	504	CLA	CHB-C4A-NA	2.25	127.63	124.51
20	B	617	BCR	C20-C21-C22	-2.25	124.10	127.31
19	A	406	PQ9	C36-C37-C38	-2.25	122.25	127.66
17	B	602	CLA	C2D-C1D-ND	-2.25	108.45	110.10
17	B	602	CLA	CMB-C2B-C3B	2.25	128.88	124.68
25	m	5101	MGE	C3G-O3G-C1D	-2.25	109.35	113.74
20	C	514	BCR	C11-C10-C9	-2.24	124.11	127.31
20	k	5502	BCR	C27-C26-C25	2.24	125.98	122.73
20	z	5101	BCR	C8-C7-C6	-2.24	120.91	127.20
17	b	5602	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
17	b	5609	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
26	a	5411	DGD	O6D-C5D-C6D	-2.24	102.14	106.67
25	D	409	MGE	C3G-C2G-C1G	-2.24	106.49	111.79
17	c	5508	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
17	C	503	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
17	B	602	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
17	c	5510	CLA	CHB-C4A-NA	2.23	127.60	124.51
17	k	5501	CLA	C1-C2-C3	-2.23	122.18	126.04
17	B	613	CLA	C2D-C1D-ND	-2.23	108.46	110.10
26	c	5515	DGD	O6E-C1E-O5D	-2.23	104.69	109.97
20	C	515	BCR	C8-C7-C6	-2.23	120.94	127.20
17	C	510	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
17	B	614	CLA	C1-C2-C3	-2.22	122.21	126.04
17	b	5609	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
17	a	5404	CLA	C2D-C1D-ND	-2.22	108.47	110.10
17	c	5503	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
20	c	5513	BCR	C11-C10-C9	-2.22	124.15	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	609	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
29	F	101	HEM	C4D-ND-C1D	2.21	107.36	105.07
17	c	5506	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
17	c	5510	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
26	C	517	DGD	O6E-C1E-O5D	-2.21	104.74	109.97
17	b	5614	CLA	C1-C2-C3	-2.21	122.23	126.04
17	b	5602	CLA	C2D-C1D-ND	-2.21	108.48	110.10
19	d	5405	PQ9	C14-C13-C15	2.20	118.98	115.27
17	a	5402	CLA	CAA-C2A-C3A	-2.20	106.75	112.78
23	A	410	SQD	O5-C5-C4	2.20	113.69	109.69
20	t	5101	BCR	C16-C15-C14	-2.20	118.97	123.47
17	C	506	CLA	CAA-C2A-C3A	-2.20	106.77	112.78
19	a	5407	PQ9	C24-C23-C25	2.19	118.96	115.27
19	a	5407	PQ9	C16-C17-C18	-2.19	122.38	127.66
20	b	5619	BCR	C16-C15-C14	-2.19	118.99	123.47
19	A	406	PQ9	C24-C23-C25	2.19	118.95	115.27
20	C	515	BCR	C35-C13-C14	-2.19	119.86	122.92
20	t	5102	BCR	C30-C25-C26	-2.19	119.53	122.61
20	T	102	BCR	C33-C5-C6	-2.19	122.07	124.53
20	c	5514	BCR	C28-C27-C26	-2.19	110.17	114.08
20	z	5101	BCR	C35-C13-C14	-2.18	119.87	122.92
19	D	406	PQ9	C34-C33-C35	2.18	118.94	115.27
19	A	406	PQ9	C16-C17-C18	-2.18	122.42	127.66
18	a	5405	PHO	CMA-C3A-C4A	-2.18	109.61	114.38
25	b	5620	MGE	O2G-C1B-O1B	-2.18	118.44	123.70
23	l	5102	SQD	O5-C1-C2	2.18	114.95	110.35
25	B	619	MGE	O2G-C1B-O1B	-2.17	118.45	123.70
17	A	403	CLA	C2D-C1D-ND	-2.17	108.50	110.10
17	A	401	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
19	d	5405	PQ9	C34-C33-C35	2.17	118.92	115.27
19	a	5407	PQ9	C30-C28-C29	2.17	119.39	114.60
19	D	406	PQ9	C14-C13-C15	2.17	118.92	115.27
26	c	5515	DGD	C5B-C4B-C3B	-2.17	103.43	114.42
20	t	5102	BCR	C35-C13-C14	-2.17	119.89	122.92
25	C	520	MGE	C2G-O2G-C1B	-2.16	112.47	117.79
20	C	516	BCR	C28-C27-C26	-2.16	110.22	114.08
20	b	5618	BCR	C33-C5-C6	-2.16	122.10	124.53
26	C	517	DGD	C5B-C4B-C3B	-2.16	103.46	114.42
25	c	5517	MGE	C2G-O2G-C1B	-2.16	112.48	117.79
20	Y	101	BCR	C15-C14-C13	-2.16	124.23	127.31
18	A	404	PHO	CMA-C3A-C4A	-2.16	109.65	114.38
20	b	5619	BCR	C15-C16-C17	-2.16	119.06	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	5618	BCR	C8-C7-C6	-2.16	121.15	127.20
20	B	618	BCR	C2-C1-C6	2.16	113.80	110.48
17	B	606	CLA	C1-C2-C3	-2.15	122.32	126.04
17	B	612	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
20	B	618	BCR	C33-C5-C6	-2.15	122.12	124.53
25	d	5409	MGE	C1D-C2D-C3D	-2.15	105.52	110.00
17	b	5612	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
20	B	618	BCR	C8-C7-C6	-2.14	121.19	127.20
20	T	102	BCR	C38-C26-C25	-2.14	122.12	124.53
20	t	5101	BCR	C15-C16-C17	-2.14	119.09	123.47
25	c	5517	MGE	O1G-C1A-O1A	-2.14	118.20	123.59
17	c	5507	CLA	C3C-C4C-NC	-2.13	108.18	110.57
25	C	520	MGE	O1G-C1A-O1A	-2.13	118.21	123.59
20	b	5618	BCR	C2-C1-C6	2.13	113.77	110.48
17	C	513	CLA	CHD-C1D-ND	-2.13	122.50	124.45
20	k	5502	BCR	C7-C8-C9	-2.13	123.02	126.23
19	d	5405	PQ9	C45-C43-C44	2.13	119.30	114.60
19	D	406	PQ9	C45-C43-C44	2.13	119.30	114.60
20	h	5101	BCR	C30-C25-C26	-2.13	119.62	122.61
17	c	5512	CLA	CHD-C1D-ND	-2.13	122.50	124.45
17	C	507	CLA	C3C-C4C-NC	-2.12	108.19	110.57
25	l	5101	MGE	O1G-C1A-O1A	-2.12	118.24	123.59
17	b	5611	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
20	b	5617	BCR	C24-C23-C22	-2.12	123.03	126.23
20	A	407	BCR	C38-C26-C25	-2.12	122.15	124.53
25	d	5409	MGE	C2G-O2G-C1B	-2.12	112.58	117.79
22	A	409	LMT	O5B-C5B-C4B	2.12	113.54	109.69
17	B	607	CLA	CAA-CBA-CGA	-2.11	107.08	113.25
17	b	5607	CLA	CAA-CBA-CGA	-2.11	107.08	113.25
17	d	5404	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
25	A	412	MGE	O1G-C1A-O1A	-2.11	118.26	123.59
17	D	405	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
17	B	611	CLA	CAA-C2A-C3A	-2.11	107.00	112.78
17	c	5502	CLA	C6-C7-C8	-2.11	109.11	115.92
21	A	408	LHG	C5-O7-C7	-2.11	112.60	117.79
25	d	5409	MGE	O1G-C1A-O1A	-2.11	118.27	123.59
20	B	617	BCR	C24-C23-C22	-2.11	123.05	126.23
20	A	407	BCR	C8-C7-C6	-2.11	121.29	127.20
17	C	502	CLA	C6-C7-C8	-2.10	109.12	115.92
21	a	5409	LHG	C5-O7-C7	-2.10	112.61	117.79
26	c	5516	DGD	O2D-C2D-C1D	-2.10	104.94	110.05
20	H	101	BCR	C30-C25-C26	-2.10	119.65	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	5610	CLA	C2D-C1D-ND	-2.10	108.55	110.10
20	a	5408	BCR	C38-C26-C25	-2.10	122.17	124.53
23	l	5102	SQD	O8-S-C6	2.10	109.08	105.74
18	D	402	PHO	O2A-CGA-O1A	-2.10	118.30	123.59
17	B	612	CLA	C11-C10-C8	-2.10	109.14	115.92
18	d	5402	PHO	O2A-CGA-O1A	-2.10	118.30	123.59
26	C	518	DGD	O2D-C2D-C1D	-2.10	104.96	110.05
17	C	510	CLA	C16-C15-C13	-2.10	109.15	115.92
23	A	410	SQD	O6-C1-C2	2.09	111.57	108.30
20	b	5617	BCR	C2-C1-C6	2.09	113.70	110.48
17	b	5606	CLA	CAA-C2A-C1A	-2.09	107.51	112.14
17	b	5612	CLA	C11-C10-C8	-2.09	109.16	115.92
17	c	5510	CLA	C16-C15-C13	-2.09	109.17	115.92
17	B	616	CLA	O2D-CGD-CBD	2.09	114.97	111.27
17	C	512	CLA	O2D-CGD-CBD	2.09	114.97	111.27
25	D	410	MGE	O2G-C1B-O1B	-2.08	118.67	123.70
22	A	409	LMT	C3'-C4'-C5'	-2.08	106.15	110.93
26	H	102	DGD	O3E-C3E-C2E	-2.08	105.54	110.35
17	c	5511	CLA	O2D-CGD-CBD	2.08	114.96	111.27
17	c	5502	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
25	d	5410	MGE	C4D-C3D-C2D	-2.08	107.20	110.82
17	C	501	CLA	CHD-C1D-ND	-2.07	122.55	124.45
20	a	5408	BCR	C8-C7-C6	-2.07	121.38	127.20
20	a	5408	BCR	C11-C10-C9	-2.07	124.36	127.31
17	C	502	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
26	h	5102	DGD	O3E-C3E-C2E	-2.07	105.57	110.35
26	h	5102	DGD	C5B-C4B-C3B	-2.06	103.95	114.42
26	C	519	DGD	C5B-C4B-C3B	-2.06	103.96	114.42
20	A	407	BCR	C11-C10-C9	-2.06	124.37	127.31
26	C	519	DGD	CAB-C9B-C8B	-2.06	103.96	114.42
17	b	5616	CLA	O2D-CGD-CBD	2.06	114.93	111.27
20	B	617	BCR	C2-C1-C6	2.06	113.65	110.48
26	a	5411	DGD	CAB-C9B-C8B	-2.06	103.99	114.42
26	H	102	DGD	C5B-C4B-C3B	-2.05	104.00	114.42
23	l	5102	SQD	O47-C7-O49	-2.05	118.74	123.70
17	C	506	CLA	O1D-CGD-CBD	2.05	128.68	124.48
17	c	5503	CLA	CHD-C1D-ND	-2.05	122.57	124.45
17	a	5404	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
20	b	5618	BCR	C38-C26-C25	-2.05	122.22	124.53
17	A	405	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
17	B	605	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
26	a	5411	DGD	C5B-C4B-C3B	-2.05	104.02	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	5602	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
20	c	5513	BCR	C20-C21-C22	-2.05	124.39	127.31
20	C	516	BCR	C8-C7-C6	-2.05	121.45	127.20
17	A	403	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
17	a	5406	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
20	B	618	BCR	C38-C26-C25	-2.05	122.23	124.53
19	D	406	PQ9	C11-C2-C1	2.05	118.54	116.88
17	c	5506	CLA	O1D-CGD-CBD	2.04	128.67	124.48
17	B	602	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
20	d	5406	BCR	C38-C26-C25	-2.04	122.23	124.53
17	a	5402	CLA	CHB-C4A-NA	2.04	127.33	124.51
17	C	503	CLA	CHD-C1D-ND	-2.04	122.58	124.45
19	a	5407	PQ9	C26-C27-C28	-2.04	120.79	127.75
20	C	516	BCR	C27-C26-C25	2.04	125.69	122.73
17	B	616	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
20	C	514	BCR	C20-C21-C22	-2.04	124.40	127.31
17	C	509	CLA	C2D-C1D-ND	-2.04	108.60	110.10
17	c	5507	CLA	CHC-C1C-NC	2.04	127.29	124.20
25	D	409	MGE	O1G-C1A-O1A	-2.04	118.45	123.59
26	c	5515	DGD	O4D-C4D-C5D	-2.03	104.25	109.30
20	c	5514	BCR	C8-C7-C6	-2.03	121.49	127.20
23	d	5407	SQD	O9-S-C6	2.03	109.35	106.94
20	t	5102	BCR	C11-C10-C9	-2.03	124.41	127.31
20	t	5102	BCR	C15-C16-C17	-2.03	119.31	123.47
17	a	5403	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
17	b	5616	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
17	c	5501	CLA	CHD-C1D-ND	-2.03	122.59	124.45
17	b	5605	CLA	C11-C10-C8	-2.02	109.38	115.92
20	t	5101	BCR	C20-C21-C22	-2.02	124.42	127.31
20	D	407	BCR	C38-C26-C25	-2.02	122.26	124.53
17	A	401	CLA	CHB-C4A-NA	2.02	127.31	124.51
17	d	5403	CLA	C1-C2-C3	-2.02	122.55	126.04
17	B	605	CLA	C3C-C4C-NC	-2.02	108.31	110.57
17	B	610	CLA	C2D-C1D-ND	-2.02	108.61	110.10
20	C	514	BCR	C35-C13-C14	-2.02	120.09	122.92
21	A	408	LHG	O8-C6-C5	-2.02	102.56	108.43
17	A	402	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
20	c	5514	BCR	C27-C26-C25	2.02	125.66	122.73
17	b	5605	CLA	C3C-C4C-NC	-2.02	108.31	110.57
25	m	5103	MGE	C3G-O3G-C1D	-2.02	109.80	113.74
17	C	507	CLA	CHC-C1C-NC	2.02	127.26	124.20
26	C	517	DGD	O4D-C4D-C5D	-2.01	104.29	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	c	5509	CLA	CHA-C1A-NA	-2.01	121.78	126.40
17	B	613	CLA	C3C-C4C-NC	-2.01	108.31	110.57
25	D	409	MGE	O2G-C1B-O1B	-2.01	118.84	123.70
17	B	605	CLA	C11-C10-C8	-2.01	109.42	115.92
19	d	5405	PQ9	C11-C2-C1	2.01	118.51	116.88
17	A	401	CLA	C1-C2-C3	-2.01	122.57	126.04
21	a	5409	LHG	O8-C6-C5	-2.01	102.59	108.43
17	c	5510	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
17	b	5605	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
17	c	5509	CLA	C2D-C1D-ND	-2.01	108.62	110.10
17	D	404	CLA	C1-C2-C3	-2.00	122.58	126.04
20	k	5502	BCR	C15-C14-C13	-2.00	124.45	127.31

All (70) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	A	401	CLA	ND
17	A	402	CLA	ND
17	A	403	CLA	ND
17	A	405	CLA	ND
17	B	601	CLA	ND
17	B	602	CLA	ND
17	B	603	CLA	ND
17	B	604	CLA	ND
17	B	605	CLA	ND
17	B	606	CLA	ND
17	B	607	CLA	ND
17	B	608	CLA	ND
17	B	609	CLA	ND
17	B	610	CLA	ND
17	B	611	CLA	ND
17	B	612	CLA	ND
17	B	613	CLA	ND
17	B	614	CLA	ND
17	B	615	CLA	ND
17	B	616	CLA	ND
17	C	501	CLA	ND
17	C	502	CLA	ND
17	C	503	CLA	ND
17	C	504	CLA	ND
17	C	505	CLA	ND
17	C	506	CLA	ND

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Mol	Chain	Res	Type	Atom
17	C	507	CLA	ND
17	C	508	CLA	ND
17	C	509	CLA	ND
17	C	510	CLA	ND
17	C	511	CLA	ND
17	C	512	CLA	ND
17	C	513	CLA	ND
17	D	404	CLA	ND
17	D	405	CLA	ND
17	a	5402	CLA	ND
17	a	5403	CLA	ND
17	a	5404	CLA	ND
17	a	5406	CLA	ND
17	b	5601	CLA	ND
17	b	5602	CLA	ND
17	b	5603	CLA	ND
17	b	5604	CLA	ND
17	b	5605	CLA	ND
17	b	5606	CLA	ND
17	b	5607	CLA	ND
17	b	5608	CLA	ND
17	b	5609	CLA	ND
17	b	5610	CLA	ND
17	b	5611	CLA	ND
17	b	5612	CLA	ND
17	b	5613	CLA	ND
17	b	5614	CLA	ND
17	b	5615	CLA	ND
17	b	5616	CLA	ND
17	c	5501	CLA	ND
17	c	5502	CLA	ND
17	c	5503	CLA	ND
17	c	5504	CLA	ND
17	c	5505	CLA	ND
17	c	5506	CLA	ND
17	c	5507	CLA	ND
17	c	5508	CLA	ND
17	c	5509	CLA	ND
17	c	5510	CLA	ND
17	c	5511	CLA	ND
17	c	5512	CLA	ND
17	d	5403	CLA	ND

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Mol	Chain	Res	Type	Atom
17	d	5404	CLA	ND
17	k	5501	CLA	ND

All (1877) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	403	CLA	CHA-CBD-CGD-O1D
17	A	403	CLA	CHA-CBD-CGD-O2D
17	B	602	CLA	C2-C3-C5-C6
17	B	602	CLA	C4-C3-C5-C6
17	B	603	CLA	CBD-CGD-O2D-CED
17	B	604	CLA	CHA-CBD-CGD-O1D
17	B	604	CLA	CHA-CBD-CGD-O2D
17	B	605	CLA	CHA-CBD-CGD-O1D
17	B	605	CLA	CHA-CBD-CGD-O2D
17	B	605	CLA	C14-C13-C15-C16
17	B	606	CLA	C1A-C2A-CAA-CBA
17	B	606	CLA	C3A-C2A-CAA-CBA
17	B	606	CLA	C4-C3-C5-C6
17	B	607	CLA	CAD-CBD-CGD-O2D
17	B	607	CLA	C2-C3-C5-C6
17	B	607	CLA	C4-C3-C5-C6
17	B	608	CLA	C1A-C2A-CAA-CBA
17	B	609	CLA	C1A-C2A-CAA-CBA
17	B	609	CLA	C3A-C2A-CAA-CBA
17	B	609	CLA	CHA-CBD-CGD-O1D
17	B	609	CLA	CHA-CBD-CGD-O2D
17	B	609	CLA	CAD-CBD-CGD-O1D
17	B	609	CLA	CAD-CBD-CGD-O2D
17	B	609	CLA	CBD-CGD-O2D-CED
17	B	609	CLA	C11-C10-C8-C9
17	B	612	CLA	C1A-C2A-CAA-CBA
17	B	612	CLA	C3A-C2A-CAA-CBA
17	B	615	CLA	CHA-CBD-CGD-O1D
17	B	615	CLA	CHA-CBD-CGD-O2D
17	B	615	CLA	CBD-CGD-O2D-CED
17	B	616	CLA	C1A-C2A-CAA-CBA
17	B	616	CLA	C3A-C2A-CAA-CBA
17	C	503	CLA	C1A-C2A-CAA-CBA
17	C	503	CLA	C2-C3-C5-C6
17	C	503	CLA	C4-C3-C5-C6
17	C	504	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	C	504	CLA	O1A-CGA-O2A-C1
17	C	505	CLA	CAD-CBD-CGD-O1D
17	C	506	CLA	C1A-C2A-CAA-CBA
17	C	507	CLA	CHA-CBD-CGD-O1D
17	C	507	CLA	CHA-CBD-CGD-O2D
17	C	510	CLA	CBD-CGD-O2D-CED
17	C	513	CLA	CHA-CBD-CGD-O1D
17	C	513	CLA	CHA-CBD-CGD-O2D
17	D	404	CLA	C1A-C2A-CAA-CBA
17	D	405	CLA	C1A-C2A-CAA-CBA
17	D	405	CLA	C3A-C2A-CAA-CBA
17	D	405	CLA	CBD-CGD-O2D-CED
17	a	5404	CLA	CHA-CBD-CGD-O1D
17	a	5404	CLA	CHA-CBD-CGD-O2D
17	b	5602	CLA	C2-C3-C5-C6
17	b	5602	CLA	C4-C3-C5-C6
17	b	5603	CLA	CBD-CGD-O2D-CED
17	b	5604	CLA	CHA-CBD-CGD-O1D
17	b	5604	CLA	CHA-CBD-CGD-O2D
17	b	5605	CLA	CHA-CBD-CGD-O1D
17	b	5605	CLA	CHA-CBD-CGD-O2D
17	b	5605	CLA	C14-C13-C15-C16
17	b	5606	CLA	C1A-C2A-CAA-CBA
17	b	5606	CLA	C3A-C2A-CAA-CBA
17	b	5607	CLA	CAD-CBD-CGD-O2D
17	b	5607	CLA	C2-C3-C5-C6
17	b	5607	CLA	C4-C3-C5-C6
17	b	5608	CLA	C1A-C2A-CAA-CBA
17	b	5609	CLA	C1A-C2A-CAA-CBA
17	b	5609	CLA	C3A-C2A-CAA-CBA
17	b	5609	CLA	CHA-CBD-CGD-O1D
17	b	5609	CLA	CHA-CBD-CGD-O2D
17	b	5609	CLA	CAD-CBD-CGD-O1D
17	b	5609	CLA	CAD-CBD-CGD-O2D
17	b	5609	CLA	CBD-CGD-O2D-CED
17	b	5609	CLA	C11-C10-C8-C9
17	b	5612	CLA	C1A-C2A-CAA-CBA
17	b	5612	CLA	C3A-C2A-CAA-CBA
17	b	5615	CLA	CHA-CBD-CGD-O1D
17	b	5615	CLA	CHA-CBD-CGD-O2D
17	b	5615	CLA	CBD-CGD-O2D-CED
17	b	5616	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	b	5616	CLA	C3A-C2A-CAA-CBA
17	c	5503	CLA	C1A-C2A-CAA-CBA
17	c	5503	CLA	C2-C3-C5-C6
17	c	5503	CLA	C4-C3-C5-C6
17	c	5504	CLA	CBA-CGA-O2A-C1
17	c	5504	CLA	O1A-CGA-O2A-C1
17	c	5505	CLA	CAD-CBD-CGD-O1D
17	c	5506	CLA	C1A-C2A-CAA-CBA
17	c	5507	CLA	CHA-CBD-CGD-O1D
17	c	5507	CLA	CHA-CBD-CGD-O2D
17	c	5510	CLA	CBD-CGD-O2D-CED
17	c	5512	CLA	CHA-CBD-CGD-O1D
17	c	5512	CLA	CHA-CBD-CGD-O2D
17	d	5403	CLA	C1A-C2A-CAA-CBA
17	d	5404	CLA	C1A-C2A-CAA-CBA
17	d	5404	CLA	C3A-C2A-CAA-CBA
17	d	5404	CLA	CBD-CGD-O2D-CED
18	D	402	PHO	C1A-C2A-CAA-CBA
18	D	402	PHO	C3A-C2A-CAA-CBA
18	D	402	PHO	CBD-CGD-O2D-CED
18	d	5402	PHO	C1A-C2A-CAA-CBA
18	d	5402	PHO	C3A-C2A-CAA-CBA
18	d	5402	PHO	CBD-CGD-O2D-CED
19	A	406	PQ9	C19-C18-C20-C21
19	A	406	PQ9	C18-C20-C21-C22
19	A	406	PQ9	C23-C25-C26-C27
19	A	406	PQ9	C27-C28-C30-C31
19	A	406	PQ9	C29-C28-C30-C31
19	A	406	PQ9	C34-C33-C35-C36
19	D	406	PQ9	C24-C23-C25-C26
19	D	406	PQ9	C34-C33-C35-C36
19	a	5407	PQ9	C19-C18-C20-C21
19	a	5407	PQ9	C18-C20-C21-C22
19	a	5407	PQ9	C23-C25-C26-C27
19	d	5405	PQ9	C24-C23-C25-C26
19	d	5405	PQ9	C34-C33-C35-C36
20	A	407	BCR	C1-C6-C7-C8
20	A	407	BCR	C9-C10-C11-C12
20	A	407	BCR	C11-C12-C13-C35
20	A	407	BCR	C18-C19-C20-C21
20	B	617	BCR	C11-C12-C13-C35
20	B	617	BCR	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
20	B	617	BCR	C21-C22-C23-C24
20	B	617	BCR	C37-C22-C23-C24
20	B	618	BCR	C11-C10-C9-C8
20	B	618	BCR	C10-C11-C12-C13
20	B	618	BCR	C21-C22-C23-C24
20	B	618	BCR	C37-C22-C23-C24
20	C	514	BCR	C7-C8-C9-C34
20	C	514	BCR	C14-C15-C16-C17
20	C	515	BCR	C1-C6-C7-C8
20	C	515	BCR	C6-C7-C8-C9
20	C	515	BCR	C11-C10-C9-C8
20	C	515	BCR	C11-C12-C13-C14
20	C	515	BCR	C11-C12-C13-C35
20	C	515	BCR	C12-C13-C14-C15
20	C	515	BCR	C14-C15-C16-C17
20	C	515	BCR	C16-C17-C18-C19
20	C	515	BCR	C16-C17-C18-C36
20	C	515	BCR	C18-C19-C20-C21
20	C	515	BCR	C22-C23-C24-C25
20	C	516	BCR	C6-C7-C8-C9
20	C	516	BCR	C7-C8-C9-C34
20	C	516	BCR	C10-C11-C12-C13
20	C	516	BCR	C11-C12-C13-C35
20	C	516	BCR	C12-C13-C14-C15
20	C	516	BCR	C35-C13-C14-C15
20	C	516	BCR	C20-C21-C22-C37
20	C	516	BCR	C21-C22-C23-C24
20	C	516	BCR	C22-C23-C24-C25
20	D	407	BCR	C7-C8-C9-C10
20	D	407	BCR	C11-C12-C13-C35
20	D	407	BCR	C23-C24-C25-C30
20	H	101	BCR	C6-C7-C8-C9
20	H	101	BCR	C16-C17-C18-C19
20	H	101	BCR	C16-C17-C18-C36
20	T	102	BCR	C16-C17-C18-C19
20	T	102	BCR	C16-C17-C18-C36
20	T	102	BCR	C23-C24-C25-C26
20	T	102	BCR	C23-C24-C25-C30
20	a	5408	BCR	C1-C6-C7-C8
20	a	5408	BCR	C9-C10-C11-C12
20	a	5408	BCR	C11-C12-C13-C35
20	a	5408	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
20	b	5617	BCR	C11-C12-C13-C35
20	b	5617	BCR	C14-C15-C16-C17
20	b	5617	BCR	C21-C22-C23-C24
20	b	5617	BCR	C37-C22-C23-C24
20	b	5618	BCR	C11-C10-C9-C8
20	b	5618	BCR	C10-C11-C12-C13
20	b	5618	BCR	C21-C22-C23-C24
20	b	5618	BCR	C37-C22-C23-C24
20	b	5619	BCR	C1-C6-C7-C8
20	b	5619	BCR	C6-C7-C8-C9
20	b	5619	BCR	C7-C8-C9-C34
20	b	5619	BCR	C22-C23-C24-C25
20	c	5513	BCR	C7-C8-C9-C34
20	c	5513	BCR	C14-C15-C16-C17
20	c	5514	BCR	C6-C7-C8-C9
20	c	5514	BCR	C7-C8-C9-C34
20	c	5514	BCR	C10-C11-C12-C13
20	c	5514	BCR	C11-C12-C13-C35
20	c	5514	BCR	C12-C13-C14-C15
20	c	5514	BCR	C35-C13-C14-C15
20	c	5514	BCR	C20-C21-C22-C37
20	c	5514	BCR	C21-C22-C23-C24
20	c	5514	BCR	C22-C23-C24-C25
20	d	5406	BCR	C7-C8-C9-C10
20	d	5406	BCR	C11-C12-C13-C35
20	d	5406	BCR	C23-C24-C25-C30
20	h	5101	BCR	C6-C7-C8-C9
20	h	5101	BCR	C16-C17-C18-C19
20	h	5101	BCR	C16-C17-C18-C36
20	k	5502	BCR	C6-C7-C8-C9
20	k	5502	BCR	C14-C15-C16-C17
20	k	5502	BCR	C18-C19-C20-C21
20	k	5502	BCR	C19-C20-C21-C22
20	k	5502	BCR	C20-C21-C22-C37
20	k	5502	BCR	C21-C22-C23-C24
20	k	5502	BCR	C22-C23-C24-C25
20	t	5101	BCR	C1-C6-C7-C8
20	t	5101	BCR	C6-C7-C8-C9
20	t	5101	BCR	C7-C8-C9-C34
20	t	5101	BCR	C22-C23-C24-C25
20	t	5102	BCR	C1-C6-C7-C8
20	t	5102	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
20	t	5102	BCR	C14-C15-C16-C17
20	t	5102	BCR	C16-C17-C18-C36
20	t	5102	BCR	C21-C22-C23-C24
20	t	5102	BCR	C37-C22-C23-C24
20	t	5102	BCR	C22-C23-C24-C25
20	z	5101	BCR	C1-C6-C7-C8
20	z	5101	BCR	C6-C7-C8-C9
20	z	5101	BCR	C11-C10-C9-C8
20	z	5101	BCR	C11-C12-C13-C14
20	z	5101	BCR	C11-C12-C13-C35
20	z	5101	BCR	C12-C13-C14-C15
20	z	5101	BCR	C14-C15-C16-C17
20	z	5101	BCR	C16-C17-C18-C19
20	z	5101	BCR	C16-C17-C18-C36
20	z	5101	BCR	C18-C19-C20-C21
20	z	5101	BCR	C22-C23-C24-C25
20	Y	101	BCR	C11-C12-C13-C14
20	Y	101	BCR	C11-C12-C13-C35
20	Y	101	BCR	C14-C15-C16-C17
20	Y	101	BCR	C17-C18-C19-C20
20	Y	101	BCR	C18-C19-C20-C21
20	Y	101	BCR	C22-C23-C24-C25
21	A	408	LHG	O1-C1-C2-C3
21	A	408	LHG	C3-O3-P-O4
21	A	408	LHG	C3-O3-P-O5
21	A	408	LHG	C4-O6-P-O3
21	A	408	LHG	C4-O6-P-O4
21	A	408	LHG	C4-O6-P-O5
21	a	5409	LHG	O1-C1-C2-C3
21	a	5409	LHG	C3-O3-P-O4
21	a	5409	LHG	C3-O3-P-O5
21	a	5409	LHG	C4-O6-P-O3
21	a	5409	LHG	C4-O6-P-O4
21	a	5409	LHG	C4-O6-P-O5
22	A	409	LMT	C2'-C1'-O1'-C1
22	A	409	LMT	O5'-C1'-O1'-C1
22	B	620	LMT	C2'-C1'-O1'-C1
22	B	620	LMT	O5'-C1'-O1'-C1
22	m	5102	LMT	C2'-C1'-O1'-C1
22	m	5102	LMT	O5'-C1'-O1'-C1
23	A	410	SQD	O5-C5-C6-S
23	D	403	SQD	O5-C5-C6-S

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Mol	Chain	Res	Type	Atoms
23	L	101	SQD	O47-C45-C46-O48
23	L	101	SQD	O49-C7-O47-C45
23	L	101	SQD	C5-C6-S-O7
23	L	101	SQD	C5-C6-S-O8
23	L	101	SQD	C5-C6-S-O9
23	a	5401	SQD	C8-C7-O47-C45
23	a	5401	SQD	O5-C5-C6-S
23	a	5401	SQD	C5-C6-S-O7
23	a	5401	SQD	C5-C6-S-O8
23	a	5401	SQD	C5-C6-S-O9
23	d	5407	SQD	O5-C1-O6-C44
23	d	5407	SQD	O5-C5-C6-S
23	l	5102	SQD	O5-C1-O6-C44
23	l	5102	SQD	O5-C5-C6-S
25	C	520	MGE	O2G-C2G-C3G-O3G
25	D	409	MGE	O2G-C2G-C3G-O3G
25	D	410	MGE	O6D-C1D-O3G-C3G
25	c	5517	MGE	O2G-C2G-C3G-O3G
25	d	5410	MGE	O6D-C1D-O3G-C3G
25	m	5103	MGE	C2B-C1B-O2G-C2G
25	m	5103	MGE	O6D-C1D-O3G-C3G
26	C	517	DGD	C2D-C1D-O3G-C3G
26	C	517	DGD	O6D-C1D-O3G-C3G
26	C	517	DGD	O6E-C1E-O5D-C6D
26	C	518	DGD	C2E-C1E-O5D-C6D
26	C	518	DGD	O6E-C1E-O5D-C6D
26	C	519	DGD	O2G-C2G-C3G-O3G
26	C	519	DGD	O6E-C1E-O5D-C6D
26	H	102	DGD	O1G-C1G-C2G-O2G
26	H	102	DGD	C2D-C1D-O3G-C3G
26	H	102	DGD	O6D-C1D-O3G-C3G
26	H	102	DGD	C2E-C1E-O5D-C6D
26	H	102	DGD	O6E-C1E-O5D-C6D
26	a	5411	DGD	O2G-C2G-C3G-O3G
26	a	5411	DGD	O6E-C1E-O5D-C6D
26	c	5515	DGD	C2D-C1D-O3G-C3G
26	c	5515	DGD	O6D-C1D-O3G-C3G
26	c	5515	DGD	O6E-C1E-O5D-C6D
26	c	5516	DGD	C2E-C1E-O5D-C6D
26	c	5516	DGD	O6E-C1E-O5D-C6D
26	h	5102	DGD	O1G-C1G-C2G-O2G
26	h	5102	DGD	C2D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
26	h	5102	DGD	O6D-C1D-O3G-C3G
26	h	5102	DGD	C2E-C1E-O5D-C6D
26	h	5102	DGD	O6E-C1E-O5D-C6D
17	B	607	CLA	O1D-CGD-O2D-CED
17	B	609	CLA	O1D-CGD-O2D-CED
17	B	611	CLA	O1D-CGD-O2D-CED
17	B	613	CLA	O1D-CGD-O2D-CED
17	B	615	CLA	O1D-CGD-O2D-CED
17	C	511	CLA	O1D-CGD-O2D-CED
17	b	5607	CLA	O1D-CGD-O2D-CED
17	b	5609	CLA	O1D-CGD-O2D-CED
17	b	5611	CLA	O1D-CGD-O2D-CED
17	b	5615	CLA	O1D-CGD-O2D-CED
17	k	5501	CLA	O1D-CGD-O2D-CED
23	a	5401	SQD	O49-C7-O47-C45
17	C	502	CLA	O1D-CGD-O2D-CED
17	b	5613	CLA	O1D-CGD-O2D-CED
17	c	5502	CLA	O1D-CGD-O2D-CED
17	A	405	CLA	CBD-CGD-O2D-CED
17	B	605	CLA	CBD-CGD-O2D-CED
17	B	606	CLA	CBD-CGD-O2D-CED
17	B	607	CLA	CBD-CGD-O2D-CED
17	B	611	CLA	CBD-CGD-O2D-CED
17	B	613	CLA	CBD-CGD-O2D-CED
17	B	614	CLA	CBD-CGD-O2D-CED
17	B	616	CLA	CBD-CGD-O2D-CED
17	C	501	CLA	CBD-CGD-O2D-CED
17	C	502	CLA	CBD-CGD-O2D-CED
17	C	503	CLA	CBD-CGD-O2D-CED
17	C	506	CLA	CBD-CGD-O2D-CED
17	C	507	CLA	CBD-CGD-O2D-CED
17	C	509	CLA	CBD-CGD-O2D-CED
17	C	511	CLA	CBD-CGD-O2D-CED
17	C	512	CLA	CBD-CGD-O2D-CED
17	a	5406	CLA	CBD-CGD-O2D-CED
17	b	5605	CLA	CBD-CGD-O2D-CED
17	b	5606	CLA	CBD-CGD-O2D-CED
17	b	5607	CLA	CBD-CGD-O2D-CED
17	b	5611	CLA	CBD-CGD-O2D-CED
17	b	5613	CLA	CBD-CGD-O2D-CED
17	b	5614	CLA	CBD-CGD-O2D-CED
17	b	5616	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	c	5501	CLA	CBD-CGD-O2D-CED
17	c	5502	CLA	CBD-CGD-O2D-CED
17	c	5503	CLA	CBD-CGD-O2D-CED
17	c	5506	CLA	CBD-CGD-O2D-CED
17	c	5507	CLA	CBD-CGD-O2D-CED
17	c	5509	CLA	CBD-CGD-O2D-CED
17	c	5511	CLA	CBD-CGD-O2D-CED
17	k	5501	CLA	CBD-CGD-O2D-CED
22	T	101	LMT	O5B-C1B-O1B-C4'
22	T	101	LMT	C4B-C5B-C6B-O6B
17	C	501	CLA	O1D-CGD-O2D-CED
17	c	5501	CLA	O1D-CGD-O2D-CED
17	B	603	CLA	O1D-CGD-O2D-CED
17	C	509	CLA	O1D-CGD-O2D-CED
17	C	510	CLA	O1D-CGD-O2D-CED
17	b	5603	CLA	O1D-CGD-O2D-CED
17	c	5509	CLA	O1D-CGD-O2D-CED
17	c	5510	CLA	O1D-CGD-O2D-CED
18	D	402	PHO	O1D-CGD-O2D-CED
18	d	5402	PHO	O1D-CGD-O2D-CED
17	B	602	CLA	CBD-CGD-O2D-CED
17	B	604	CLA	CBD-CGD-O2D-CED
17	C	508	CLA	CBD-CGD-O2D-CED
17	b	5602	CLA	CBD-CGD-O2D-CED
17	b	5604	CLA	CBD-CGD-O2D-CED
17	c	5508	CLA	CBD-CGD-O2D-CED
17	C	507	CLA	O1A-CGA-O2A-C1
17	D	405	CLA	O1A-CGA-O2A-C1
17	c	5507	CLA	O1A-CGA-O2A-C1
17	d	5404	CLA	O1A-CGA-O2A-C1
23	L	101	SQD	O10-C23-O48-C46
25	D	409	MGE	C4D-C5D-C6D-O5D
17	D	405	CLA	O1D-CGD-O2D-CED
17	d	5404	CLA	O1D-CGD-O2D-CED
22	T	101	LMT	C2B-C1B-O1B-C4'
17	A	401	CLA	CBD-CGD-O2D-CED
17	a	5402	CLA	CBD-CGD-O2D-CED
25	m	5103	MGE	O1B-C1B-O2G-C2G
26	C	517	DGD	O1B-C1B-O2G-C2G
26	C	518	DGD	O1B-C1B-O2G-C2G
26	c	5515	DGD	O1B-C1B-O2G-C2G
26	c	5516	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
17	B	602	CLA	C3-C5-C6-C7
17	B	606	CLA	C3-C5-C6-C7
17	B	608	CLA	C3-C5-C6-C7
17	B	614	CLA	C3-C5-C6-C7
17	b	5602	CLA	C3-C5-C6-C7
17	b	5608	CLA	C3-C5-C6-C7
17	b	5614	CLA	C3-C5-C6-C7
17	C	507	CLA	CBA-CGA-O2A-C1
17	D	405	CLA	CBA-CGA-O2A-C1
17	c	5507	CLA	CBA-CGA-O2A-C1
17	d	5404	CLA	CBA-CGA-O2A-C1
26	C	519	DGD	C2A-C1A-O1G-C1G
26	a	5411	DGD	C2A-C1A-O1G-C1G
23	L	101	SQD	C8-C7-O47-C45
17	c	5505	CLA	C2C-C3C-CAC-CBC
17	B	606	CLA	C2-C3-C5-C6
19	A	406	PQ9	C17-C18-C20-C21
19	A	406	PQ9	C32-C33-C35-C36
19	D	406	PQ9	C32-C33-C35-C36
19	a	5407	PQ9	C17-C18-C20-C21
19	d	5405	PQ9	C32-C33-C35-C36
17	B	601	CLA	CBD-CGD-O2D-CED
17	C	513	CLA	CBD-CGD-O2D-CED
17	b	5601	CLA	CBD-CGD-O2D-CED
17	c	5512	CLA	CBD-CGD-O2D-CED
17	B	602	CLA	C2A-CAA-CBA-CGA
17	C	508	CLA	C2A-CAA-CBA-CGA
17	b	5602	CLA	C2A-CAA-CBA-CGA
17	c	5508	CLA	C2A-CAA-CBA-CGA
17	C	506	CLA	O1D-CGD-O2D-CED
17	c	5506	CLA	O1D-CGD-O2D-CED
17	C	505	CLA	C2C-C3C-CAC-CBC
17	A	402	CLA	C3-C5-C6-C7
17	B	612	CLA	C3-C5-C6-C7
17	C	505	CLA	C3-C5-C6-C7
17	a	5403	CLA	C3-C5-C6-C7
17	b	5612	CLA	C3-C5-C6-C7
17	c	5505	CLA	C3-C5-C6-C7
23	L	101	SQD	C24-C23-O48-C46
26	H	102	DGD	C4D-C5D-C6D-O5D
26	h	5102	DGD	C4D-C5D-C6D-O5D
17	B	605	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	b	5605	CLA	O1D-CGD-O2D-CED
25	D	409	MGE	O6D-C5D-C6D-O5D
23	a	5401	SQD	C24-C23-O48-C46
20	A	407	BCR	C13-C14-C15-C16
20	C	514	BCR	C9-C10-C11-C12
20	C	515	BCR	C19-C20-C21-C22
20	D	407	BCR	C9-C10-C11-C12
20	T	102	BCR	C9-C10-C11-C12
20	a	5408	BCR	C13-C14-C15-C16
20	c	5513	BCR	C9-C10-C11-C12
20	d	5406	BCR	C9-C10-C11-C12
20	t	5102	BCR	C15-C16-C17-C18
20	z	5101	BCR	C19-C20-C21-C22
20	Y	101	BCR	C19-C20-C21-C22
22	A	409	LMT	O5B-C5B-C6B-O6B
22	B	620	LMT	O5'-C5'-C6'-O6'
22	A	409	LMT	C4B-C5B-C6B-O6B
17	C	504	CLA	CBD-CGD-O2D-CED
17	D	404	CLA	CBD-CGD-O2D-CED
17	c	5504	CLA	CBD-CGD-O2D-CED
17	d	5403	CLA	CBD-CGD-O2D-CED
17	A	405	CLA	O1D-CGD-O2D-CED
17	B	614	CLA	O1D-CGD-O2D-CED
17	a	5406	CLA	O1D-CGD-O2D-CED
17	b	5614	CLA	O1D-CGD-O2D-CED
22	T	101	LMT	O5B-C5B-C6B-O6B
22	a	5410	LMT	O5'-C5'-C6'-O6'
22	m	5102	LMT	O5B-C5B-C6B-O6B
22	m	5102	LMT	C4B-C5B-C6B-O6B
17	c	5503	CLA	O1D-CGD-O2D-CED
25	D	409	MGE	C2B-C1B-O2G-C2G
17	C	503	CLA	O1D-CGD-O2D-CED
22	M	101	LMT	O5B-C5B-C6B-O6B
17	C	507	CLA	O1D-CGD-O2D-CED
17	c	5507	CLA	O1D-CGD-O2D-CED
22	T	101	LMT	O5'-C5'-C6'-O6'
17	b	5616	CLA	O1D-CGD-O2D-CED
17	C	505	CLA	C5-C6-C7-C8
17	c	5505	CLA	C5-C6-C7-C8
17	A	403	CLA	C3-C5-C6-C7
17	a	5404	CLA	C3-C5-C6-C7
23	a	5401	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
17	B	616	CLA	O1D-CGD-O2D-CED
26	C	519	DGD	O6E-C5E-C6E-O5E
26	a	5411	DGD	O6E-C5E-C6E-O5E
17	B	605	CLA	C4-C3-C5-C6
17	D	404	CLA	C4-C3-C5-C6
17	b	5605	CLA	C4-C3-C5-C6
17	d	5403	CLA	C4-C3-C5-C6
19	A	406	PQ9	C14-C13-C15-C16
19	D	406	PQ9	C19-C18-C20-C21
19	a	5407	PQ9	C14-C13-C15-C16
19	d	5405	PQ9	C19-C18-C20-C21
17	B	605	CLA	C2-C3-C5-C6
17	D	404	CLA	C2-C3-C5-C6
17	b	5605	CLA	C2-C3-C5-C6
17	d	5403	CLA	C2-C3-C5-C6
19	A	406	PQ9	C12-C13-C15-C16
19	D	406	PQ9	C17-C18-C20-C21
19	D	406	PQ9	C22-C23-C25-C26
19	a	5407	PQ9	C12-C13-C15-C16
19	d	5405	PQ9	C17-C18-C20-C21
19	d	5405	PQ9	C22-C23-C25-C26
26	H	102	DGD	O6D-C5D-C6D-O5D
26	h	5102	DGD	O6D-C5D-C6D-O5D
17	B	606	CLA	C2A-CAA-CBA-CGA
17	C	509	CLA	C2A-CAA-CBA-CGA
17	c	5509	CLA	C2A-CAA-CBA-CGA
22	M	101	LMT	O5'-C1'-O1'-C1
23	D	403	SQD	O5-C1-O6-C44
19	A	406	PQ9	C38-C40-C41-C42
17	B	606	CLA	O1D-CGD-O2D-CED
17	C	512	CLA	O1D-CGD-O2D-CED
17	b	5606	CLA	O1D-CGD-O2D-CED
17	c	5511	CLA	O1D-CGD-O2D-CED
17	C	505	CLA	C4C-C3C-CAC-CBC
17	c	5505	CLA	C4C-C3C-CAC-CBC
17	C	508	CLA	O1D-CGD-O2D-CED
17	c	5508	CLA	O1D-CGD-O2D-CED
17	A	401	CLA	CBA-CGA-O2A-C1
17	B	607	CLA	CBA-CGA-O2A-C1
17	C	506	CLA	CBA-CGA-O2A-C1
17	a	5402	CLA	CBA-CGA-O2A-C1
17	b	5607	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	c	5506	CLA	CBA-CGA-O2A-C1
22	B	620	LMT	C4'-C5'-C6'-O6'
20	B	617	BCR	C9-C10-C11-C12
20	C	516	BCR	C9-C10-C11-C12
20	C	516	BCR	C13-C14-C15-C16
20	b	5617	BCR	C9-C10-C11-C12
20	c	5514	BCR	C9-C10-C11-C12
20	c	5514	BCR	C13-C14-C15-C16
22	M	101	LMT	O5'-C5'-C6'-O6'
26	C	519	DGD	O1A-C1A-O1G-C1G
26	a	5411	DGD	O1A-C1A-O1G-C1G
17	C	503	CLA	C10-C11-C12-C13
17	c	5503	CLA	C10-C11-C12-C13
23	A	410	SQD	C2-C1-O6-C44
26	C	519	DGD	C2E-C1E-O5D-C6D
26	a	5411	DGD	C2E-C1E-O5D-C6D
23	l	5102	SQD	O47-C45-C46-O48
17	B	607	CLA	O1A-CGA-O2A-C1
17	b	5607	CLA	O1A-CGA-O2A-C1
17	B	603	CLA	C4-C3-C5-C6
17	b	5603	CLA	C4-C3-C5-C6
17	B	604	CLA	C14-C13-C15-C16
17	C	501	CLA	C11-C12-C13-C14
17	C	506	CLA	C11-C10-C8-C9
17	C	507	CLA	C11-C10-C8-C9
17	C	508	CLA	C11-C10-C8-C9
17	C	511	CLA	C6-C7-C8-C9
17	D	404	CLA	C6-C7-C8-C9
17	b	5604	CLA	C14-C13-C15-C16
17	c	5501	CLA	C11-C12-C13-C14
17	c	5506	CLA	C11-C10-C8-C9
17	c	5507	CLA	C11-C10-C8-C9
17	c	5508	CLA	C11-C10-C8-C9
17	d	5403	CLA	C6-C7-C8-C9
17	k	5501	CLA	C6-C7-C8-C9
18	A	404	PHO	C11-C10-C8-C9
18	a	5405	PHO	C11-C10-C8-C9
17	B	602	CLA	O1D-CGD-O2D-CED
17	b	5602	CLA	O1D-CGD-O2D-CED
17	A	403	CLA	CBD-CGD-O2D-CED
17	a	5404	CLA	CBD-CGD-O2D-CED
17	C	510	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
17	c	5510	CLA	C15-C16-C17-C18
17	A	405	CLA	C2A-CAA-CBA-CGA
17	a	5406	CLA	C2A-CAA-CBA-CGA
20	C	515	BCR	C7-C8-C9-C34
20	D	407	BCR	C7-C8-C9-C34
20	d	5406	BCR	C7-C8-C9-C34
20	z	5101	BCR	C7-C8-C9-C34
20	A	407	BCR	C11-C12-C13-C14
20	C	515	BCR	C7-C8-C9-C10
20	T	102	BCR	C7-C8-C9-C10
20	a	5408	BCR	C11-C12-C13-C14
20	z	5101	BCR	C7-C8-C9-C10
25	D	409	MGE	O1B-C1B-O2G-C2G
23	d	5407	SQD	C8-C7-O47-C45
23	L	101	SQD	C9-C10-C11-C12
25	d	5409	MGE	C1B-C2B-C3B-C4B
25	m	5103	MGE	C1A-C2A-C3A-C4A
17	C	506	CLA	C15-C16-C17-C18
17	c	5506	CLA	C15-C16-C17-C18
22	m	5102	LMT	O5'-C5'-C6'-O6'
22	a	5410	LMT	C4'-C5'-C6'-O6'
17	A	402	CLA	C15-C16-C17-C18
17	B	609	CLA	C10-C11-C12-C13
17	B	609	CLA	C13-C15-C16-C17
17	C	505	CLA	C13-C15-C16-C17
17	D	404	CLA	C13-C15-C16-C17
17	a	5403	CLA	C15-C16-C17-C18
17	c	5505	CLA	C13-C15-C16-C17
17	d	5403	CLA	C13-C15-C16-C17
18	D	402	PHO	C5-C6-C7-C8
18	d	5402	PHO	C5-C6-C7-C8
17	A	401	CLA	O1A-CGA-O2A-C1
17	a	5402	CLA	O1A-CGA-O2A-C1
17	A	402	CLA	C5-C6-C7-C8
17	A	403	CLA	C8-C10-C11-C12
17	A	405	CLA	C5-C6-C7-C8
17	C	508	CLA	C10-C11-C12-C13
17	C	511	CLA	C10-C11-C12-C13
17	a	5403	CLA	C5-C6-C7-C8
17	a	5404	CLA	C8-C10-C11-C12
17	a	5406	CLA	C5-C6-C7-C8
17	b	5609	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
17	b	5609	CLA	C13-C15-C16-C17
17	c	5508	CLA	C10-C11-C12-C13
17	k	5501	CLA	C10-C11-C12-C13
23	A	410	SQD	O10-C23-O48-C46
17	C	506	CLA	O1A-CGA-O2A-C1
17	c	5506	CLA	O1A-CGA-O2A-C1
21	A	408	LHG	C23-C24-C25-C26
21	a	5409	LHG	C23-C24-C25-C26
25	D	409	MGE	C1B-C2B-C3B-C4B
17	B	611	CLA	C13-C15-C16-C17
17	b	5611	CLA	C13-C15-C16-C17
25	d	5410	MGE	C2A-C3A-C4A-C5A
17	B	603	CLA	C10-C11-C12-C13
17	B	611	CLA	C15-C16-C17-C18
17	D	404	CLA	C15-C16-C17-C18
17	b	5603	CLA	C10-C11-C12-C13
17	b	5611	CLA	C15-C16-C17-C18
17	d	5403	CLA	C15-C16-C17-C18
18	D	402	PHO	C15-C16-C17-C18
18	d	5402	PHO	C15-C16-C17-C18
25	A	412	MGE	C1A-C2A-C3A-C4A
25	A	412	MGE	C1B-C2B-C3B-C4B
25	l	5101	MGE	C1A-C2A-C3A-C4A
25	l	5101	MGE	C1B-C2B-C3B-C4B
17	B	612	CLA	CBD-CGD-O2D-CED
17	b	5612	CLA	CBD-CGD-O2D-CED
26	C	517	DGD	C2B-C1B-O2G-C2G
26	c	5515	DGD	C2B-C1B-O2G-C2G
17	B	601	CLA	O1D-CGD-O2D-CED
17	b	5601	CLA	O1D-CGD-O2D-CED
17	B	606	CLA	C12-C13-C15-C16
17	B	612	CLA	C11-C10-C8-C7
17	C	503	CLA	C12-C13-C15-C16
17	b	5612	CLA	C11-C10-C8-C7
17	c	5503	CLA	C12-C13-C15-C16
18	A	404	PHO	C11-C10-C8-C7
18	A	404	PHO	C12-C13-C15-C16
18	a	5405	PHO	C11-C10-C8-C7
18	a	5405	PHO	C12-C13-C15-C16
20	k	5502	BCR	C9-C10-C11-C12
17	A	401	CLA	O1D-CGD-O2D-CED
17	a	5402	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	b	5604	CLA	O1D-CGD-O2D-CED
17	B	611	CLA	C5-C6-C7-C8
17	b	5611	CLA	C5-C6-C7-C8
22	M	101	LMT	O1'-C1-C2-C3
20	T	102	BCR	C22-C23-C24-C25
17	B	610	CLA	C15-C16-C17-C18
17	b	5610	CLA	C15-C16-C17-C18
17	B	604	CLA	O1D-CGD-O2D-CED
19	A	406	PQ9	C13-C15-C16-C17
19	D	406	PQ9	C13-C15-C16-C17
19	a	5407	PQ9	C13-C15-C16-C17
19	d	5405	PQ9	C13-C15-C16-C17
23	L	101	SQD	C14-C15-C16-C17
20	B	617	BCR	C10-C11-C12-C13
20	B	618	BCR	C18-C19-C20-C21
20	D	407	BCR	C10-C11-C12-C13
20	H	101	BCR	C18-C19-C20-C21
20	b	5617	BCR	C10-C11-C12-C13
20	b	5618	BCR	C18-C19-C20-C21
20	d	5406	BCR	C10-C11-C12-C13
20	h	5101	BCR	C18-C19-C20-C21
20	k	5502	BCR	C10-C11-C12-C13
17	A	401	CLA	C13-C15-C16-C17
17	a	5402	CLA	C13-C15-C16-C17
23	l	5102	SQD	C23-C24-C25-C26
17	A	401	CLA	C5-C6-C7-C8
17	B	602	CLA	C15-C16-C17-C18
17	B	612	CLA	C10-C11-C12-C13
17	B	616	CLA	C13-C15-C16-C17
17	C	508	CLA	C15-C16-C17-C18
17	a	5402	CLA	C5-C6-C7-C8
17	b	5602	CLA	C15-C16-C17-C18
17	b	5612	CLA	C10-C11-C12-C13
17	b	5616	CLA	C13-C15-C16-C17
17	c	5508	CLA	C15-C16-C17-C18
26	C	518	DGD	C2B-C1B-O2G-C2G
26	c	5516	DGD	C2B-C1B-O2G-C2G
21	A	408	LHG	C3-O3-P-O6
21	a	5409	LHG	C3-O3-P-O6
17	C	506	CLA	C3-C5-C6-C7
17	c	5506	CLA	C3-C5-C6-C7
23	D	403	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
25	D	410	MGE	C1B-C2B-C3B-C4B
17	B	614	CLA	C2A-CAA-CBA-CGA
17	b	5614	CLA	C2A-CAA-CBA-CGA
17	B	605	CLA	CBA-CGA-O2A-C1
17	C	512	CLA	CBA-CGA-O2A-C1
17	b	5605	CLA	CBA-CGA-O2A-C1
17	c	5511	CLA	CBA-CGA-O2A-C1
23	l	5102	SQD	C24-C25-C26-C27
23	D	403	SQD	C8-C7-O47-C45
25	D	410	MGE	C2B-C1B-O2G-C2G
25	d	5408	MGE	C2B-C1B-O2G-C2G
25	d	5410	MGE	C2B-C1B-O2G-C2G
20	A	407	BCR	C11-C10-C9-C34
20	A	407	BCR	C16-C17-C18-C36
20	B	618	BCR	C11-C10-C9-C34
20	C	515	BCR	C11-C10-C9-C34
20	D	407	BCR	C35-C13-C14-C15
20	H	101	BCR	C20-C21-C22-C37
20	T	102	BCR	C20-C21-C22-C37
20	a	5408	BCR	C11-C10-C9-C34
20	a	5408	BCR	C16-C17-C18-C36
20	b	5618	BCR	C11-C10-C9-C34
20	d	5406	BCR	C35-C13-C14-C15
20	h	5101	BCR	C20-C21-C22-C37
20	z	5101	BCR	C11-C10-C9-C34
20	Y	101	BCR	C20-C21-C22-C37
22	B	620	LMT	C4-C5-C6-C7
26	C	517	DGD	C4A-C5A-C6A-C7A
26	C	518	DGD	C8A-C9A-CAA-CBA
26	c	5515	DGD	C4A-C5A-C6A-C7A
26	c	5516	DGD	C8A-C9A-CAA-CBA
26	C	519	DGD	C5A-C6A-C7A-C8A
26	a	5411	DGD	C5A-C6A-C7A-C8A
17	C	513	CLA	O1D-CGD-O2D-CED
17	c	5512	CLA	O1D-CGD-O2D-CED
25	C	520	MGE	O6D-C5D-C6D-O5D
25	D	410	MGE	O1B-C1B-O2G-C2G
25	d	5408	MGE	O1B-C1B-O2G-C2G
25	d	5410	MGE	O1B-C1B-O2G-C2G
26	C	517	DGD	O1A-C1A-O1G-C1G
17	D	404	CLA	O1D-CGD-O2D-CED
17	d	5403	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	D	410	MGE	C2B-C3B-C4B-C5B
17	B	605	CLA	C3-C5-C6-C7
17	b	5605	CLA	C3-C5-C6-C7
25	c	5517	MGE	O6D-C5D-C6D-O5D
17	C	504	CLA	O1D-CGD-O2D-CED
17	c	5504	CLA	O1D-CGD-O2D-CED
20	B	618	BCR	C12-C13-C14-C15
20	C	514	BCR	C16-C17-C18-C19
20	C	516	BCR	C20-C21-C22-C23
20	T	102	BCR	C20-C21-C22-C23
20	b	5618	BCR	C12-C13-C14-C15
20	c	5513	BCR	C16-C17-C18-C19
20	c	5514	BCR	C20-C21-C22-C23
20	k	5502	BCR	C20-C21-C22-C23
20	t	5102	BCR	C12-C13-C14-C15
23	L	101	SQD	C2-C1-O6-C44
23	l	5102	SQD	C27-C28-C29-C30
17	A	402	CLA	C8-C10-C11-C12
17	B	605	CLA	C8-C10-C11-C12
17	a	5403	CLA	C8-C10-C11-C12
17	b	5605	CLA	C8-C10-C11-C12
26	c	5515	DGD	O1A-C1A-O1G-C1G
17	A	403	CLA	C16-C17-C18-C19
17	B	609	CLA	C16-C17-C18-C20
17	a	5404	CLA	C16-C17-C18-C19
17	b	5609	CLA	C16-C17-C18-C20
22	A	409	LMT	C5'-C4'-O1B-C1B
23	D	403	SQD	C15-C16-C17-C18
26	C	517	DGD	C3A-C4A-C5A-C6A
26	c	5515	DGD	C3A-C4A-C5A-C6A
17	B	602	CLA	C6-C7-C8-C9
17	b	5602	CLA	C6-C7-C8-C9
26	C	518	DGD	C1A-C2A-C3A-C4A
26	c	5516	DGD	C1A-C2A-C3A-C4A
23	D	403	SQD	C17-C18-C19-C20
25	D	409	MGE	C9B-CAB-CBB-CCB
25	m	5103	MGE	C2A-C3A-C4A-C5A
26	C	517	DGD	C2B-C3B-C4B-C5B
26	C	518	DGD	C2A-C3A-C4A-C5A
26	H	102	DGD	C2A-C3A-C4A-C5A
26	c	5515	DGD	C2B-C3B-C4B-C5B
26	c	5516	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
26	h	5102	DGD	C2A-C3A-C4A-C5A
17	C	503	CLA	C13-C15-C16-C17
17	c	5503	CLA	C13-C15-C16-C17
17	B	610	CLA	C2A-CAA-CBA-CGA
17	b	5610	CLA	C2A-CAA-CBA-CGA
26	C	517	DGD	C4D-C5D-C6D-O5D
26	c	5515	DGD	C4D-C5D-C6D-O5D
20	T	102	BCR	C7-C8-C9-C34
20	B	617	BCR	C7-C8-C9-C10
20	B	617	BCR	C11-C12-C13-C14
20	C	514	BCR	C7-C8-C9-C10
20	C	516	BCR	C7-C8-C9-C10
20	b	5617	BCR	C7-C8-C9-C10
20	b	5617	BCR	C11-C12-C13-C14
20	c	5513	BCR	C7-C8-C9-C10
20	c	5514	BCR	C7-C8-C9-C10
17	D	404	CLA	C3-C5-C6-C7
17	d	5403	CLA	C3-C5-C6-C7
23	D	403	SQD	C34-C35-C36-C37
25	d	5409	MGE	C9B-CAB-CBB-CCB
23	d	5407	SQD	C11-C12-C13-C14
26	C	519	DGD	C6A-C7A-C8A-C9A
26	H	102	DGD	C4A-C5A-C6A-C7A
26	a	5411	DGD	C6A-C7A-C8A-C9A
26	h	5102	DGD	C4A-C5A-C6A-C7A
17	B	606	CLA	C16-C17-C18-C19
18	A	404	PHO	C16-C17-C18-C19
18	a	5405	PHO	C16-C17-C18-C19
23	L	101	SQD	O5-C1-O6-C44
17	B	615	CLA	C5-C6-C7-C8
17	C	506	CLA	C13-C15-C16-C17
17	D	404	CLA	C5-C6-C7-C8
17	b	5615	CLA	C5-C6-C7-C8
17	c	5506	CLA	C13-C15-C16-C17
17	d	5403	CLA	C5-C6-C7-C8
22	a	5410	LMT	C4-C5-C6-C7
26	C	517	DGD	C3B-C4B-C5B-C6B
26	C	519	DGD	C2B-C3B-C4B-C5B
26	a	5411	DGD	C2B-C3B-C4B-C5B
26	c	5515	DGD	C3B-C4B-C5B-C6B
23	D	403	SQD	C27-C28-C29-C30
23	L	101	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
17	B	605	CLA	O1A-CGA-O2A-C1
17	b	5605	CLA	O1A-CGA-O2A-C1
17	B	613	CLA	CBA-CGA-O2A-C1
17	b	5613	CLA	CBA-CGA-O2A-C1
23	d	5407	SQD	C24-C25-C26-C27
17	C	503	CLA	C3A-C2A-CAA-CBA
17	C	512	CLA	C3A-C2A-CAA-CBA
17	D	404	CLA	C3A-C2A-CAA-CBA
17	c	5503	CLA	C3A-C2A-CAA-CBA
17	c	5511	CLA	C3A-C2A-CAA-CBA
17	d	5403	CLA	C3A-C2A-CAA-CBA
22	T	101	LMT	C2-C1-O1'-C1'
23	D	403	SQD	C11-C12-C13-C14
17	A	403	CLA	C16-C17-C18-C20
17	B	606	CLA	C16-C17-C18-C20
17	a	5404	CLA	C16-C17-C18-C20
18	A	404	PHO	C16-C17-C18-C20
18	a	5405	PHO	C16-C17-C18-C20
25	d	5408	MGE	C7A-C8A-C9A-CAA
21	A	408	LHG	C4-C5-C6-O8
21	a	5409	LHG	C4-C5-C6-O8
23	L	101	SQD	O6-C44-C45-C46
25	D	409	MGE	O1G-C1G-C2G-C3G
25	d	5409	MGE	C1G-C2G-C3G-O3G
25	d	5410	MGE	O1G-C1G-C2G-C3G
17	B	608	CLA	CBD-CGD-O2D-CED
17	b	5608	CLA	CBD-CGD-O2D-CED
21	A	408	LHG	C25-C26-C27-C28
21	a	5409	LHG	C25-C26-C27-C28
26	C	517	DGD	C6A-C7A-C8A-C9A
26	C	519	DGD	C4A-C5A-C6A-C7A
26	a	5411	DGD	C4A-C5A-C6A-C7A
26	c	5515	DGD	C6A-C7A-C8A-C9A
20	B	618	BCR	C14-C15-C16-C17
20	b	5618	BCR	C14-C15-C16-C17
17	C	508	CLA	C3-C5-C6-C7
17	c	5508	CLA	C3-C5-C6-C7
25	D	409	MGE	C2B-C3B-C4B-C5B
17	B	611	CLA	CBA-CGA-O2A-C1
17	b	5611	CLA	CBA-CGA-O2A-C1
26	C	519	DGD	C4E-C5E-C6E-O5E
26	a	5411	DGD	C4E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
25	A	412	MGE	C2B-C1B-O2G-C2G
25	l	5101	MGE	C2B-C1B-O2G-C2G
26	C	519	DGD	C2B-C1B-O2G-C2G
26	a	5411	DGD	C2B-C1B-O2G-C2G
22	M	101	LMT	C4B-C5B-C6B-O6B
21	A	408	LHG	O1-C1-C2-O2
21	a	5409	LHG	O1-C1-C2-O2
17	B	609	CLA	C16-C17-C18-C19
17	b	5609	CLA	C16-C17-C18-C19
25	m	5103	MGE	C6B-C7B-C8B-C9B
17	C	512	CLA	O1A-CGA-O2A-C1
17	c	5511	CLA	O1A-CGA-O2A-C1
23	D	403	SQD	C13-C14-C15-C16
17	B	615	CLA	C2-C1-O2A-CGA
17	b	5615	CLA	C2-C1-O2A-CGA
26	C	517	DGD	O6D-C5D-C6D-O5D
26	c	5515	DGD	O6D-C5D-C6D-O5D
22	T	101	LMT	C4'-C5'-C6'-O6'
25	B	619	MGE	C8A-C9A-CAA-CBA
25	C	520	MGE	C6A-C7A-C8A-C9A
25	b	5620	MGE	C8A-C9A-CAA-CBA
25	c	5517	MGE	C6A-C7A-C8A-C9A
22	T	101	LMT	C1-C2-C3-C4
25	d	5408	MGE	C5B-C6B-C7B-C8B
20	A	407	BCR	C5-C6-C7-C8
20	C	514	BCR	C1-C6-C7-C8
20	C	514	BCR	C5-C6-C7-C8
20	C	515	BCR	C5-C6-C7-C8
20	C	516	BCR	C1-C6-C7-C8
20	C	516	BCR	C23-C24-C25-C30
20	D	407	BCR	C1-C6-C7-C8
20	D	407	BCR	C5-C6-C7-C8
20	D	407	BCR	C23-C24-C25-C26
20	a	5408	BCR	C5-C6-C7-C8
20	b	5619	BCR	C5-C6-C7-C8
20	b	5619	BCR	C23-C24-C25-C26
20	b	5619	BCR	C23-C24-C25-C30
20	c	5513	BCR	C1-C6-C7-C8
20	c	5513	BCR	C5-C6-C7-C8
20	c	5514	BCR	C1-C6-C7-C8
20	c	5514	BCR	C23-C24-C25-C30
20	d	5406	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	d	5406	BCR	C5-C6-C7-C8
20	d	5406	BCR	C23-C24-C25-C26
20	t	5101	BCR	C5-C6-C7-C8
20	t	5101	BCR	C23-C24-C25-C26
20	t	5101	BCR	C23-C24-C25-C30
20	t	5102	BCR	C5-C6-C7-C8
20	z	5101	BCR	C5-C6-C7-C8
25	D	410	MGE	O6D-C5D-C6D-O5D
25	d	5409	MGE	O6D-C5D-C6D-O5D
26	h	5102	DGD	C8A-C9A-CAA-CBA
17	C	505	CLA	CBA-CGA-O2A-C1
17	c	5505	CLA	CBA-CGA-O2A-C1
17	C	503	CLA	C8-C10-C11-C12
17	C	511	CLA	C8-C10-C11-C12
17	c	5503	CLA	C8-C10-C11-C12
17	k	5501	CLA	C8-C10-C11-C12
18	D	402	PHO	C10-C11-C12-C13
18	d	5402	PHO	C10-C11-C12-C13
23	A	410	SQD	C24-C23-O48-C46
25	m	5103	MGE	C3A-C4A-C5A-C6A
26	H	102	DGD	C8A-C9A-CAA-CBA
17	B	613	CLA	O1A-CGA-O2A-C1
17	b	5613	CLA	O1A-CGA-O2A-C1
17	B	604	CLA	C4-C3-C5-C6
17	b	5604	CLA	C4-C3-C5-C6
17	A	402	CLA	C11-C12-C13-C15
17	A	403	CLA	C2-C3-C5-C6
17	B	602	CLA	C6-C7-C8-C10
17	B	605	CLA	C12-C13-C15-C16
17	B	609	CLA	C12-C13-C15-C16
17	B	613	CLA	C12-C13-C15-C16
17	C	503	CLA	C11-C12-C13-C15
17	D	404	CLA	C6-C7-C8-C10
17	a	5403	CLA	C11-C12-C13-C15
17	a	5404	CLA	C2-C3-C5-C6
17	b	5602	CLA	C6-C7-C8-C10
17	b	5605	CLA	C12-C13-C15-C16
17	b	5609	CLA	C12-C13-C15-C16
17	b	5613	CLA	C12-C13-C15-C16
17	c	5503	CLA	C11-C12-C13-C15
17	d	5403	CLA	C6-C7-C8-C10
18	A	404	PHO	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
18	a	5405	PHO	C6-C7-C8-C10
17	B	611	CLA	O1A-CGA-O2A-C1
17	b	5611	CLA	O1A-CGA-O2A-C1
17	B	613	CLA	C5-C6-C7-C8
17	C	507	CLA	C10-C11-C12-C13
17	b	5613	CLA	C5-C6-C7-C8
17	c	5507	CLA	C10-C11-C12-C13
17	k	5501	CLA	C5-C6-C7-C8
17	B	609	CLA	CBA-CGA-O2A-C1
17	B	615	CLA	CBA-CGA-O2A-C1
17	b	5609	CLA	CBA-CGA-O2A-C1
17	b	5615	CLA	CBA-CGA-O2A-C1
17	C	504	CLA	C2A-CAA-CBA-CGA
17	c	5504	CLA	C2A-CAA-CBA-CGA
17	B	608	CLA	C8-C10-C11-C12
17	C	511	CLA	C5-C6-C7-C8
17	b	5608	CLA	C8-C10-C11-C12
17	B	611	CLA	C10-C11-C12-C13
17	b	5611	CLA	C10-C11-C12-C13
23	l	5102	SQD	C11-C12-C13-C14
20	B	617	BCR	C6-C7-C8-C9
20	B	618	BCR	C6-C7-C8-C9
20	b	5617	BCR	C6-C7-C8-C9
20	b	5618	BCR	C6-C7-C8-C9
17	B	612	CLA	C5-C6-C7-C8
17	b	5612	CLA	C5-C6-C7-C8
23	L	101	SQD	C27-C28-C29-C30
22	T	101	LMT	C4-C5-C6-C7
23	d	5407	SQD	C14-C15-C16-C17
23	l	5102	SQD	C9-C10-C11-C12
26	C	519	DGD	O1B-C1B-O2G-C2G
26	a	5411	DGD	O1B-C1B-O2G-C2G
17	B	604	CLA	C3-C5-C6-C7
17	b	5604	CLA	C3-C5-C6-C7
25	A	412	MGE	C2D-C1D-O3G-C3G
25	l	5101	MGE	C2D-C1D-O3G-C3G
25	D	410	MGE	O1G-C1G-C2G-O2G
25	d	5410	MGE	O1G-C1G-C2G-O2G
25	d	5410	MGE	O6D-C5D-C6D-O5D
25	m	5101	MGE	O6D-C5D-C6D-O5D
23	D	403	SQD	C14-C15-C16-C17
26	h	5102	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
17	C	511	CLA	C16-C17-C18-C20
17	k	5501	CLA	C16-C17-C18-C20
25	D	410	MGE	C6B-C7B-C8B-C9B
26	C	517	DGD	C5B-C6B-C7B-C8B
26	H	102	DGD	CBA-CCA-CDA-CEA
26	c	5515	DGD	C5B-C6B-C7B-C8B
17	B	610	CLA	C8-C10-C11-C12
17	B	612	CLA	C8-C10-C11-C12
17	b	5610	CLA	C8-C10-C11-C12
17	b	5612	CLA	C8-C10-C11-C12
17	B	603	CLA	C2-C3-C5-C6
17	b	5603	CLA	C2-C3-C5-C6
23	L	101	SQD	C11-C10-C9-C8
17	B	603	CLA	C14-C13-C15-C16
17	B	609	CLA	C14-C13-C15-C16
17	B	613	CLA	C14-C13-C15-C16
17	C	501	CLA	C14-C13-C15-C16
17	C	503	CLA	C11-C12-C13-C14
17	C	503	CLA	C14-C13-C15-C16
17	b	5603	CLA	C14-C13-C15-C16
17	b	5609	CLA	C14-C13-C15-C16
17	b	5613	CLA	C14-C13-C15-C16
17	c	5501	CLA	C14-C13-C15-C16
17	c	5503	CLA	C11-C12-C13-C14
17	c	5503	CLA	C14-C13-C15-C16
18	A	404	PHO	C6-C7-C8-C9
18	A	404	PHO	C14-C13-C15-C16
18	a	5405	PHO	C6-C7-C8-C9
18	a	5405	PHO	C14-C13-C15-C16
26	H	102	DGD	C3B-C4B-C5B-C6B
26	h	5102	DGD	C3B-C4B-C5B-C6B
17	C	505	CLA	C2A-CAA-CBA-CGA
17	c	5505	CLA	C2A-CAA-CBA-CGA
25	D	408	MGE	O6D-C5D-C6D-O5D
18	A	404	PHO	C5-C6-C7-C8
18	a	5405	PHO	C5-C6-C7-C8
22	a	5410	LMT	C3-C4-C5-C6
23	D	403	SQD	C32-C33-C34-C35
20	B	618	BCR	C17-C18-C19-C20
20	b	5618	BCR	C17-C18-C19-C20
17	C	505	CLA	O1A-CGA-O2A-C1
17	c	5505	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	D	403	SQD	O10-C23-O48-C46
17	A	405	CLA	C1A-C2A-CAA-CBA
17	C	504	CLA	C1A-C2A-CAA-CBA
17	C	512	CLA	C1A-C2A-CAA-CBA
17	a	5406	CLA	C1A-C2A-CAA-CBA
17	c	5504	CLA	C1A-C2A-CAA-CBA
17	c	5511	CLA	C1A-C2A-CAA-CBA
17	C	511	CLA	C16-C17-C18-C19
17	k	5501	CLA	C16-C17-C18-C19
23	d	5407	SQD	O49-C7-O47-C45
25	A	412	MGE	O1B-C1B-O2G-C2G
25	l	5101	MGE	O1B-C1B-O2G-C2G
22	a	5410	LMT	C2-C3-C4-C5
17	B	613	CLA	C10-C11-C12-C13
17	b	5613	CLA	C10-C11-C12-C13
21	a	5409	LHG	C24-C25-C26-C27
22	T	101	LMT	O1'-C1-C2-C3
22	M	101	LMT	C4'-C5'-C6'-O6'
21	A	408	LHG	C24-C25-C26-C27
26	h	5102	DGD	C5B-C6B-C7B-C8B
17	A	403	CLA	C4-C3-C5-C6
17	a	5404	CLA	C4-C3-C5-C6
18	A	404	PHO	C4-C3-C5-C6
18	a	5405	PHO	C4-C3-C5-C6
26	C	518	DGD	C5A-C6A-C7A-C8A
26	H	102	DGD	C5B-C6B-C7B-C8B
26	c	5516	DGD	C5A-C6A-C7A-C8A
23	d	5407	SQD	C12-C13-C14-C15
17	B	609	CLA	O1A-CGA-O2A-C1
25	d	5410	MGE	C3A-C4A-C5A-C6A
23	A	410	SQD	C44-C45-C46-O48
23	D	403	SQD	O6-C44-C45-C46
23	L	101	SQD	C44-C45-C46-O48
23	l	5102	SQD	C44-C45-C46-O48
25	d	5408	MGE	C1G-C2G-C3G-O3G
25	d	5409	MGE	O1G-C1G-C2G-C3G
25	m	5103	MGE	C1G-C2G-C3G-O3G
26	C	519	DGD	C1G-C2G-C3G-O3G
26	H	102	DGD	O1G-C1G-C2G-C3G
26	a	5411	DGD	C1G-C2G-C3G-O3G
26	h	5102	DGD	O1G-C1G-C2G-C3G
23	L	101	SQD	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
17	b	5609	CLA	O1A-CGA-O2A-C1
25	d	5408	MGE	C2G-C3G-O3G-C1D
17	A	403	CLA	O1D-CGD-O2D-CED
17	a	5404	CLA	O1D-CGD-O2D-CED
23	l	5102	SQD	C19-C20-C21-C22
22	B	620	LMT	C2-C3-C4-C5
17	C	505	CLA	C16-C17-C18-C20
17	c	5505	CLA	C16-C17-C18-C20
26	H	102	DGD	O6E-C5E-C6E-O5E
26	h	5102	DGD	O6E-C5E-C6E-O5E
17	B	615	CLA	O1A-CGA-O2A-C1
17	b	5615	CLA	O1A-CGA-O2A-C1
17	B	605	CLA	C13-C15-C16-C17
17	b	5605	CLA	C13-C15-C16-C17
20	B	618	BCR	C20-C21-C22-C37
20	C	514	BCR	C11-C10-C9-C34
20	C	515	BCR	C35-C13-C14-C15
20	b	5618	BCR	C20-C21-C22-C37
20	b	5619	BCR	C16-C17-C18-C36
20	c	5513	BCR	C11-C10-C9-C34
20	t	5101	BCR	C16-C17-C18-C36
20	t	5102	BCR	C11-C10-C9-C34
20	z	5101	BCR	C35-C13-C14-C15
25	D	408	MGE	C1B-C2B-C3B-C4B
17	D	404	CLA	CBA-CGA-O2A-C1
17	d	5403	CLA	CBA-CGA-O2A-C1
25	d	5408	MGE	O6D-C5D-C6D-O5D
17	b	5607	CLA	C15-C16-C17-C18
23	d	5407	SQD	C17-C18-C19-C20
17	c	5507	CLA	C2A-CAA-CBA-CGA
17	B	604	CLA	C15-C16-C17-C18
17	B	607	CLA	C5-C6-C7-C8
17	B	607	CLA	C15-C16-C17-C18
17	C	508	CLA	C8-C10-C11-C12
17	b	5604	CLA	C15-C16-C17-C18
17	b	5613	CLA	C13-C15-C16-C17
17	c	5508	CLA	C8-C10-C11-C12
17	A	403	CLA	C2-C1-O2A-CGA
17	a	5404	CLA	C2-C1-O2A-CGA
17	b	5607	CLA	C5-C6-C7-C8
17	B	613	CLA	C13-C15-C16-C17
20	B	617	BCR	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
20	b	5617	BCR	C12-C13-C14-C15
25	D	409	MGE	C2D-C1D-O3G-C3G
25	m	5103	MGE	C2D-C1D-O3G-C3G
21	A	408	LHG	O7-C5-C6-O8
21	a	5409	LHG	O7-C5-C6-O8
25	d	5408	MGE	O1G-C1G-C2G-O2G
26	C	518	DGD	O1G-C1G-C2G-O2G
26	c	5516	DGD	O1G-C1G-C2G-O2G
25	B	619	MGE	C7A-C8A-C9A-CAA
25	b	5620	MGE	C7A-C8A-C9A-CAA
25	d	5409	MGE	C2B-C3B-C4B-C5B
17	B	603	CLA	C6-C7-C8-C10
17	B	603	CLA	C12-C13-C15-C16
17	B	608	CLA	C12-C13-C15-C16
17	B	609	CLA	C11-C10-C8-C7
17	B	610	CLA	C6-C7-C8-C10
17	B	612	CLA	C12-C13-C15-C16
17	B	615	CLA	C6-C7-C8-C10
17	B	615	CLA	C12-C13-C15-C16
17	C	501	CLA	C11-C12-C13-C15
17	C	501	CLA	C12-C13-C15-C16
17	C	505	CLA	C11-C10-C8-C7
17	C	506	CLA	C6-C7-C8-C10
17	D	404	CLA	C12-C13-C15-C16
17	b	5603	CLA	C6-C7-C8-C10
17	b	5603	CLA	C12-C13-C15-C16
17	b	5608	CLA	C12-C13-C15-C16
17	b	5609	CLA	C11-C10-C8-C7
17	b	5610	CLA	C6-C7-C8-C10
17	b	5612	CLA	C12-C13-C15-C16
17	b	5615	CLA	C6-C7-C8-C10
17	b	5615	CLA	C12-C13-C15-C16
17	c	5501	CLA	C11-C12-C13-C15
17	c	5501	CLA	C12-C13-C15-C16
17	c	5505	CLA	C11-C10-C8-C7
17	c	5506	CLA	C6-C7-C8-C10
17	d	5403	CLA	C12-C13-C15-C16
17	B	602	CLA	C11-C10-C8-C9
17	B	602	CLA	C11-C12-C13-C14
17	B	602	CLA	C14-C13-C15-C16
17	B	603	CLA	C6-C7-C8-C9
17	B	605	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
17	B	610	CLA	C6-C7-C8-C9
17	B	612	CLA	C11-C10-C8-C9
17	B	612	CLA	C14-C13-C15-C16
17	B	615	CLA	C11-C10-C8-C9
17	B	615	CLA	C14-C13-C15-C16
17	C	503	CLA	C6-C7-C8-C9
17	C	505	CLA	C11-C10-C8-C9
17	C	508	CLA	C14-C13-C15-C16
17	D	404	CLA	C14-C13-C15-C16
17	b	5602	CLA	C11-C10-C8-C9
17	b	5602	CLA	C11-C12-C13-C14
17	b	5602	CLA	C14-C13-C15-C16
17	b	5603	CLA	C6-C7-C8-C9
17	b	5605	CLA	C11-C12-C13-C14
17	b	5610	CLA	C6-C7-C8-C9
17	b	5612	CLA	C11-C10-C8-C9
17	b	5612	CLA	C14-C13-C15-C16
17	b	5615	CLA	C11-C10-C8-C9
17	b	5615	CLA	C14-C13-C15-C16
17	c	5503	CLA	C6-C7-C8-C9
17	c	5505	CLA	C11-C10-C8-C9
17	c	5508	CLA	C14-C13-C15-C16
17	d	5403	CLA	C14-C13-C15-C16
18	D	402	PHO	C11-C12-C13-C14
18	d	5402	PHO	C11-C12-C13-C14
25	d	5409	MGE	C2A-C1A-O1G-C1G
17	C	507	CLA	C2A-CAA-CBA-CGA
20	D	407	BCR	C11-C12-C13-C14
20	d	5406	BCR	C11-C12-C13-C14
22	A	409	LMT	C3'-C4'-O1B-C1B
18	D	402	PHO	C3-C5-C6-C7
18	d	5402	PHO	C3-C5-C6-C7
25	C	520	MGE	C2B-C1B-O2G-C2G
25	c	5517	MGE	C2B-C1B-O2G-C2G
25	d	5410	MGE	C8B-C9B-CAB-CBB
26	C	517	DGD	C2A-C1A-O1G-C1G
26	c	5515	DGD	C2A-C1A-O1G-C1G
25	D	408	MGE	C5B-C6B-C7B-C8B
21	a	5409	LHG	C32-C33-C34-C35
21	A	408	LHG	C32-C33-C34-C35
26	C	518	DGD	C1B-C2B-C3B-C4B
26	c	5516	DGD	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
21	A	408	LHG	C33-C34-C35-C36
21	a	5409	LHG	C33-C34-C35-C36
22	a	5410	LMT	C7-C8-C9-C10
23	l	5102	SQD	C11-C10-C9-C8
25	D	408	MGE	C2A-C3A-C4A-C5A
17	A	405	CLA	C3A-C2A-CAA-CBA
17	B	607	CLA	C3A-C2A-CAA-CBA
17	a	5406	CLA	C3A-C2A-CAA-CBA
17	b	5607	CLA	C3A-C2A-CAA-CBA
18	A	404	PHO	C3A-C2A-CAA-CBA
18	a	5405	PHO	C3A-C2A-CAA-CBA
25	A	412	MGE	C2A-C3A-C4A-C5A
25	l	5101	MGE	C2A-C3A-C4A-C5A
25	m	5103	MGE	C4A-C5A-C6A-C7A
17	B	615	CLA	C15-C16-C17-C18
18	A	404	PHO	C15-C16-C17-C18
18	a	5405	PHO	C15-C16-C17-C18
23	D	403	SQD	C33-C34-C35-C36
17	B	609	CLA	C5-C6-C7-C8
17	b	5609	CLA	C5-C6-C7-C8
17	b	5615	CLA	C15-C16-C17-C18
23	d	5407	SQD	O6-C44-C45-C46
25	C	520	MGE	C1G-C2G-C3G-O3G
25	D	410	MGE	O1G-C1G-C2G-C3G
25	c	5517	MGE	C1G-C2G-C3G-O3G
25	d	5408	MGE	O1G-C1G-C2G-C3G
26	C	519	DGD	O1G-C1G-C2G-C3G
26	a	5411	DGD	O1G-C1G-C2G-C3G
22	A	409	LMT	C5-C6-C7-C8
17	C	510	CLA	C3-C5-C6-C7
17	c	5510	CLA	C3-C5-C6-C7
17	D	404	CLA	O1A-CGA-O2A-C1
17	d	5403	CLA	O1A-CGA-O2A-C1
22	B	620	LMT	C5-C6-C7-C8
25	m	5103	MGE	O6D-C5D-C6D-O5D
17	B	607	CLA	C8-C10-C11-C12
17	b	5607	CLA	C8-C10-C11-C12
25	C	520	MGE	C1A-C2A-C3A-C4A
25	c	5517	MGE	C1A-C2A-C3A-C4A
26	C	518	DGD	O1A-C1A-O1G-C1G
26	c	5516	DGD	O1A-C1A-O1G-C1G
25	A	412	MGE	C7A-C8A-C9A-CAA

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Mol	Chain	Res	Type	Atoms
17	b	5613	CLA	C8-C10-C11-C12
17	B	612	CLA	O1D-CGD-O2D-CED
17	C	505	CLA	C16-C17-C18-C19
17	c	5505	CLA	C16-C17-C18-C19
17	B	613	CLA	C8-C10-C11-C12
25	l	5101	MGE	C7A-C8A-C9A-CAA
17	b	5612	CLA	O1D-CGD-O2D-CED
17	b	5610	CLA	CBD-CGD-O2D-CED
23	A	410	SQD	O6-C44-C45-O47
23	a	5401	SQD	O6-C44-C45-O47
25	d	5409	MGE	O1G-C1G-C2G-O2G
17	B	610	CLA	CBD-CGD-O2D-CED
22	m	5102	LMT	C4'-C5'-C6'-O6'
25	D	410	MGE	C5A-C6A-C7A-C8A
17	C	501	CLA	C10-C11-C12-C13
17	c	5501	CLA	C10-C11-C12-C13
26	H	102	DGD	CCA-CDA-CEA-CFA
26	h	5102	DGD	CCA-CDA-CEA-CFA
17	B	608	CLA	C2-C1-O2A-CGA
17	b	5608	CLA	C2-C1-O2A-CGA
17	A	401	CLA	C11-C10-C8-C9
17	A	402	CLA	C14-C13-C15-C16
17	B	606	CLA	C14-C13-C15-C16
17	B	611	CLA	C6-C7-C8-C9
17	B	612	CLA	C6-C7-C8-C9
17	C	501	CLA	C6-C7-C8-C9
17	C	506	CLA	C6-C7-C8-C9
17	a	5402	CLA	C11-C10-C8-C9
17	a	5403	CLA	C14-C13-C15-C16
17	b	5611	CLA	C6-C7-C8-C9
17	b	5612	CLA	C6-C7-C8-C9
17	c	5501	CLA	C6-C7-C8-C9
17	c	5506	CLA	C6-C7-C8-C9
22	A	409	LMT	C1-C2-C3-C4
22	m	5102	LMT	C1-C2-C3-C4
25	d	5409	MGE	O1A-C1A-O1G-C1G
17	B	615	CLA	C16-C17-C18-C19
17	B	615	CLA	C16-C17-C18-C20
17	b	5615	CLA	C16-C17-C18-C19
17	b	5615	CLA	C16-C17-C18-C20
20	B	617	BCR	C5-C6-C7-C8
20	B	618	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
20	C	514	BCR	C23-C24-C25-C26
20	C	515	BCR	C23-C24-C25-C26
20	C	515	BCR	C23-C24-C25-C30
20	C	516	BCR	C5-C6-C7-C8
20	H	101	BCR	C5-C6-C7-C8
20	b	5617	BCR	C5-C6-C7-C8
20	b	5618	BCR	C23-C24-C25-C30
20	c	5513	BCR	C23-C24-C25-C26
20	c	5514	BCR	C5-C6-C7-C8
20	h	5101	BCR	C5-C6-C7-C8
20	z	5101	BCR	C23-C24-C25-C26
20	z	5101	BCR	C23-C24-C25-C30
17	B	603	CLA	C15-C16-C17-C18
20	k	5502	BCR	C11-C12-C13-C14
17	b	5603	CLA	C15-C16-C17-C18
20	H	101	BCR	C14-C15-C16-C17
20	h	5101	BCR	C14-C15-C16-C17
25	m	5103	MGE	CCB-CDB-CEB-CFB
17	D	404	CLA	C8-C10-C11-C12
17	d	5403	CLA	C8-C10-C11-C12
17	C	501	CLA	C13-C15-C16-C17
17	c	5501	CLA	C13-C15-C16-C17
25	B	619	MGE	C3A-C4A-C5A-C6A
25	b	5620	MGE	C3A-C4A-C5A-C6A
17	A	401	CLA	C6-C7-C8-C10
17	A	402	CLA	C12-C13-C15-C16
17	B	602	CLA	C11-C10-C8-C7
17	B	602	CLA	C11-C12-C13-C15
17	B	602	CLA	C12-C13-C15-C16
17	B	606	CLA	C11-C12-C13-C15
17	B	611	CLA	C6-C7-C8-C10
17	B	615	CLA	C11-C10-C8-C7
17	C	501	CLA	C6-C7-C8-C10
17	C	503	CLA	C6-C7-C8-C10
17	C	506	CLA	C11-C10-C8-C7
17	C	506	CLA	C11-C12-C13-C15
17	C	508	CLA	C12-C13-C15-C16
17	a	5402	CLA	C6-C7-C8-C10
17	a	5403	CLA	C12-C13-C15-C16
17	b	5602	CLA	C11-C10-C8-C7
17	b	5602	CLA	C11-C12-C13-C15
17	b	5602	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
17	b	5611	CLA	C6-C7-C8-C10
17	b	5615	CLA	C11-C10-C8-C7
17	c	5501	CLA	C6-C7-C8-C10
17	c	5503	CLA	C6-C7-C8-C10
17	c	5506	CLA	C11-C10-C8-C7
17	c	5506	CLA	C11-C12-C13-C15
17	c	5508	CLA	C12-C13-C15-C16
25	D	410	MGE	C6A-C7A-C8A-C9A
20	A	407	BCR	C19-C20-C21-C22
20	a	5408	BCR	C19-C20-C21-C22
21	A	408	LHG	C29-C30-C31-C32
21	a	5409	LHG	C29-C30-C31-C32
20	A	407	BCR	C35-C13-C14-C15
20	B	618	BCR	C16-C17-C18-C36
20	a	5408	BCR	C35-C13-C14-C15
20	b	5618	BCR	C16-C17-C18-C36
17	C	501	CLA	CBA-CGA-O2A-C1
17	c	5501	CLA	CBA-CGA-O2A-C1
23	l	5102	SQD	C24-C23-O48-C46
22	M	101	LMT	C9-C10-C11-C12
25	A	412	MGE	C3A-C4A-C5A-C6A
25	l	5101	MGE	C3A-C4A-C5A-C6A
17	C	502	CLA	C10-C11-C12-C13
17	c	5502	CLA	C10-C11-C12-C13
17	B	606	CLA	CAD-CBD-CGD-O2D
17	B	612	CLA	CAD-CBD-CGD-O2D
17	C	504	CLA	CAD-CBD-CGD-O2D
17	C	512	CLA	CAD-CBD-CGD-O2D
17	b	5606	CLA	CAD-CBD-CGD-O2D
17	b	5612	CLA	CAD-CBD-CGD-O2D
17	c	5504	CLA	CAD-CBD-CGD-O2D
17	c	5511	CLA	CAD-CBD-CGD-O2D
22	a	5410	LMT	C1-C2-C3-C4
20	D	407	BCR	C6-C7-C8-C9
25	A	412	MGE	O6D-C1D-O3G-C3G
25	l	5101	MGE	O6D-C1D-O3G-C3G
23	A	410	SQD	O6-C44-C45-C46
25	D	409	MGE	C1G-C2G-C3G-O3G
26	C	517	DGD	C1G-C2G-C3G-O3G
26	c	5515	DGD	C1G-C2G-C3G-O3G
21	A	408	LHG	O6-C4-C5-O7
21	a	5409	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
25	d	5408	MGE	O2G-C1B-C2B-C3B
20	D	407	BCR	C14-C15-C16-C17
20	d	5406	BCR	C14-C15-C16-C17
25	C	520	MGE	O1B-C1B-O2G-C2G
25	c	5517	MGE	O1B-C1B-O2G-C2G
17	A	402	CLA	CHA-CBD-CGD-O1D
17	A	402	CLA	CHA-CBD-CGD-O2D
17	A	405	CLA	CHA-CBD-CGD-O1D
17	B	602	CLA	CHA-CBD-CGD-O1D
17	B	608	CLA	CHA-CBD-CGD-O1D
17	B	608	CLA	CHA-CBD-CGD-O2D
17	B	610	CLA	CHA-CBD-CGD-O1D
17	B	610	CLA	CHA-CBD-CGD-O2D
17	B	614	CLA	CHA-CBD-CGD-O1D
17	C	502	CLA	CHA-CBD-CGD-O1D
17	C	502	CLA	CHA-CBD-CGD-O2D
17	C	503	CLA	CHA-CBD-CGD-O1D
17	C	503	CLA	CHA-CBD-CGD-O2D
17	C	506	CLA	CHA-CBD-CGD-O1D
17	C	506	CLA	CHA-CBD-CGD-O2D
17	C	508	CLA	CHA-CBD-CGD-O1D
17	C	508	CLA	CHA-CBD-CGD-O2D
17	C	510	CLA	CHA-CBD-CGD-O1D
17	C	510	CLA	CHA-CBD-CGD-O2D
17	D	405	CLA	CHA-CBD-CGD-O1D
17	D	405	CLA	CHA-CBD-CGD-O2D
17	a	5403	CLA	CHA-CBD-CGD-O1D
17	a	5403	CLA	CHA-CBD-CGD-O2D
17	a	5406	CLA	CHA-CBD-CGD-O1D
17	b	5602	CLA	CHA-CBD-CGD-O1D
17	b	5608	CLA	CHA-CBD-CGD-O1D
17	b	5608	CLA	CHA-CBD-CGD-O2D
17	b	5610	CLA	CHA-CBD-CGD-O1D
17	b	5610	CLA	CHA-CBD-CGD-O2D
17	b	5614	CLA	CHA-CBD-CGD-O1D
17	c	5502	CLA	CHA-CBD-CGD-O1D
17	c	5502	CLA	CHA-CBD-CGD-O2D
17	c	5503	CLA	CHA-CBD-CGD-O1D
17	c	5503	CLA	CHA-CBD-CGD-O2D
17	c	5506	CLA	CHA-CBD-CGD-O1D
17	c	5506	CLA	CHA-CBD-CGD-O2D
17	c	5508	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
17	c	5508	CLA	CHA-CBD-CGD-O2D
17	c	5510	CLA	CHA-CBD-CGD-O1D
17	c	5510	CLA	CHA-CBD-CGD-O2D
17	d	5404	CLA	CHA-CBD-CGD-O1D
17	d	5404	CLA	CHA-CBD-CGD-O2D
23	L	101	SQD	C28-C29-C30-C31
20	t	5102	BCR	C16-C17-C18-C19
25	D	410	MGE	CCB-CDB-CEB-CFB
25	d	5410	MGE	C3B-C4B-C5B-C6B
23	L	101	SQD	O6-C44-C45-O47
25	B	619	MGE	O2G-C2G-C3G-O3G
25	D	409	MGE	O1G-C1G-C2G-O2G
25	b	5620	MGE	O2G-C2G-C3G-O3G
25	d	5408	MGE	O2G-C2G-C3G-O3G
25	m	5103	MGE	O2G-C2G-C3G-O3G
26	C	517	DGD	O2G-C2G-C3G-O3G
26	c	5515	DGD	O2G-C2G-C3G-O3G
17	B	608	CLA	O1D-CGD-O2D-CED
17	b	5608	CLA	O1D-CGD-O2D-CED
23	D	403	SQD	O49-C7-O47-C45
17	A	402	CLA	C11-C10-C8-C9
17	a	5403	CLA	C11-C10-C8-C9
26	H	102	DGD	C5A-C6A-C7A-C8A
26	h	5102	DGD	C5A-C6A-C7A-C8A
23	A	410	SQD	C4-C5-C6-S
23	D	403	SQD	C4-C5-C6-S
23	d	5407	SQD	C4-C5-C6-S
23	l	5102	SQD	C28-C29-C30-C31
17	C	501	CLA	O1A-CGA-O2A-C1
17	c	5501	CLA	O1A-CGA-O2A-C1
17	B	607	CLA	C3-C5-C6-C7
25	A	412	MGE	C7B-C8B-C9B-CAB
25	l	5101	MGE	C7B-C8B-C9B-CAB
17	B	604	CLA	C1A-C2A-CAA-CBA
17	C	513	CLA	C1A-C2A-CAA-CBA
17	b	5604	CLA	C1A-C2A-CAA-CBA
17	c	5512	CLA	C1A-C2A-CAA-CBA
25	m	5101	MGE	C4A-C5A-C6A-C7A
17	B	612	CLA	C2-C1-O2A-CGA
17	C	502	CLA	C2-C1-O2A-CGA
17	b	5612	CLA	C2-C1-O2A-CGA
17	c	5502	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
17	b	5607	CLA	C3-C5-C6-C7
17	B	604	CLA	C2-C3-C5-C6
17	b	5604	CLA	C2-C3-C5-C6
25	d	5408	MGE	C4B-C5B-C6B-C7B
23	D	403	SQD	C11-C10-C9-C8
23	d	5407	SQD	C11-C10-C9-C8
25	C	520	MGE	O6D-C1D-O3G-C3G
25	c	5517	MGE	O6D-C1D-O3G-C3G
21	A	408	LHG	O6-C4-C5-C6
21	a	5409	LHG	O6-C4-C5-C6
17	b	5616	CLA	C10-C11-C12-C13
23	D	403	SQD	C26-C27-C28-C29
17	B	603	CLA	CAD-CBD-CGD-O1D
17	B	605	CLA	CAD-CBD-CGD-O1D
17	B	607	CLA	CAD-CBD-CGD-O1D
17	B	613	CLA	CAD-CBD-CGD-O1D
17	C	501	CLA	CAD-CBD-CGD-O1D
17	C	502	CLA	CAD-CBD-CGD-O1D
17	C	506	CLA	CAD-CBD-CGD-O1D
17	C	510	CLA	CAD-CBD-CGD-O1D
17	b	5603	CLA	CAD-CBD-CGD-O1D
17	b	5605	CLA	CAD-CBD-CGD-O1D
17	b	5607	CLA	CAD-CBD-CGD-O1D
17	b	5613	CLA	CAD-CBD-CGD-O1D
17	c	5501	CLA	CAD-CBD-CGD-O1D
17	c	5502	CLA	CAD-CBD-CGD-O1D
17	c	5506	CLA	CAD-CBD-CGD-O1D
17	c	5510	CLA	CAD-CBD-CGD-O1D
17	B	616	CLA	C10-C11-C12-C13
26	a	5411	DGD	C5B-C6B-C7B-C8B
25	C	520	MGE	C5A-C6A-C7A-C8A
26	C	519	DGD	C5B-C6B-C7B-C8B
25	B	619	MGE	CAA-CBA-CCA-CDA
25	c	5517	MGE	C5A-C6A-C7A-C8A
26	C	518	DGD	C4A-C5A-C6A-C7A
26	H	102	DGD	C3A-C4A-C5A-C6A
26	c	5516	DGD	C4A-C5A-C6A-C7A
26	h	5102	DGD	C3A-C4A-C5A-C6A
17	A	402	CLA	C11-C10-C8-C7
17	B	604	CLA	C12-C13-C15-C16
17	B	607	CLA	C11-C10-C8-C7
17	C	505	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
17	a	5403	CLA	C11-C10-C8-C7
17	b	5604	CLA	C12-C13-C15-C16
17	b	5607	CLA	C11-C10-C8-C7
17	c	5505	CLA	C11-C12-C13-C15
18	D	402	PHO	C12-C13-C15-C16
18	d	5402	PHO	C12-C13-C15-C16
25	b	5620	MGE	CAA-CBA-CCA-CDA
17	B	610	CLA	C5-C6-C7-C8
17	b	5610	CLA	C5-C6-C7-C8
25	B	619	MGE	C1B-C2B-C3B-C4B
25	b	5620	MGE	C1B-C2B-C3B-C4B
17	D	405	CLA	C2A-CAA-CBA-CGA
17	d	5404	CLA	C2A-CAA-CBA-CGA
17	B	604	CLA	C16-C17-C18-C20
17	b	5604	CLA	C16-C17-C18-C20
23	D	403	SQD	O6-C44-C45-O47
23	d	5407	SQD	O6-C44-C45-O47
25	d	5409	MGE	O2G-C2G-C3G-O3G
26	C	518	DGD	O2G-C2G-C3G-O3G
26	C	519	DGD	O1G-C1G-C2G-O2G
26	a	5411	DGD	O1G-C1G-C2G-O2G
26	c	5516	DGD	O2G-C2G-C3G-O3G
22	A	409	LMT	C3-C4-C5-C6
25	D	408	MGE	C2G-C3G-O3G-C1D
17	A	402	CLA	C10-C11-C12-C13
17	a	5403	CLA	C10-C11-C12-C13
21	A	408	LHG	C2-C3-O3-P
21	a	5409	LHG	C2-C3-O3-P
25	m	5103	MGE	O1A-C1A-O1G-C1G
25	m	5103	MGE	C2A-C1A-O1G-C1G
23	L	101	SQD	C17-C18-C19-C20
17	A	401	CLA	C6-C7-C8-C9
17	B	607	CLA	C11-C10-C8-C9
17	B	610	CLA	C14-C13-C15-C16
17	B	615	CLA	C6-C7-C8-C9
17	C	507	CLA	C6-C7-C8-C9
17	a	5402	CLA	C6-C7-C8-C9
17	b	5607	CLA	C11-C10-C8-C9
17	b	5608	CLA	C6-C7-C8-C9
17	b	5615	CLA	C6-C7-C8-C9
17	c	5507	CLA	C6-C7-C8-C9
20	A	407	BCR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
20	a	5408	BCR	C22-C23-C24-C25
20	d	5406	BCR	C6-C7-C8-C9
25	D	410	MGE	CBB-CCB-CDB-CEB
21	a	5409	LHG	O10-C23-O8-C6
20	k	5502	BCR	C16-C17-C18-C36
26	C	518	DGD	C9A-CAA-CBA-CCA
26	c	5516	DGD	C9A-CAA-CBA-CCA
21	A	408	LHG	O10-C23-O8-C6
18	a	5405	PHO	C2-C3-C5-C6
17	C	510	CLA	C13-C15-C16-C17
17	c	5510	CLA	C13-C15-C16-C17
23	l	5102	SQD	C18-C19-C20-C21
25	B	619	MGE	C1A-C2A-C3A-C4A
25	b	5620	MGE	C1A-C2A-C3A-C4A
17	C	503	CLA	CBA-CGA-O2A-C1
17	c	5503	CLA	CBA-CGA-O2A-C1
23	D	403	SQD	C25-C26-C27-C28
20	A	407	BCR	C23-C24-C25-C30
20	B	617	BCR	C1-C6-C7-C8
20	B	618	BCR	C1-C6-C7-C8
20	B	618	BCR	C23-C24-C25-C26
20	C	514	BCR	C23-C24-C25-C30
20	C	516	BCR	C23-C24-C25-C26
20	H	101	BCR	C1-C6-C7-C8
20	T	102	BCR	C1-C6-C7-C8
20	T	102	BCR	C5-C6-C7-C8
20	a	5408	BCR	C23-C24-C25-C30
20	b	5617	BCR	C1-C6-C7-C8
20	b	5618	BCR	C1-C6-C7-C8
20	b	5618	BCR	C5-C6-C7-C8
20	b	5618	BCR	C23-C24-C25-C26
20	c	5513	BCR	C23-C24-C25-C30
20	c	5514	BCR	C23-C24-C25-C26
20	h	5101	BCR	C1-C6-C7-C8
18	A	404	PHO	C2-C3-C5-C6
17	D	404	CLA	C2A-CAA-CBA-CGA
17	d	5403	CLA	C2A-CAA-CBA-CGA
19	D	406	PQ9	C18-C20-C21-C22
19	d	5405	PQ9	C18-C20-C21-C22
25	D	410	MGE	C2D-C1D-O3G-C3G
25	B	619	MGE	O1G-C1G-C2G-O2G
25	D	408	MGE	O1G-C1G-C2G-O2G

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Mol	Chain	Res	Type	Atoms
25	b	5620	MGE	O1G-C1G-C2G-O2G
17	C	505	CLA	C15-C16-C17-C18
17	c	5505	CLA	C15-C16-C17-C18
25	d	5409	MGE	C6B-C7B-C8B-C9B
18	A	404	PHO	CHA-CBD-CGD-O1D
18	A	404	PHO	CHA-CBD-CGD-O2D
18	a	5405	PHO	CHA-CBD-CGD-O1D
18	a	5405	PHO	CHA-CBD-CGD-O2D
17	b	5615	CLA	C13-C15-C16-C17
25	B	619	MGE	C1G-C2G-C3G-O3G
26	C	518	DGD	C1G-C2G-C3G-O3G
26	c	5516	DGD	C1G-C2G-C3G-O3G
17	C	507	CLA	C6-C7-C8-C10
17	C	511	CLA	C12-C13-C15-C16
17	D	404	CLA	C11-C10-C8-C7
17	c	5507	CLA	C6-C7-C8-C10
17	d	5403	CLA	C11-C10-C8-C7
17	k	5501	CLA	C12-C13-C15-C16
17	B	606	CLA	C11-C12-C13-C14
17	B	608	CLA	C6-C7-C8-C9
17	C	506	CLA	C11-C12-C13-C14
17	C	511	CLA	C14-C13-C15-C16
17	b	5610	CLA	C14-C13-C15-C16
17	c	5506	CLA	C11-C12-C13-C14
17	k	5501	CLA	C14-C13-C15-C16
20	B	617	BCR	C15-C16-C17-C18
20	C	514	BCR	C13-C14-C15-C16
20	b	5617	BCR	C15-C16-C17-C18
20	c	5513	BCR	C13-C14-C15-C16
17	B	615	CLA	C13-C15-C16-C17
25	c	5517	MGE	C5B-C6B-C7B-C8B
25	C	520	MGE	C5B-C6B-C7B-C8B
25	m	5103	MGE	C5B-C6B-C7B-C8B
17	B	612	CLA	C4-C3-C5-C6
17	b	5612	CLA	C4-C3-C5-C6
17	C	503	CLA	O1A-CGA-O2A-C1
17	B	604	CLA	C16-C17-C18-C19
17	b	5604	CLA	C16-C17-C18-C19
17	c	5503	CLA	O1A-CGA-O2A-C1
17	C	511	CLA	C15-C16-C17-C18
17	B	607	CLA	C2A-CAA-CBA-CGA
17	b	5607	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
17	k	5501	CLA	C15-C16-C17-C18
20	H	101	BCR	C15-C16-C17-C18
20	h	5101	BCR	C15-C16-C17-C18
18	D	402	PHO	C13-C15-C16-C17
18	d	5402	PHO	C13-C15-C16-C17
17	B	613	CLA	C4-C3-C5-C6
17	b	5613	CLA	C4-C3-C5-C6
17	B	612	CLA	C2-C3-C5-C6
17	b	5612	CLA	C2-C3-C5-C6
17	D	404	CLA	C2-C1-O2A-CGA
17	d	5403	CLA	C2-C1-O2A-CGA
17	b	5610	CLA	O1D-CGD-O2D-CED
25	d	5410	MGE	C2D-C1D-O3G-C3G
21	A	408	LHG	C26-C27-C28-C29
17	C	507	CLA	C8-C10-C11-C12
17	c	5507	CLA	C8-C10-C11-C12
17	B	603	CLA	C2A-CAA-CBA-CGA
17	C	501	CLA	C2A-CAA-CBA-CGA
17	b	5603	CLA	C2A-CAA-CBA-CGA
17	c	5501	CLA	C2A-CAA-CBA-CGA
25	m	5101	MGE	O1G-C1G-C2G-O2G
21	a	5409	LHG	C26-C27-C28-C29
25	m	5101	MGE	C2B-C3B-C4B-C5B
17	B	608	CLA	C3A-C2A-CAA-CBA
17	C	505	CLA	C3A-C2A-CAA-CBA
17	C	506	CLA	C3A-C2A-CAA-CBA
17	b	5608	CLA	C3A-C2A-CAA-CBA
17	c	5505	CLA	C3A-C2A-CAA-CBA
17	c	5506	CLA	C3A-C2A-CAA-CBA
17	B	613	CLA	C16-C17-C18-C20
17	b	5613	CLA	C16-C17-C18-C20
26	C	519	DGD	O2G-C1B-C2B-C3B
26	a	5411	DGD	O2G-C1B-C2B-C3B
20	H	101	BCR	C9-C10-C11-C12
20	h	5101	BCR	C9-C10-C11-C12
17	A	403	CLA	CBA-CGA-O2A-C1
17	a	5404	CLA	CBA-CGA-O2A-C1
17	B	607	CLA	C6-C7-C8-C9
17	B	611	CLA	C14-C13-C15-C16
17	b	5607	CLA	C6-C7-C8-C9
17	b	5611	CLA	C14-C13-C15-C16
25	D	410	MGE	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
26	H	102	DGD	C6B-C7B-C8B-C9B
17	B	610	CLA	O1D-CGD-O2D-CED
26	h	5102	DGD	C6B-C7B-C8B-C9B
20	b	5619	BCR	C20-C21-C22-C37
20	t	5101	BCR	C20-C21-C22-C37
25	B	619	MGE	O1G-C1G-C2G-C3G
25	b	5620	MGE	O1G-C1G-C2G-C3G
25	b	5620	MGE	C1G-C2G-C3G-O3G
22	a	5410	LMT	O5'-C1'-O1'-C1
25	D	409	MGE	O6D-C1D-O3G-C3G
26	C	518	DGD	O6D-C1D-O3G-C3G
26	c	5516	DGD	O6D-C1D-O3G-C3G
26	C	517	DGD	CBA-CCA-CDA-CEA
26	c	5515	DGD	CBA-CCA-CDA-CEA
25	d	5408	MGE	C2A-C3A-C4A-C5A
17	B	607	CLA	C1A-C2A-CAA-CBA
17	C	501	CLA	C1A-C2A-CAA-CBA
17	b	5607	CLA	C1A-C2A-CAA-CBA
17	c	5501	CLA	C1A-C2A-CAA-CBA
25	l	5101	MGE	C5A-C6A-C7A-C8A
17	C	502	CLA	C6-C7-C8-C10
17	C	507	CLA	C11-C10-C8-C7
17	c	5502	CLA	C6-C7-C8-C10
17	c	5507	CLA	C11-C10-C8-C7
17	A	402	CLA	C2C-C3C-CAC-CBC
25	A	412	MGE	C5A-C6A-C7A-C8A
17	A	403	CLA	O1A-CGA-O2A-C1
17	a	5404	CLA	O1A-CGA-O2A-C1
17	C	506	CLA	C16-C17-C18-C20
17	c	5506	CLA	C16-C17-C18-C20
22	m	5102	LMT	O1'-C1-C2-C3
17	a	5403	CLA	C2C-C3C-CAC-CBC
25	d	5409	MGE	C2A-C3A-C4A-C5A
20	C	516	BCR	C16-C17-C18-C19
20	c	5514	BCR	C16-C17-C18-C19
20	C	515	BCR	C13-C14-C15-C16
20	D	407	BCR	C19-C20-C21-C22
20	d	5406	BCR	C19-C20-C21-C22
20	z	5101	BCR	C13-C14-C15-C16
20	Y	101	BCR	C9-C10-C11-C12
17	B	610	CLA	O1A-CGA-O2A-C1
17	A	401	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
17	C	502	CLA	C4-C3-C5-C6
17	c	5502	CLA	C4-C3-C5-C6
17	B	613	CLA	C2-C1-O2A-CGA
17	b	5613	CLA	C2-C1-O2A-CGA
25	D	409	MGE	C6B-C7B-C8B-C9B
17	b	5610	CLA	O1A-CGA-O2A-C1
17	a	5402	CLA	C15-C16-C17-C18
22	M	101	LMT	C1-C2-C3-C4
23	d	5407	SQD	C10-C11-C12-C13
20	A	407	BCR	C23-C24-C25-C26
20	B	618	BCR	C5-C6-C7-C8
20	a	5408	BCR	C23-C24-C25-C26
20	k	5502	BCR	C1-C6-C7-C8
20	Y	101	BCR	C1-C6-C7-C8
25	D	408	MGE	O1G-C1G-C2G-C3G
26	C	518	DGD	O1G-C1G-C2G-C3G
26	c	5516	DGD	O1G-C1G-C2G-C3G
20	C	514	BCR	C15-C16-C17-C18
20	C	515	BCR	C15-C16-C17-C18
20	c	5513	BCR	C15-C16-C17-C18
20	z	5101	BCR	C15-C16-C17-C18
20	D	407	BCR	C17-C18-C19-C20
20	d	5406	BCR	C17-C18-C19-C20
17	B	602	CLA	CAA-CBA-CGA-O2A
17	b	5602	CLA	CAA-CBA-CGA-O2A
17	B	610	CLA	CBA-CGA-O2A-C1
17	b	5610	CLA	CBA-CGA-O2A-C1
17	A	402	CLA	C4C-C3C-CAC-CBC
17	B	612	CLA	C6-C7-C8-C10
17	b	5612	CLA	C6-C7-C8-C10
18	D	402	PHO	C11-C12-C13-C15
18	d	5402	PHO	C11-C12-C13-C15
17	a	5403	CLA	C4C-C3C-CAC-CBC
23	l	5102	SQD	O48-C23-C24-C25
17	B	605	CLA	C16-C17-C18-C20
17	b	5605	CLA	C16-C17-C18-C20
17	B	614	CLA	CBA-CGA-O2A-C1
17	b	5614	CLA	CBA-CGA-O2A-C1
17	C	507	CLA	CAA-CBA-CGA-O2A
17	c	5507	CLA	CAA-CBA-CGA-O2A
17	C	502	CLA	C2-C3-C5-C6
17	c	5502	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	m	5103	MGE	O2G-C1B-C2B-C3B
17	B	605	CLA	C11-C10-C8-C9
17	C	505	CLA	C6-C7-C8-C9
17	C	505	CLA	C11-C12-C13-C14
17	D	404	CLA	C11-C10-C8-C9
17	b	5605	CLA	C11-C10-C8-C9
17	c	5505	CLA	C6-C7-C8-C9
17	c	5505	CLA	C11-C12-C13-C14
17	d	5403	CLA	C11-C10-C8-C9
25	d	5410	MGE	C6B-C7B-C8B-C9B
25	D	409	MGE	C2A-C3A-C4A-C5A
26	H	102	DGD	C4B-C5B-C6B-C7B
17	B	602	CLA	CAD-CBD-CGD-O2D
17	B	614	CLA	CAD-CBD-CGD-O2D
17	B	616	CLA	CAD-CBD-CGD-O2D
17	C	505	CLA	CAD-CBD-CGD-O2D
17	C	511	CLA	CAD-CBD-CGD-O2D
17	b	5602	CLA	CAD-CBD-CGD-O2D
17	b	5614	CLA	CAD-CBD-CGD-O2D
17	b	5616	CLA	CAD-CBD-CGD-O2D
17	c	5505	CLA	CAD-CBD-CGD-O2D
17	k	5501	CLA	CAD-CBD-CGD-O2D
25	m	5103	MGE	C1G-C2G-O2G-C1B
25	m	5103	MGE	C3G-C2G-O2G-C1B
26	h	5102	DGD	C4B-C5B-C6B-C7B
25	m	5101	MGE	O1B-C1B-O2G-C2G
17	B	614	CLA	C4C-C3C-CAC-CBC
17	b	5614	CLA	C4C-C3C-CAC-CBC
25	m	5101	MGE	C4B-C5B-C6B-C7B
23	L	101	SQD	O48-C23-C24-C25
25	d	5408	MGE	C9A-CAA-CBA-CCA
23	a	5401	SQD	O6-C44-C45-C46
17	B	614	CLA	O1A-CGA-O2A-C1
23	D	403	SQD	C12-C13-C14-C15
17	A	401	CLA	O2A-C1-C2-C3
17	C	512	CLA	O2A-C1-C2-C3
17	a	5402	CLA	O2A-C1-C2-C3
17	c	5511	CLA	O2A-C1-C2-C3
25	D	409	MGE	C3B-C4B-C5B-C6B
17	b	5614	CLA	O1A-CGA-O2A-C1
17	A	405	CLA	CHA-CBD-CGD-O2D
17	B	602	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	B	614	CLA	CHA-CBD-CGD-O2D
17	B	616	CLA	CHA-CBD-CGD-O1D
17	C	509	CLA	CHA-CBD-CGD-O1D
17	C	511	CLA	CHA-CBD-CGD-O1D
17	a	5406	CLA	CHA-CBD-CGD-O2D
17	b	5602	CLA	CHA-CBD-CGD-O2D
17	b	5614	CLA	CHA-CBD-CGD-O2D
17	b	5616	CLA	CHA-CBD-CGD-O1D
17	c	5509	CLA	CHA-CBD-CGD-O1D
17	k	5501	CLA	CHA-CBD-CGD-O1D
17	C	512	CLA	CAA-CBA-CGA-O2A
17	c	5511	CLA	CAA-CBA-CGA-O2A
17	C	506	CLA	C10-C11-C12-C13
17	B	613	CLA	CAA-CBA-CGA-O2A
17	b	5613	CLA	CAA-CBA-CGA-O2A
25	m	5103	MGE	O1G-C1G-C2G-O2G
17	c	5506	CLA	C10-C11-C12-C13
26	H	102	DGD	O2G-C1B-C2B-C3B
26	h	5102	DGD	O2G-C1B-C2B-C3B
25	D	408	MGE	C2B-C1B-O2G-C2G
17	B	614	CLA	CAA-CBA-CGA-O2A
17	b	5614	CLA	CAA-CBA-CGA-O2A
17	B	609	CLA	C2-C3-C5-C6
17	C	508	CLA	C11-C10-C8-C7
17	b	5609	CLA	C2-C3-C5-C6
17	c	5508	CLA	C11-C10-C8-C7
17	B	610	CLA	C16-C17-C18-C19
17	b	5610	CLA	C16-C17-C18-C19
20	B	617	BCR	C19-C20-C21-C22
20	b	5617	BCR	C19-C20-C21-C22
20	k	5502	BCR	C15-C16-C17-C18
17	C	504	CLA	CAA-CBA-CGA-O2A
17	c	5504	CLA	CAA-CBA-CGA-O2A
23	L	101	SQD	C4-C5-C6-S
17	B	610	CLA	C16-C17-C18-C20
17	b	5610	CLA	C16-C17-C18-C20
25	m	5101	MGE	C2B-C1B-O2G-C2G
17	A	401	CLA	C2A-CAA-CBA-CGA
17	a	5402	CLA	C2A-CAA-CBA-CGA
20	C	516	BCR	C37-C22-C23-C24
20	c	5514	BCR	C37-C22-C23-C24
25	d	5410	MGE	C9B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
17	C	503	CLA	CAA-CBA-CGA-O2A
17	C	507	CLA	CAA-CBA-CGA-O1A
17	c	5507	CLA	CAA-CBA-CGA-O1A
17	C	509	CLA	C1A-C2A-CAA-CBA
17	c	5509	CLA	C1A-C2A-CAA-CBA
25	m	5103	MGE	O1B-C1B-C2B-C3B
17	c	5503	CLA	CAA-CBA-CGA-O2A
25	m	5101	MGE	O1G-C1G-C2G-C3G
22	A	409	LMT	C9-C10-C11-C12
21	A	408	LHG	C30-C31-C32-C33
17	B	611	CLA	C4-C3-C5-C6
17	b	5611	CLA	C4-C3-C5-C6
25	B	619	MGE	C7B-C8B-C9B-CAB
17	B	613	CLA	C2-C3-C5-C6
21	a	5409	LHG	C30-C31-C32-C33
25	b	5620	MGE	C7B-C8B-C9B-CAB
17	C	504	CLA	CAA-CBA-CGA-O1A
17	C	512	CLA	CAA-CBA-CGA-O1A
17	c	5504	CLA	CAA-CBA-CGA-O1A
17	c	5511	CLA	CAA-CBA-CGA-O1A
20	c	5513	BCR	C16-C17-C18-C36
20	k	5502	BCR	C5-C6-C7-C8
20	Y	101	BCR	C5-C6-C7-C8
25	l	5101	MGE	CDB-CEB-CFB-CGB
25	C	520	MGE	C8A-C9A-CAA-CBA
25	c	5517	MGE	C8A-C9A-CAA-CBA
25	D	408	MGE	O1B-C1B-O2G-C2G
17	B	604	CLA	C2C-C3C-CAC-CBC
17	b	5604	CLA	C2C-C3C-CAC-CBC
17	b	5613	CLA	CAA-CBA-CGA-O1A
25	A	412	MGE	CDB-CEB-CFB-CGB
17	B	613	CLA	CAA-CBA-CGA-O1A
17	B	614	CLA	CAA-CBA-CGA-O1A
17	b	5613	CLA	C2-C3-C5-C6
17	B	606	CLA	CAD-CBD-CGD-O1D
17	B	612	CLA	CAD-CBD-CGD-O1D
17	C	507	CLA	CAD-CBD-CGD-O1D
17	C	509	CLA	CAD-CBD-CGD-O1D
17	b	5606	CLA	CAD-CBD-CGD-O1D
17	b	5612	CLA	CAD-CBD-CGD-O1D
17	c	5507	CLA	CAD-CBD-CGD-O1D
17	c	5509	CLA	CAD-CBD-CGD-O1D

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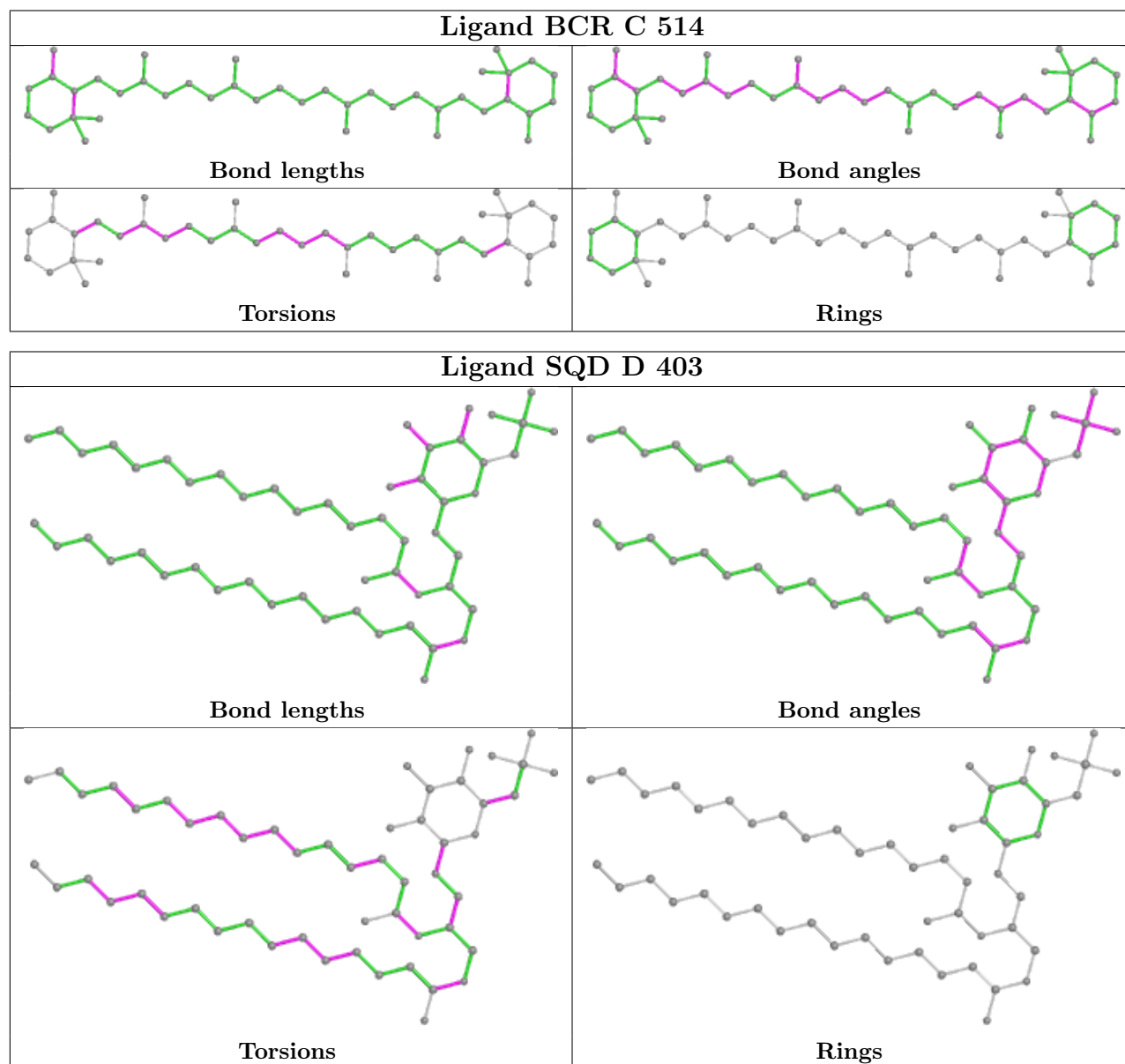
Mol	Chain	Res	Type	Atoms
17	b	5614	CLA	CAA-CBA-CGA-O1A
25	d	5408	MGE	O1B-C1B-C2B-C3B
25	b	5620	MGE	C2B-C3B-C4B-C5B
17	A	402	CLA	C11-C12-C13-C14
17	a	5403	CLA	C11-C12-C13-C14
22	m	5102	LMT	C11-C10-C9-C8
25	B	619	MGE	C2B-C3B-C4B-C5B
25	d	5410	MGE	CBB-CCB-CDB-CEB
17	B	609	CLA	C4-C3-C5-C6
17	b	5609	CLA	C4-C3-C5-C6
19	D	406	PQ9	C39-C38-C40-C41
19	d	5405	PQ9	C39-C38-C40-C41
17	B	605	CLA	C11-C10-C8-C7
17	C	505	CLA	C6-C7-C8-C10
17	C	505	CLA	C12-C13-C15-C16
17	C	511	CLA	C6-C7-C8-C10
17	b	5605	CLA	C11-C10-C8-C7
17	c	5505	CLA	C6-C7-C8-C10
17	c	5505	CLA	C12-C13-C15-C16
17	k	5501	CLA	C6-C7-C8-C10
25	D	410	MGE	C9A-CAA-CBA-CCA
25	D	410	MGE	O2G-C1B-C2B-C3B
17	B	602	CLA	C10-C11-C12-C13
17	b	5602	CLA	C10-C11-C12-C13
20	b	5619	BCR	C7-C8-C9-C10
20	t	5101	BCR	C7-C8-C9-C10
22	a	5410	LMT	C2-C1-O1'-C1'
17	D	404	CLA	CAA-CBA-CGA-O2A
17	d	5403	CLA	CAA-CBA-CGA-O2A
29	F	101	HEM	CAA-CBA-CGA-O1A
29	f	5101	HEM	CAA-CBA-CGA-O1A
17	B	606	CLA	C8-C10-C11-C12
26	c	5515	DGD	C9A-CAA-CBA-CCA
26	C	517	DGD	C9A-CAA-CBA-CCA
17	b	5613	CLA	C3-C5-C6-C7

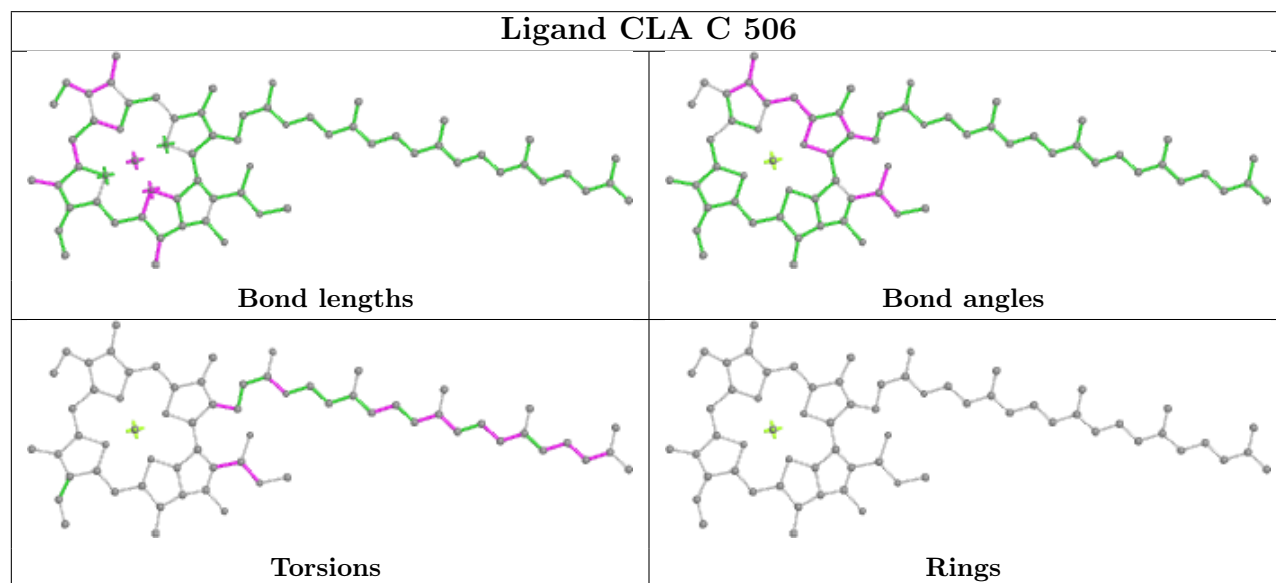
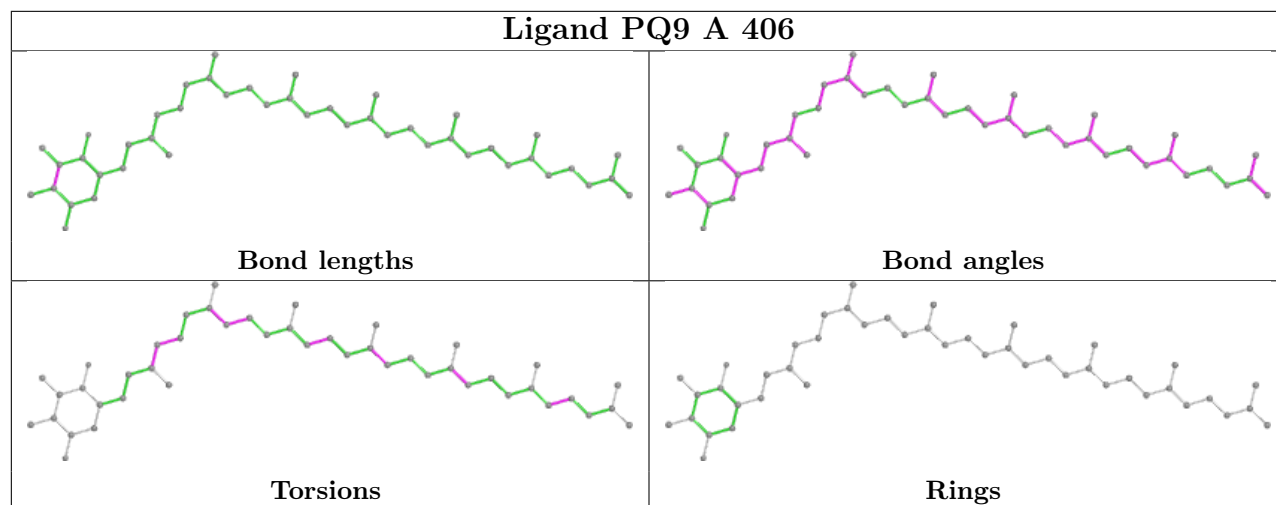
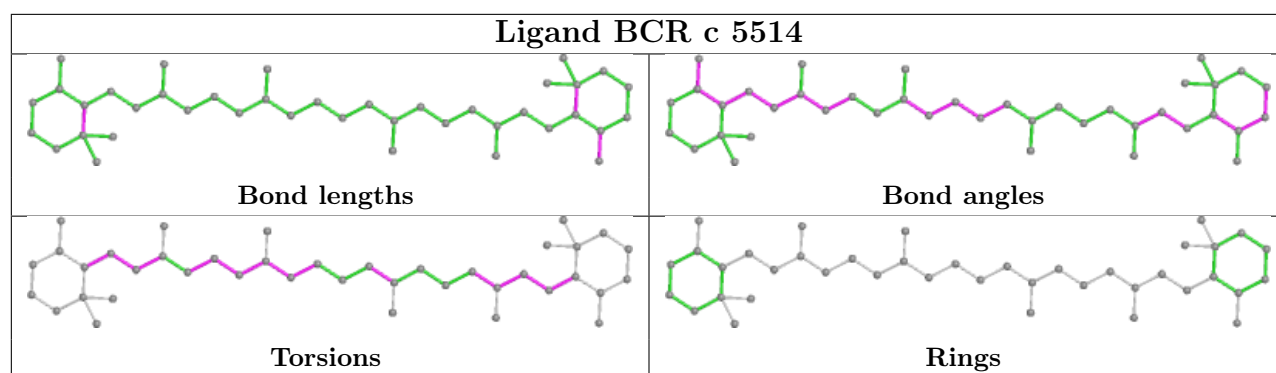
There are no ring outliers.

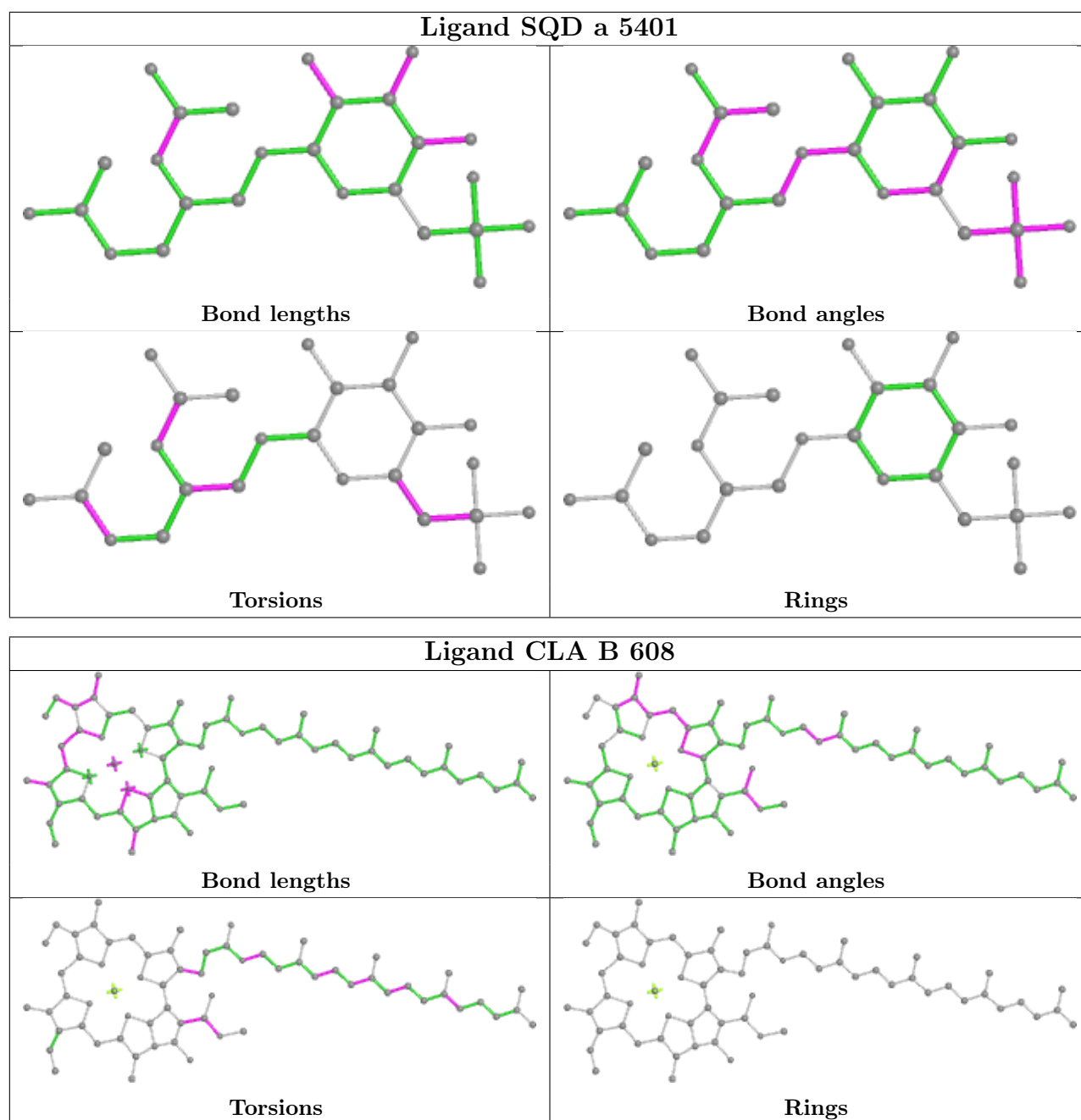
No monomer is involved in short contacts.

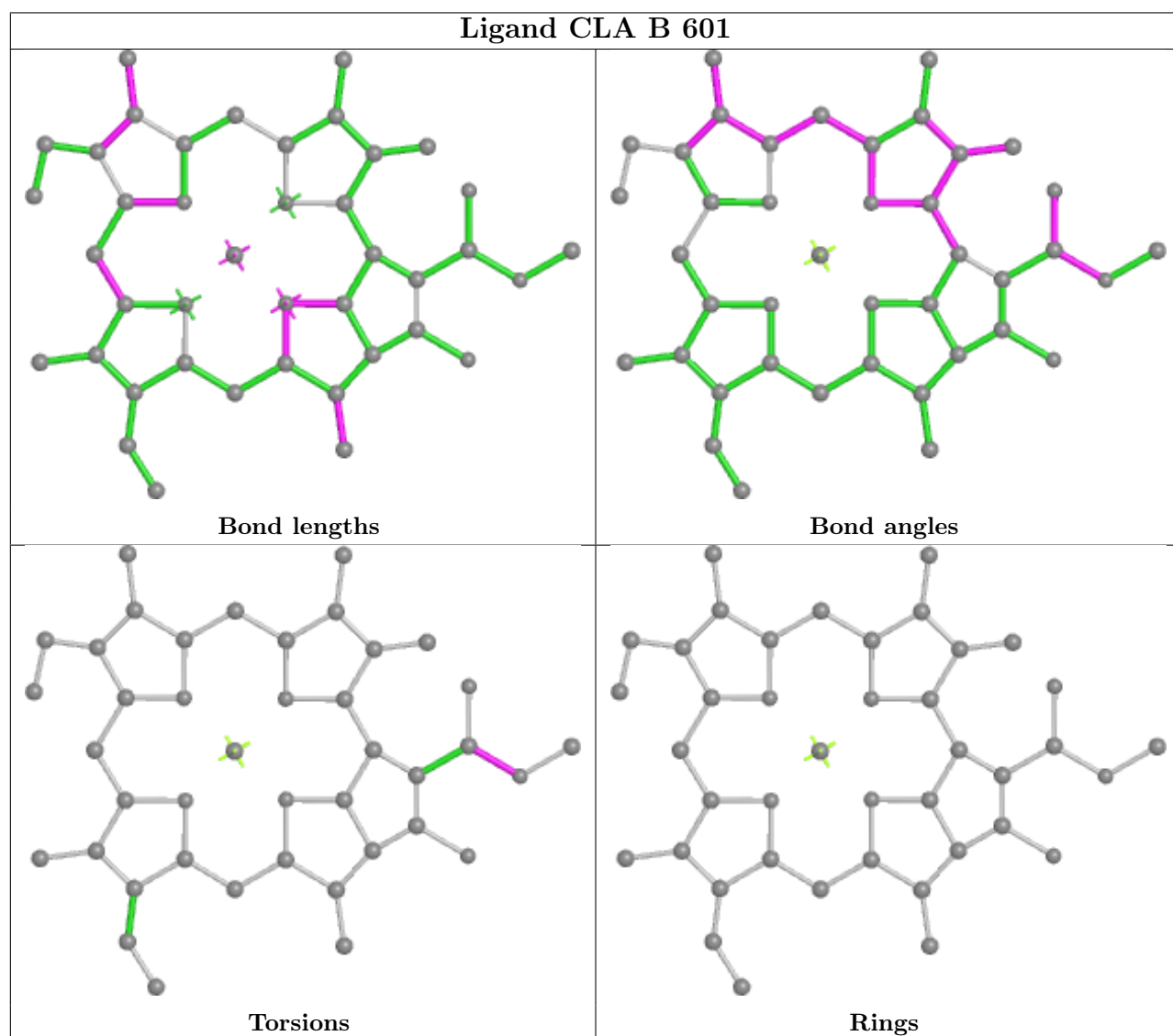
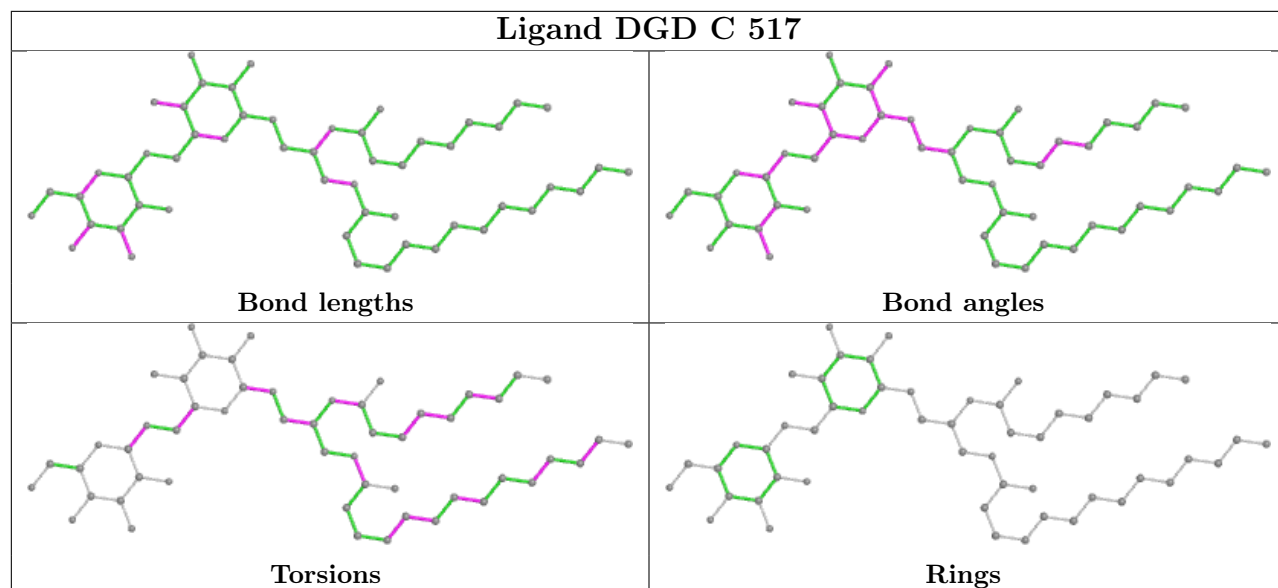
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

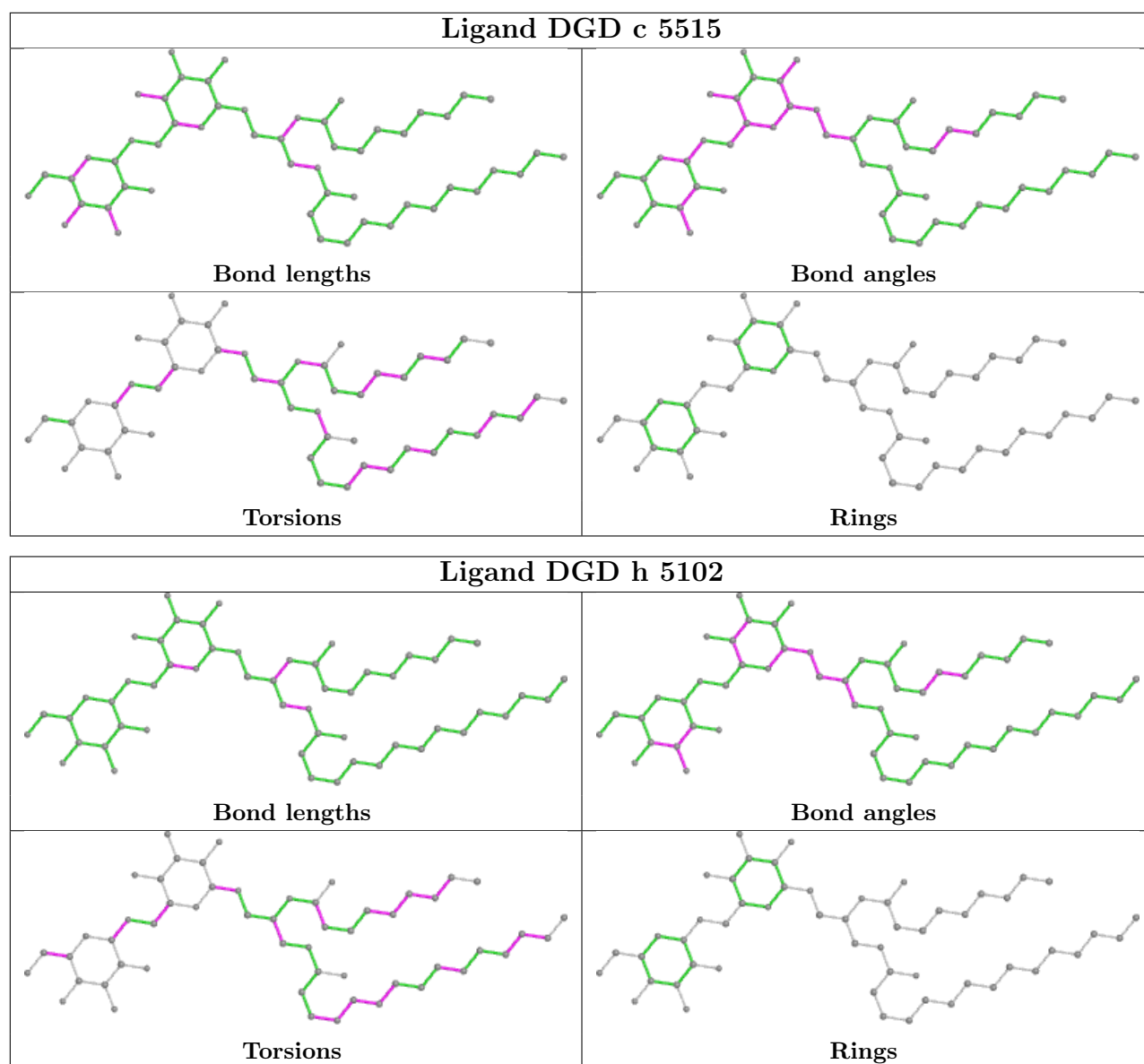
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

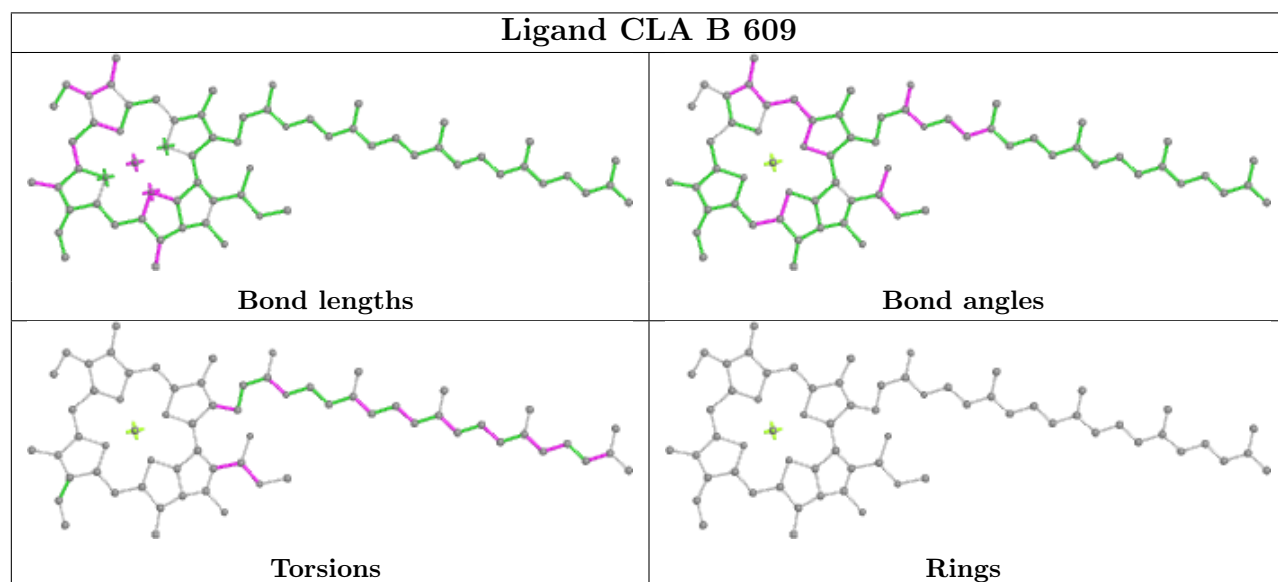
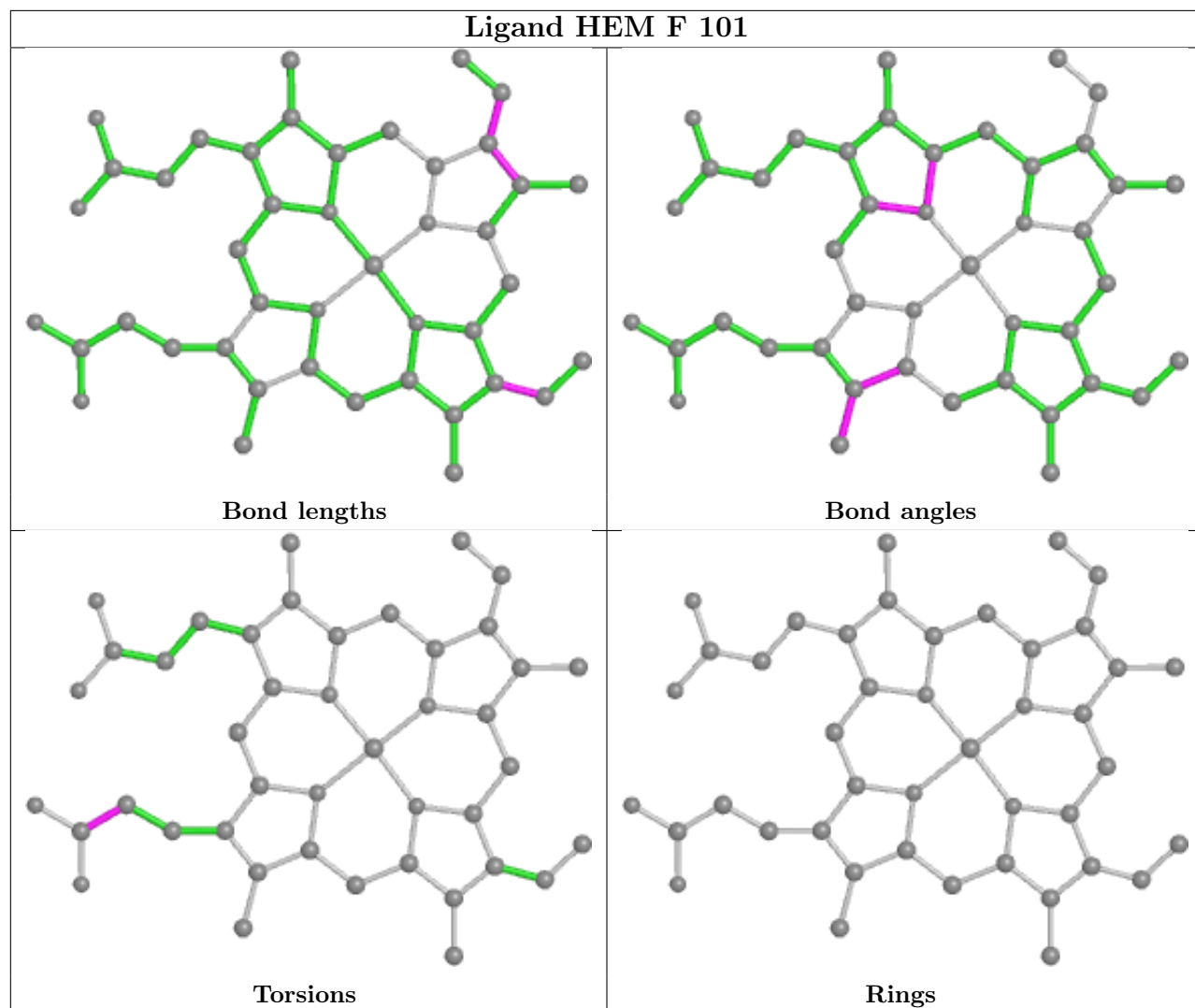


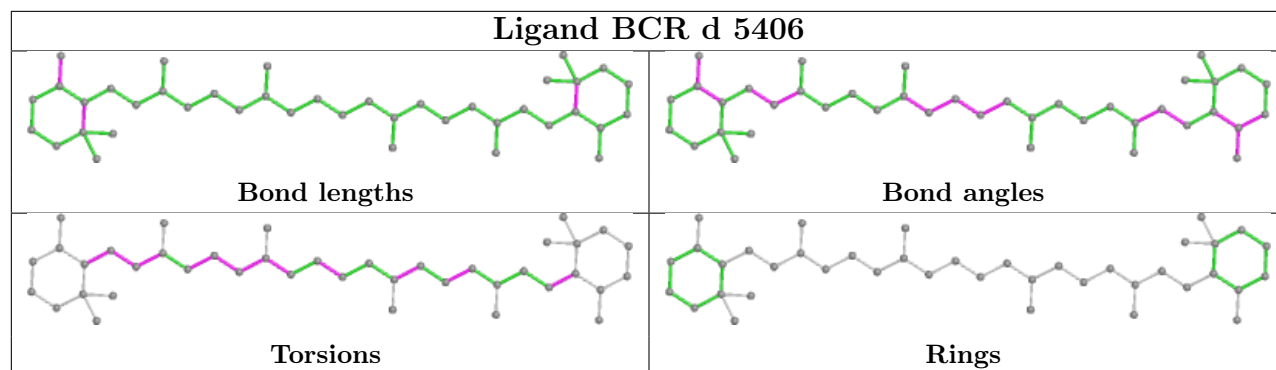


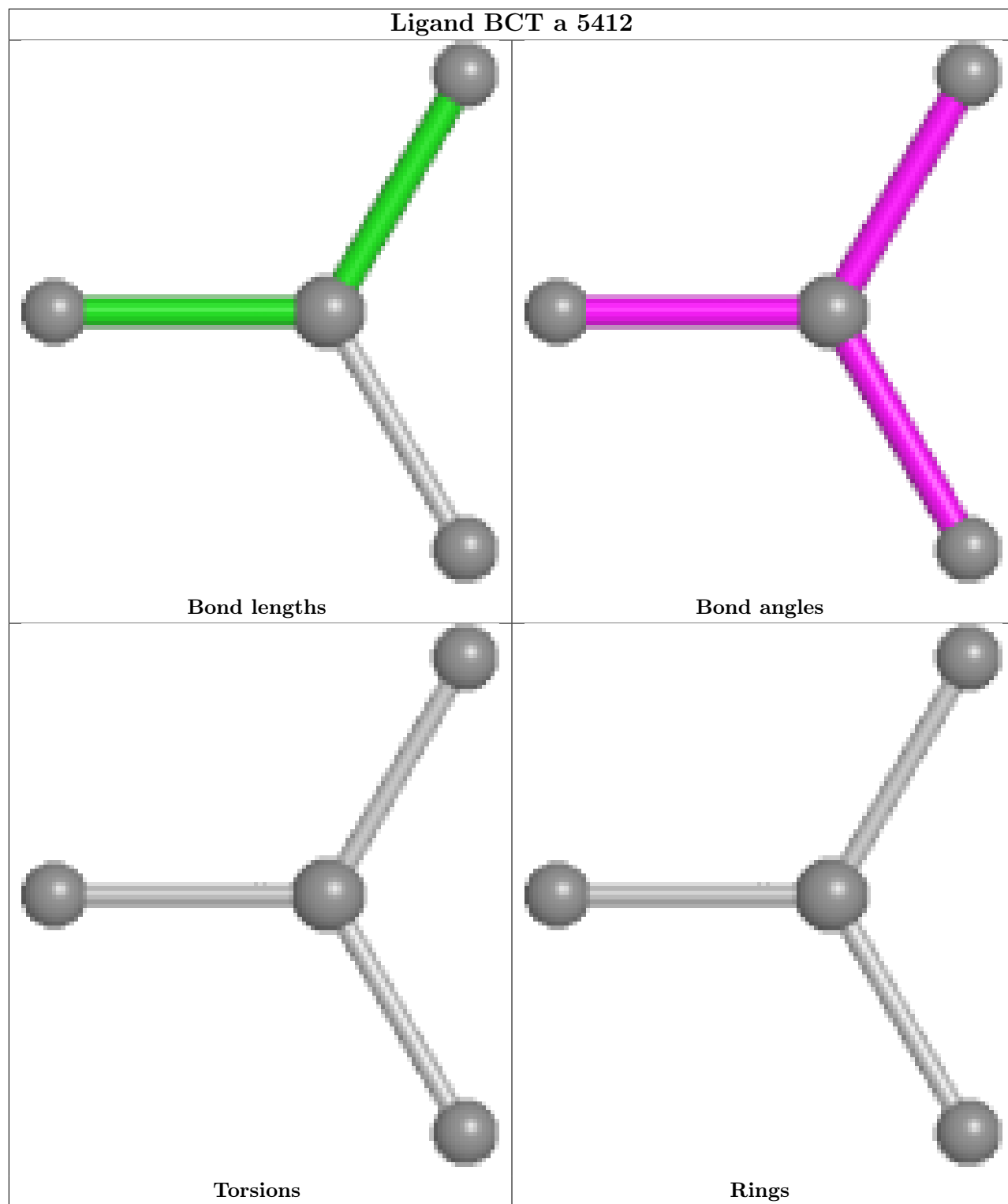


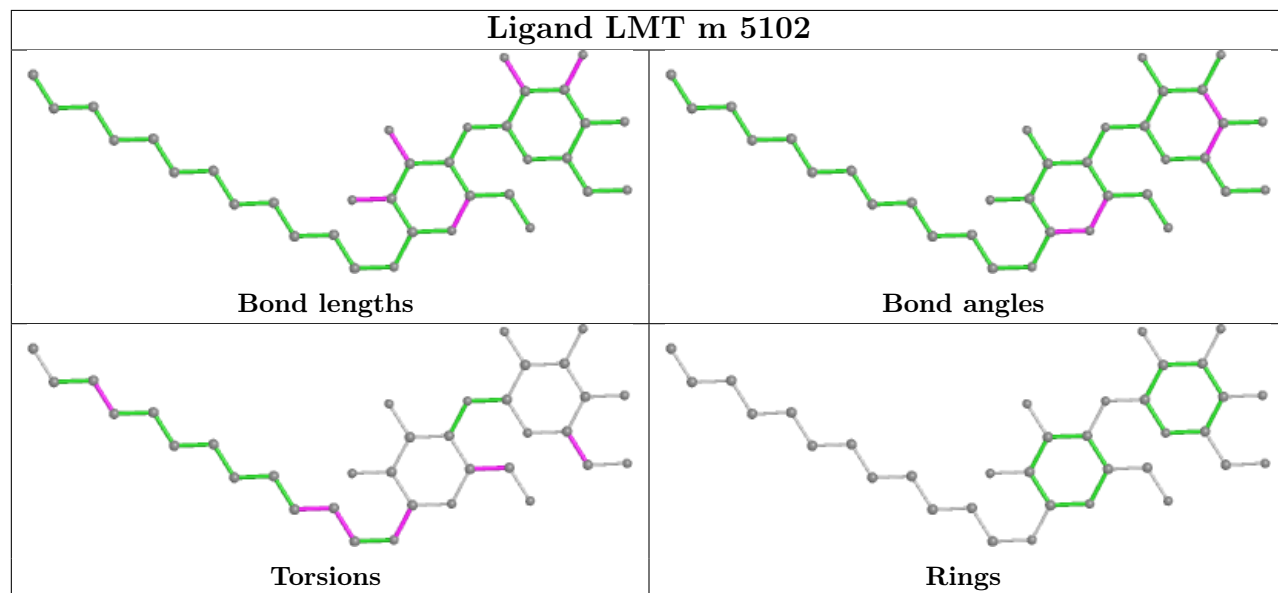
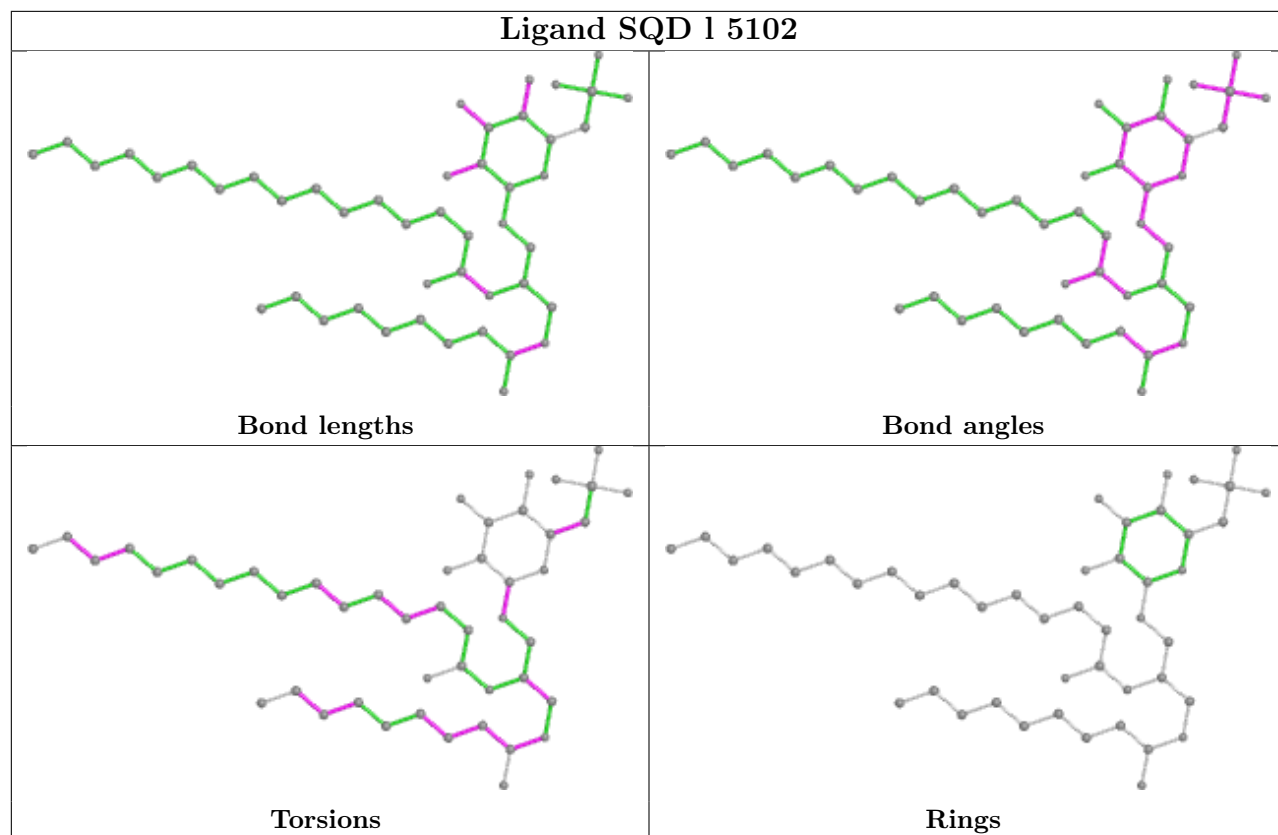


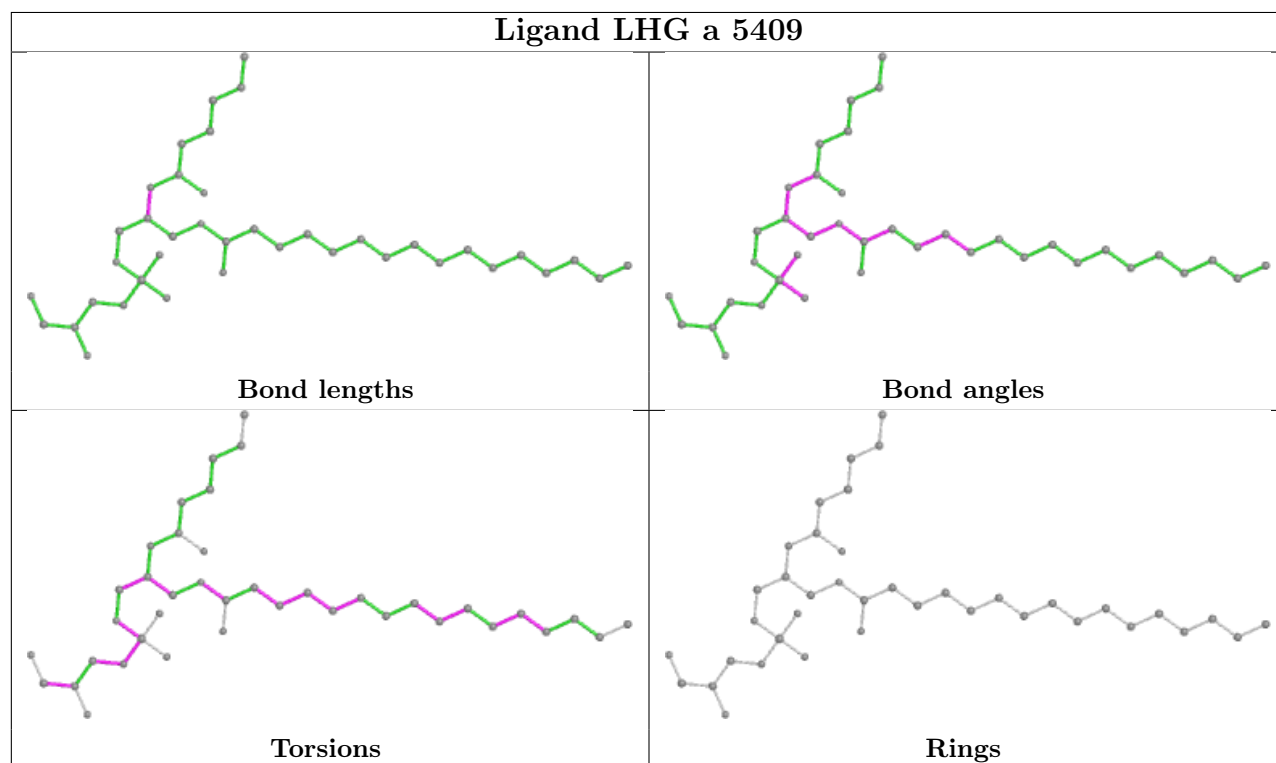
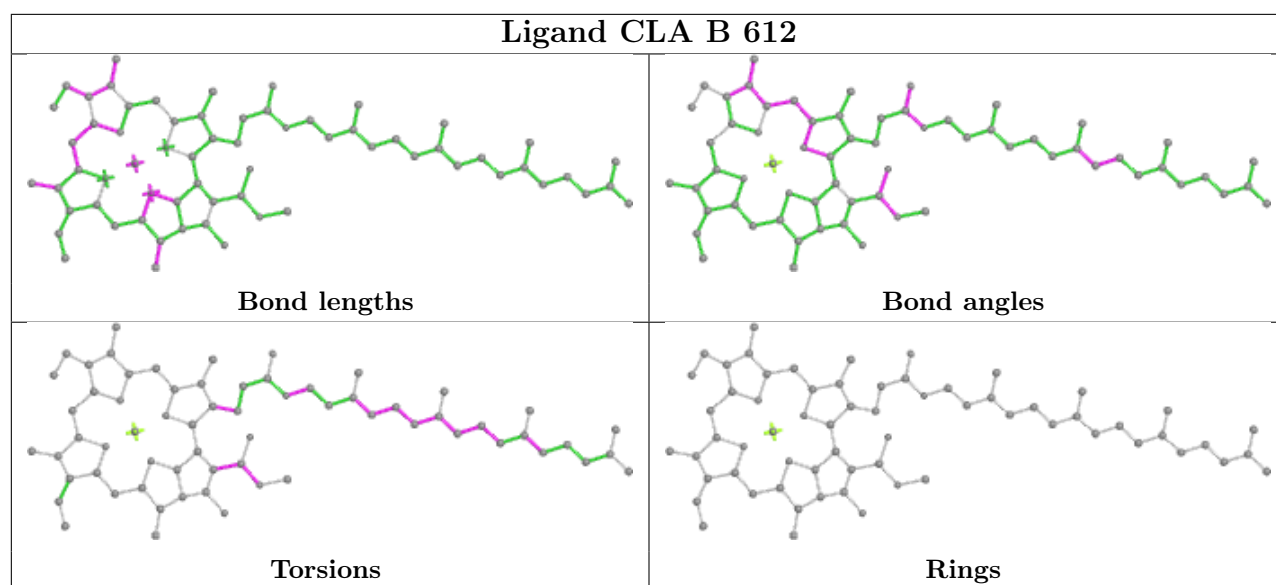


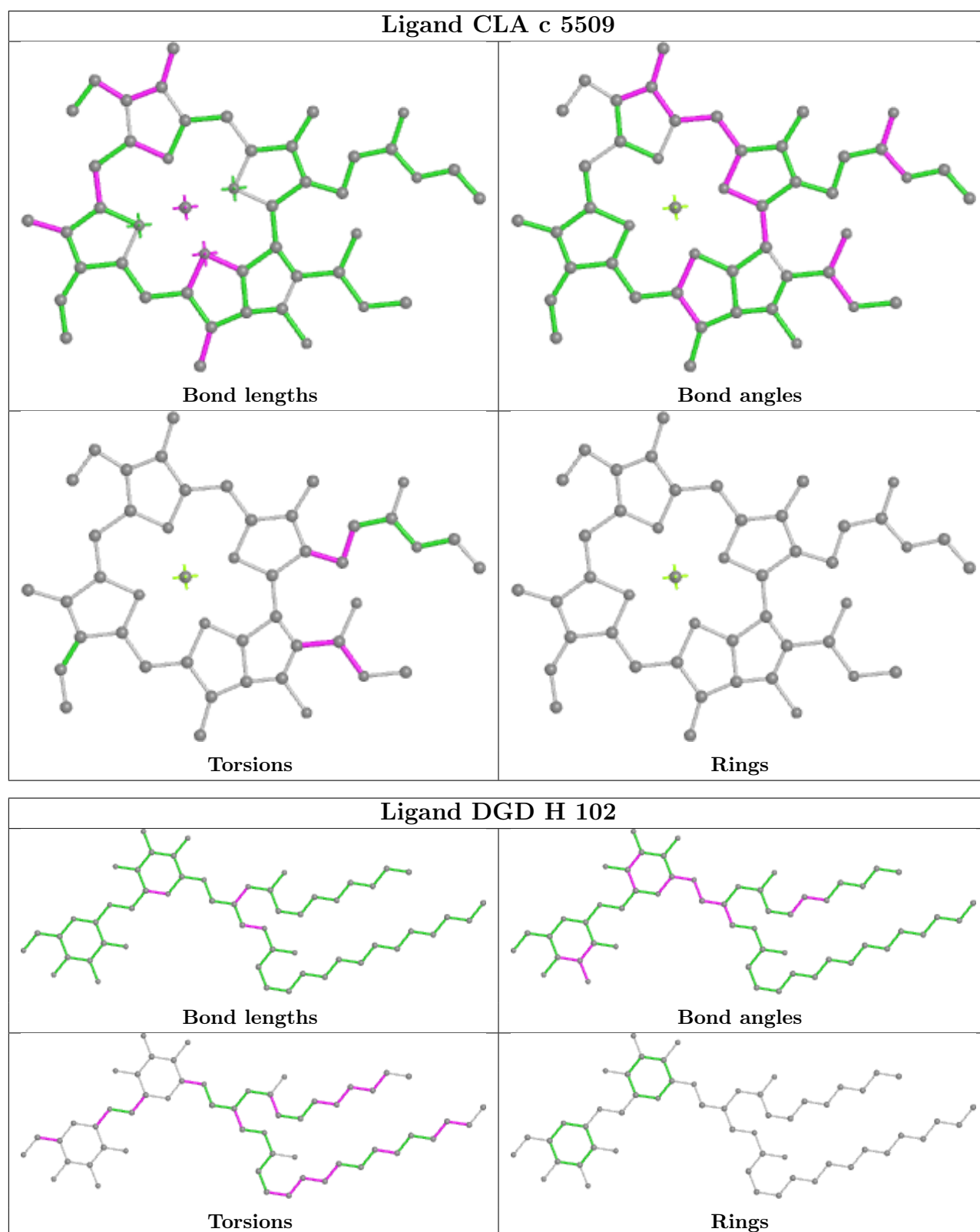


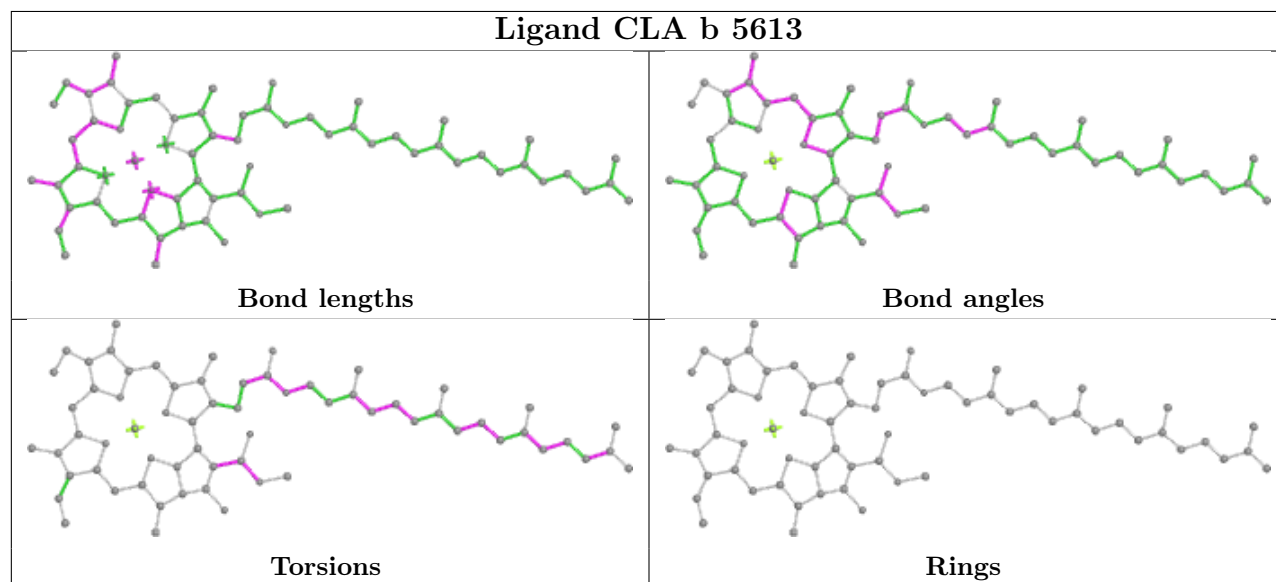
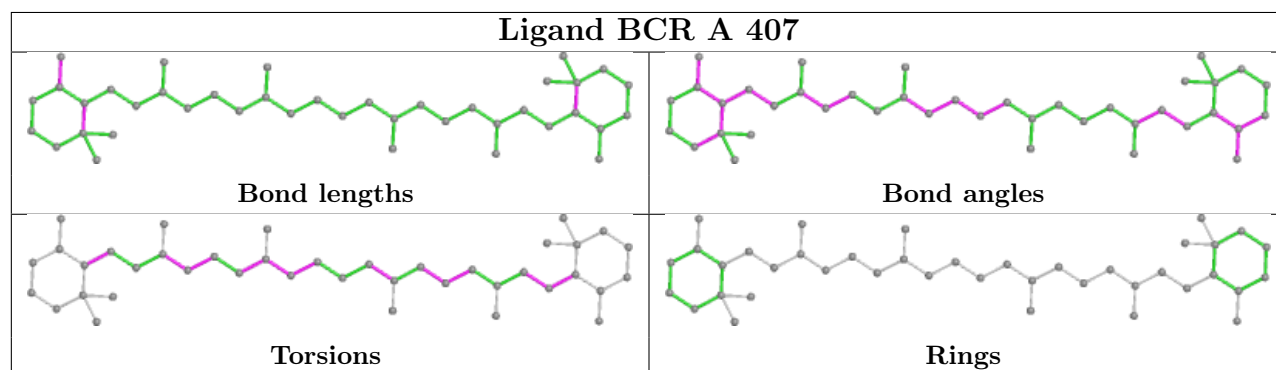
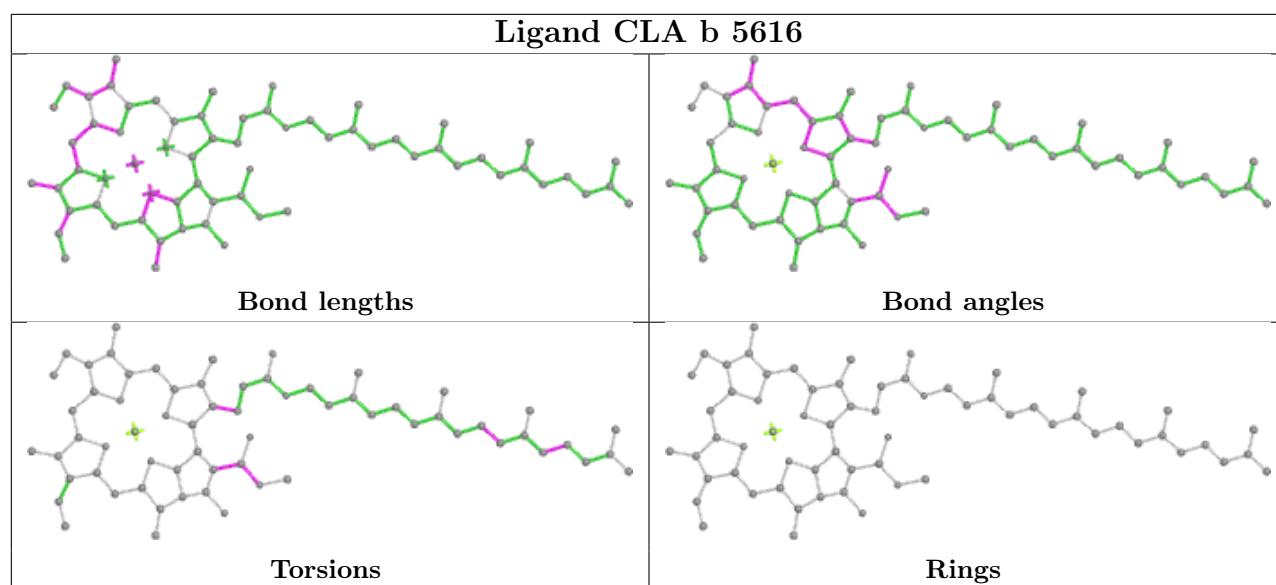


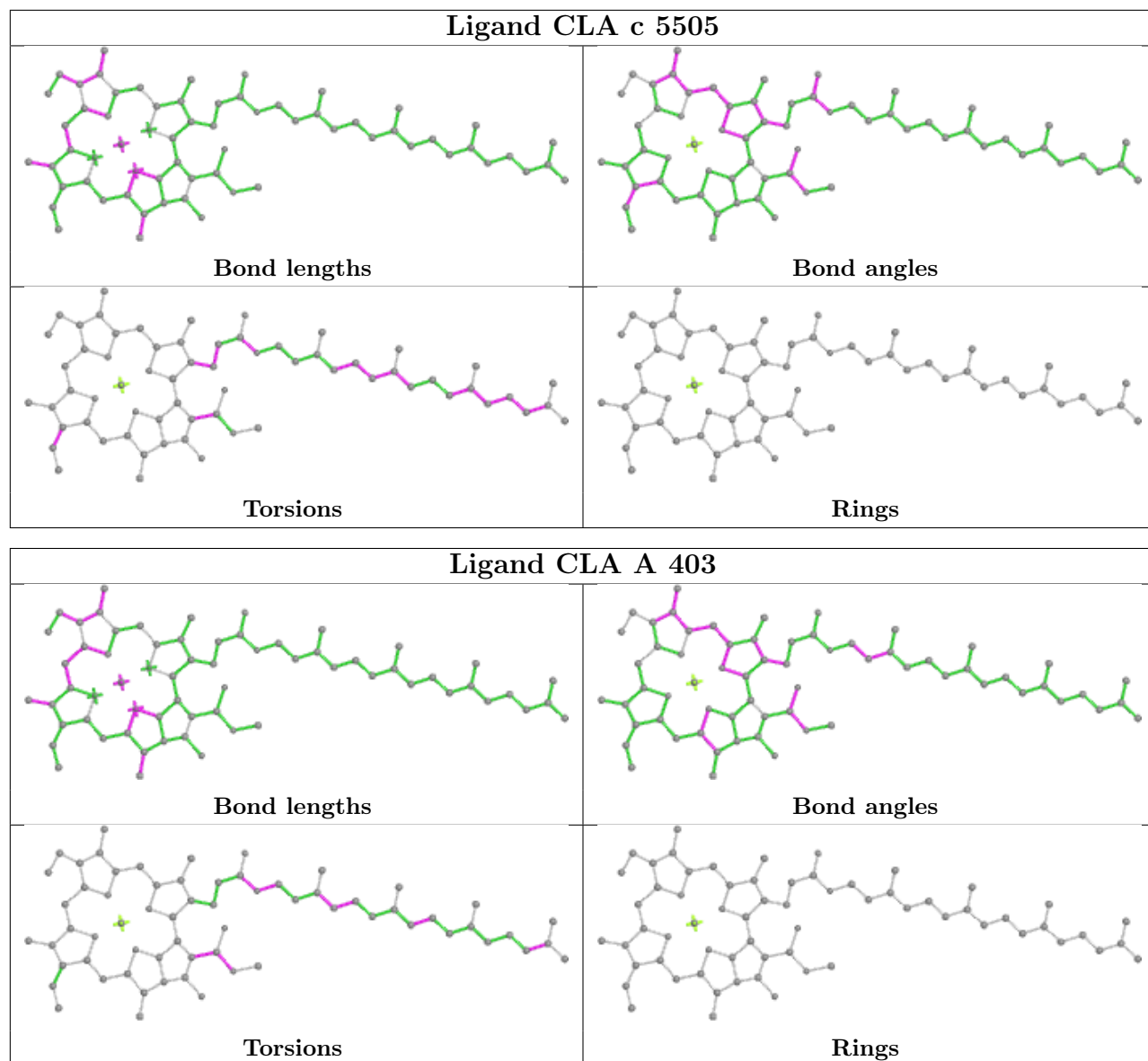


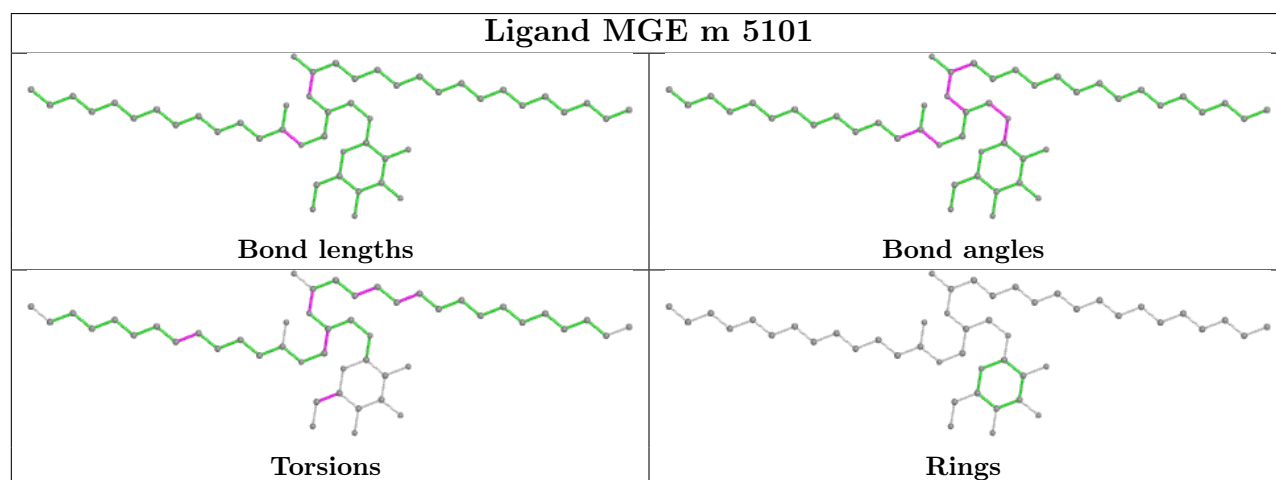
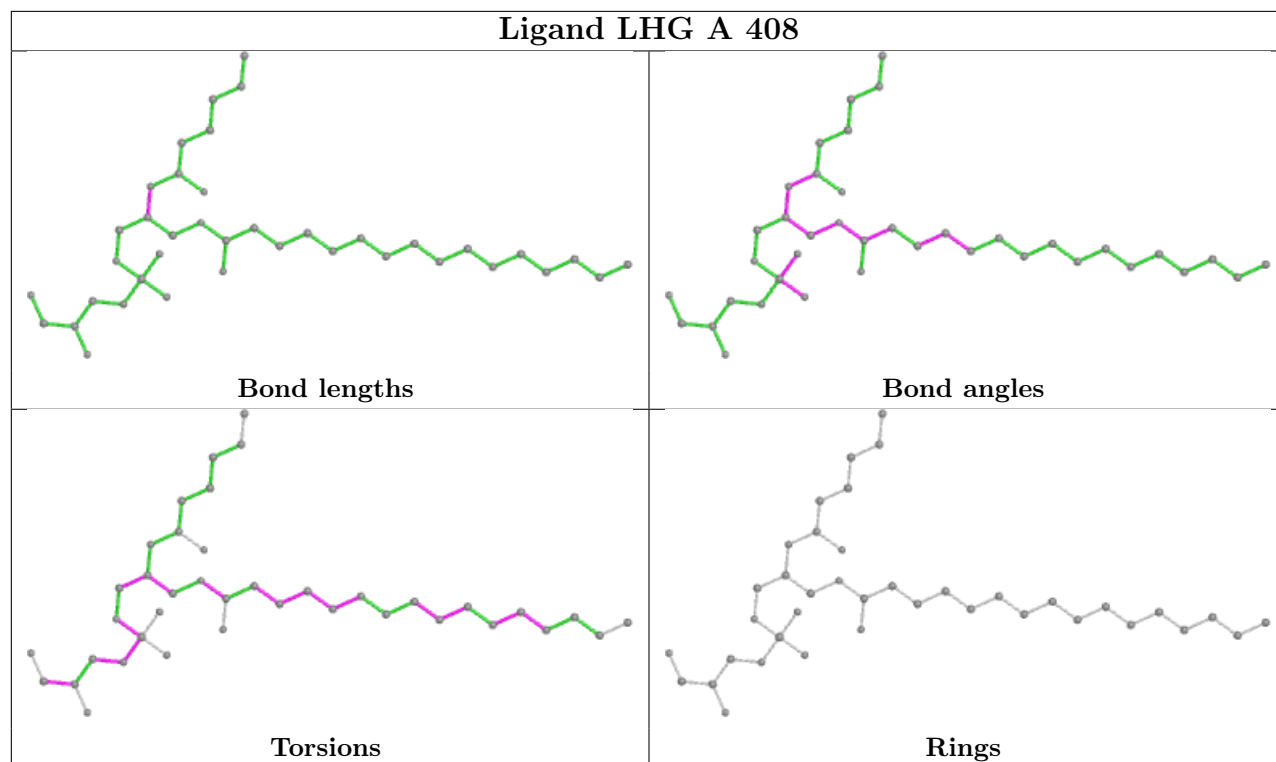


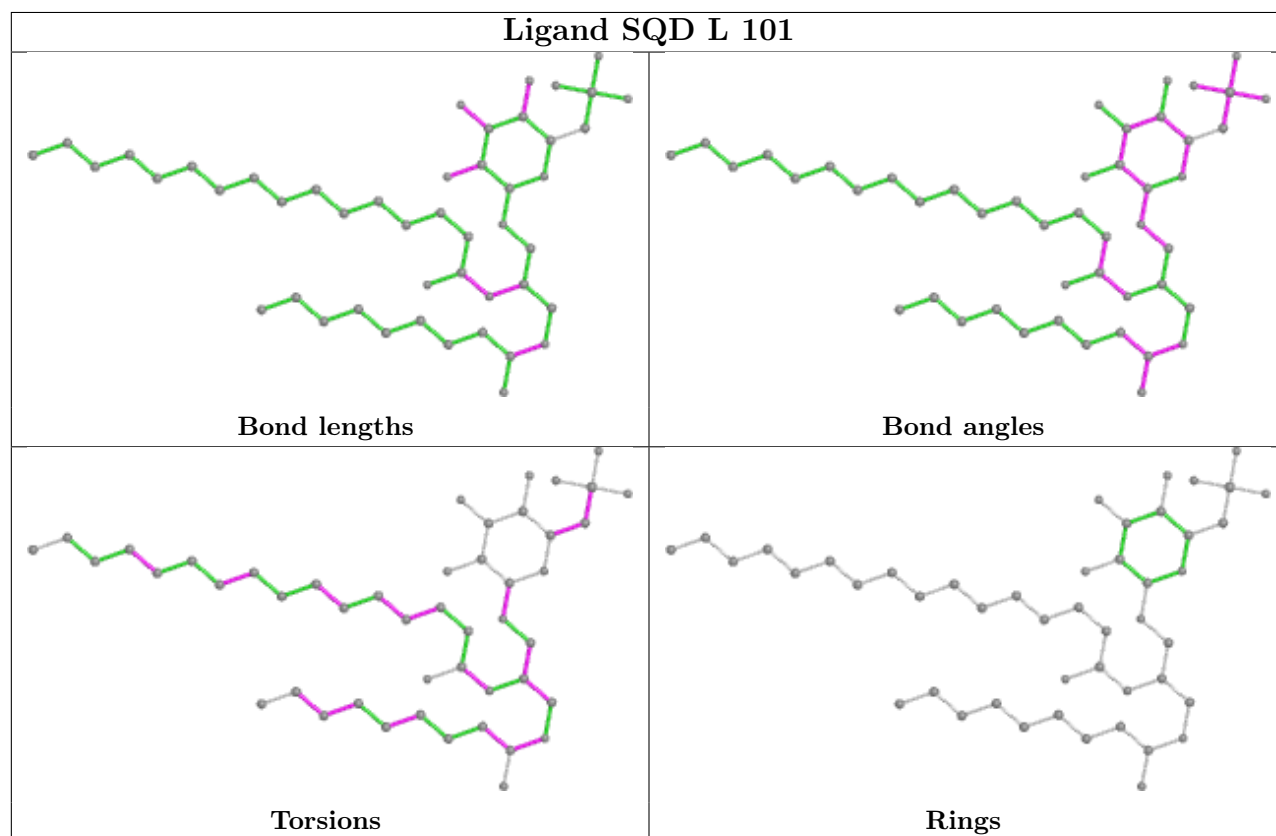
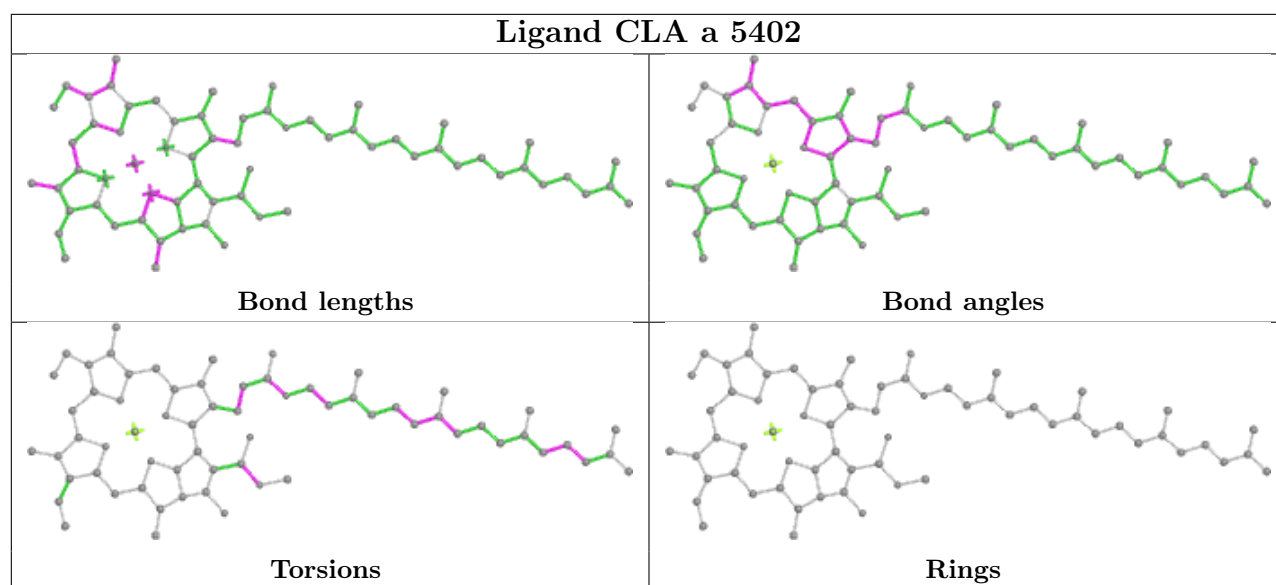




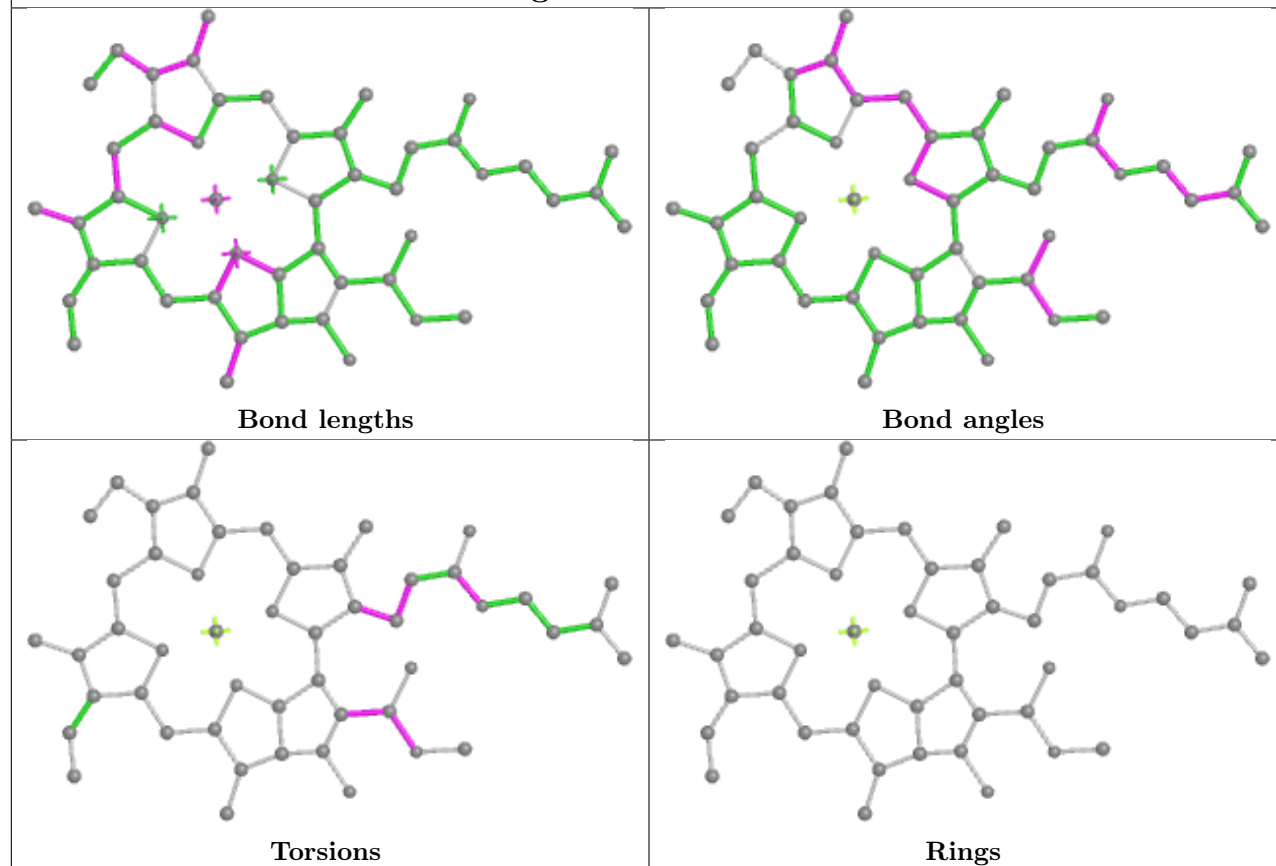




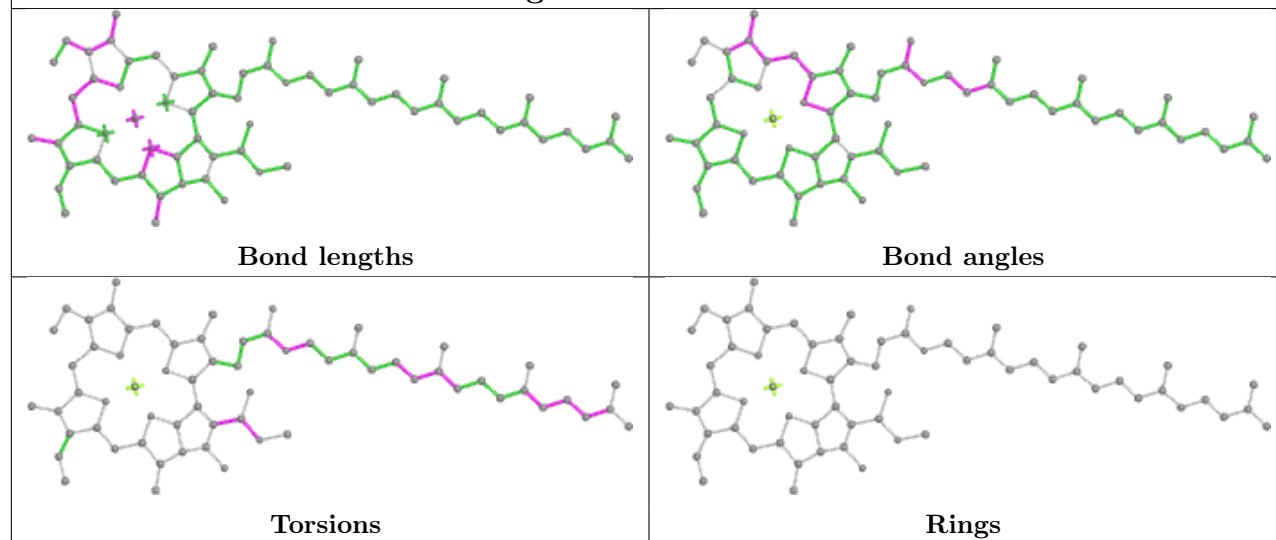


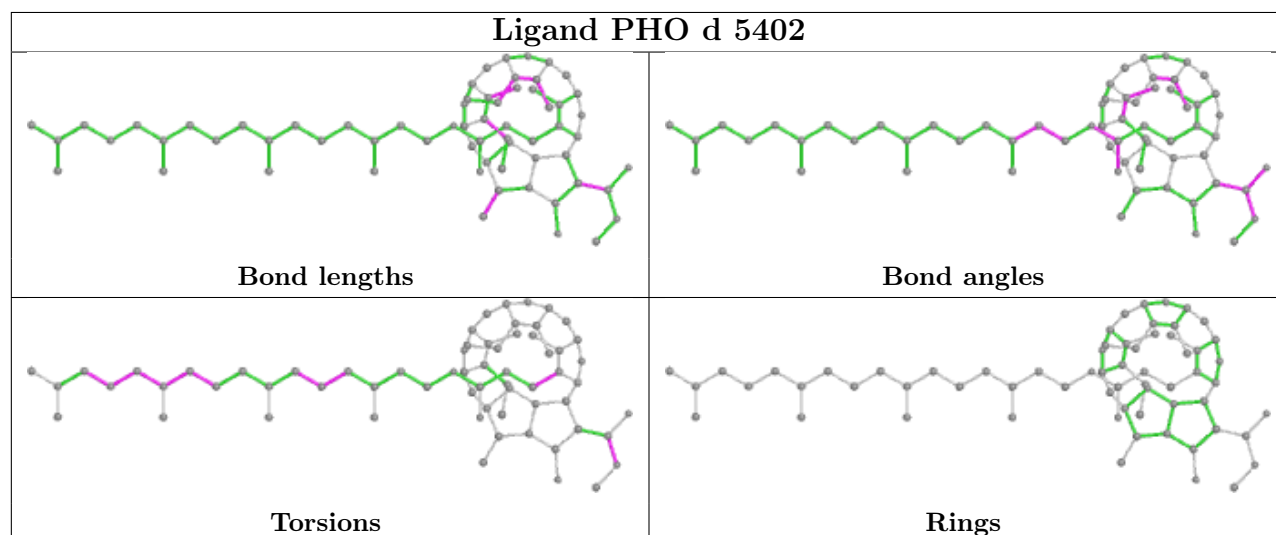
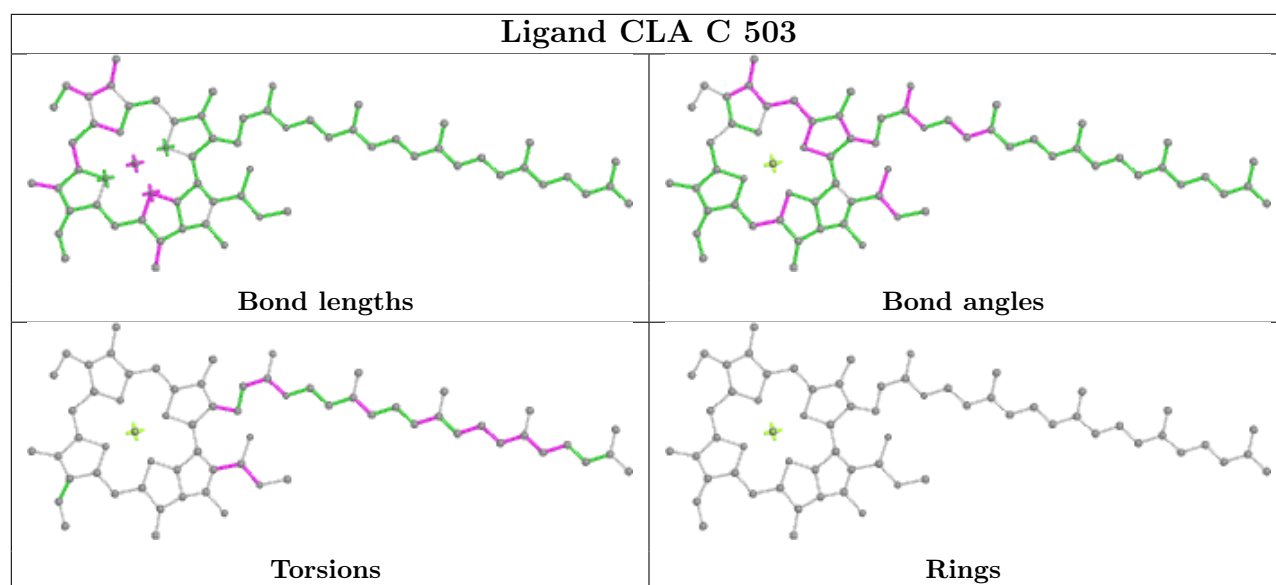


Ligand CLA D 405

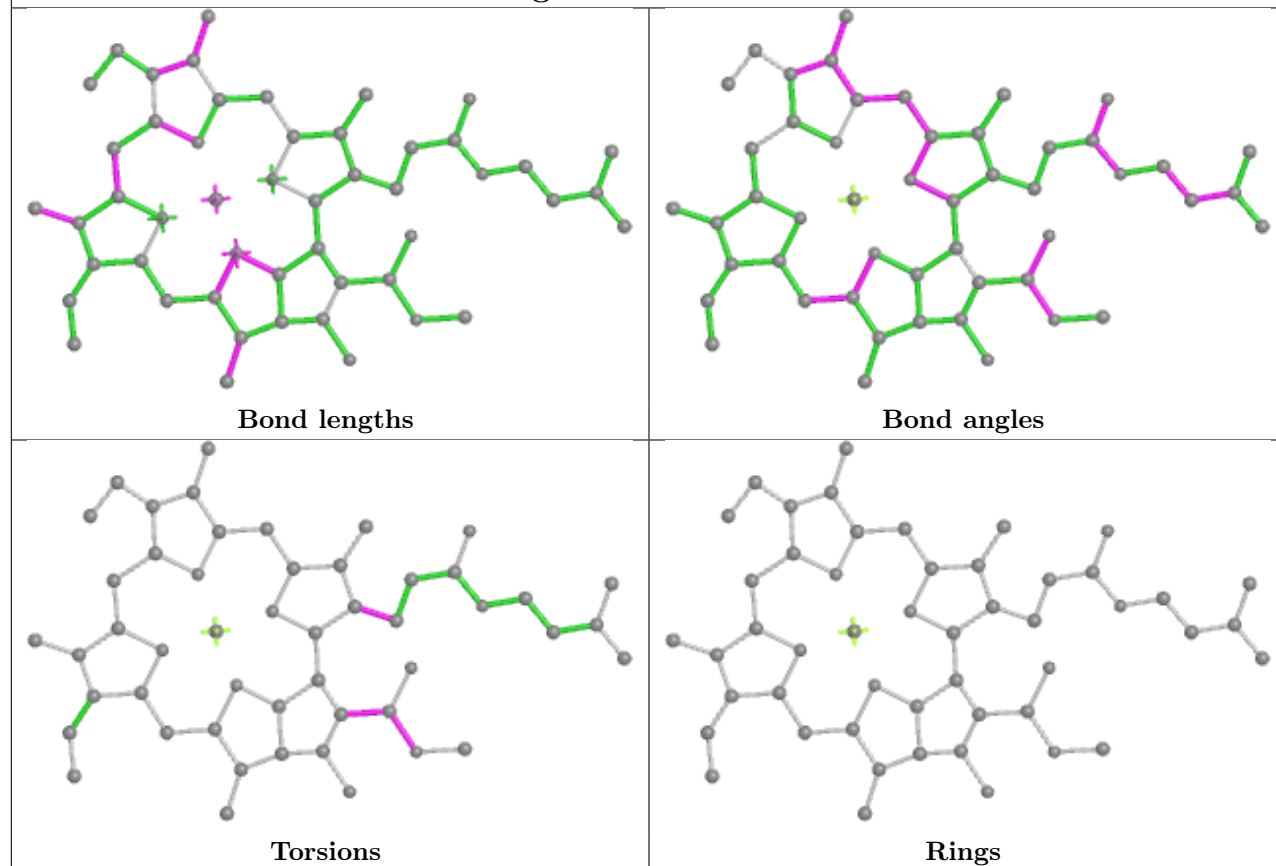


Ligand CLA b 5615

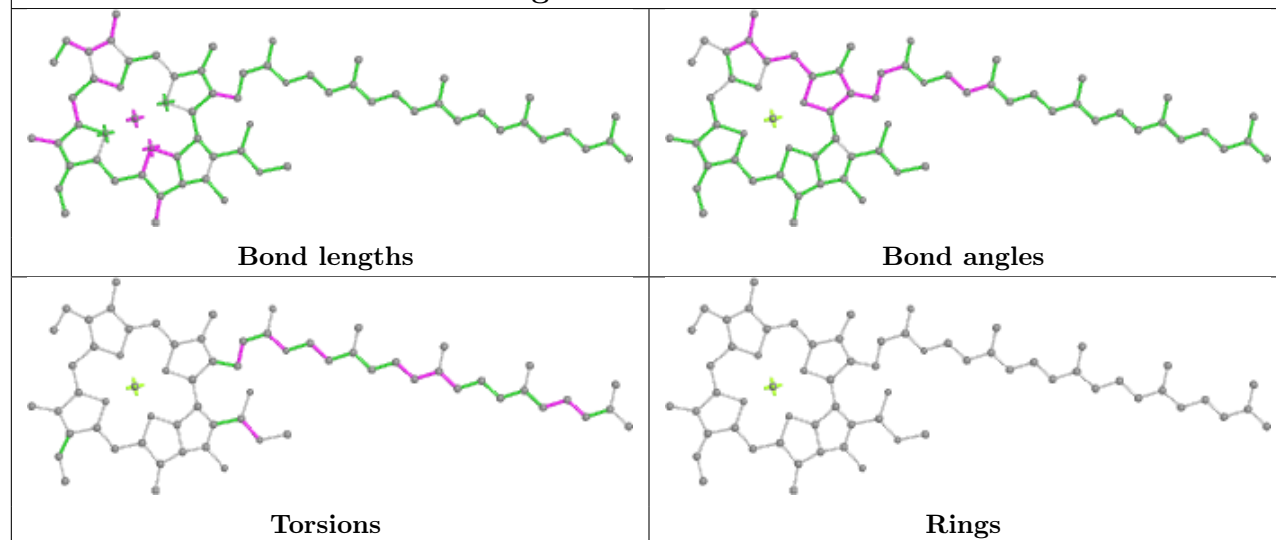


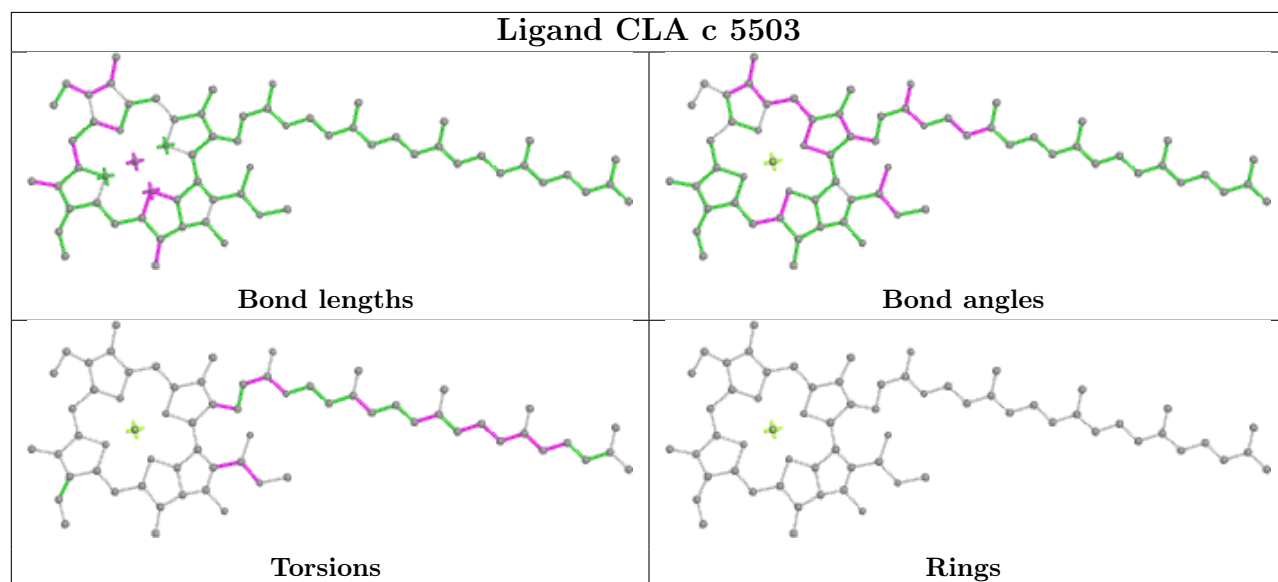
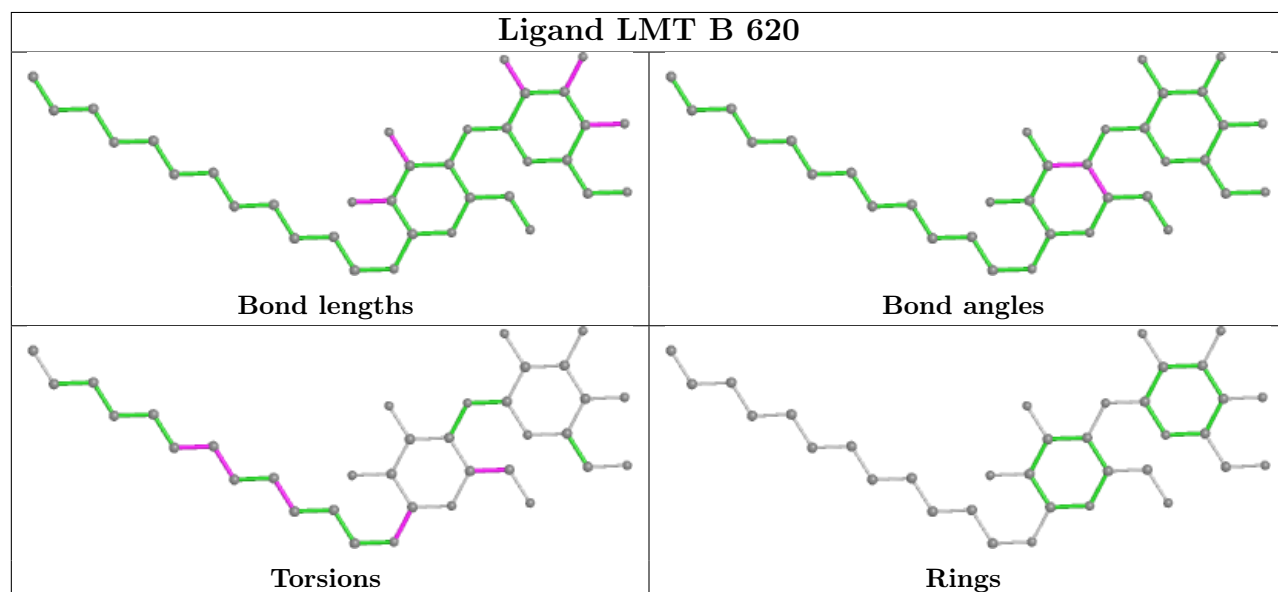
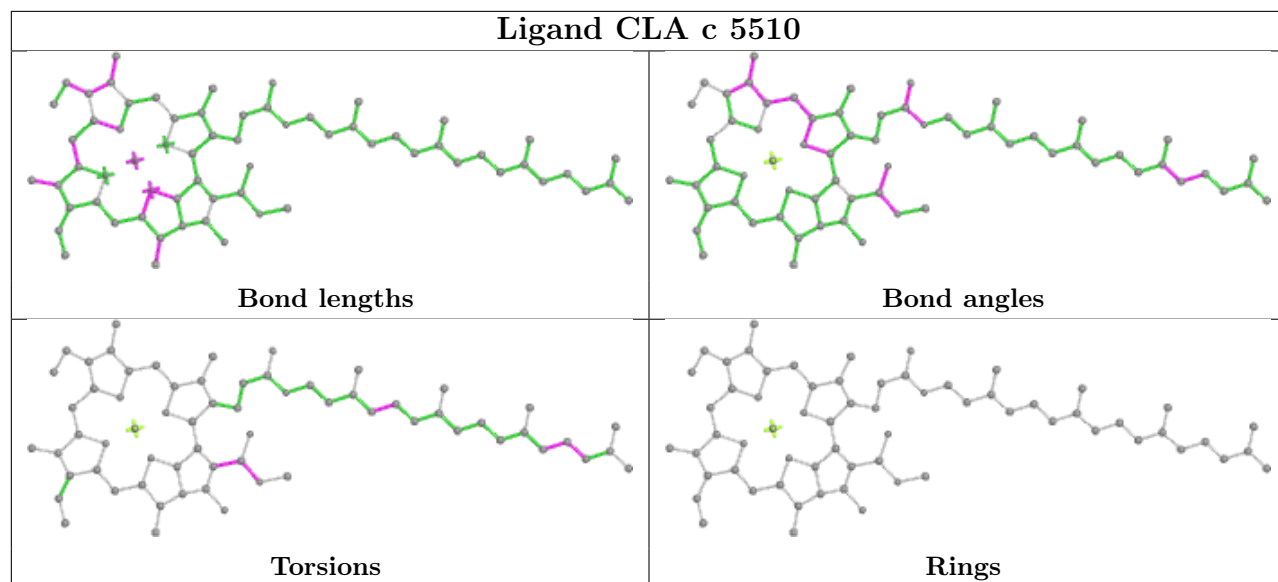


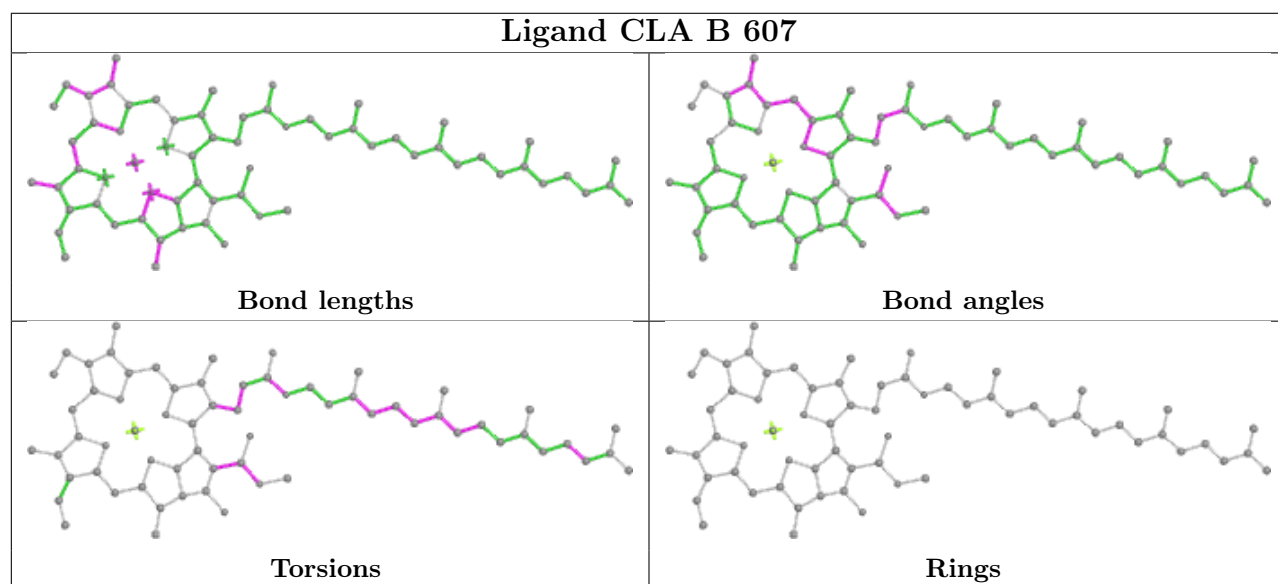
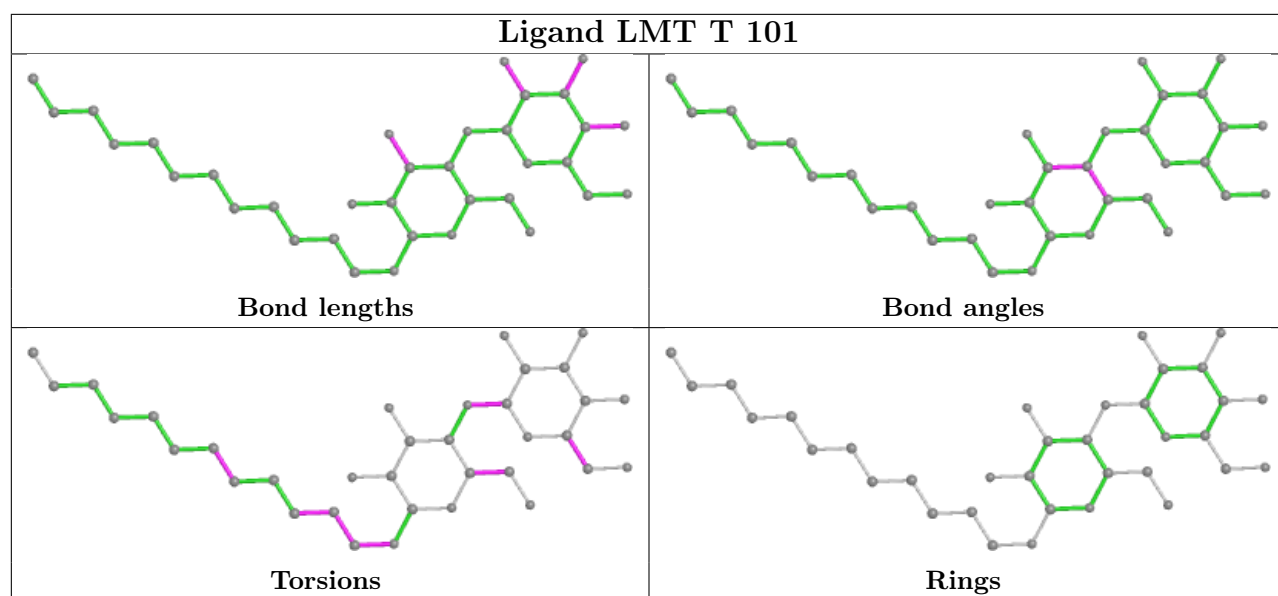
Ligand CLA C 513

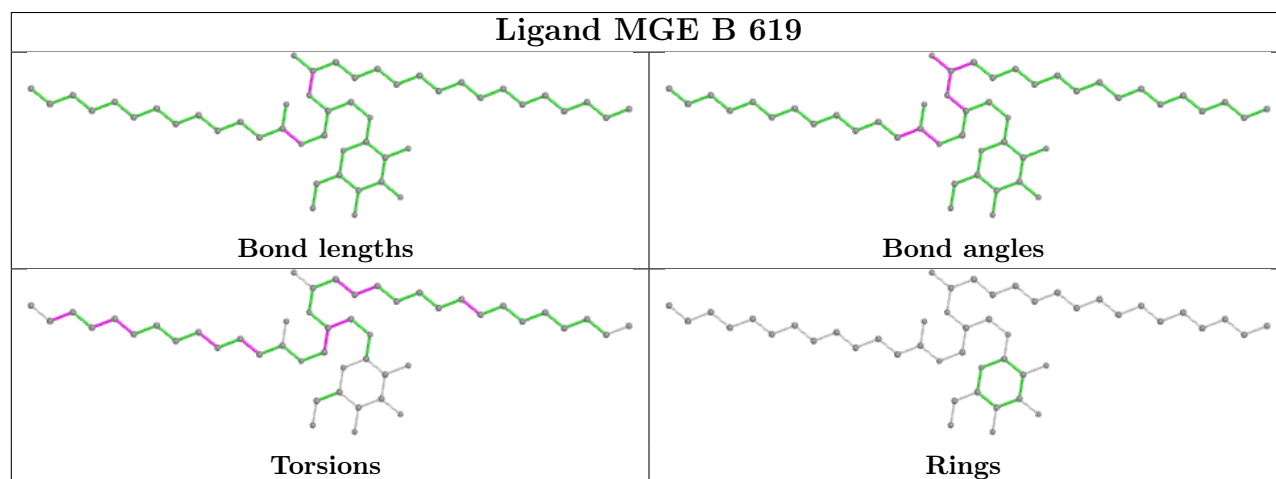
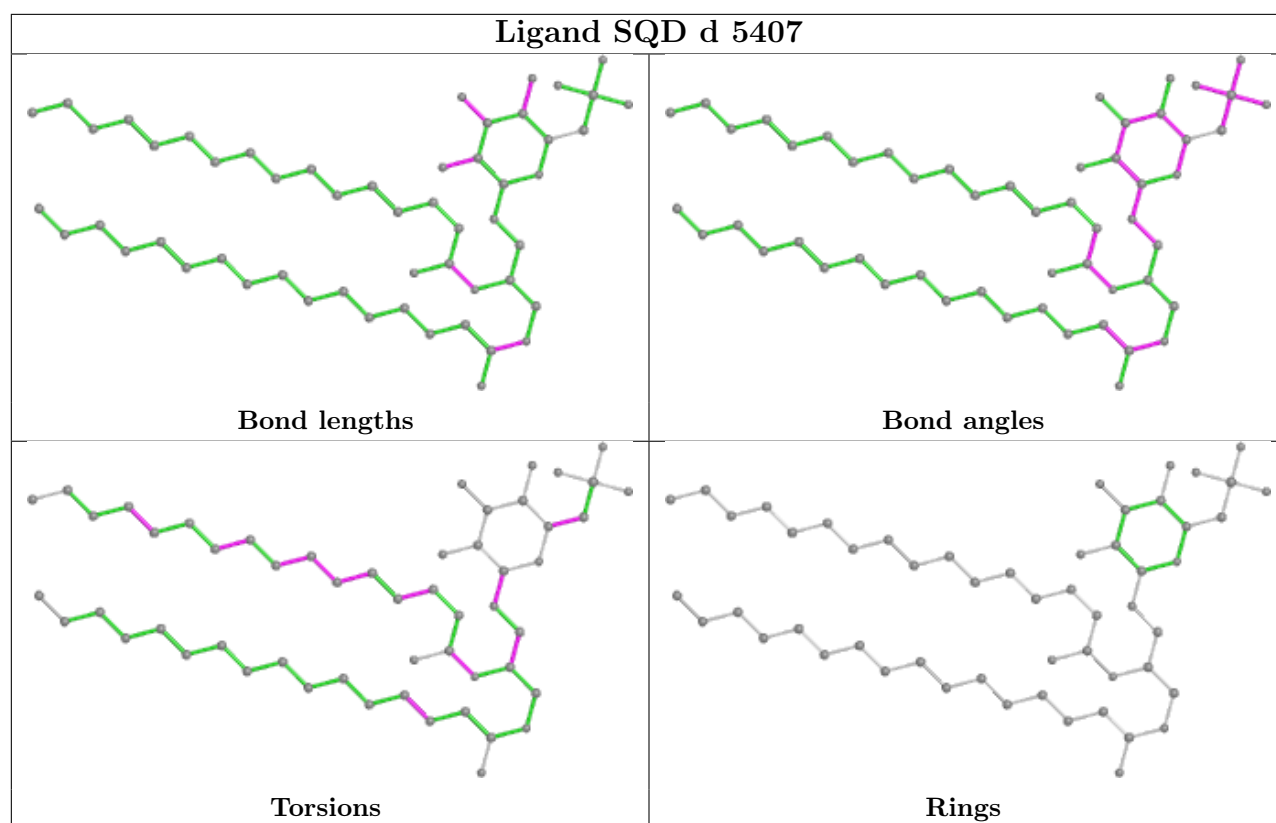


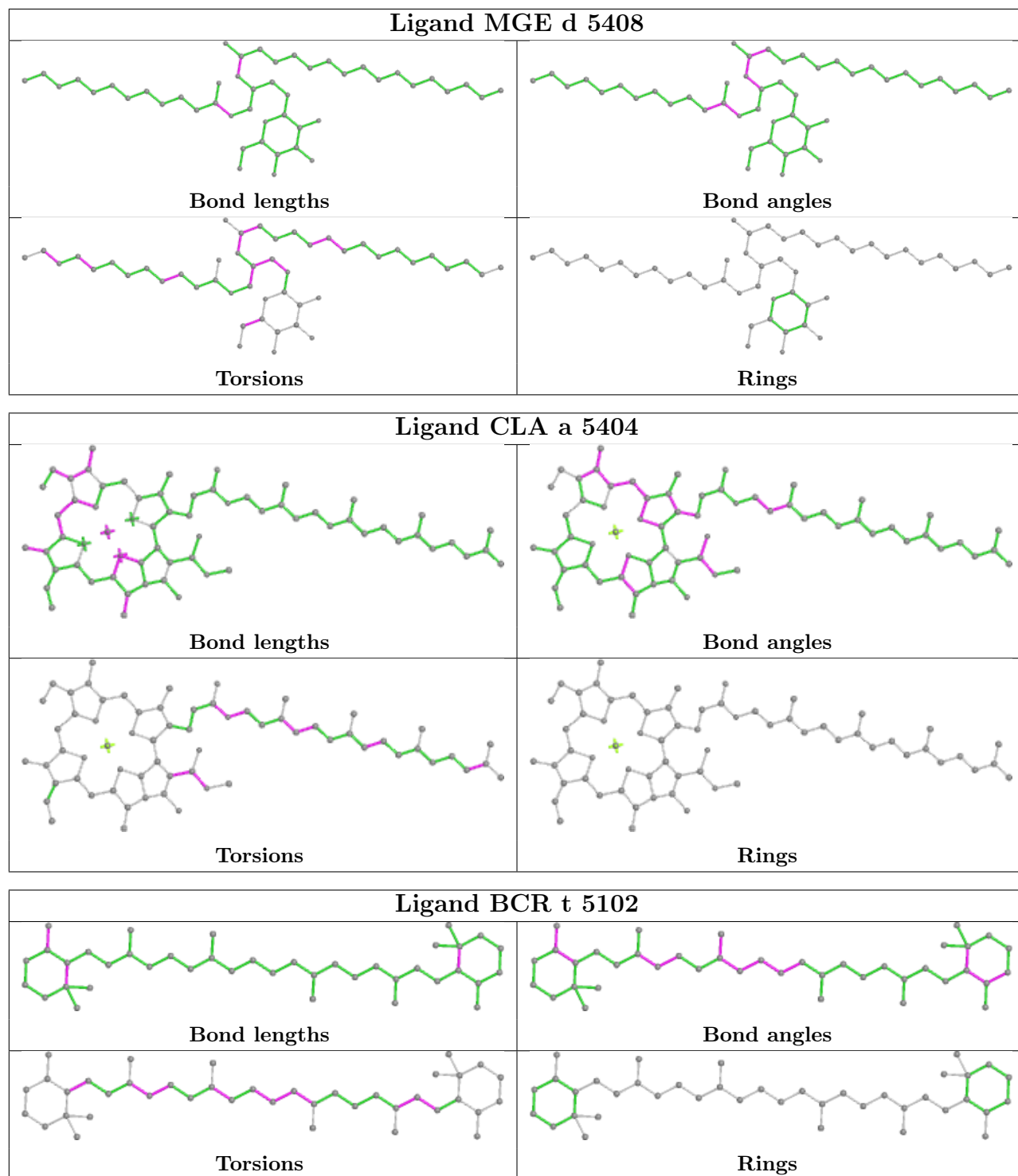
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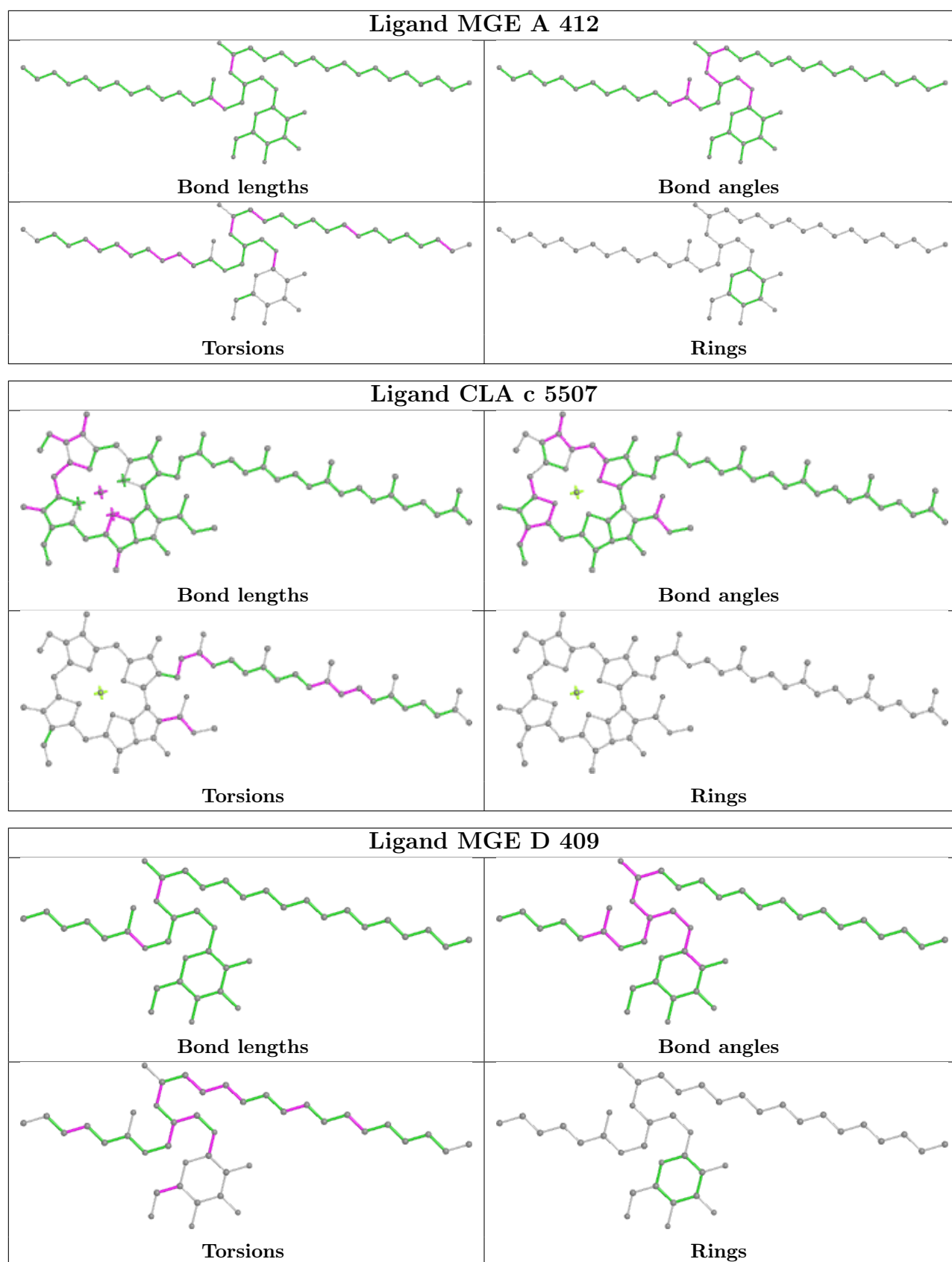




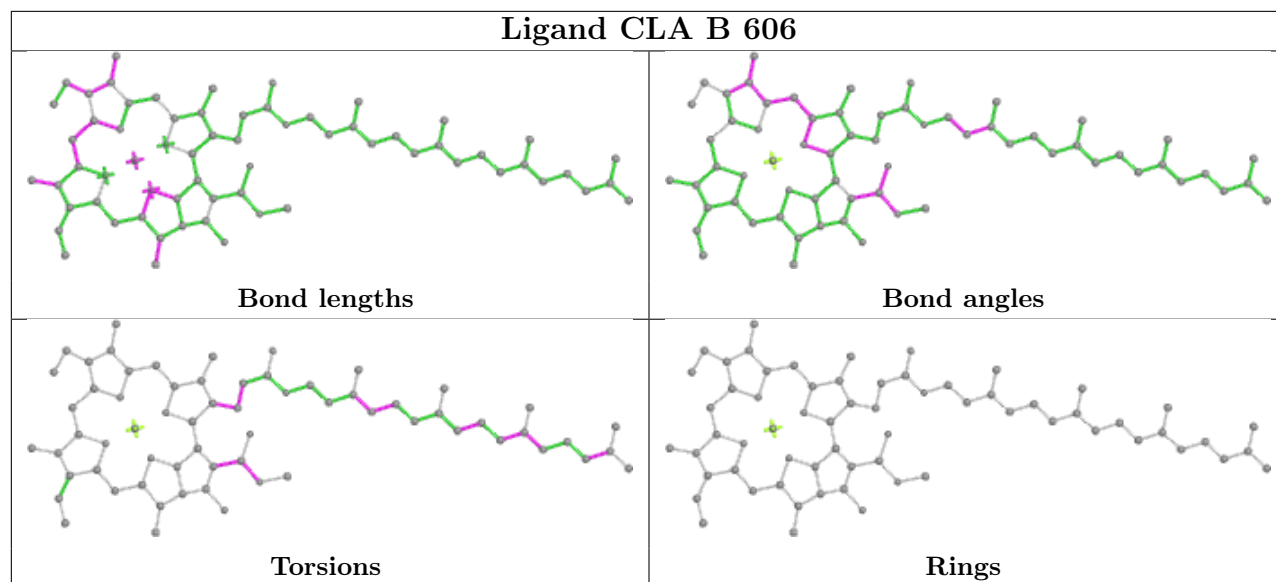




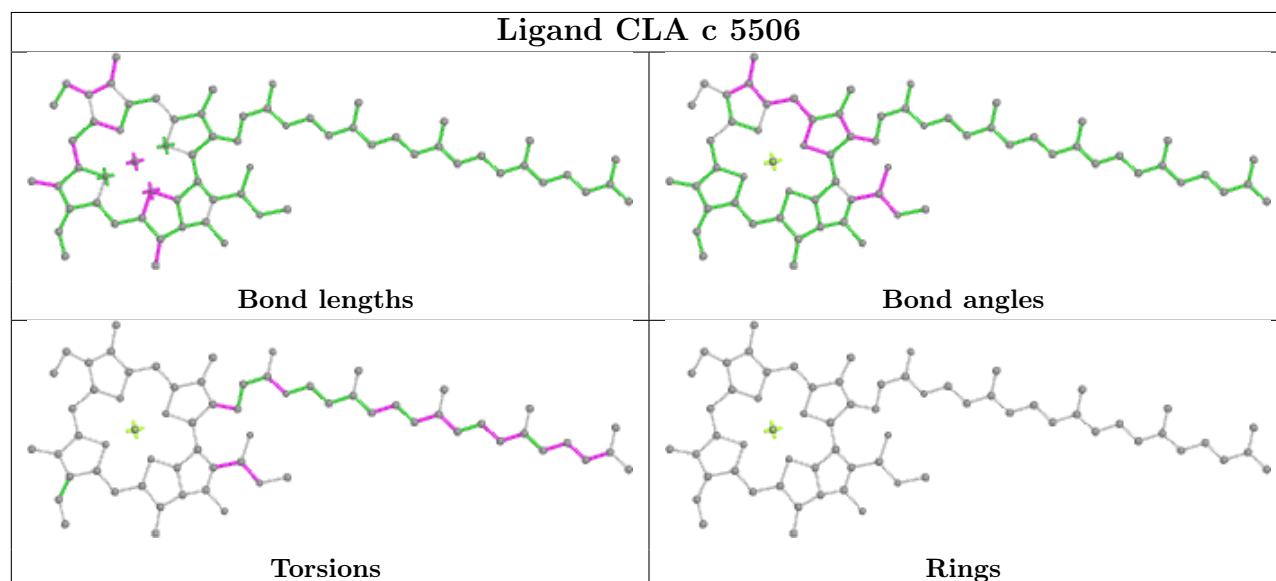




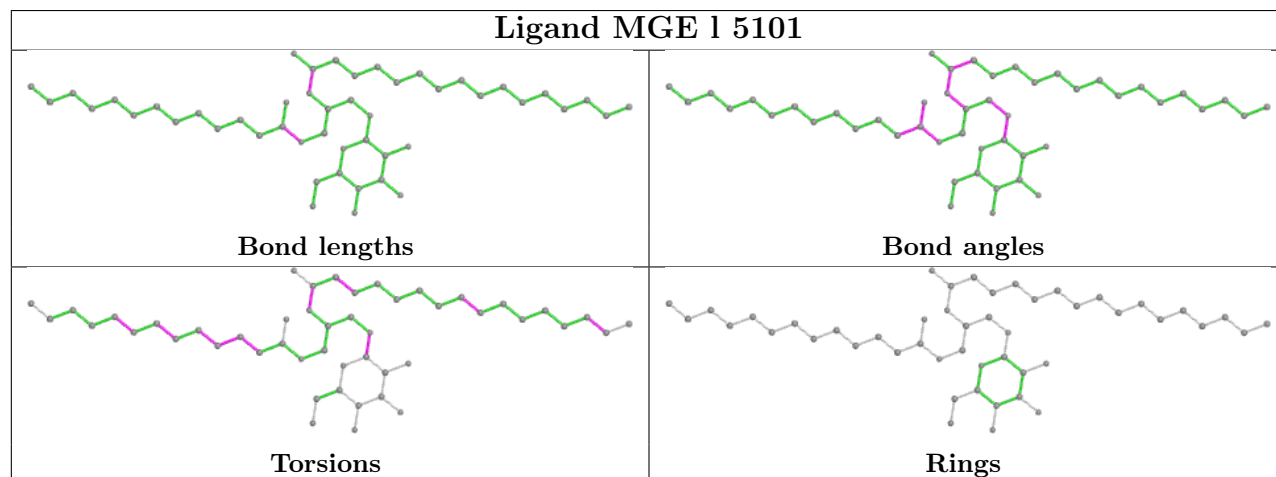
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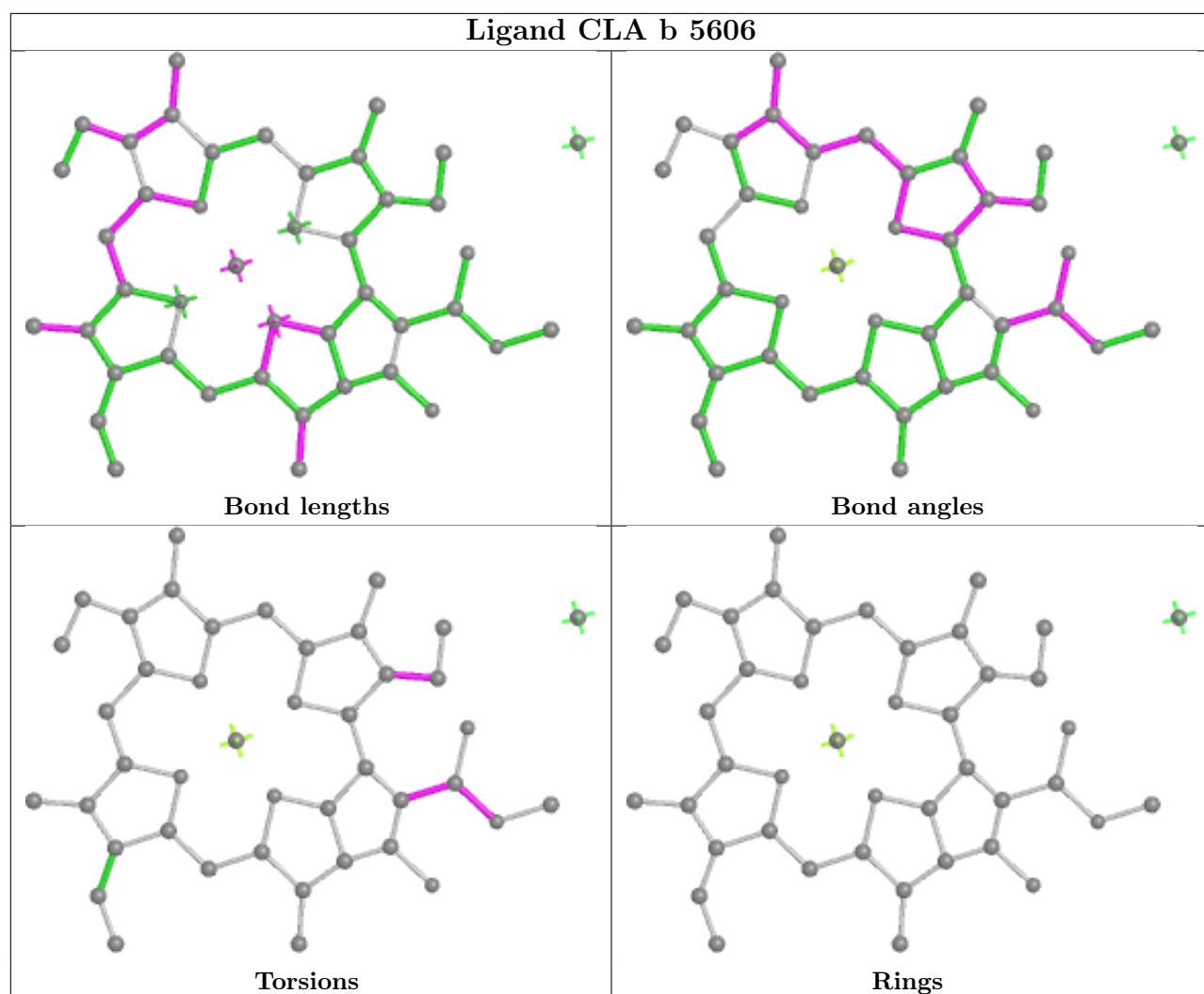


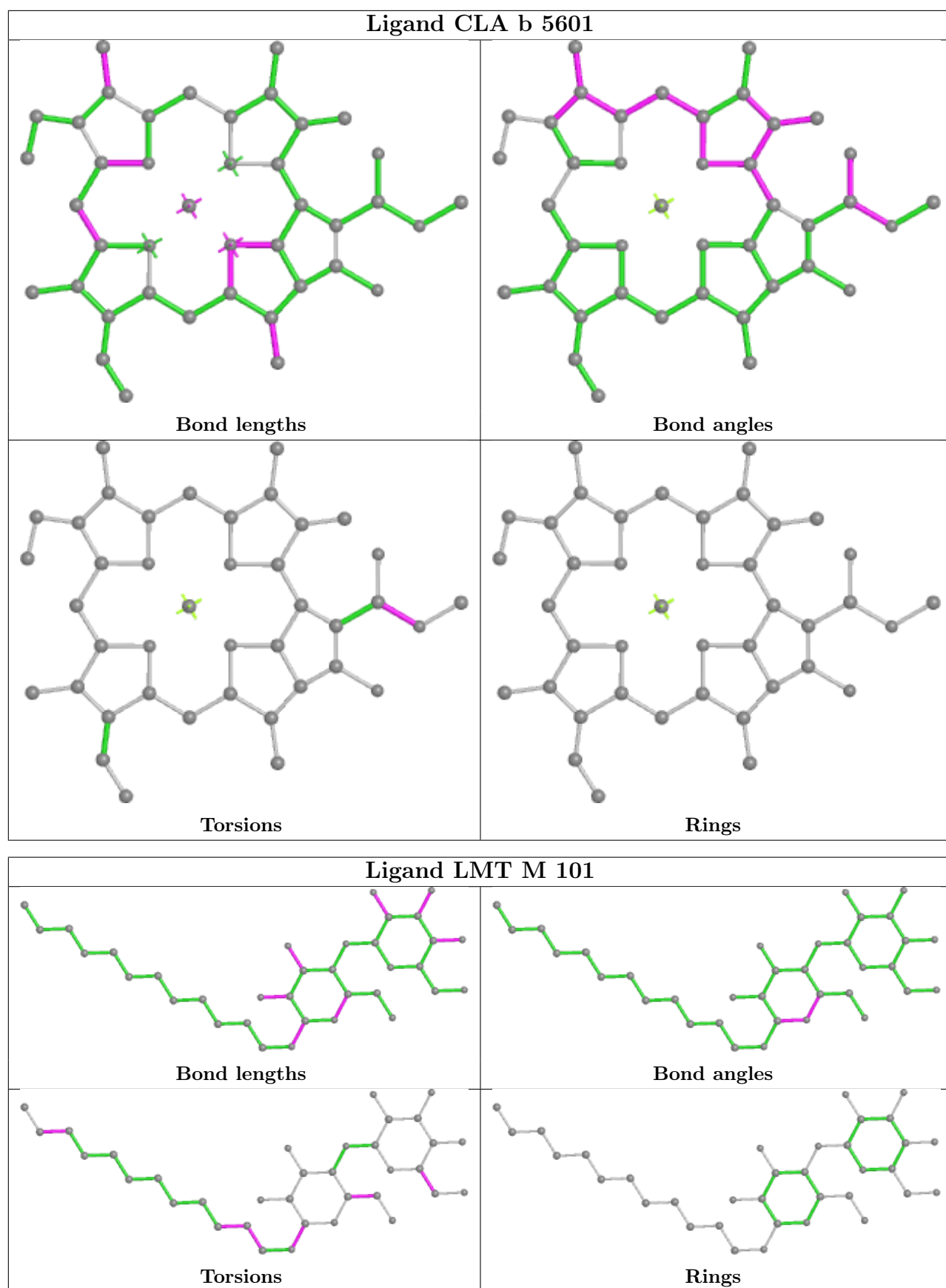
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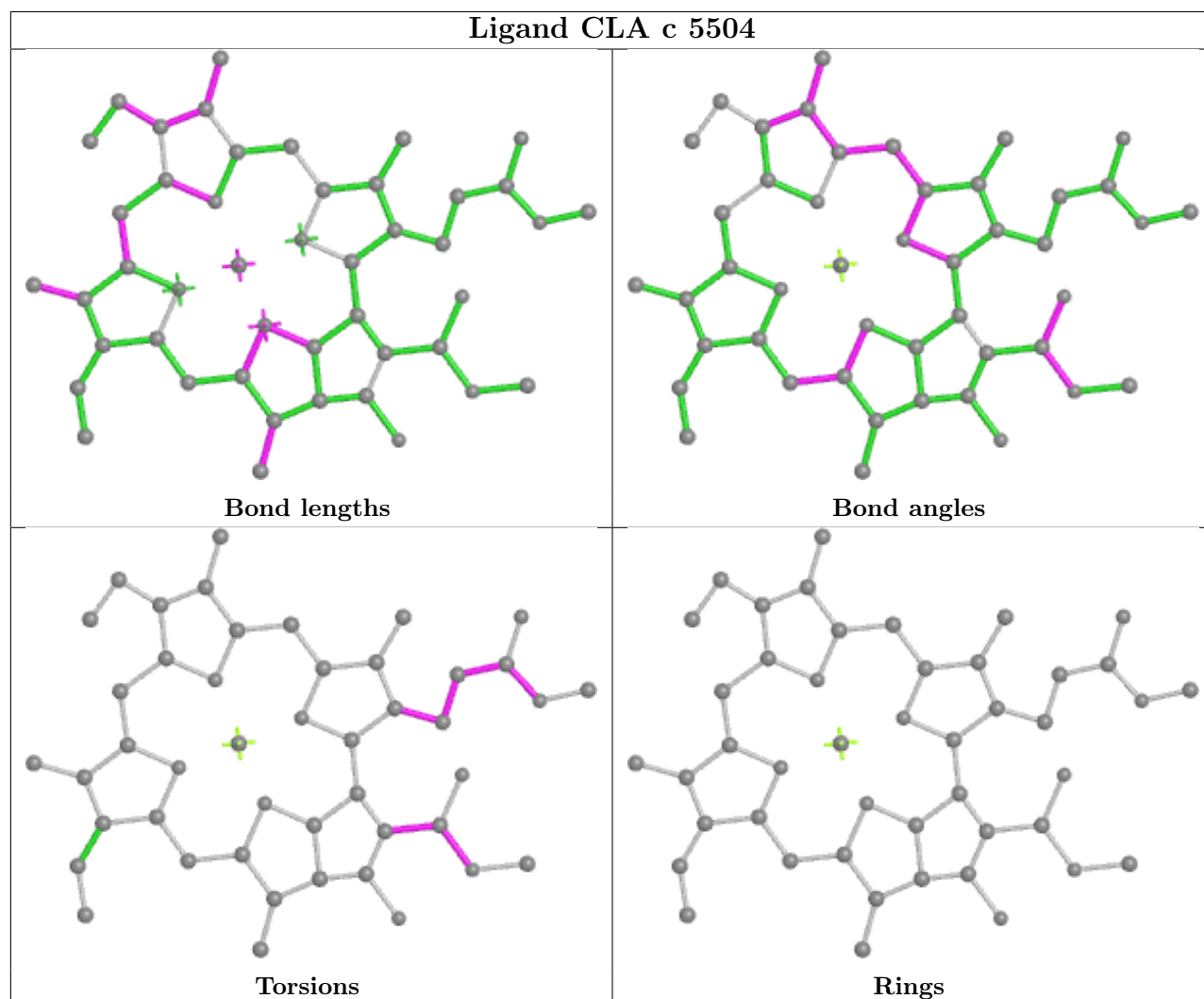
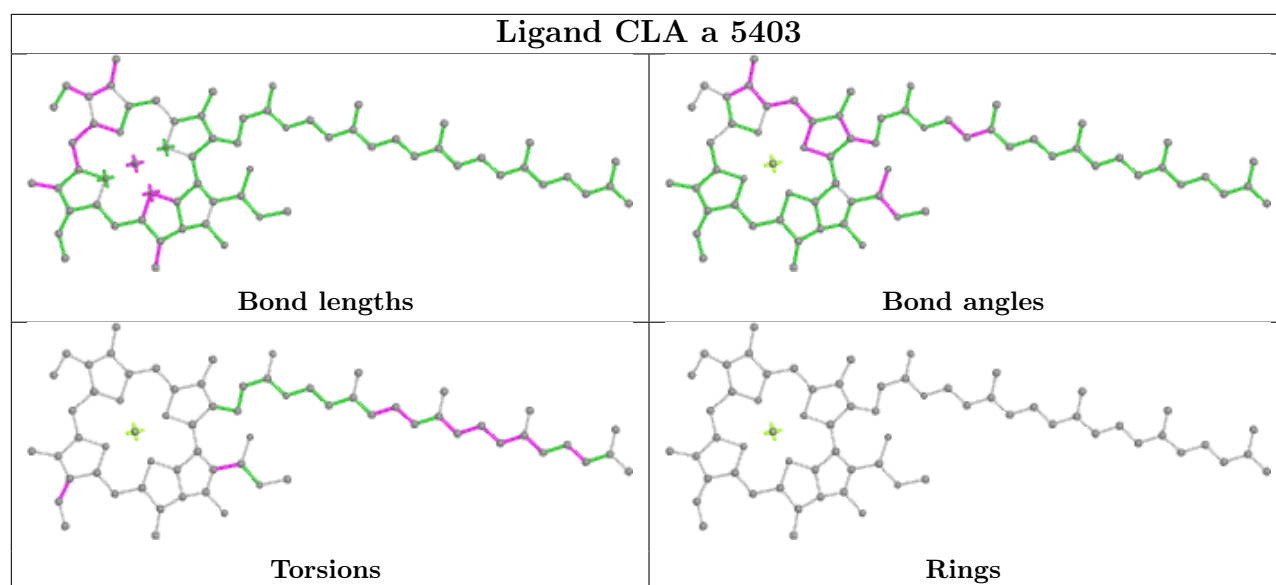


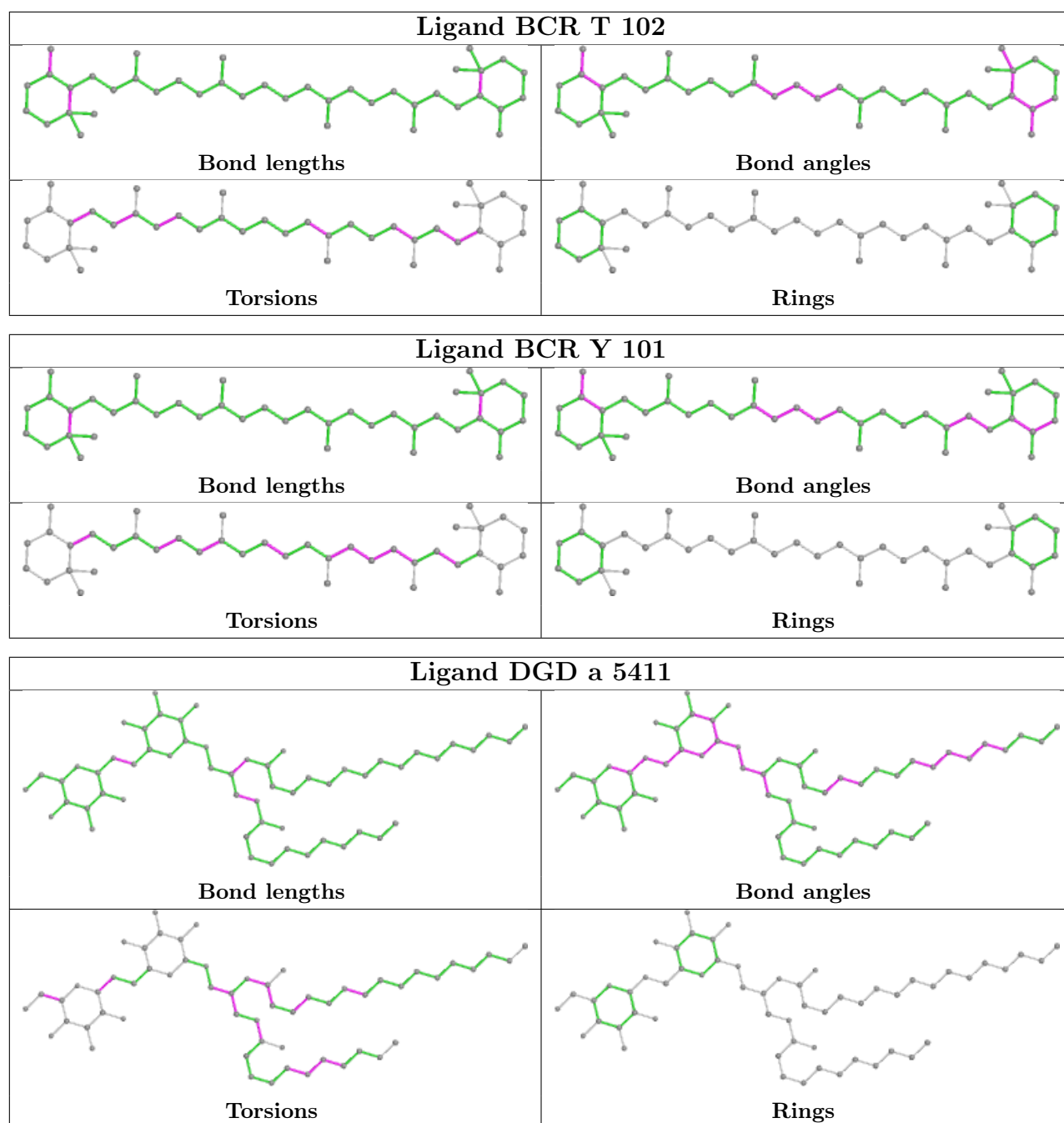
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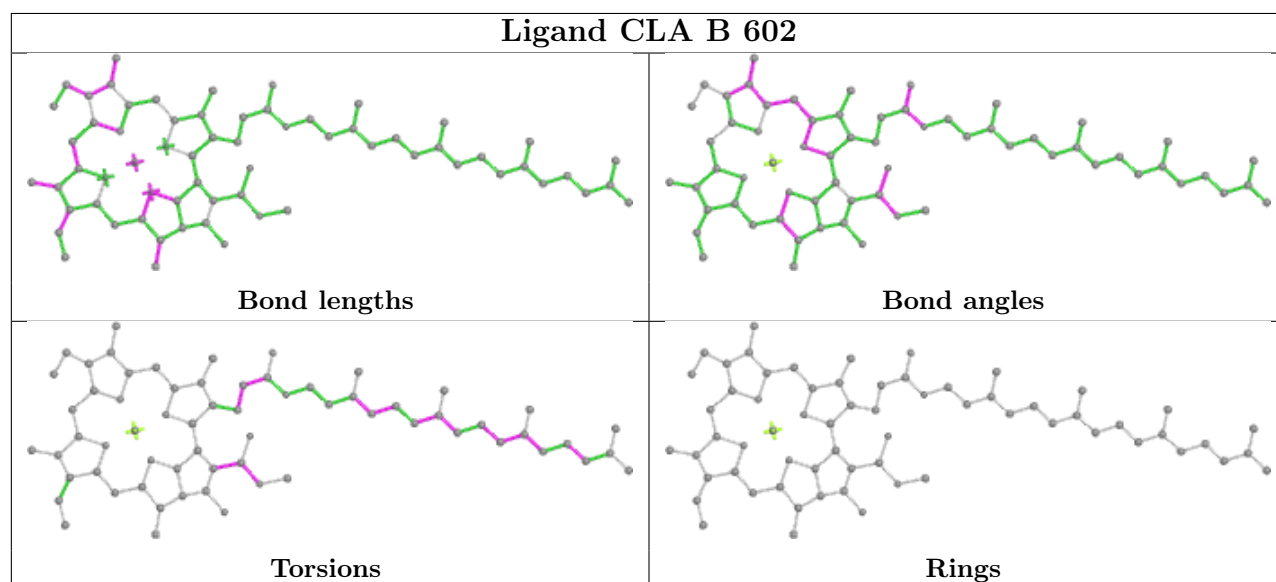
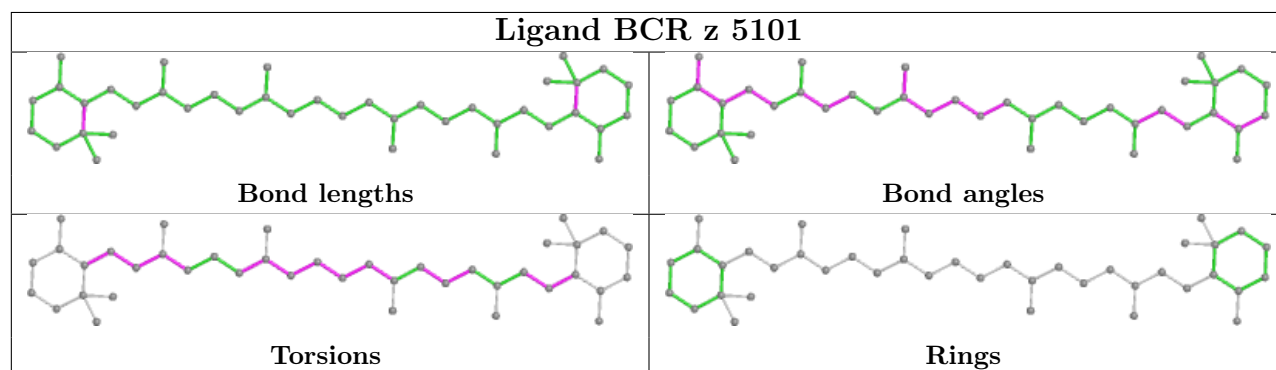
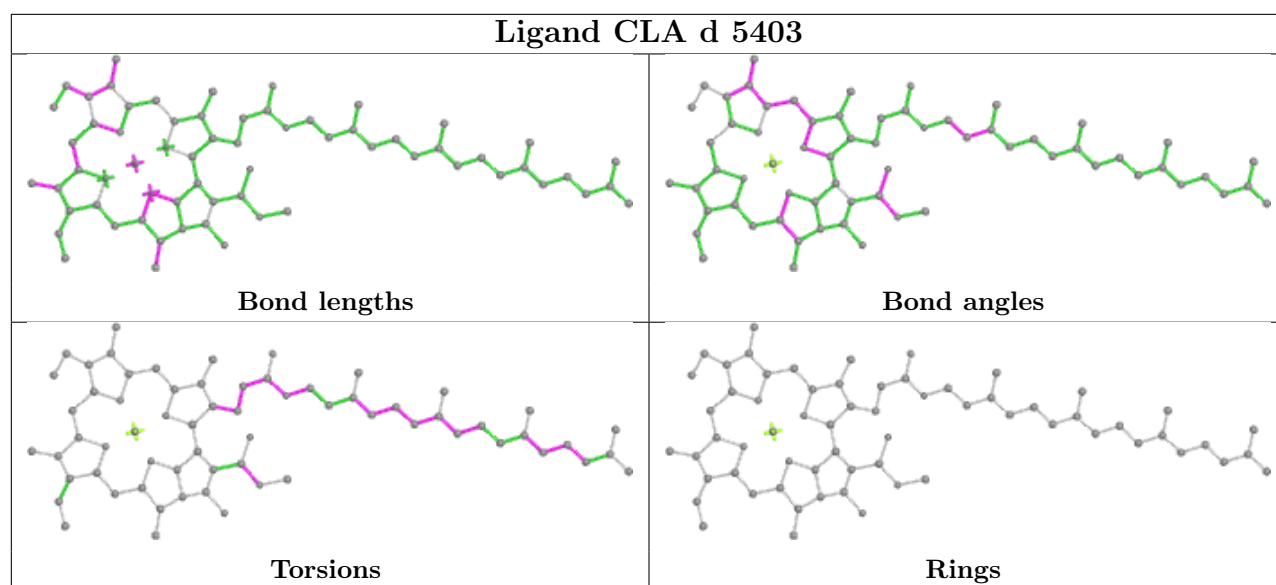


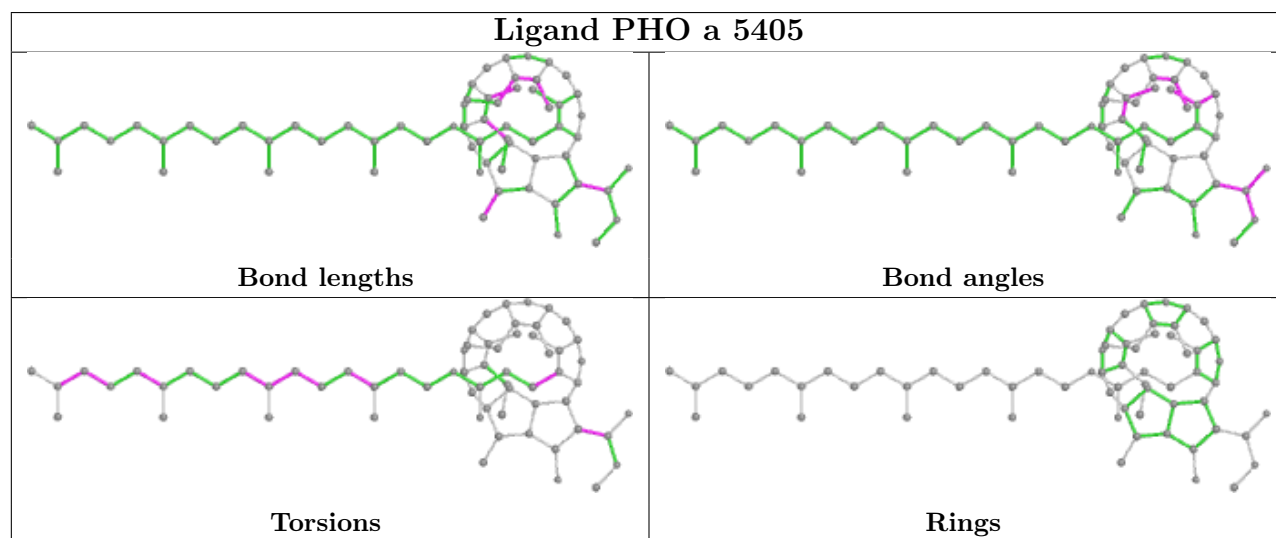
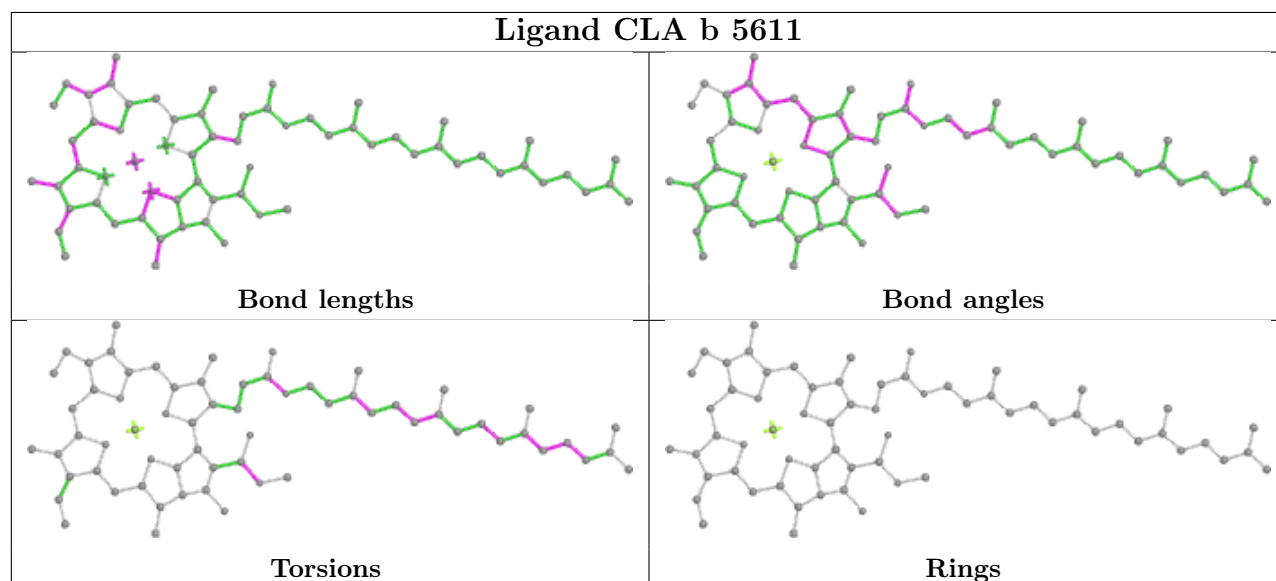
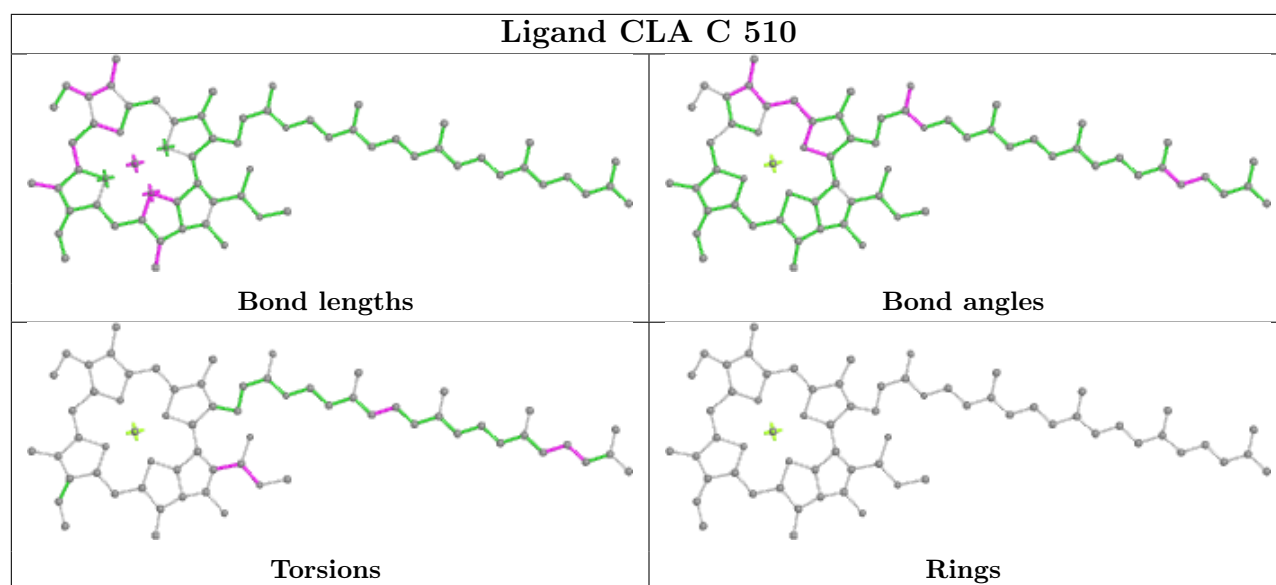


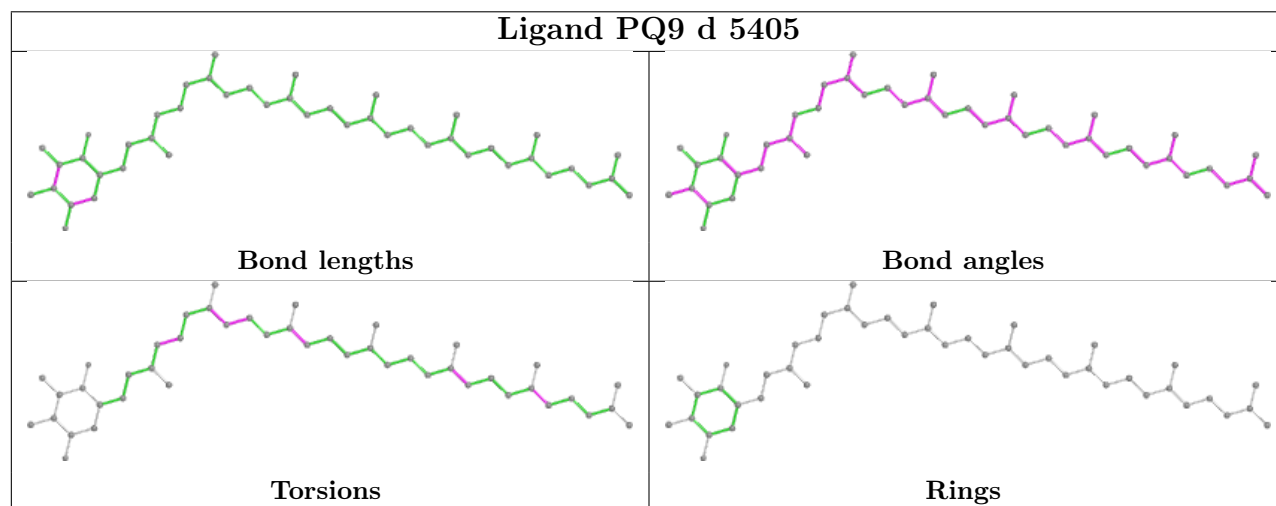
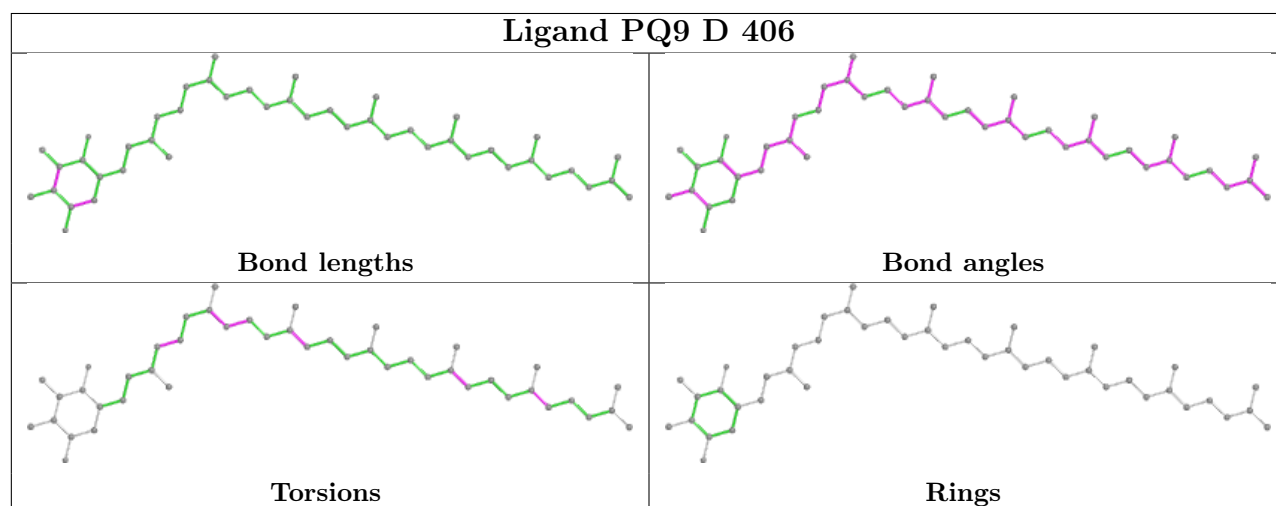
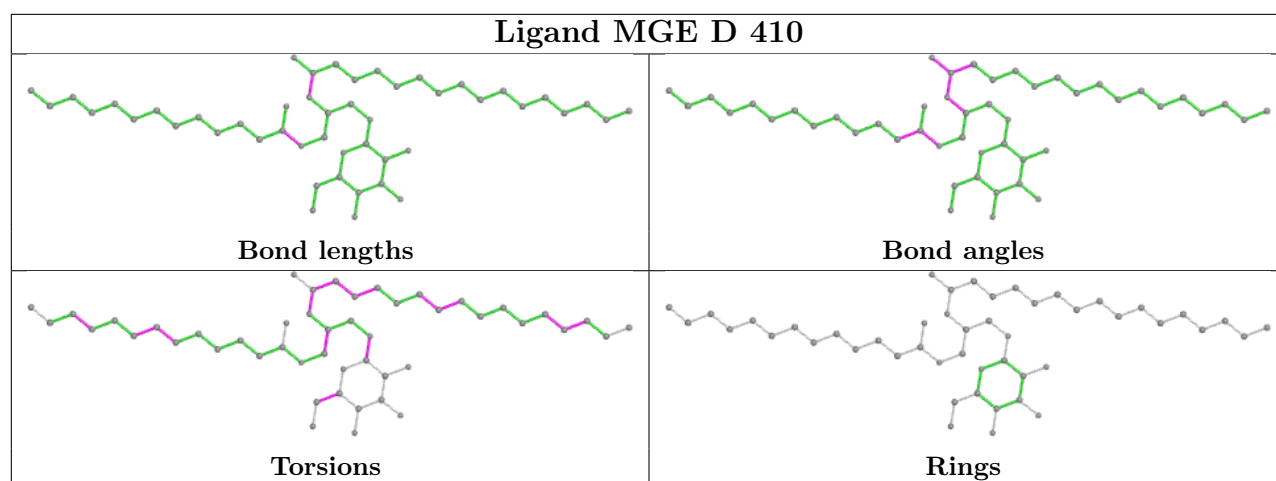




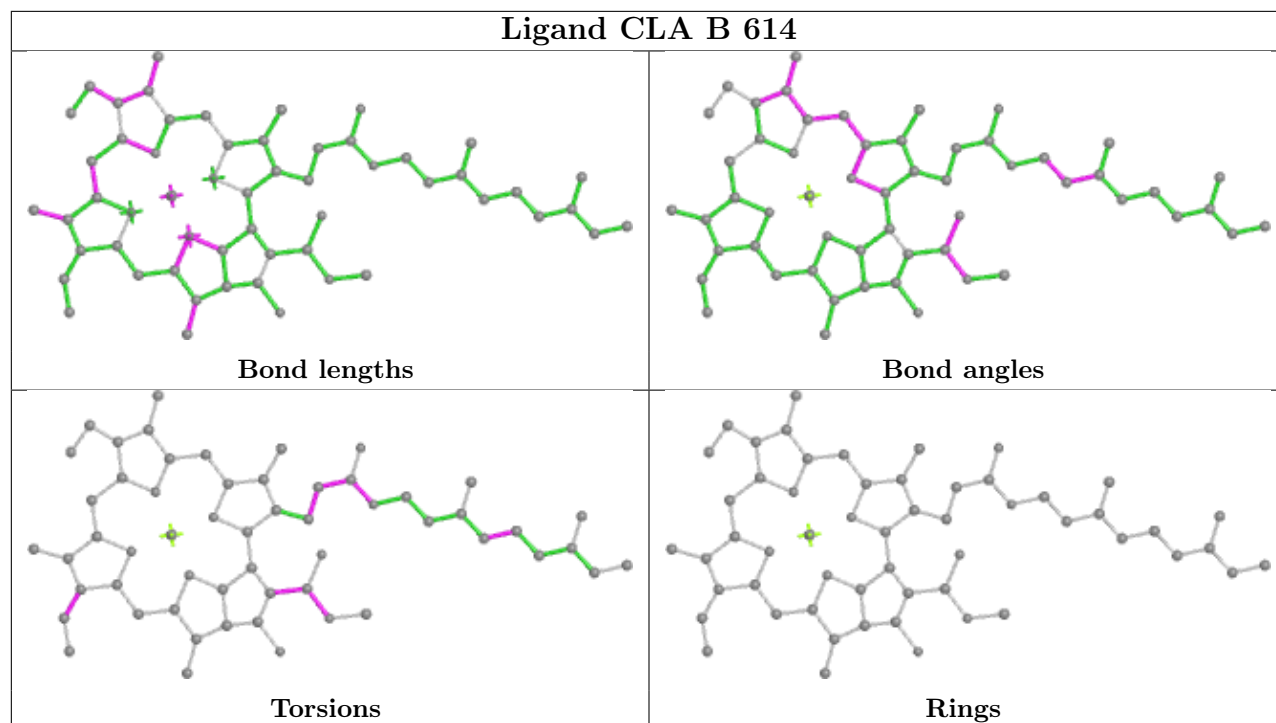




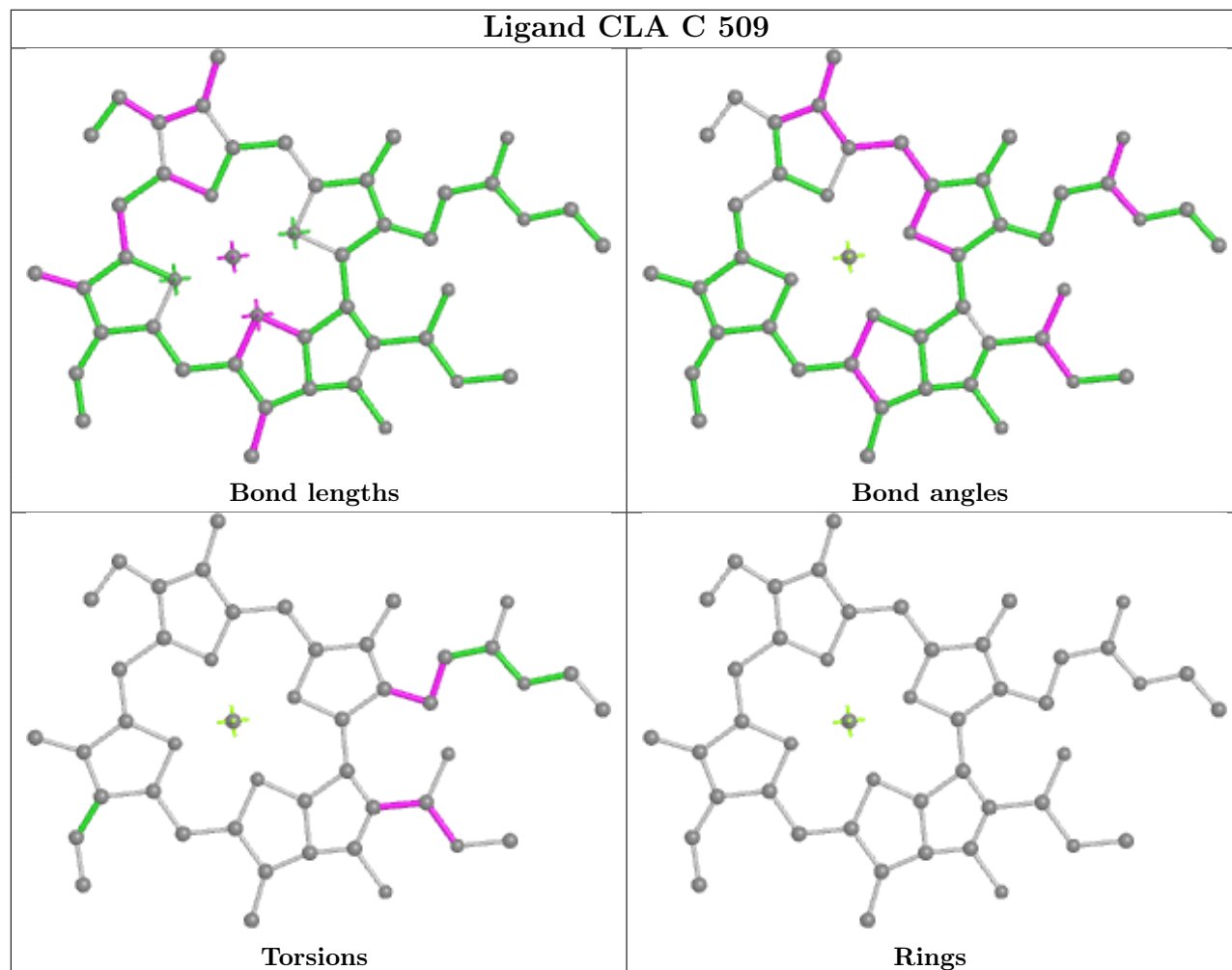


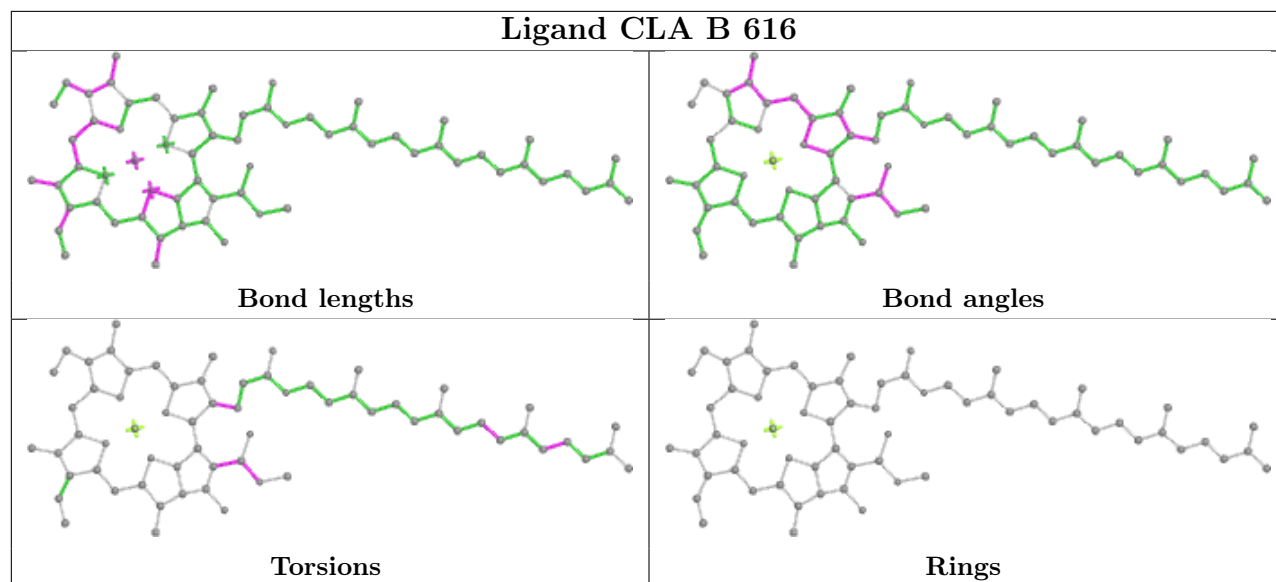
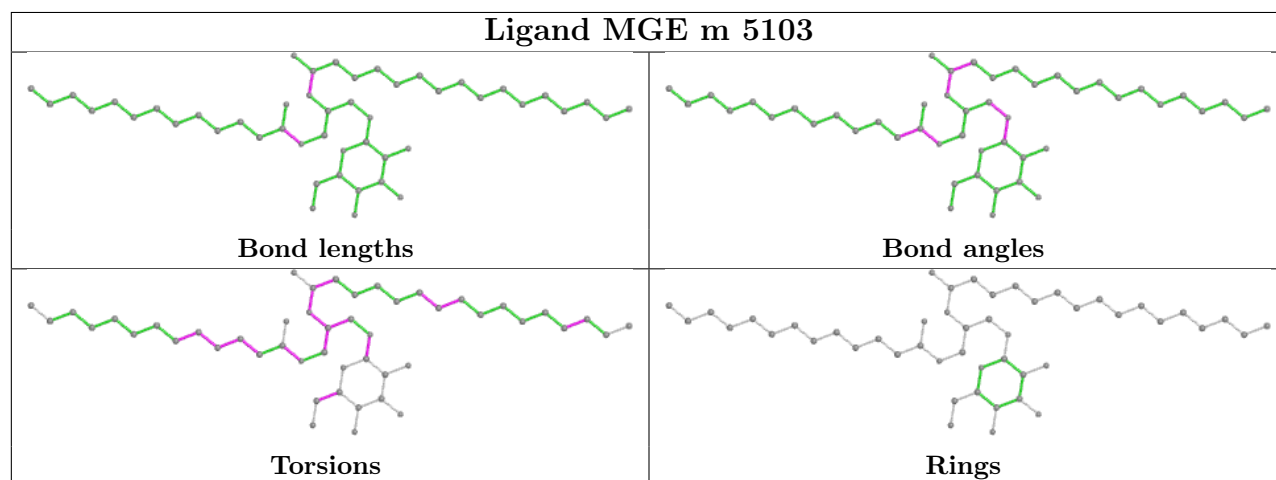
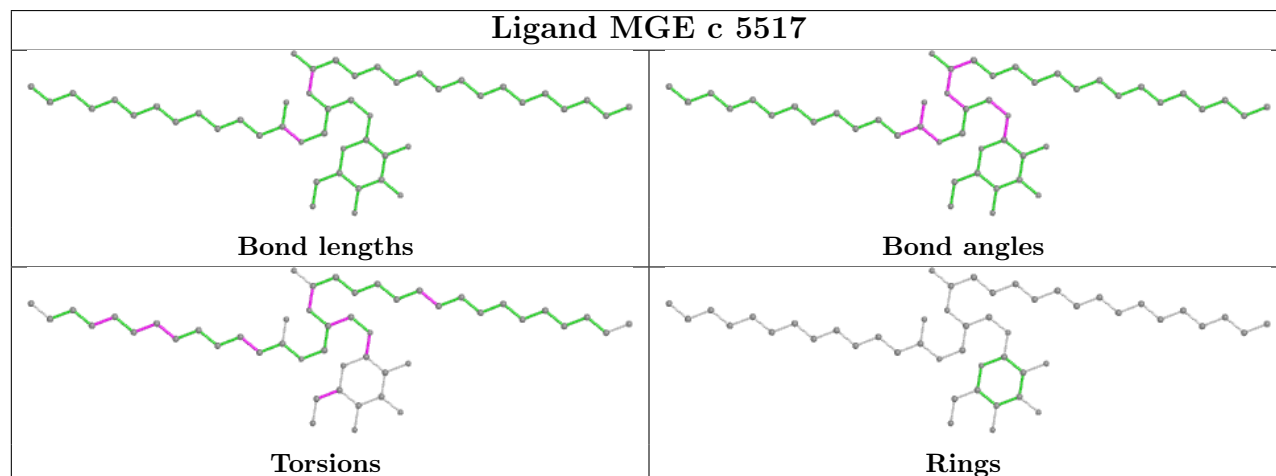


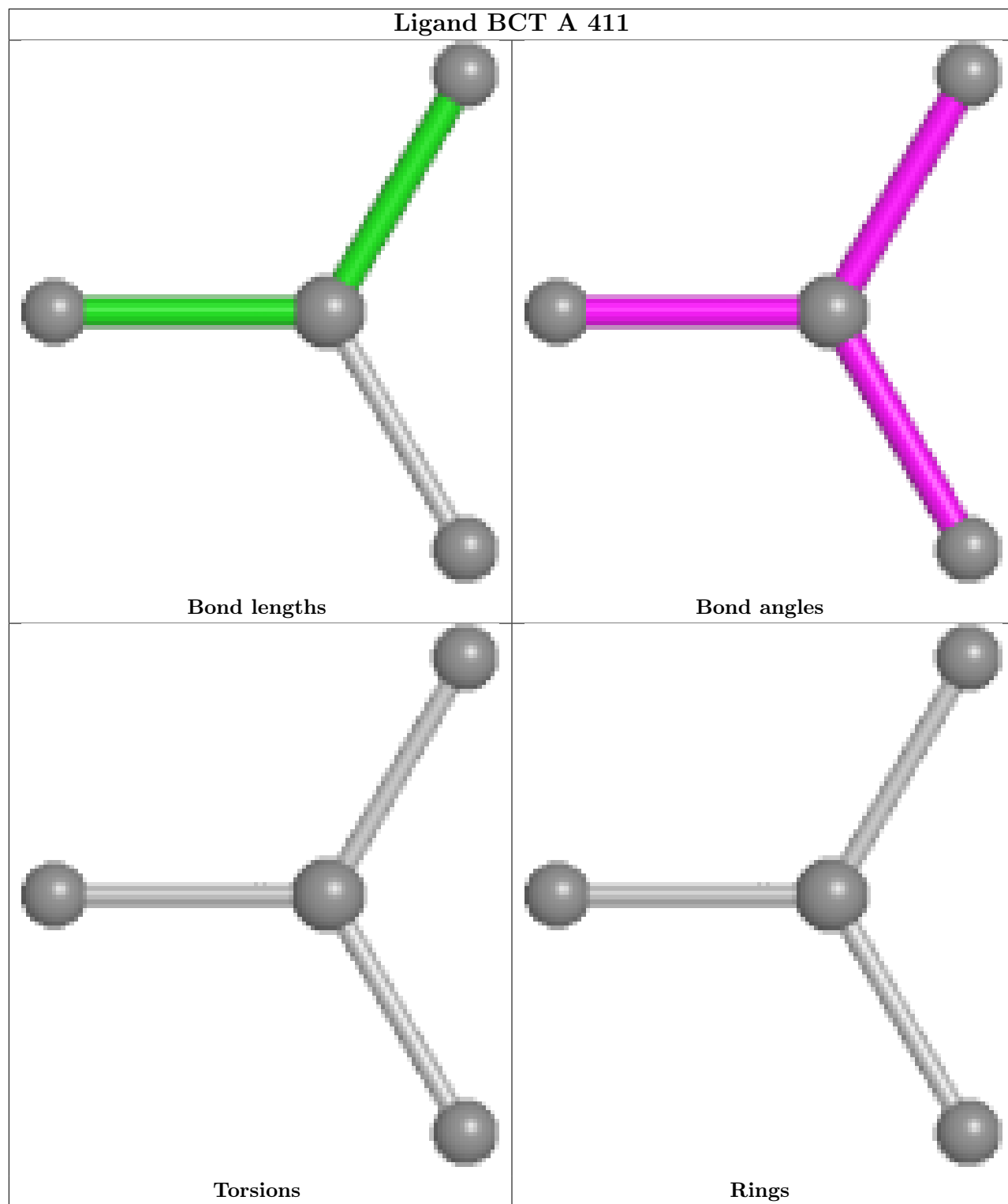
Ligand CLA B 614



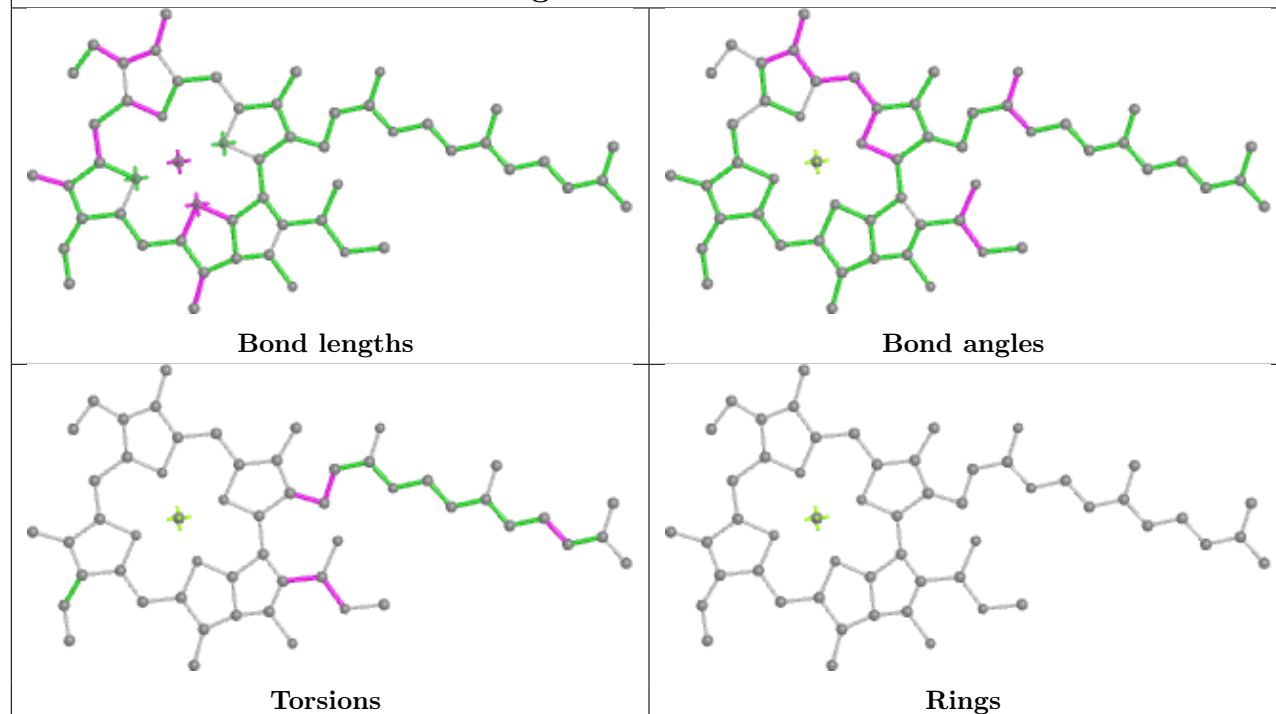
Ligand CLA C 509



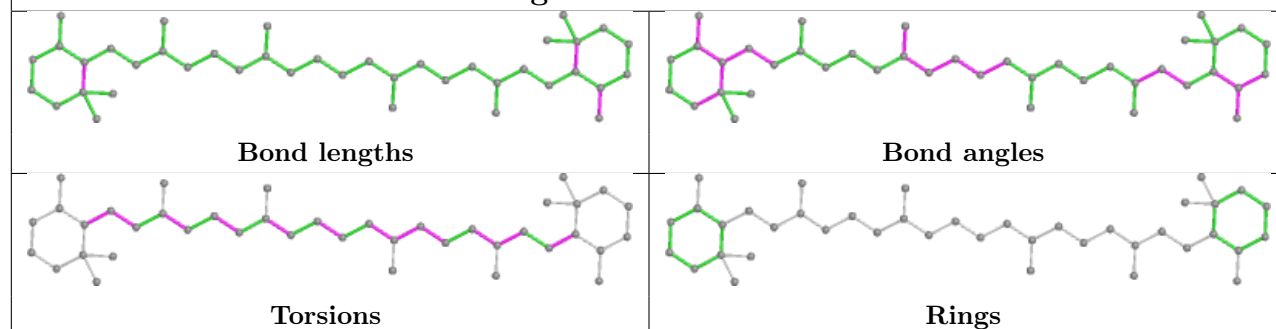
Ligand CLA B 616**Ligand MGE m 5103****Ligand MGE c 5517**



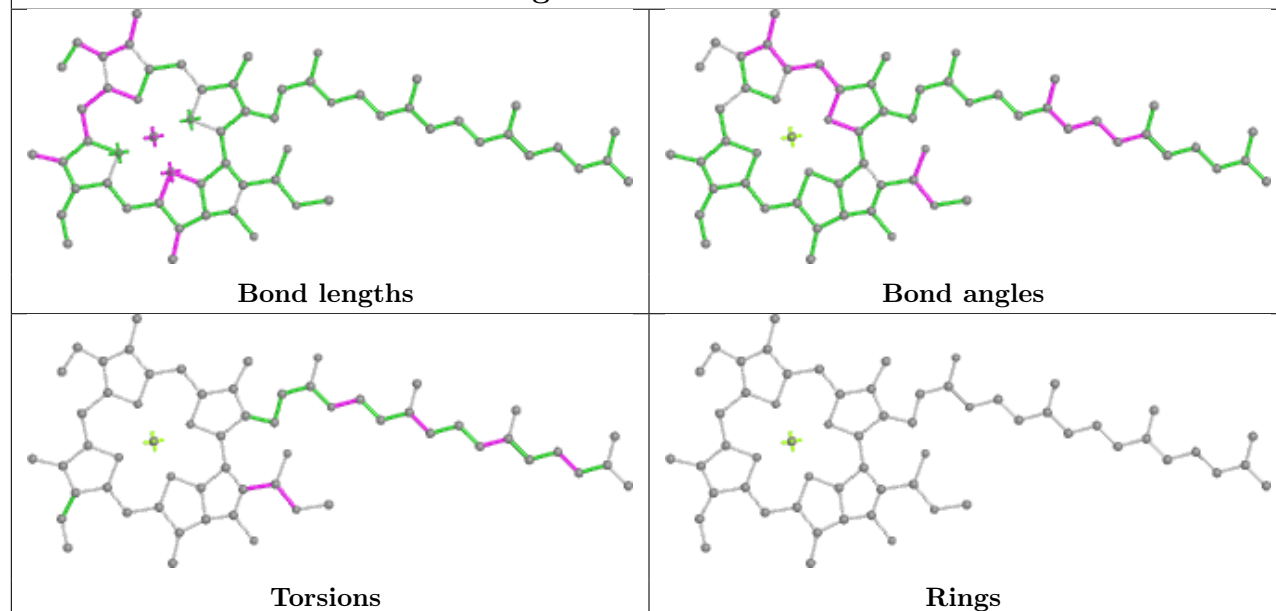
Ligand CLA A 405



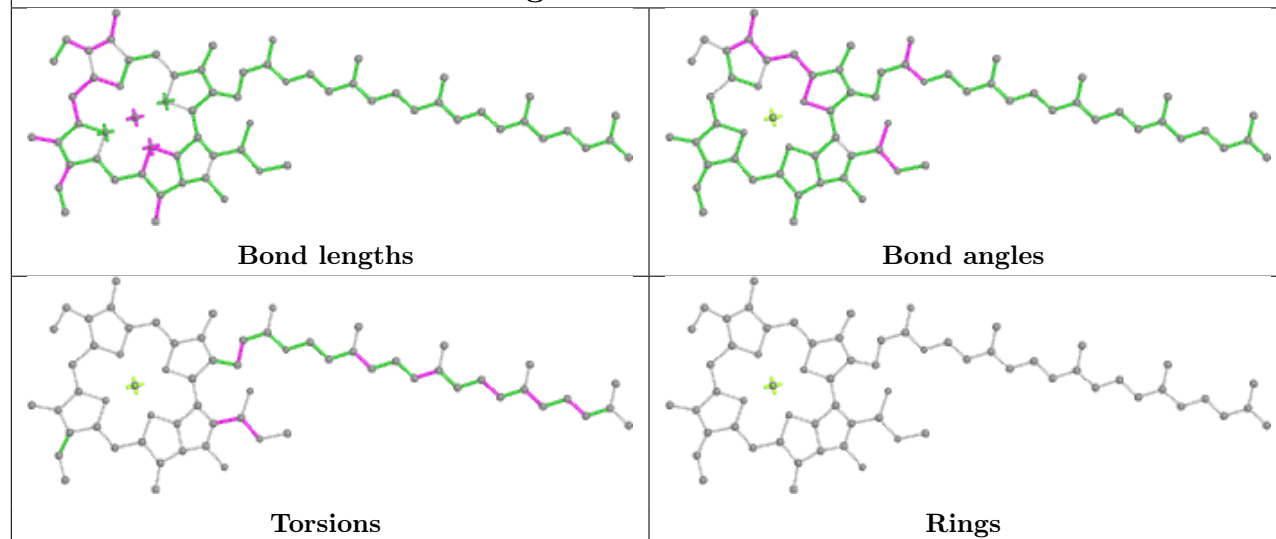
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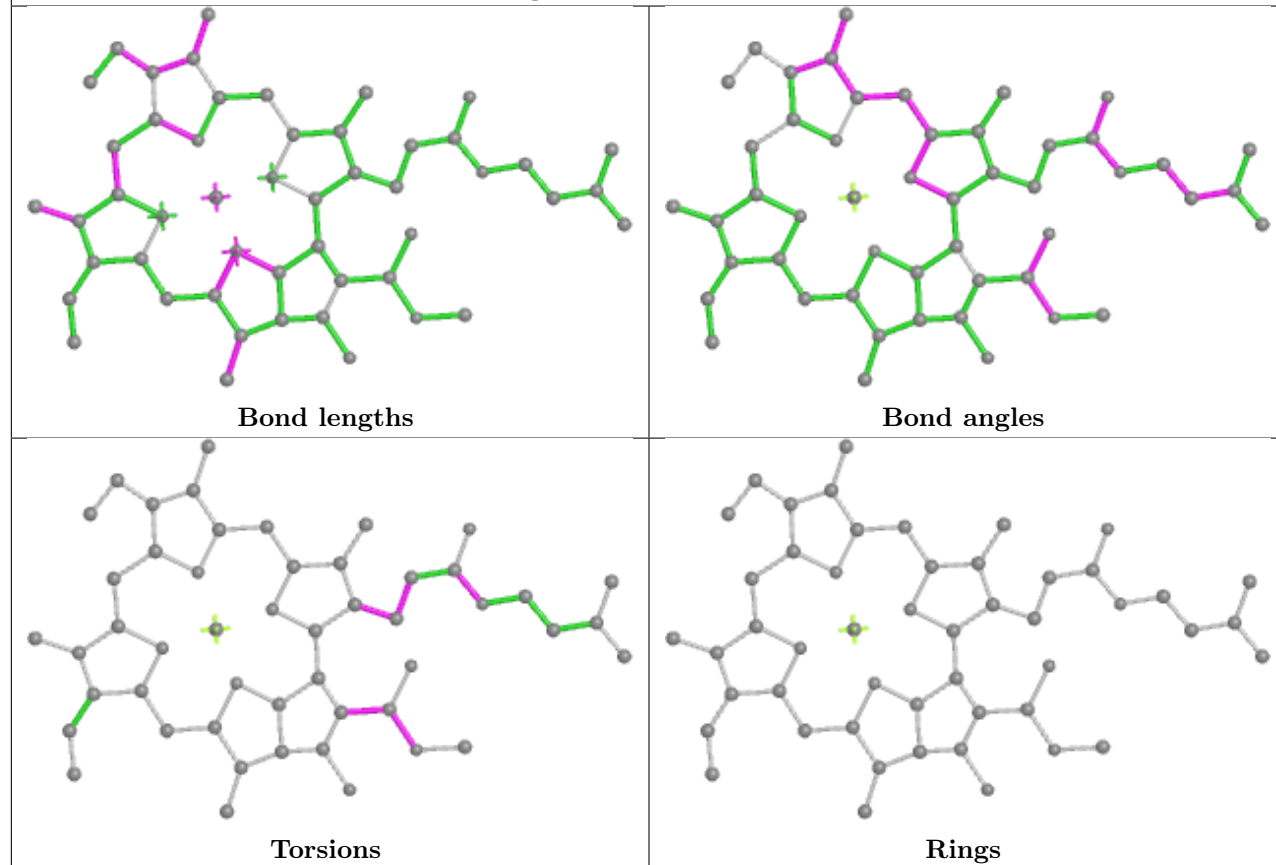
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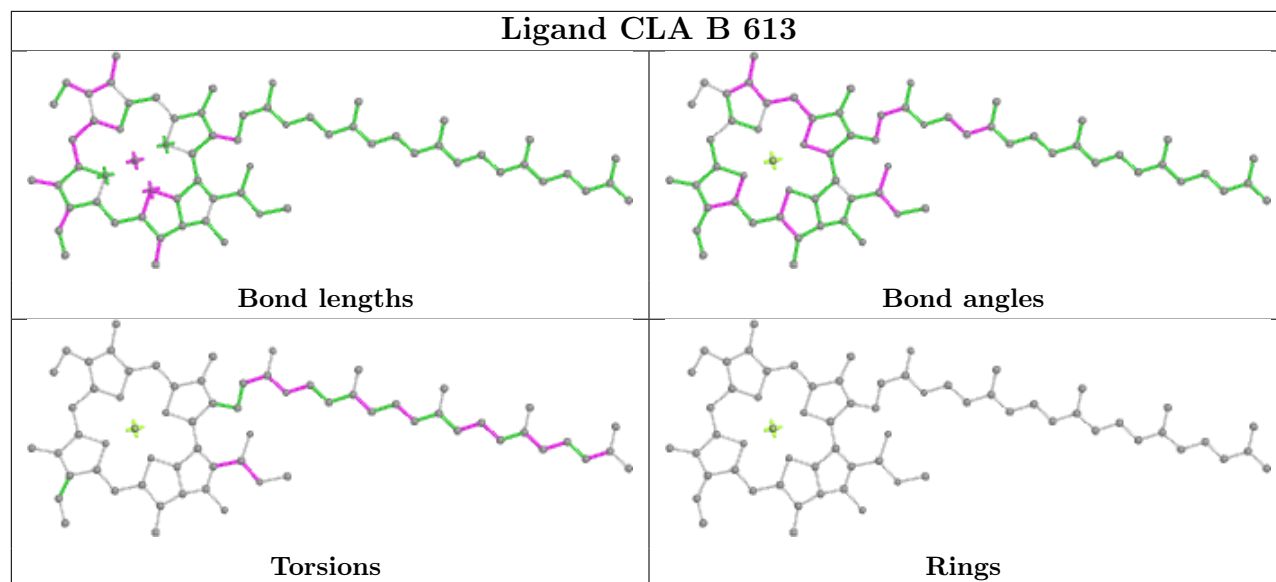
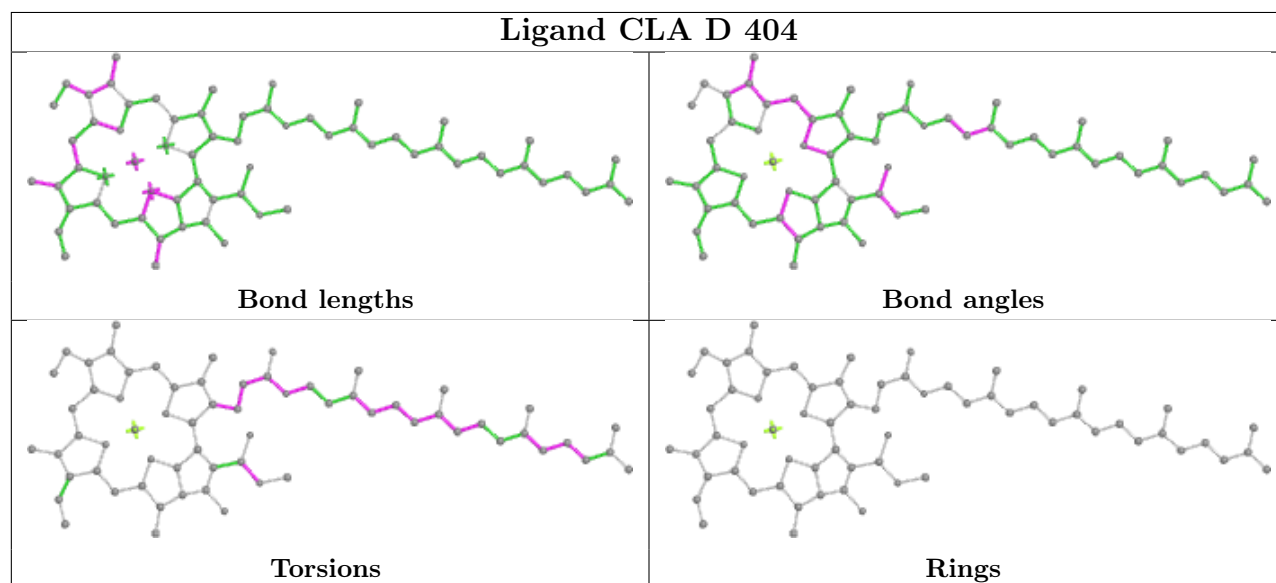


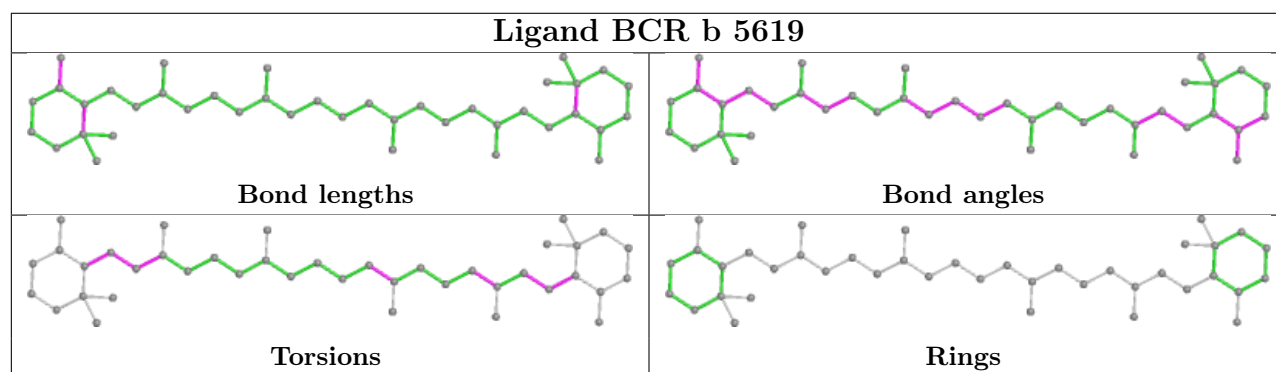
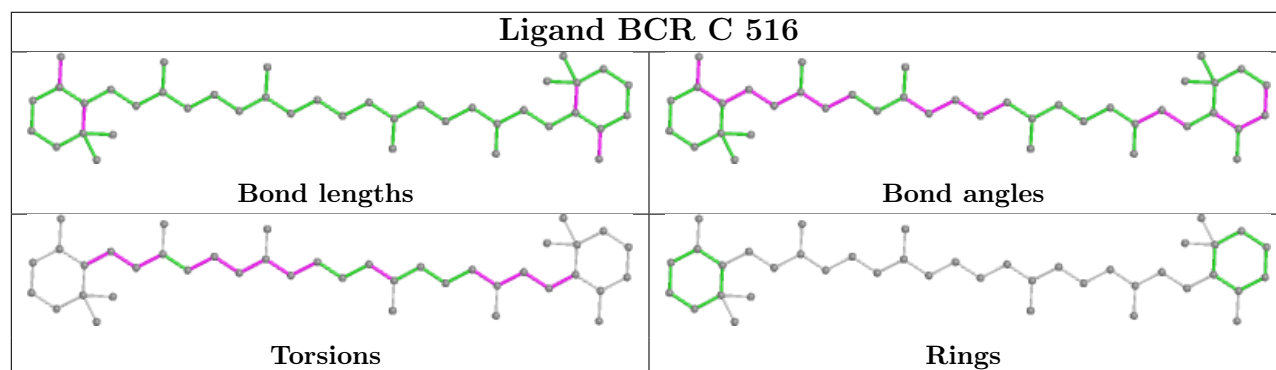
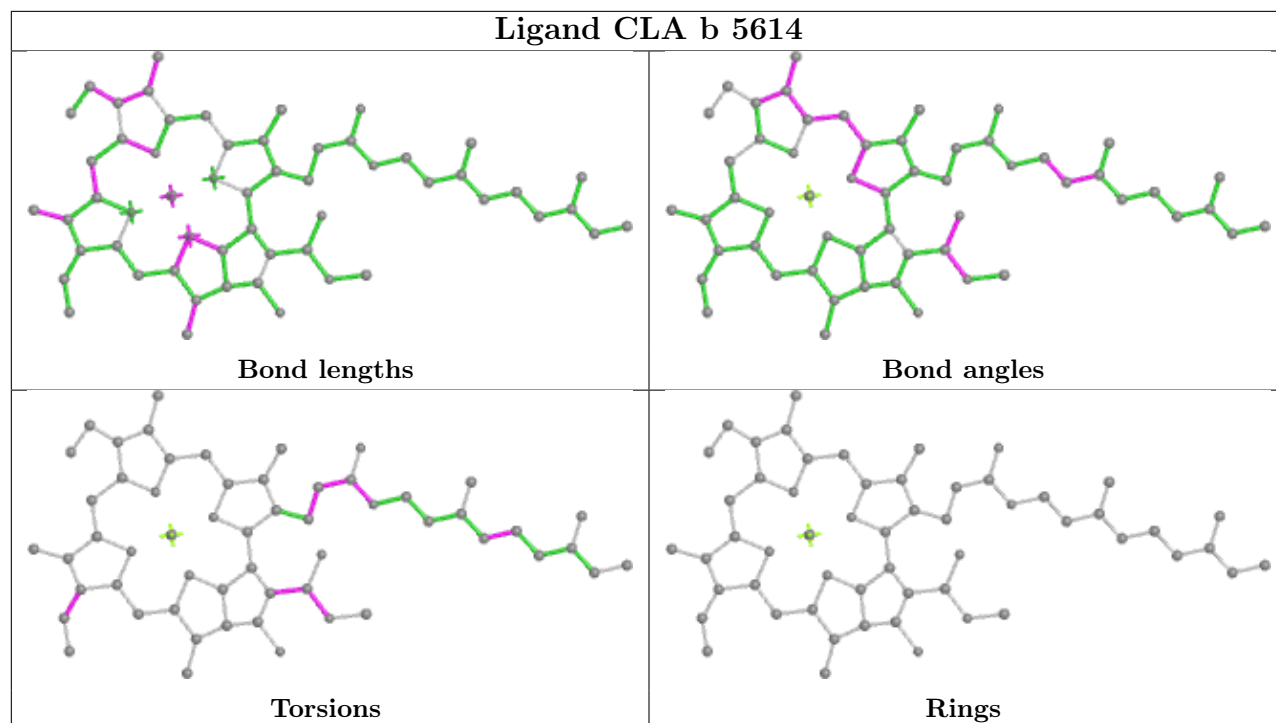
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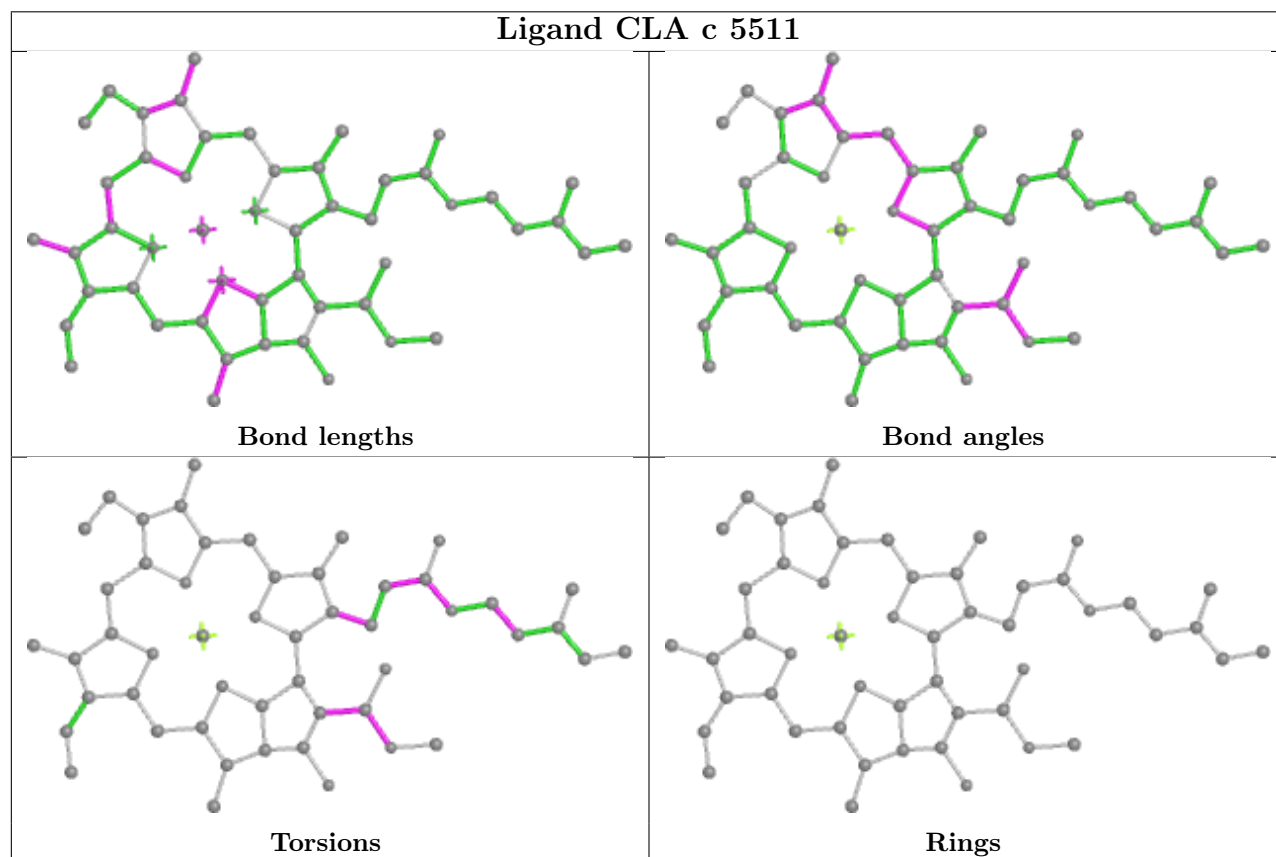
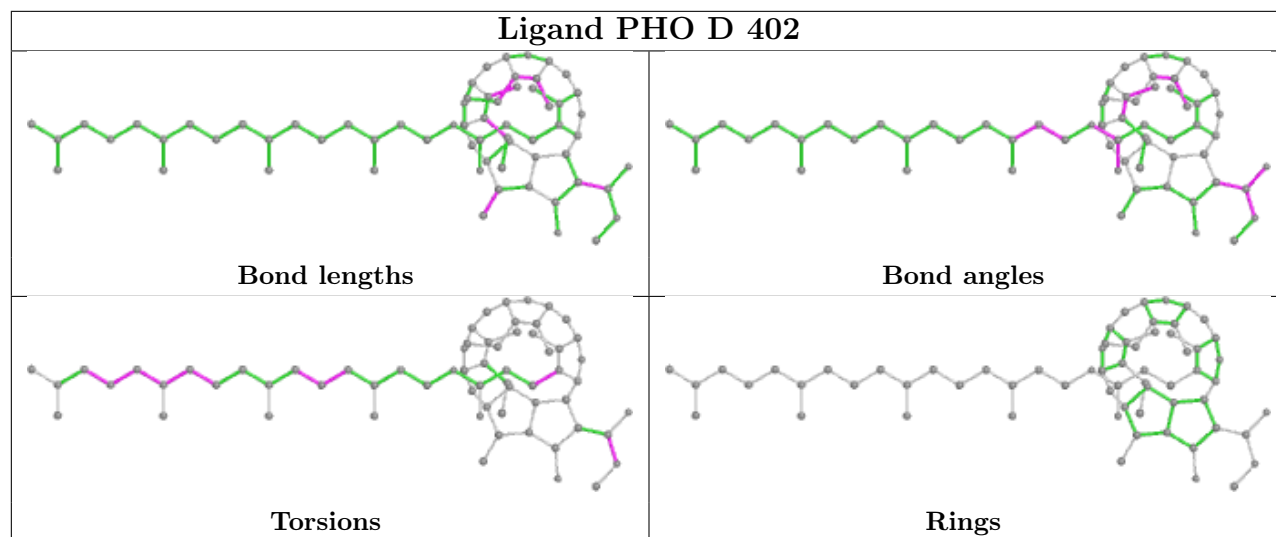
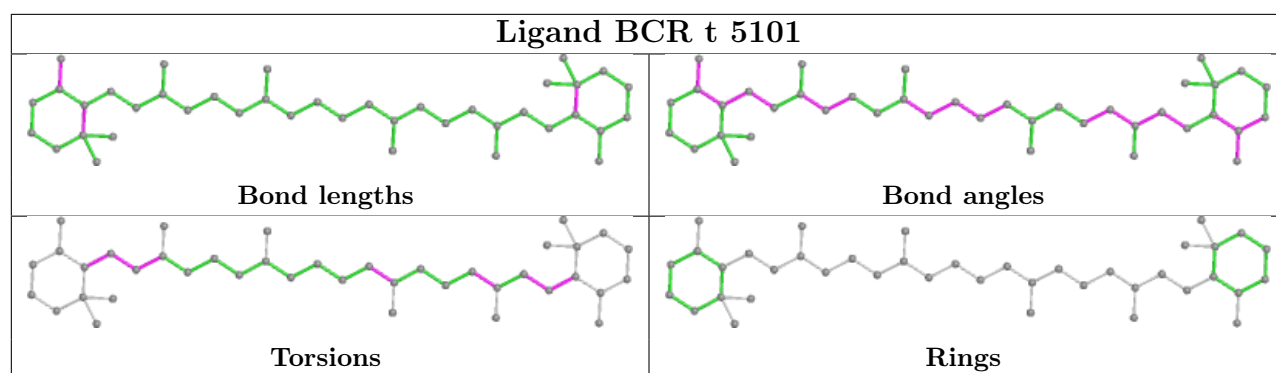


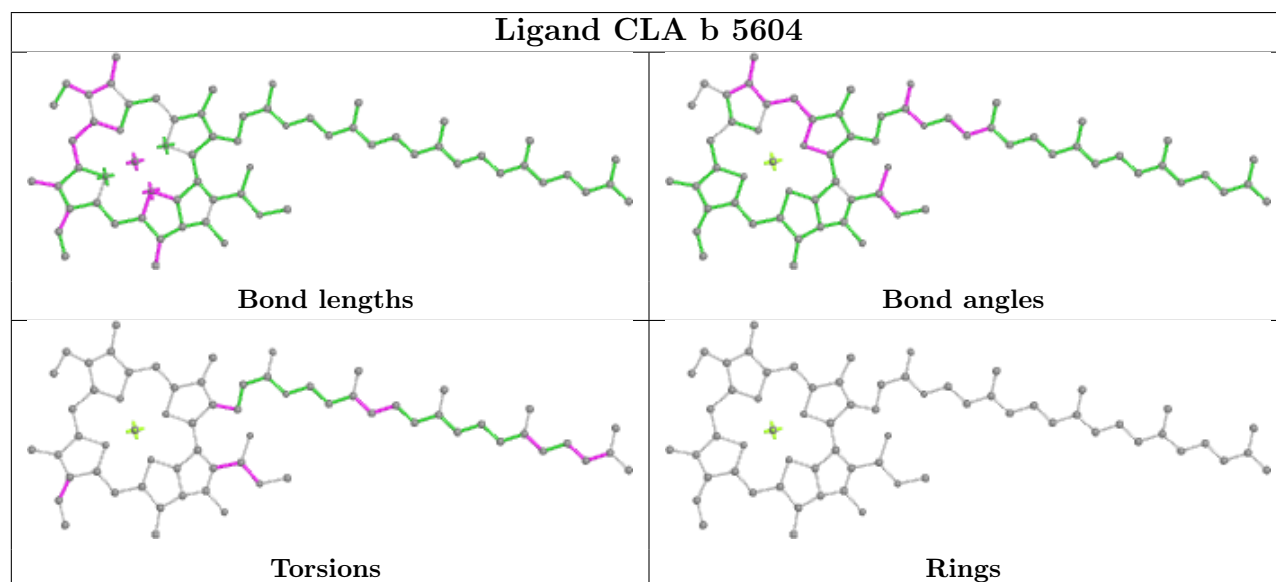
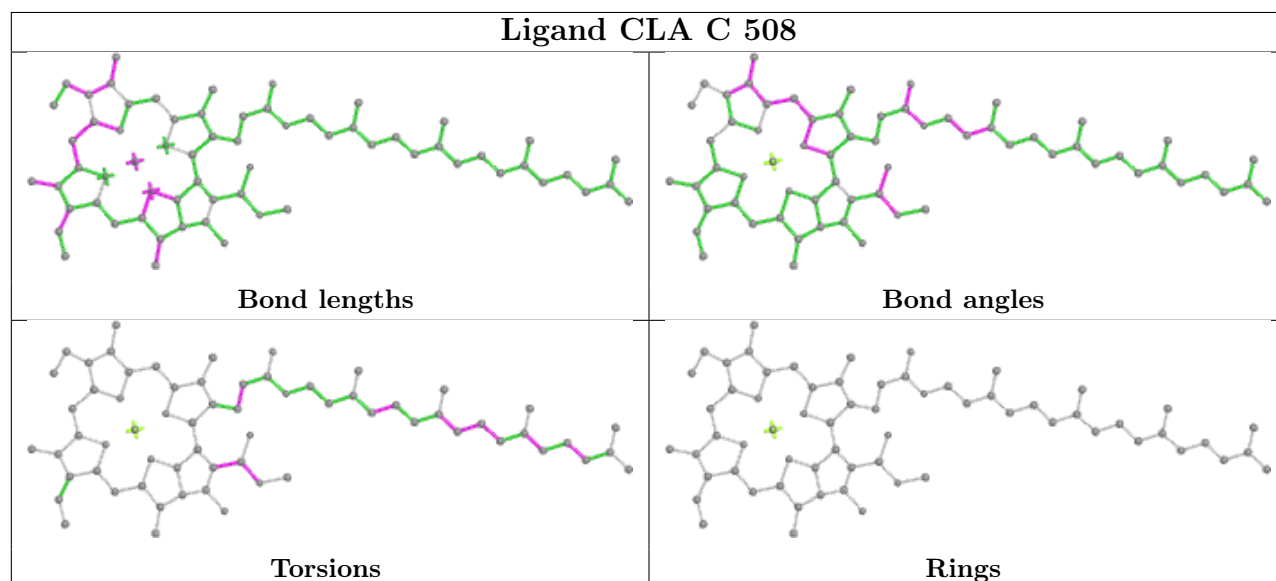
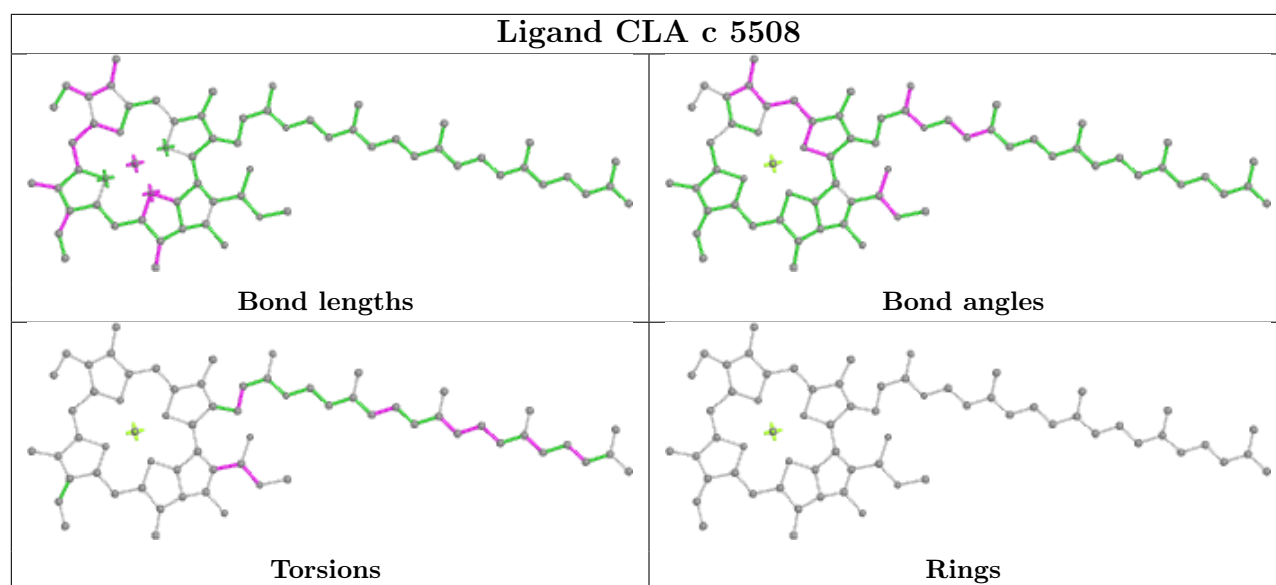
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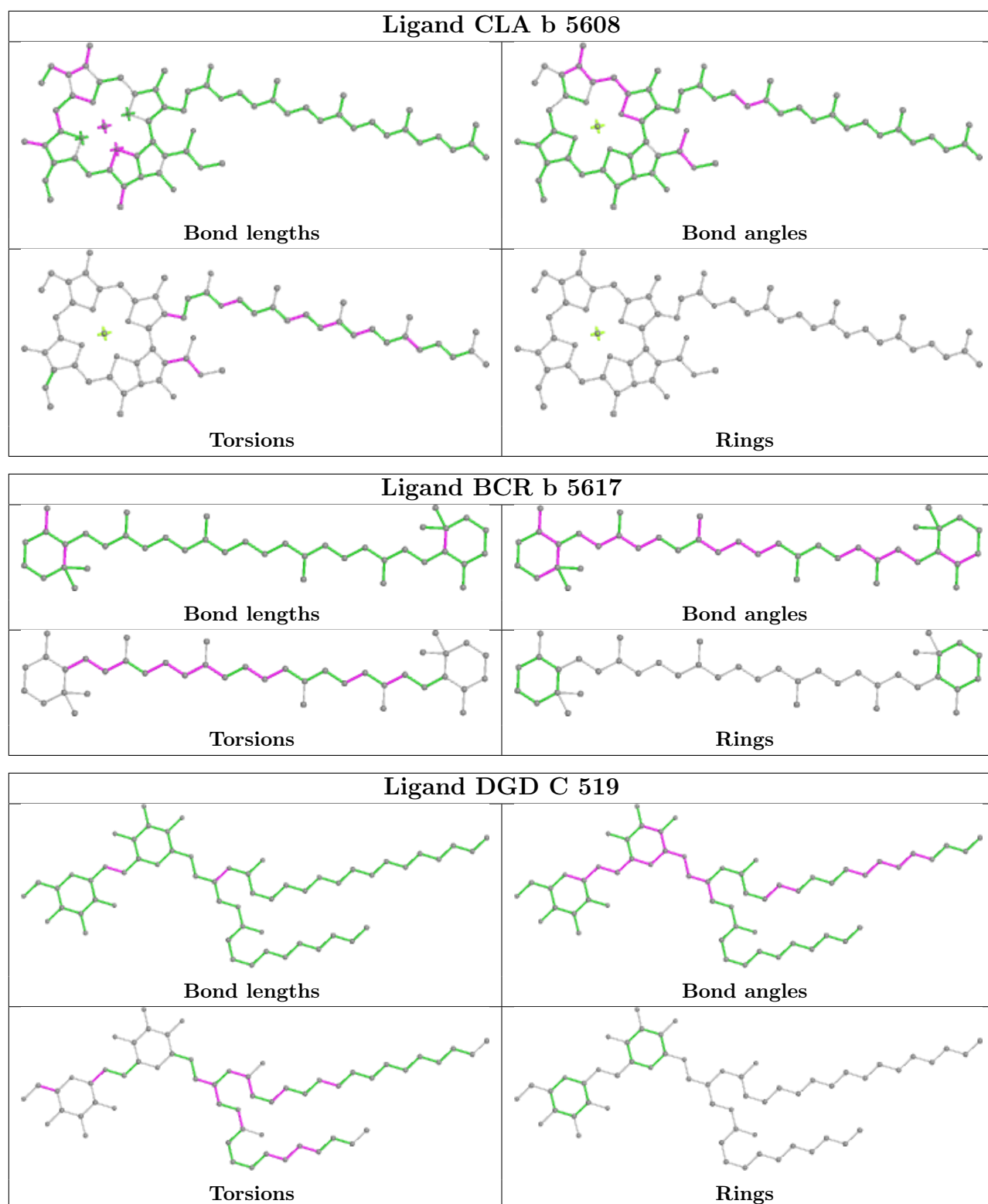


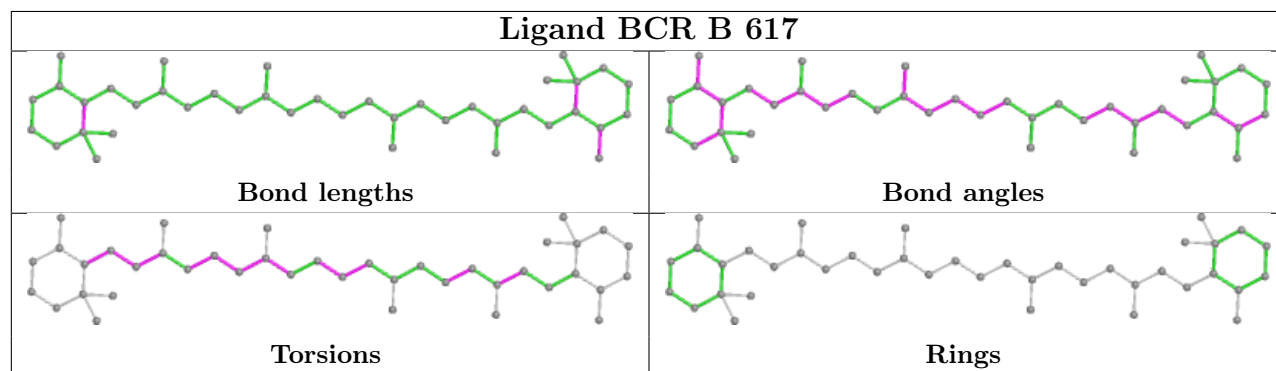
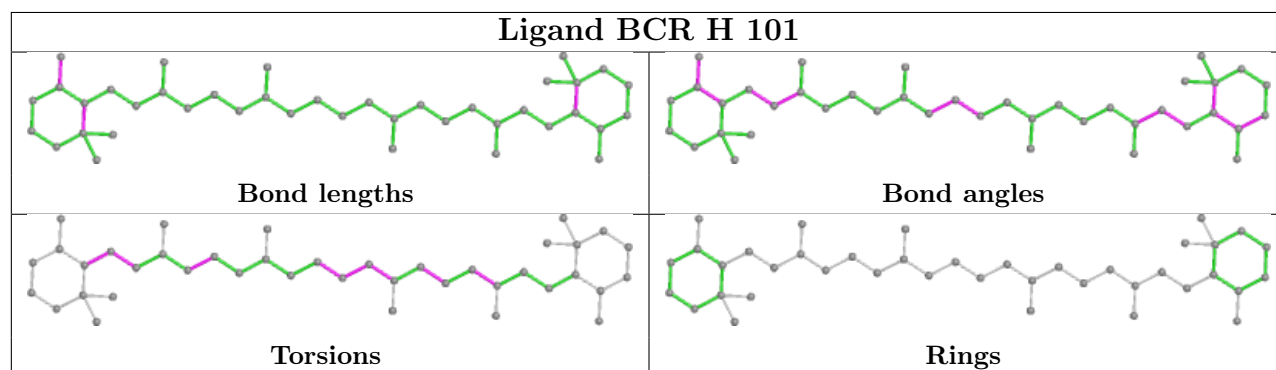
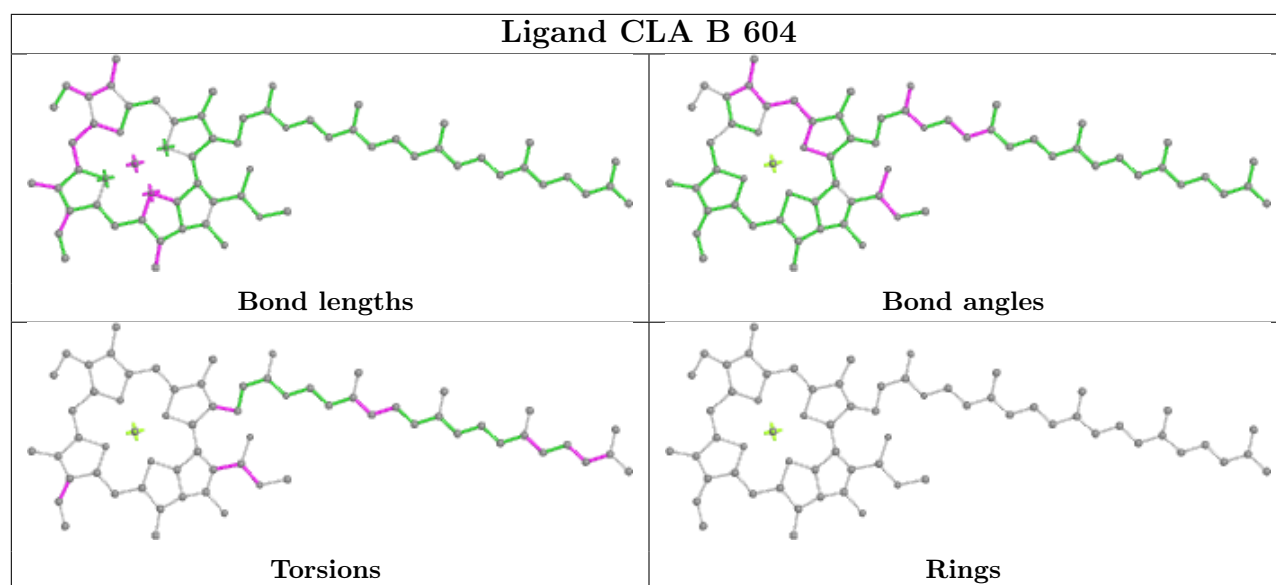
Ligand CLA B 613**Ligand CLA D 404**

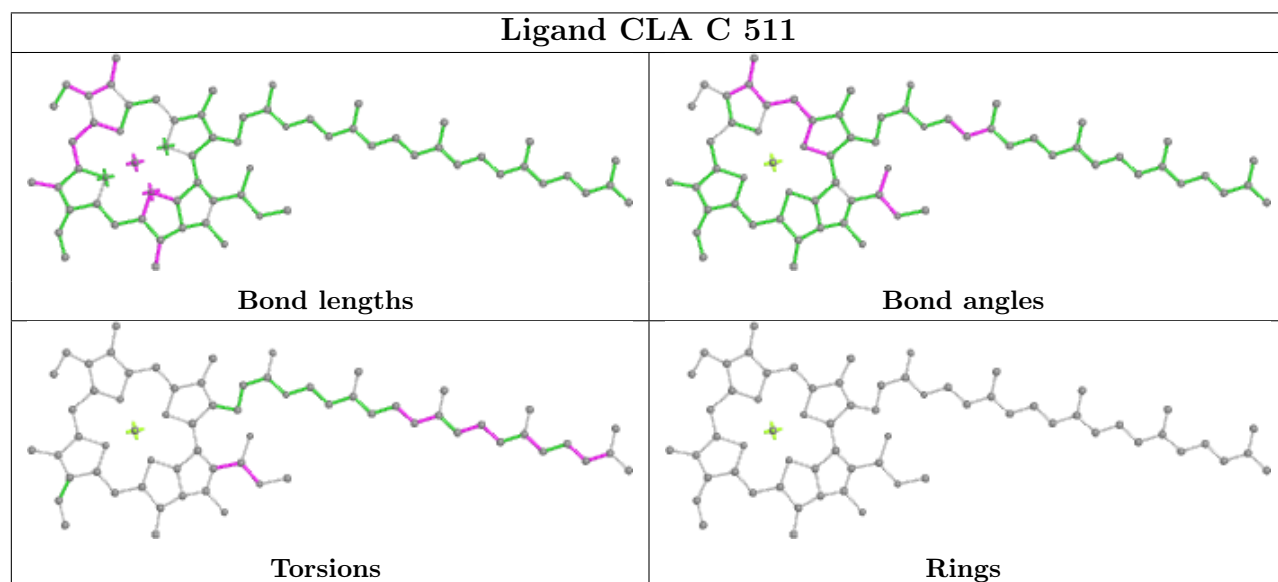
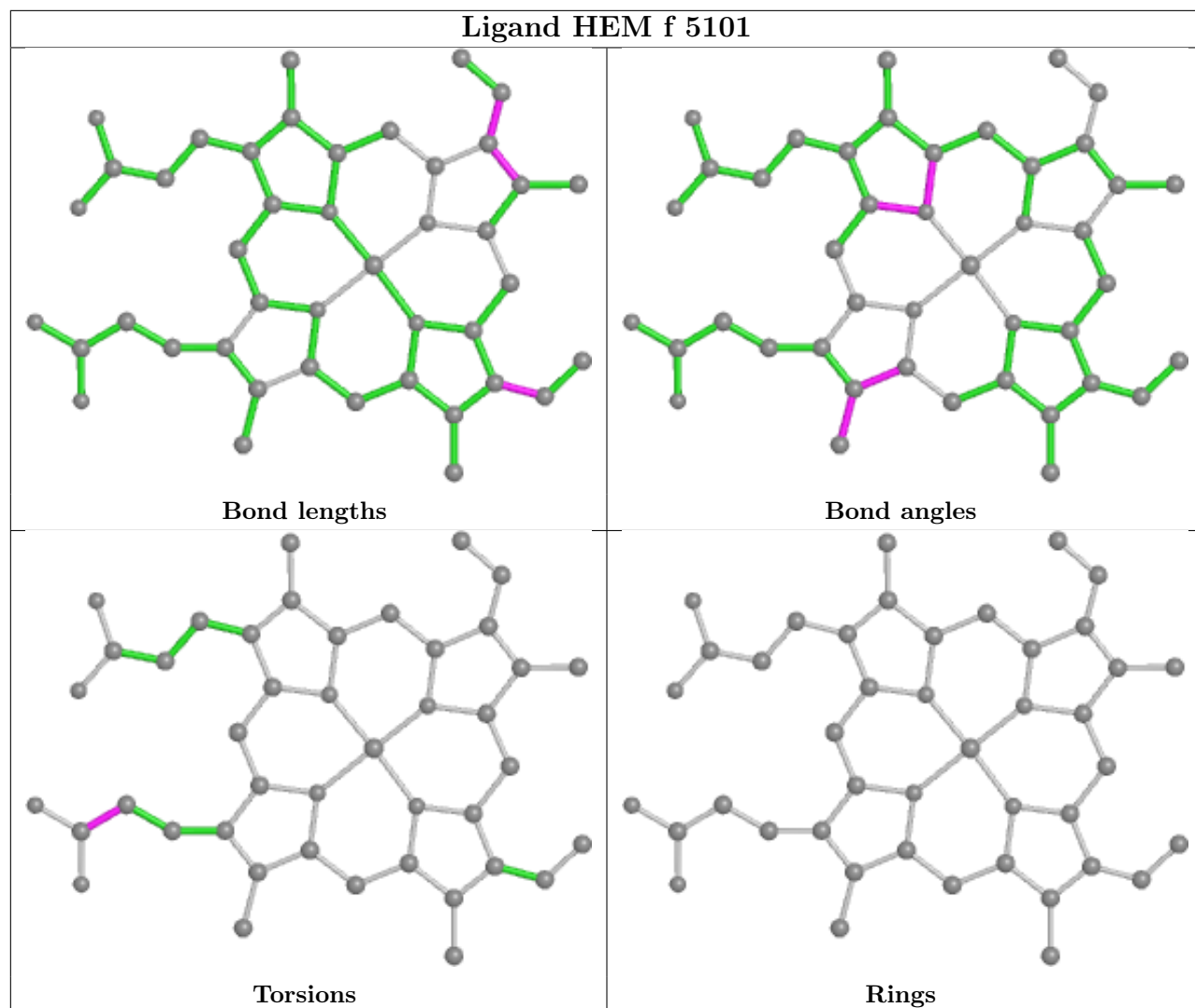


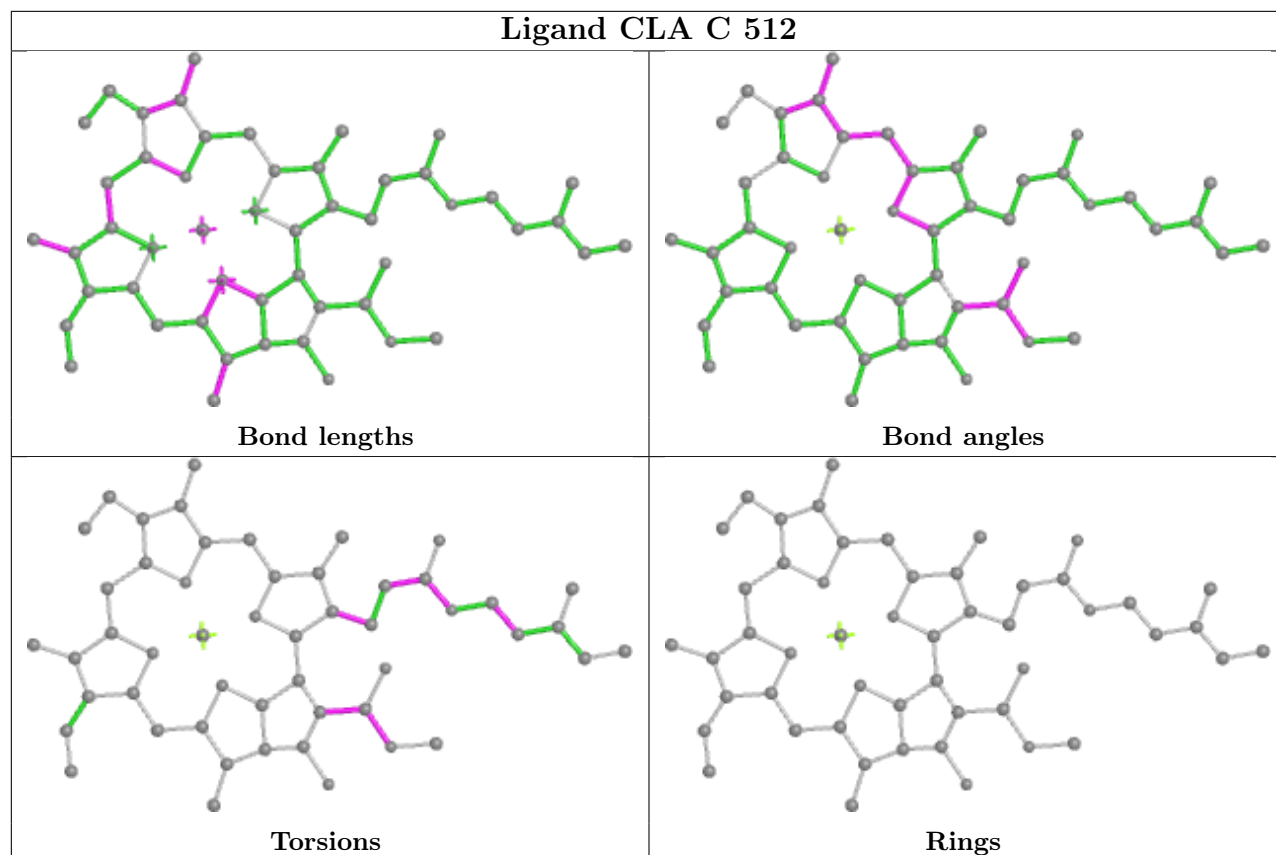
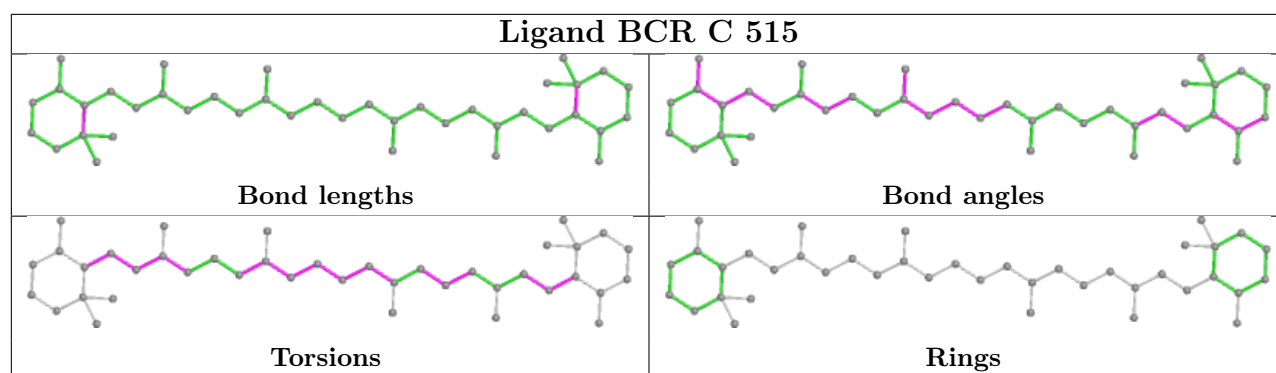


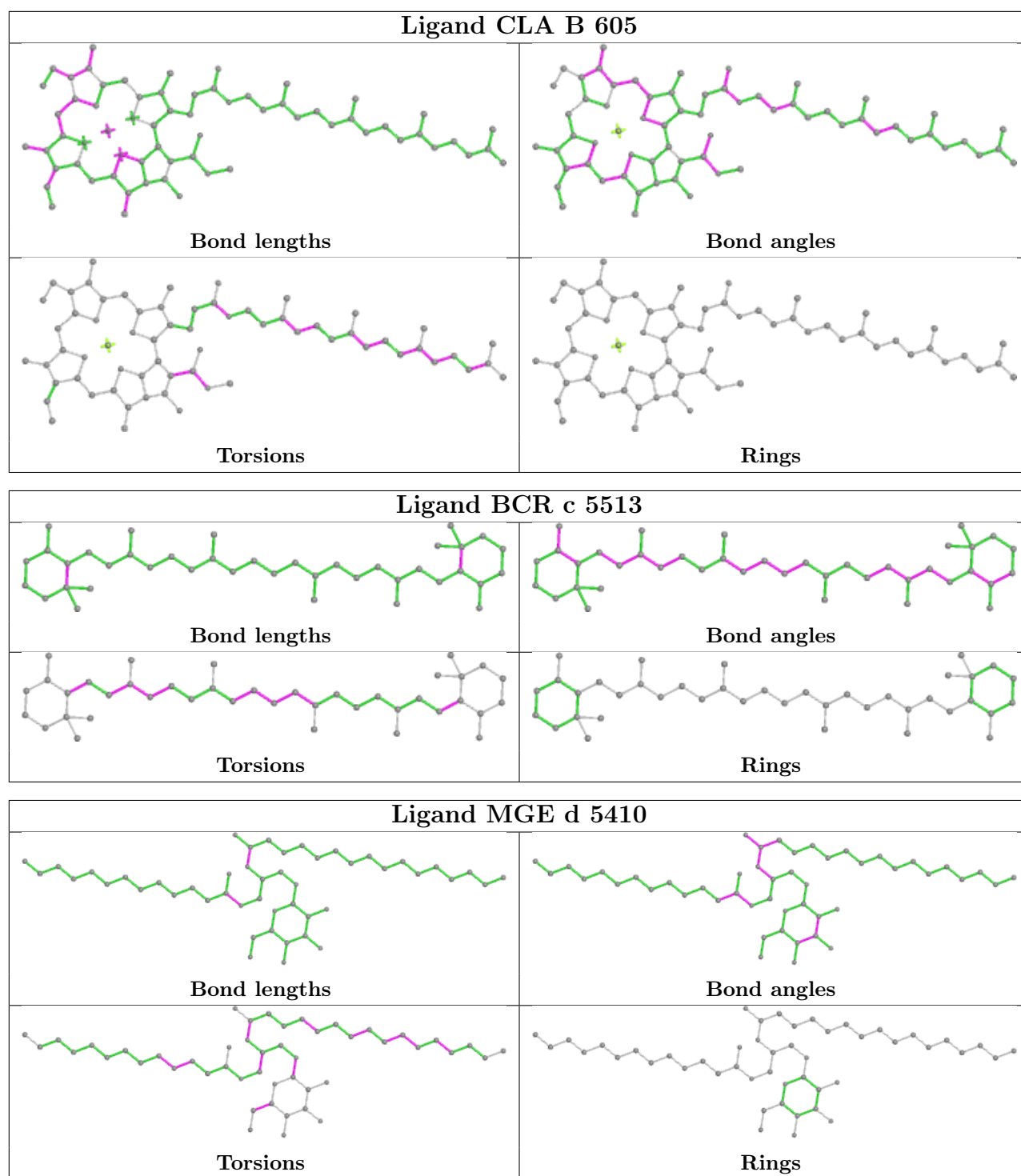




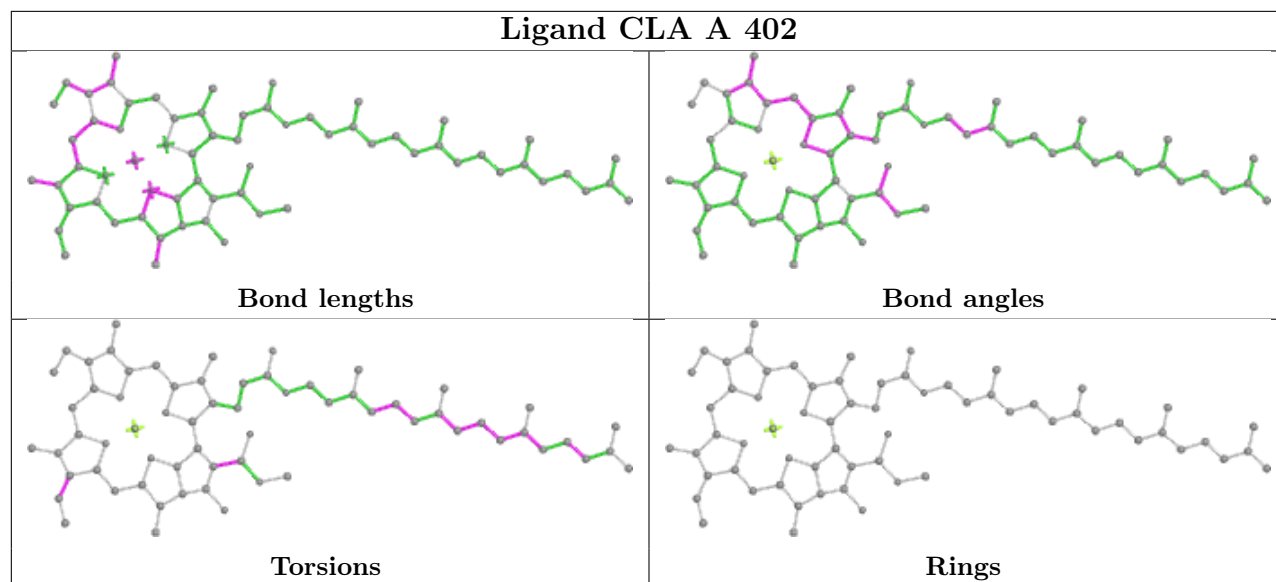




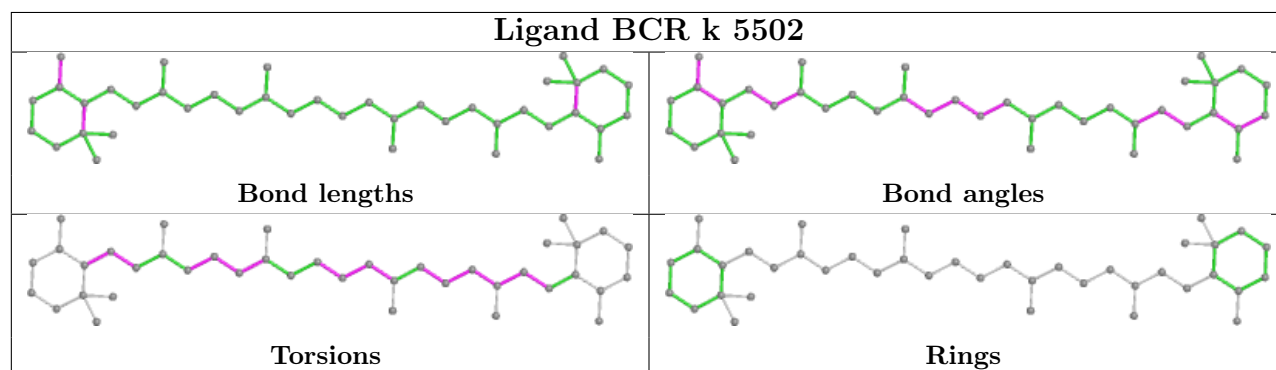




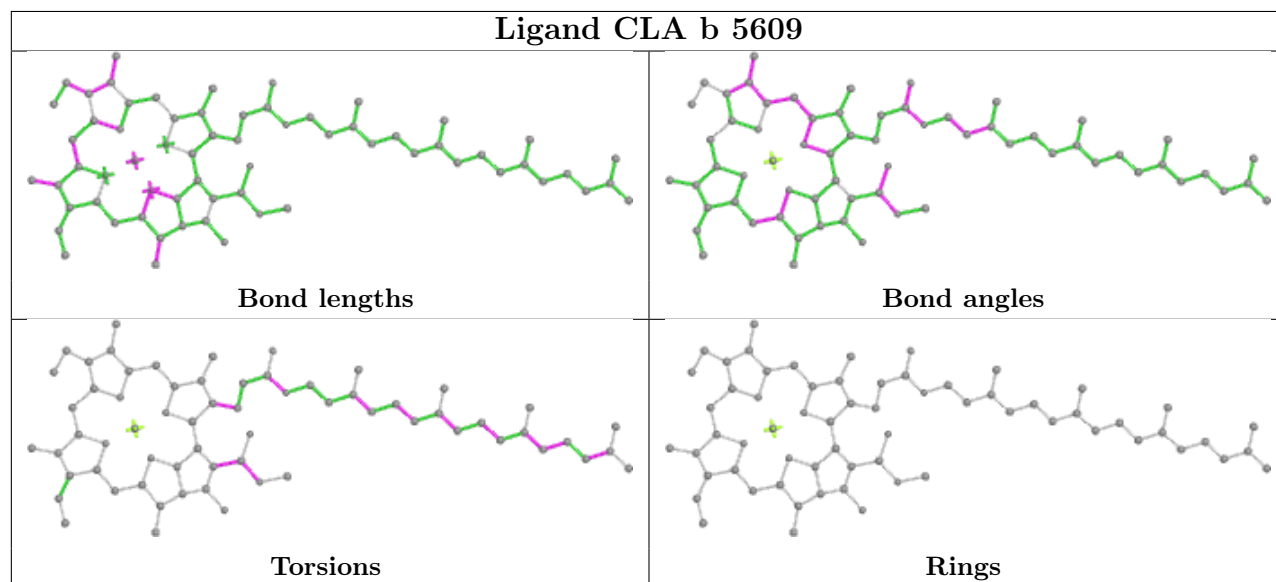
Ligand CLA A 402



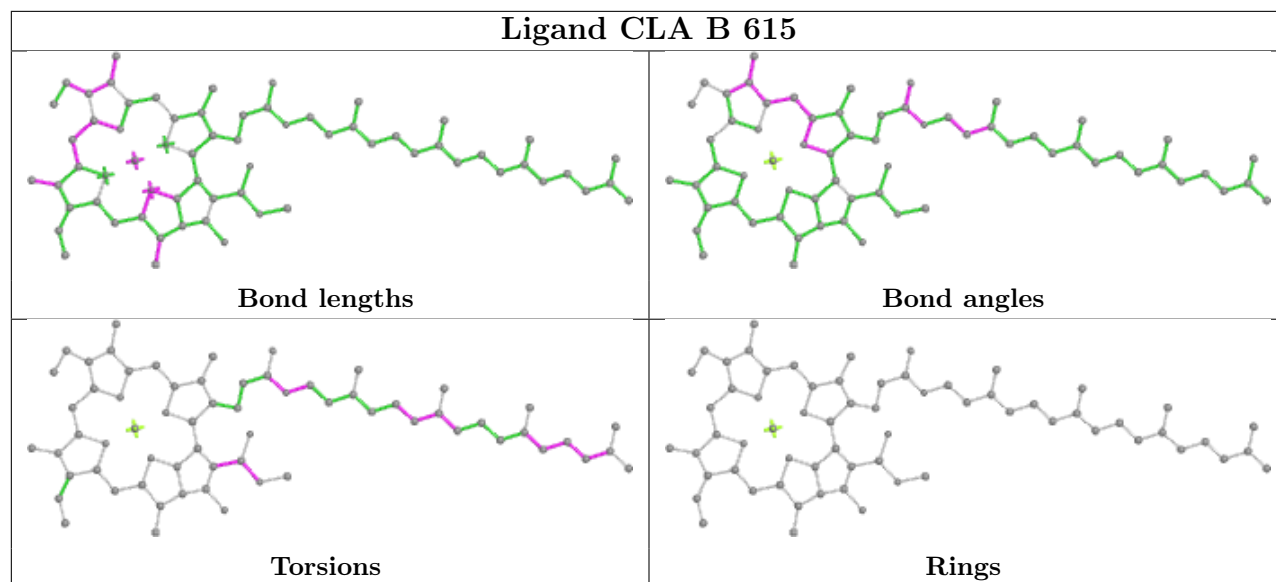
Ligand BCR k 5502



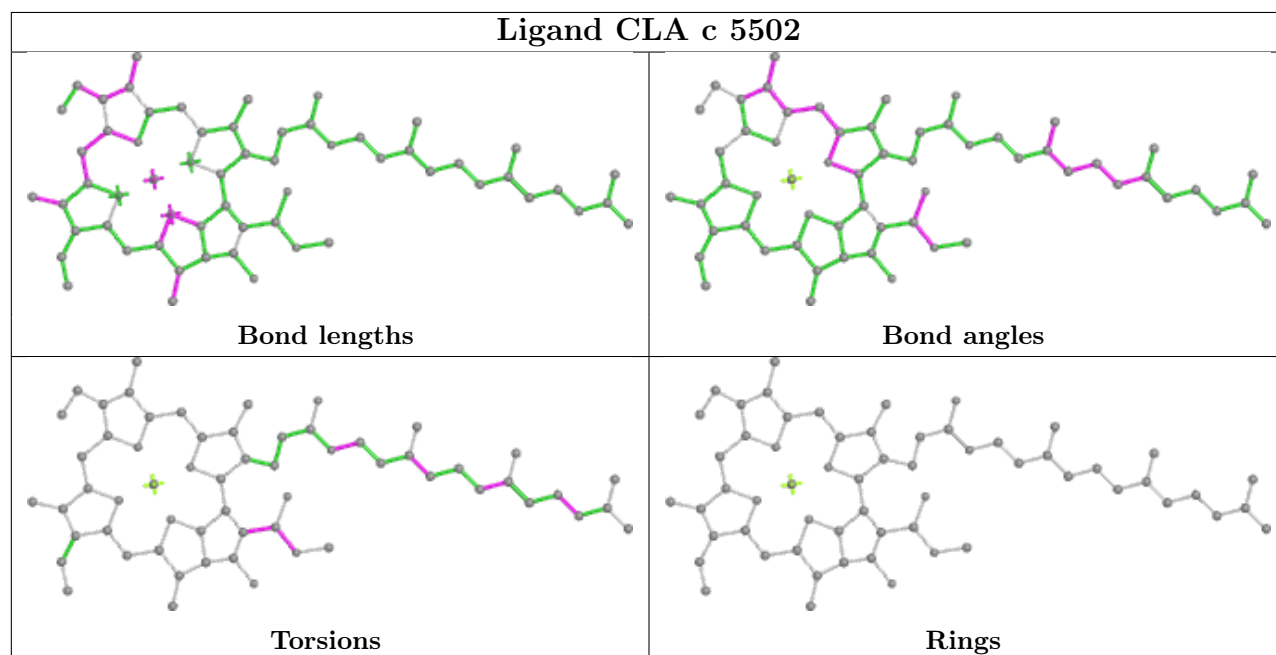
Ligand CLA b 5609

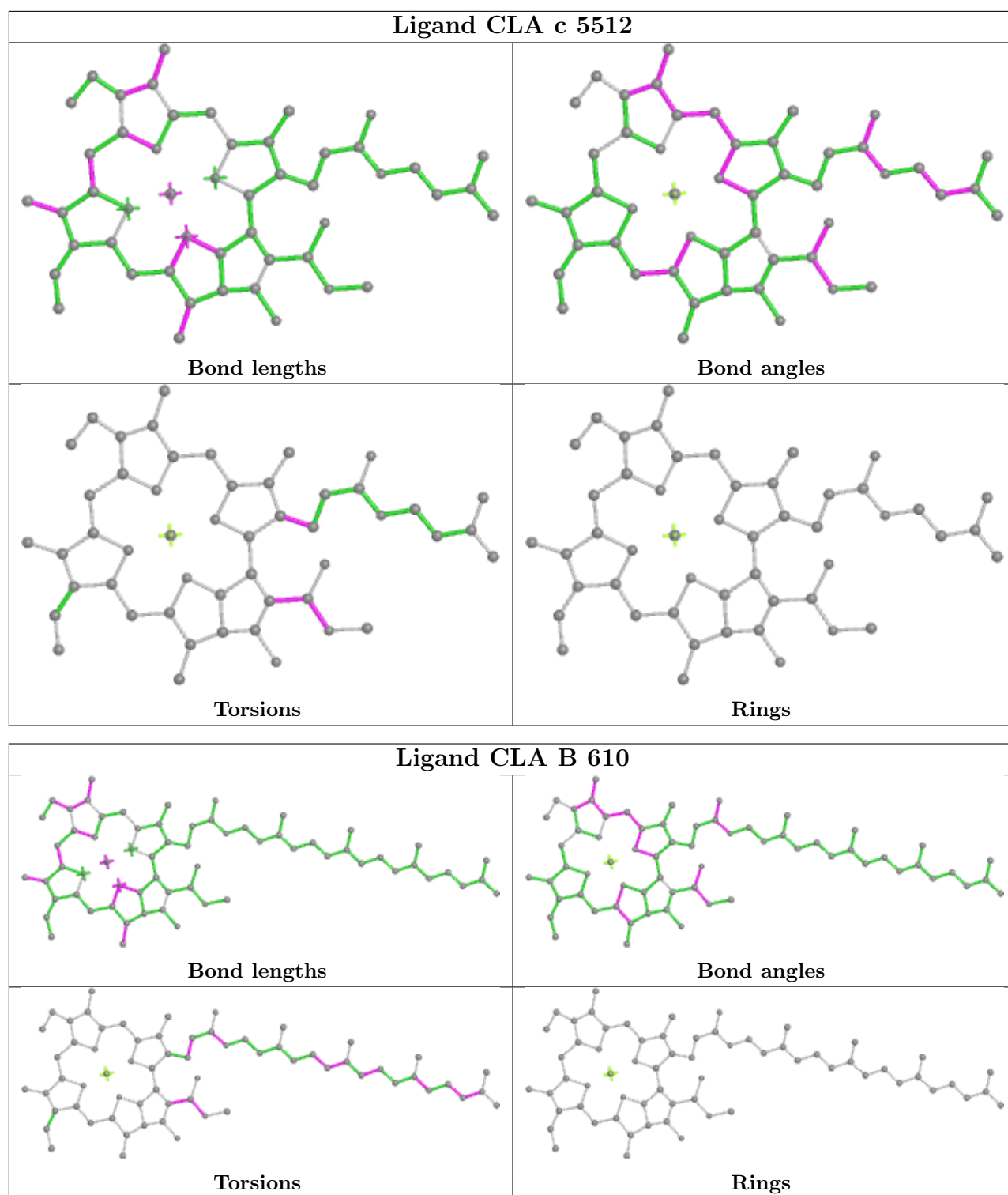


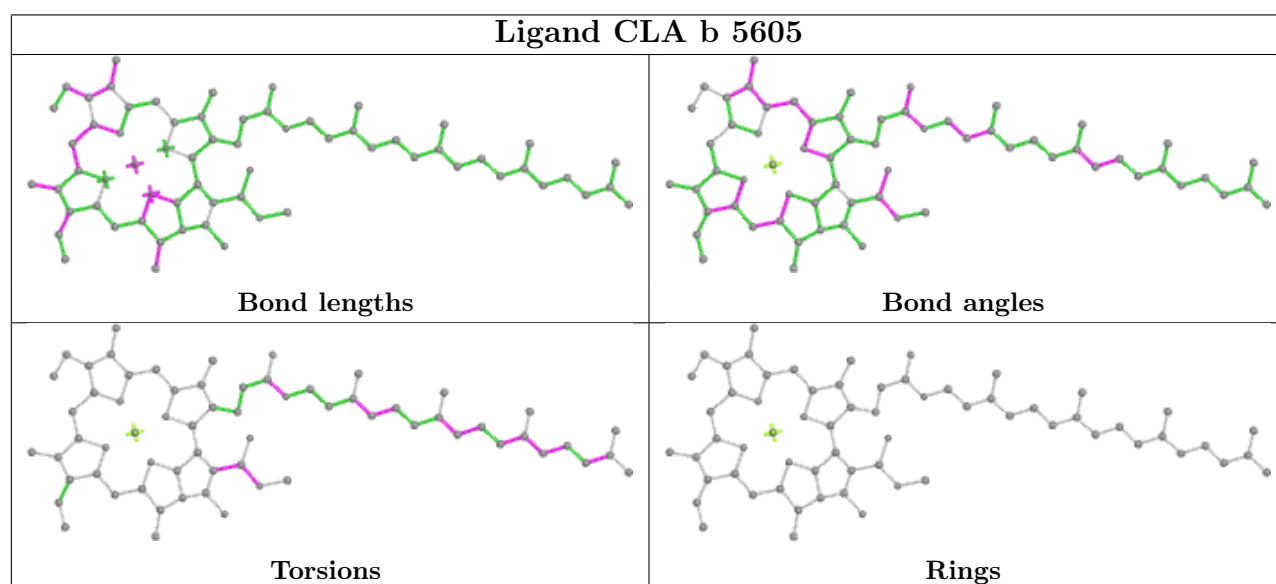
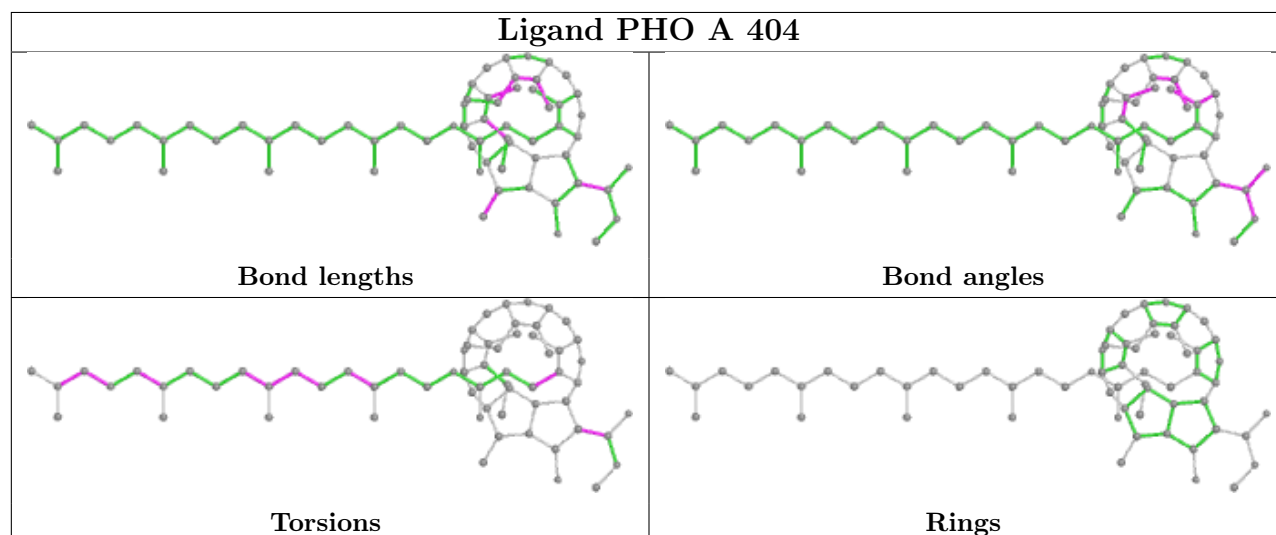
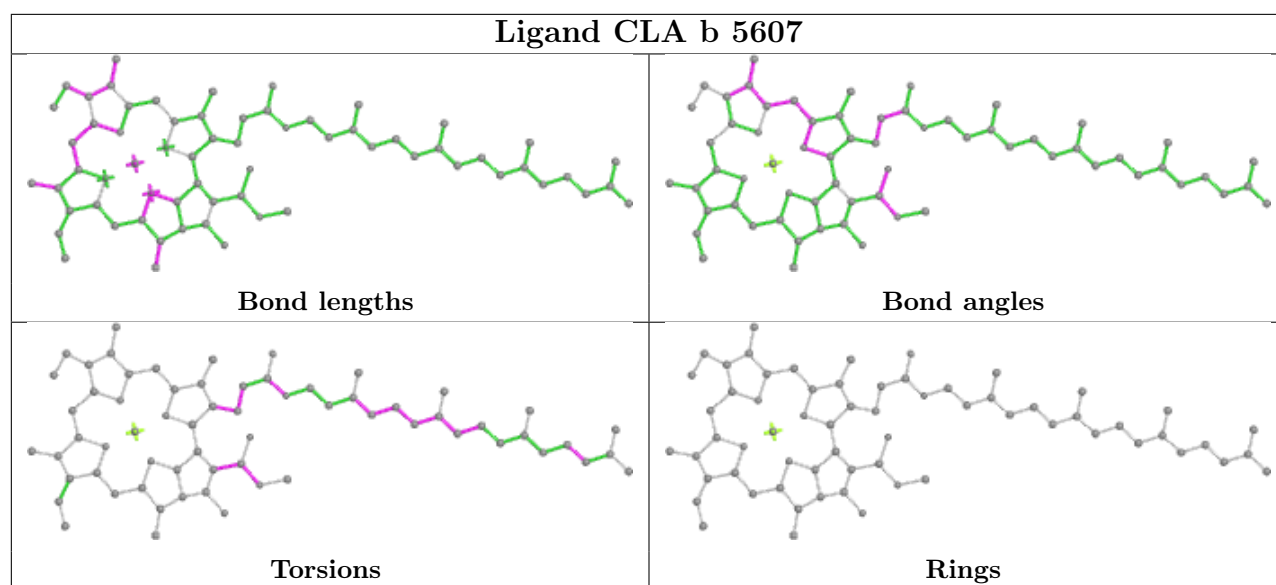
Ligand CLA B 615

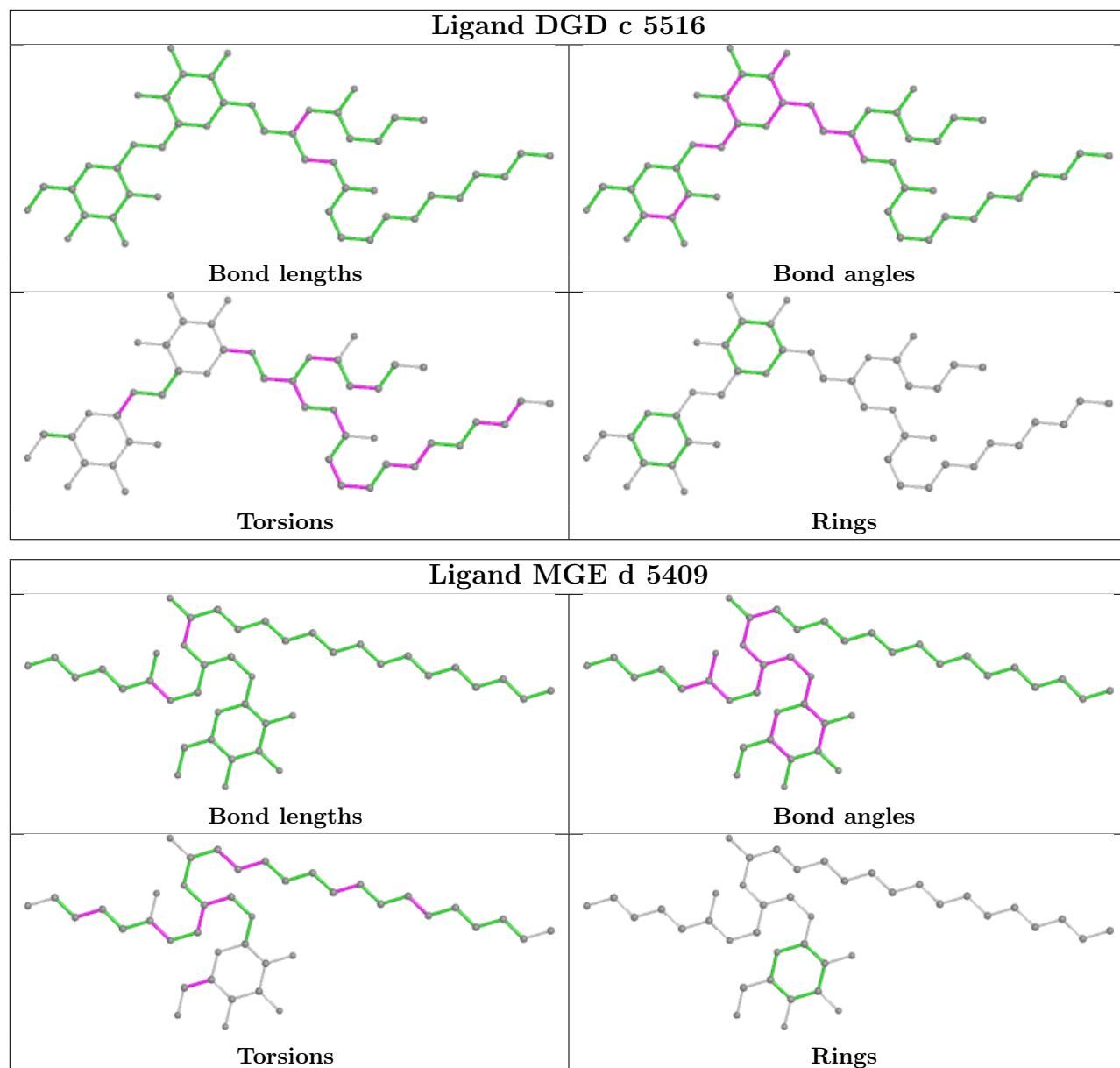


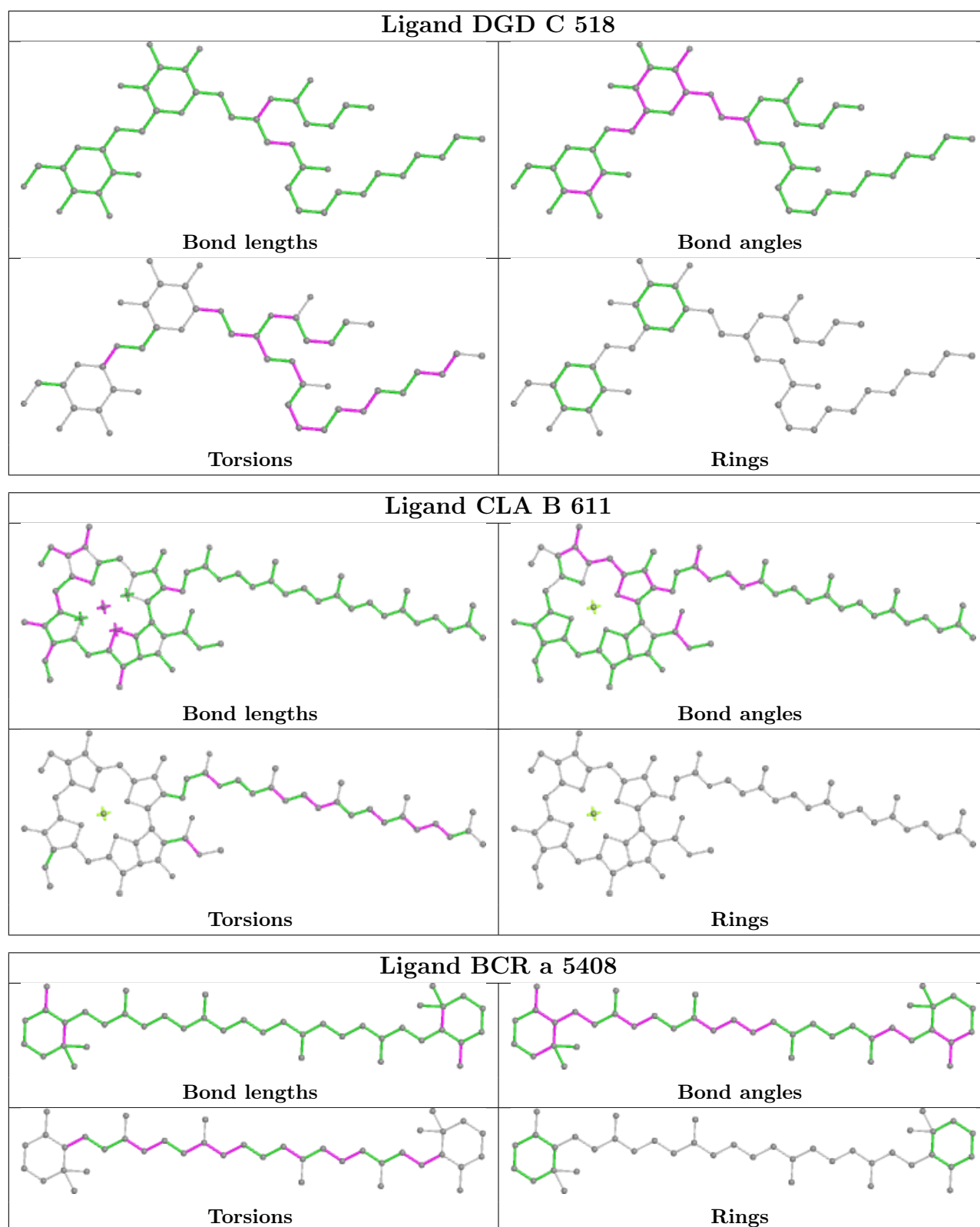
Ligand CLA c 5502



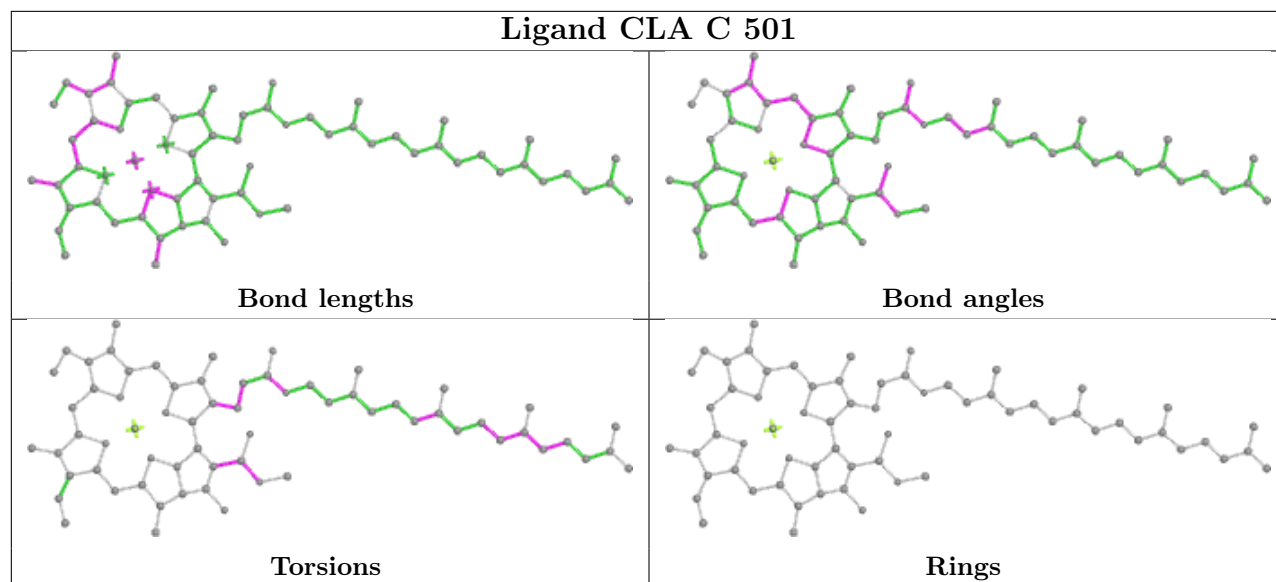




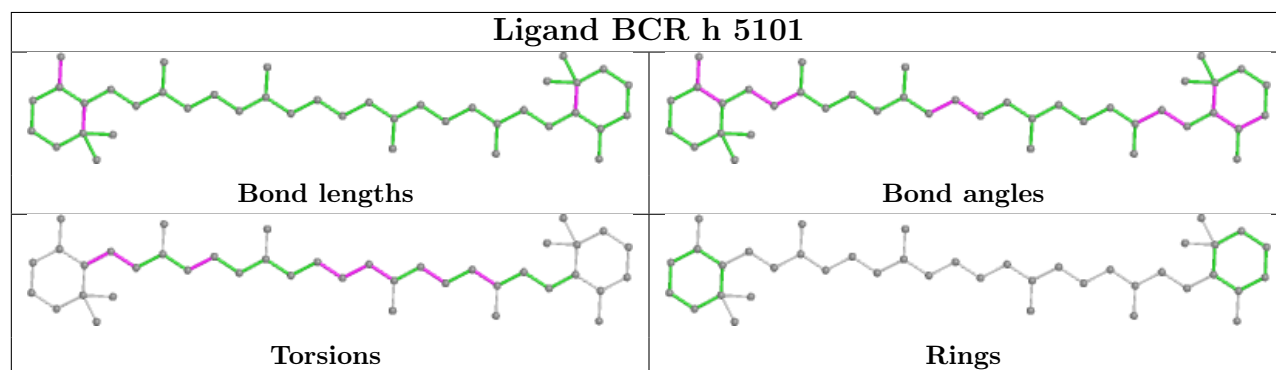




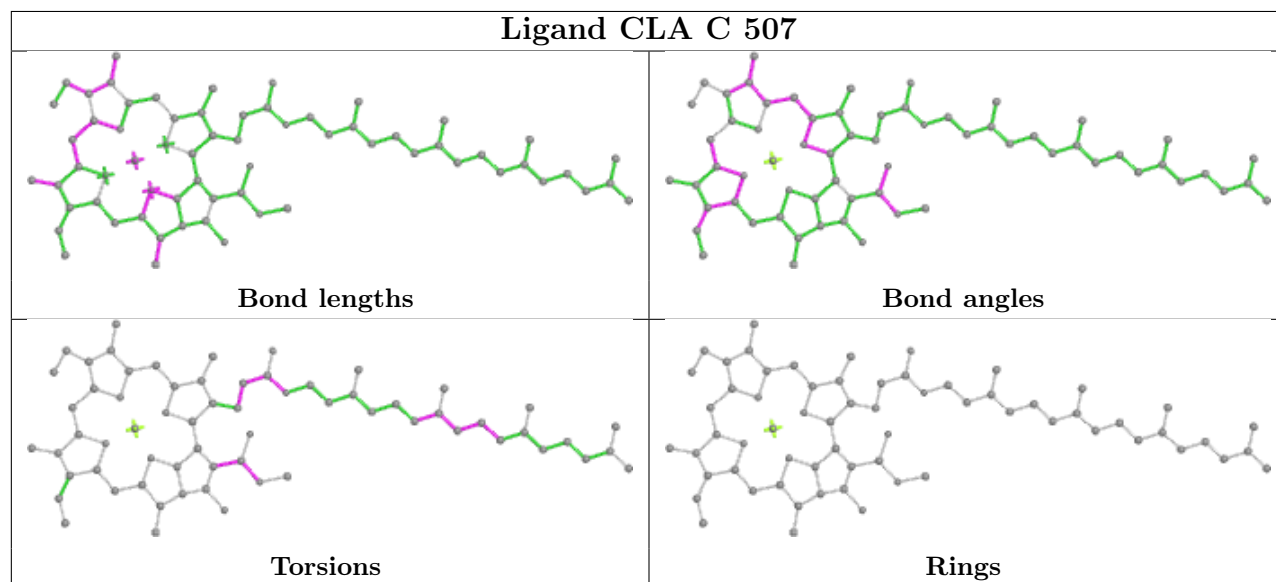
Ligand CLA C 501

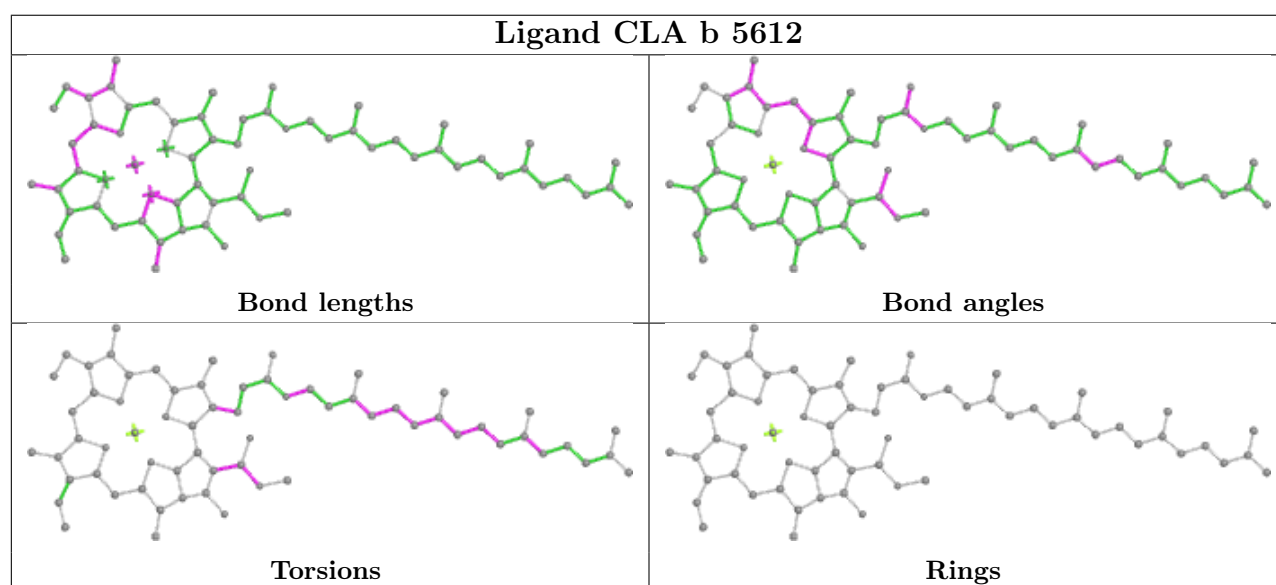
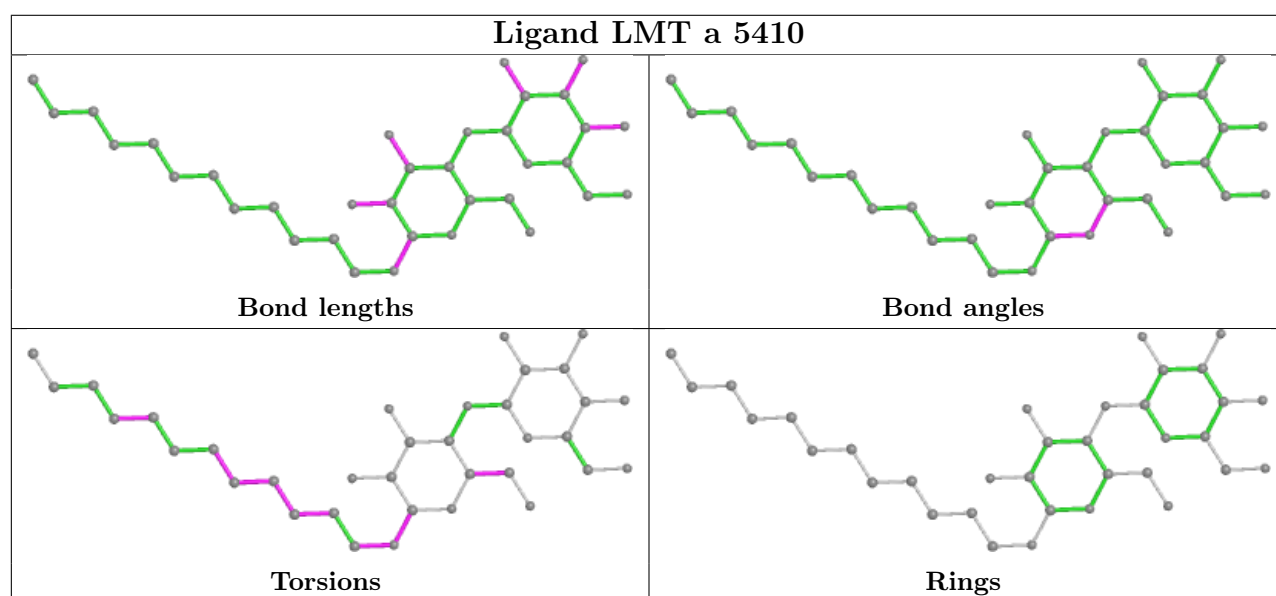
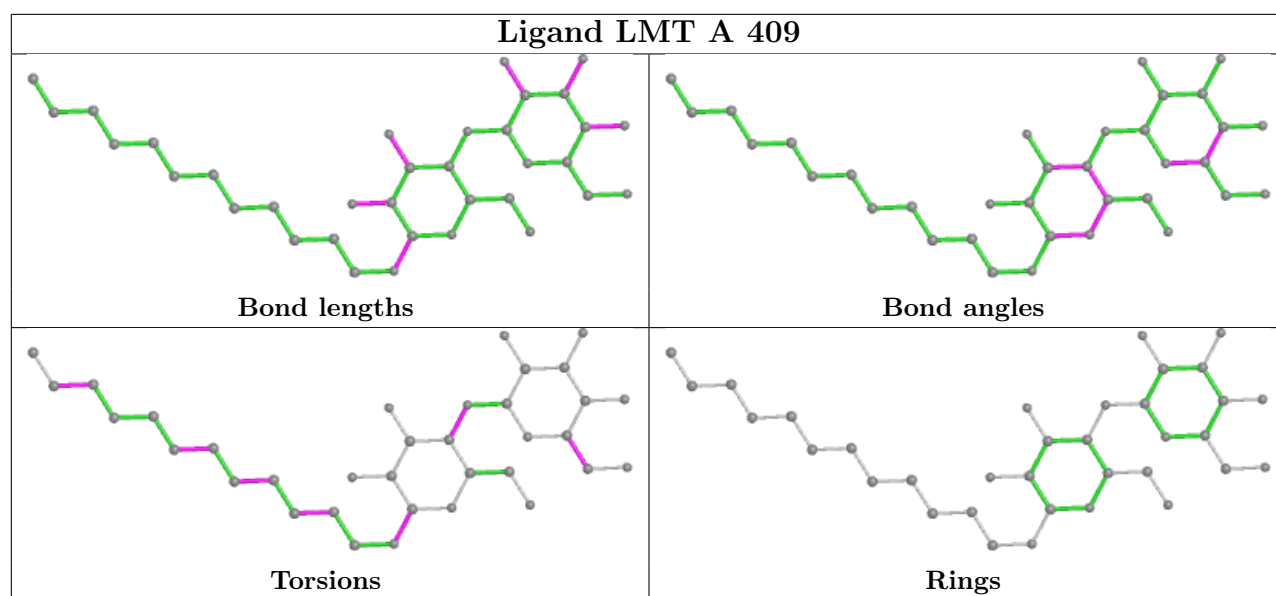


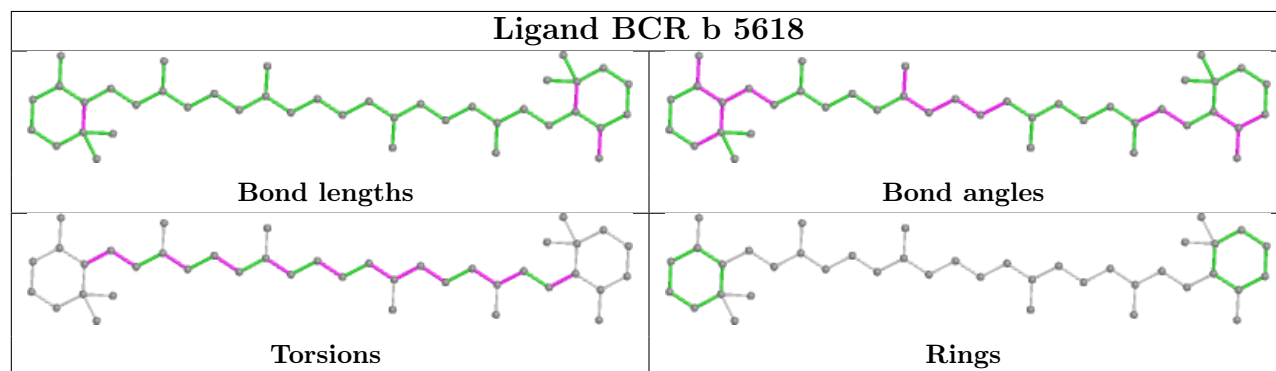
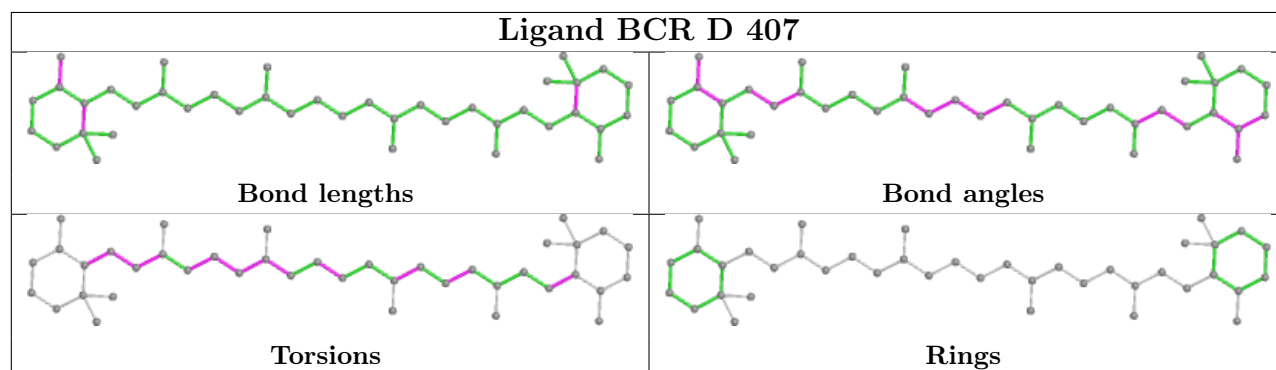
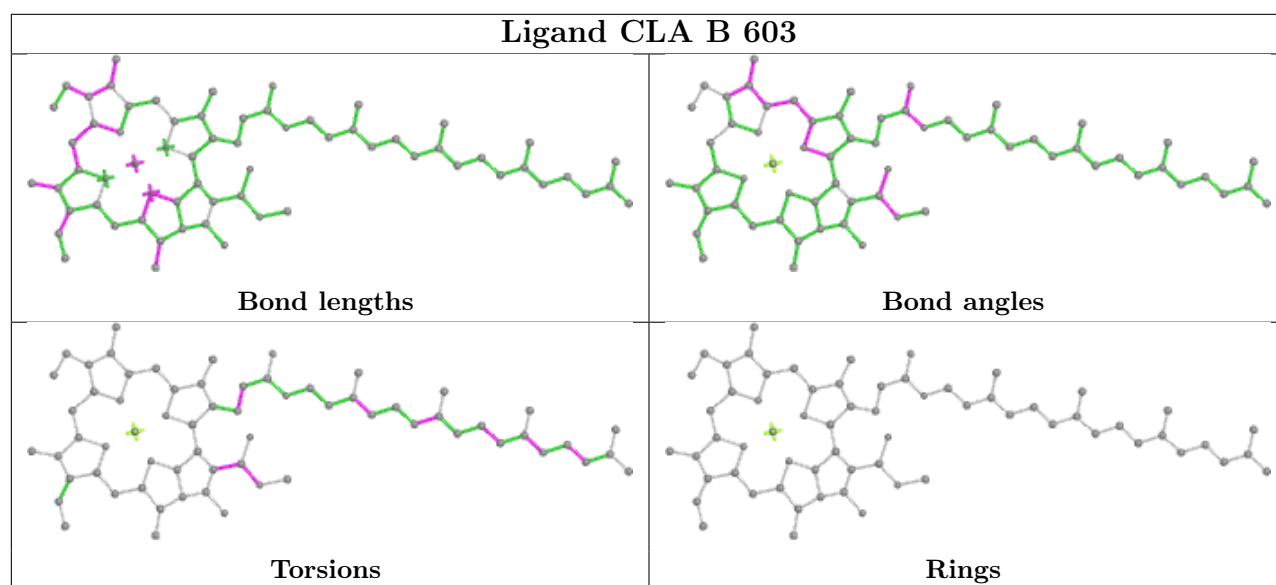
Ligand BCR h 5101

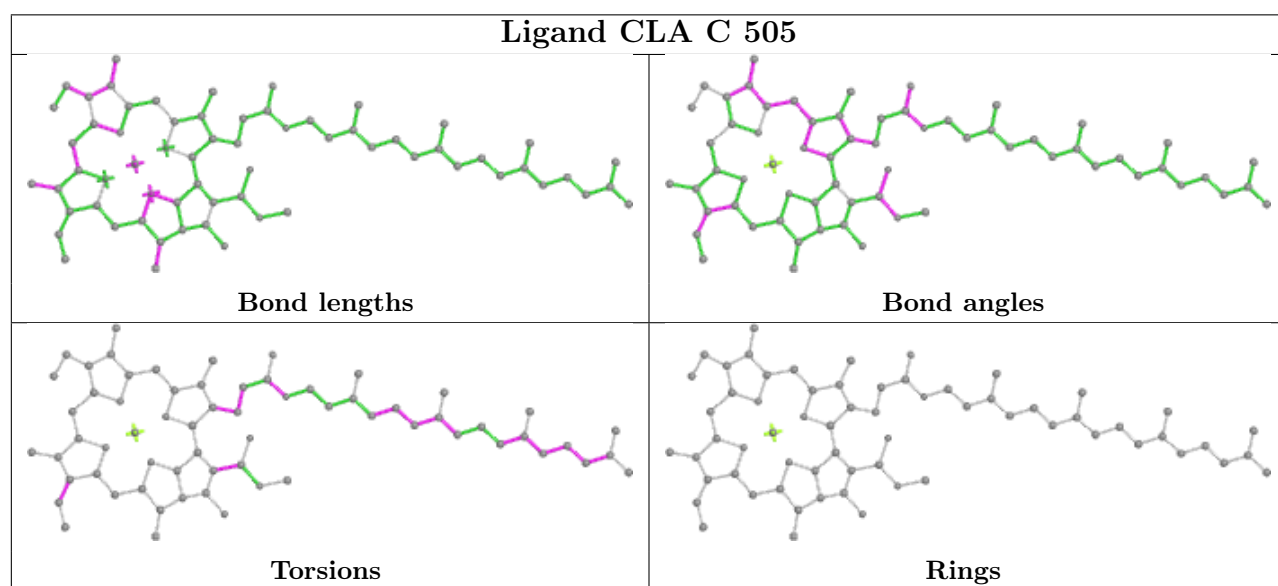
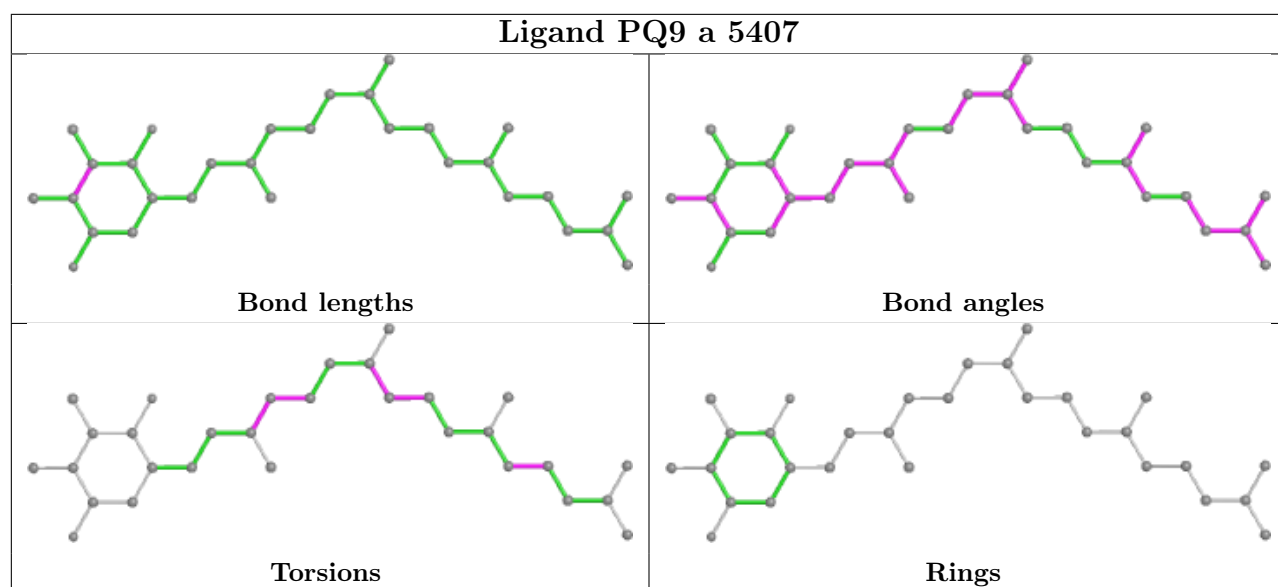


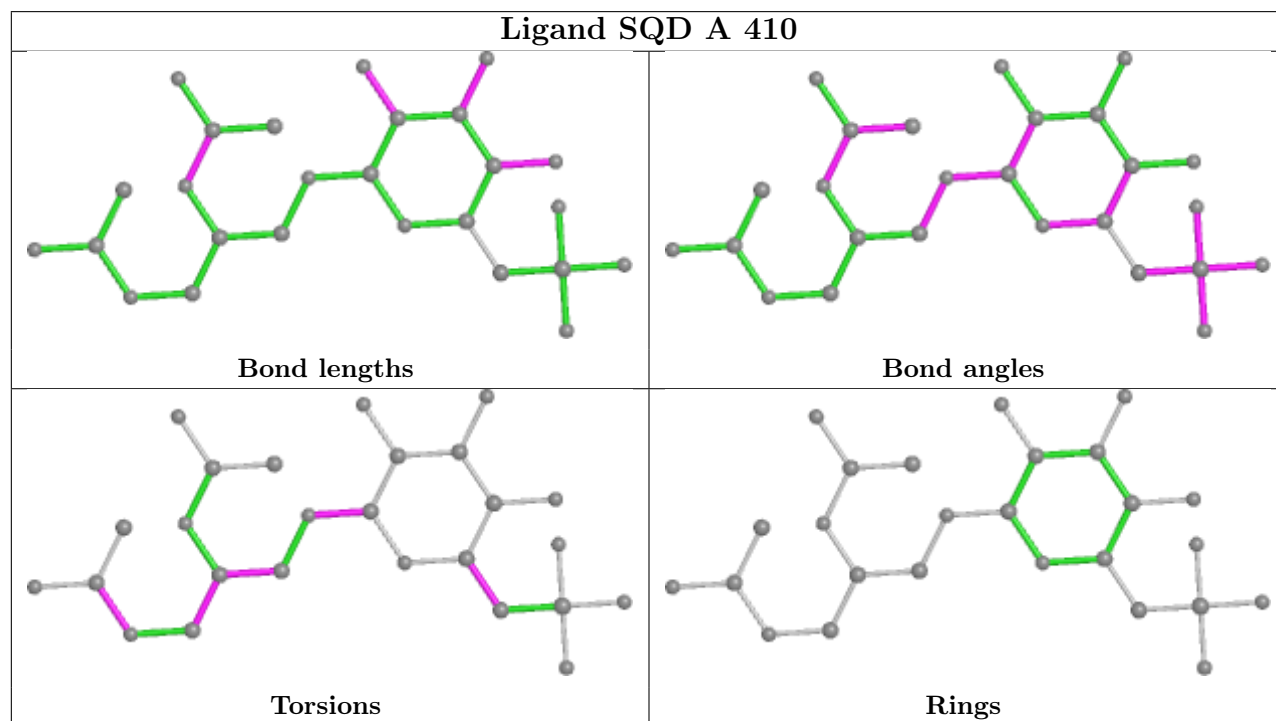
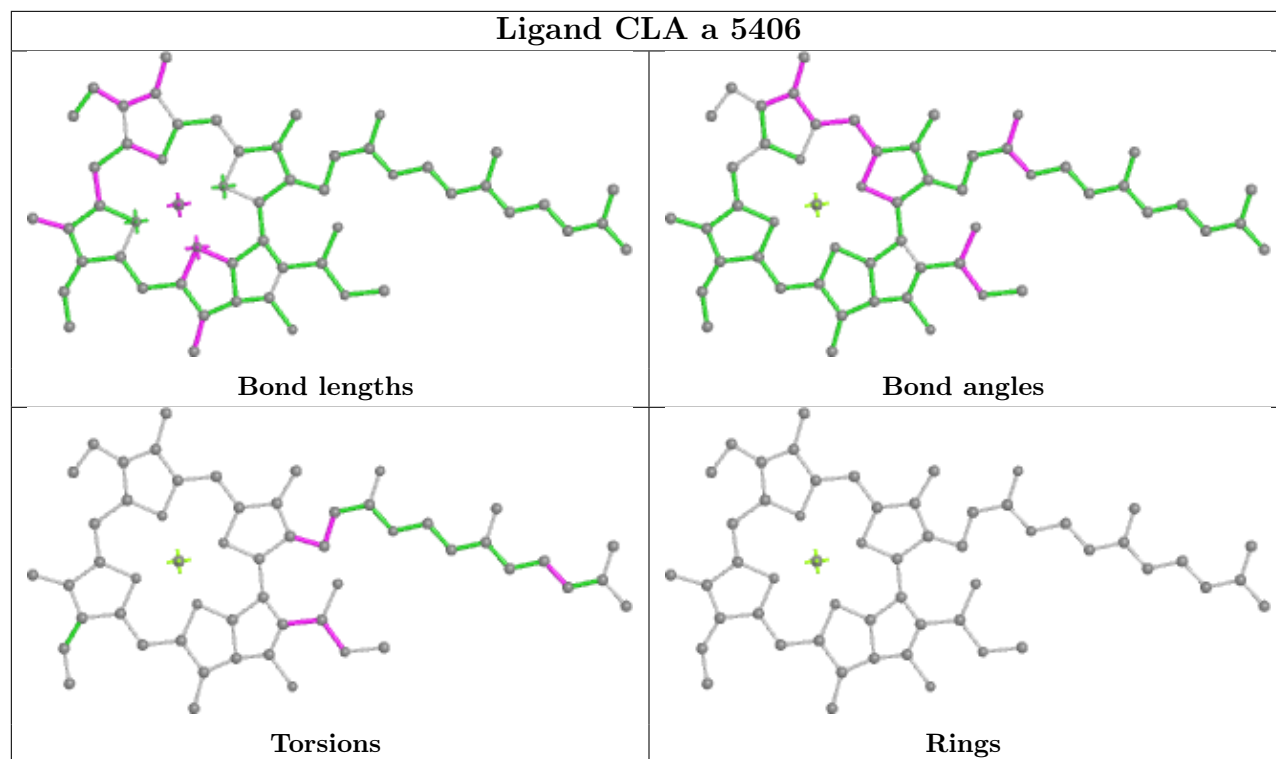
Ligand CLA C 507

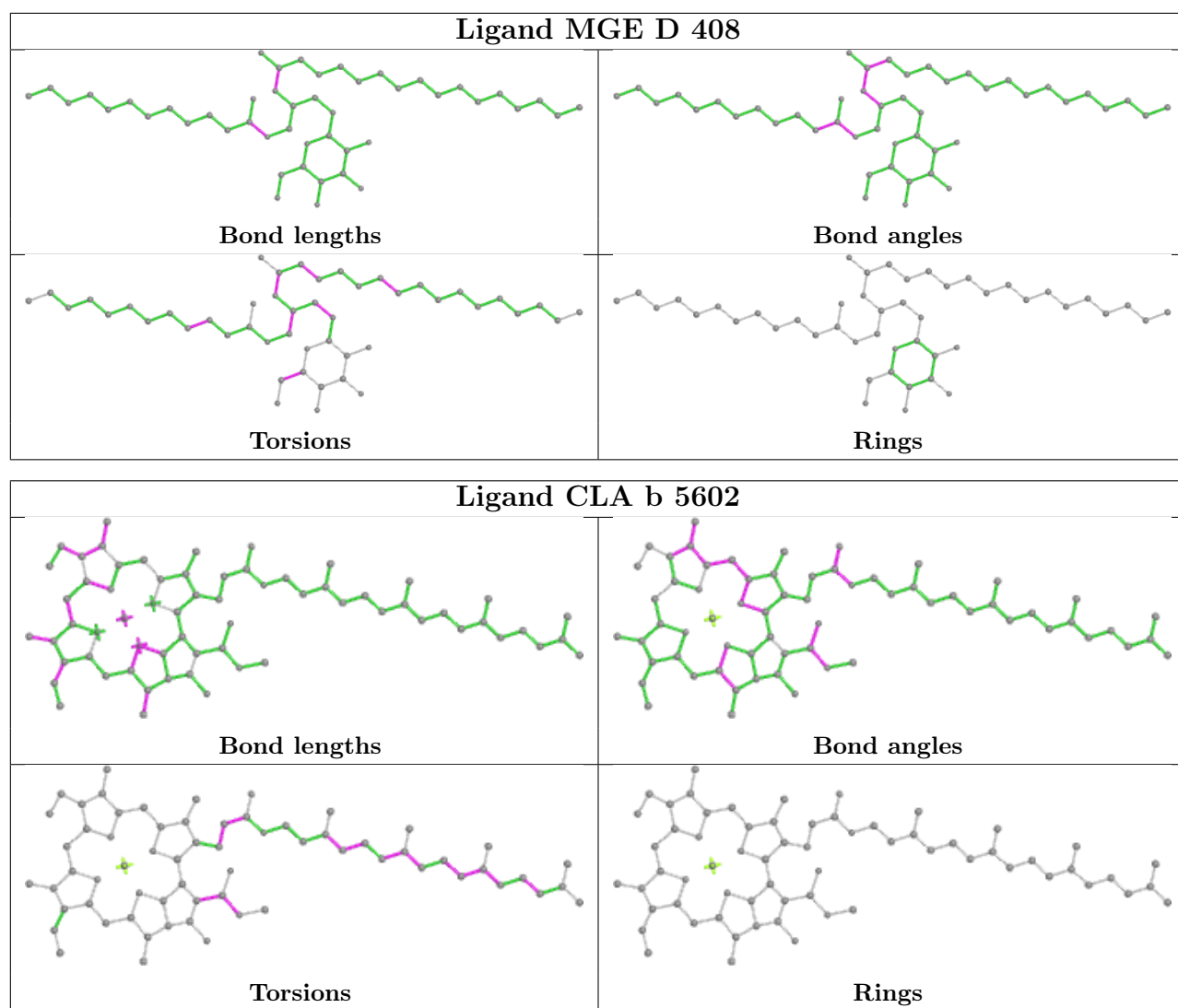




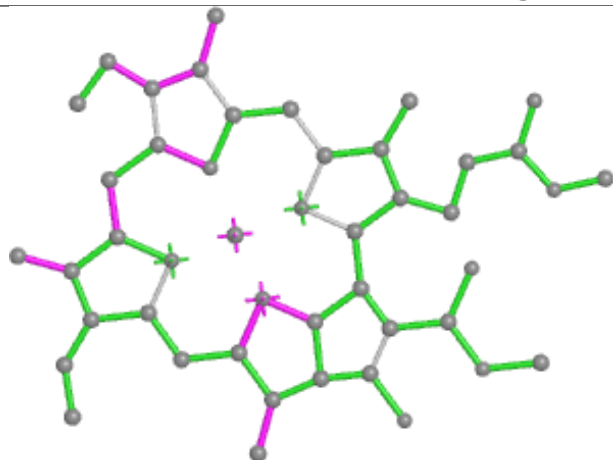




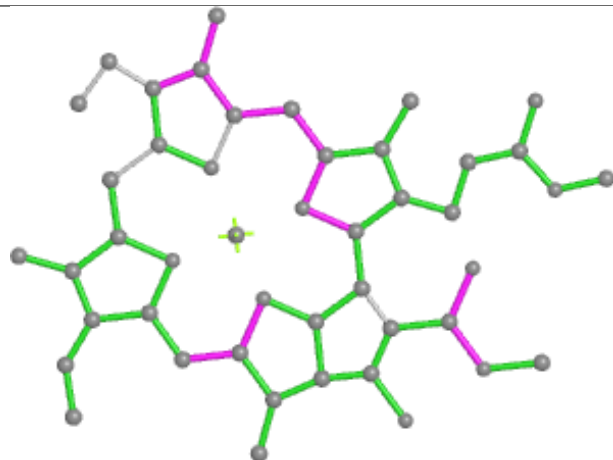




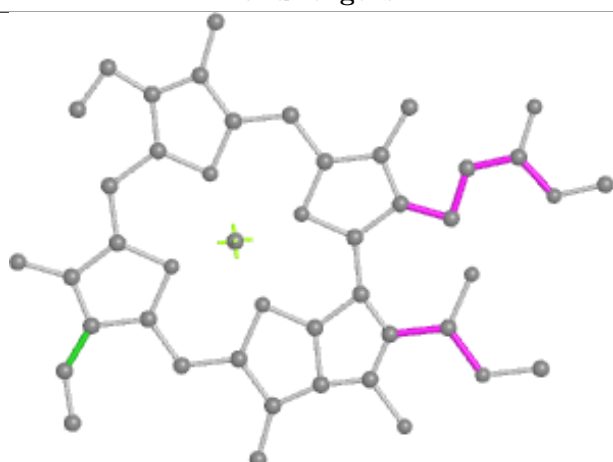
Ligand CLA C 504



Bond lengths



Bond angles

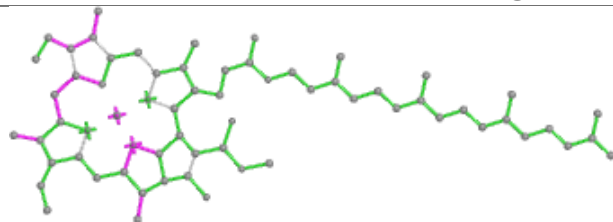


Torsions

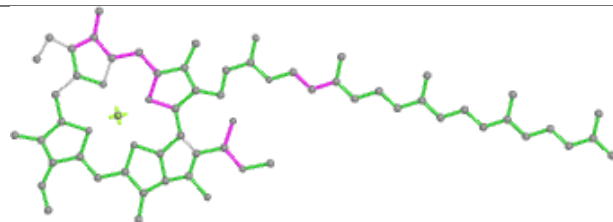


Rings

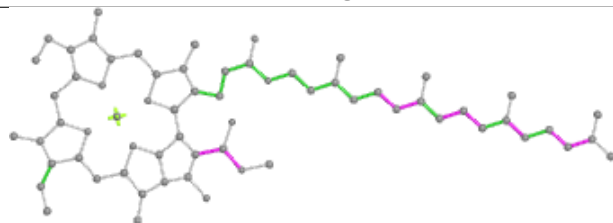
Ligand CLA k 5501



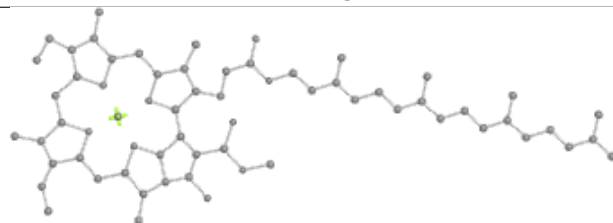
Bond lengths



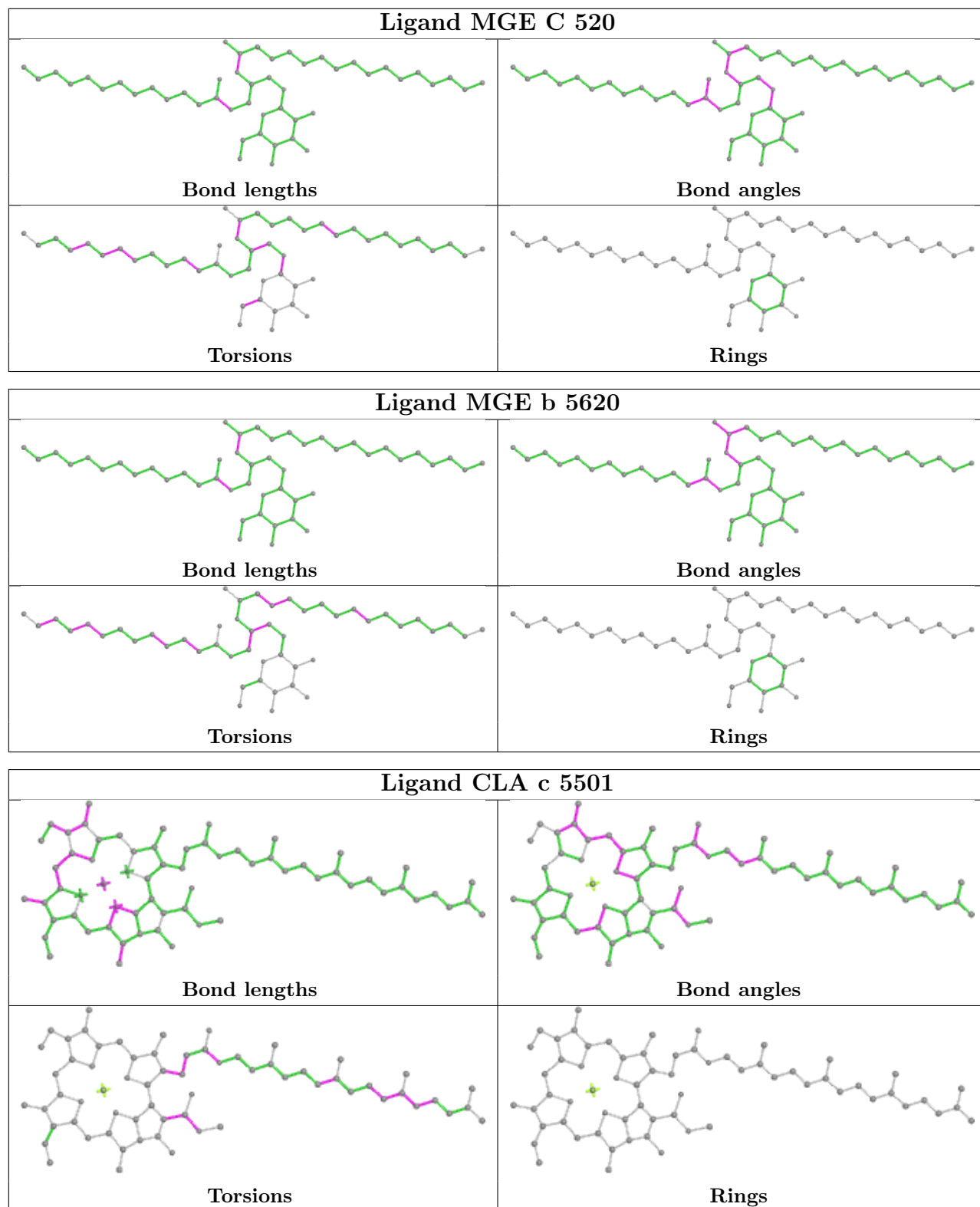
Bond angles

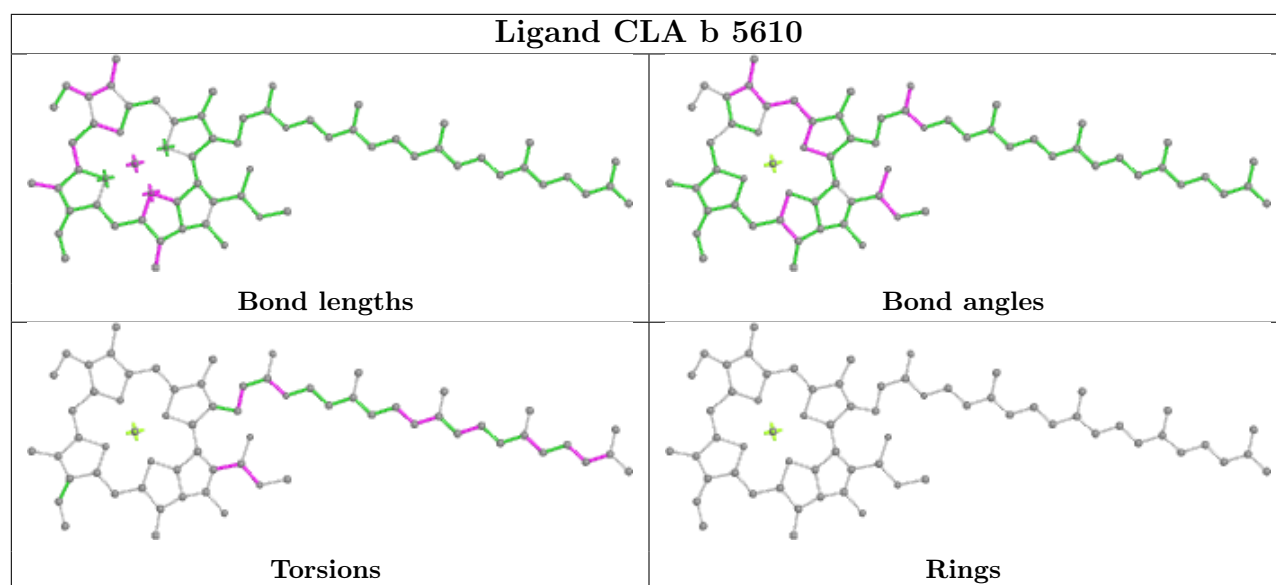


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

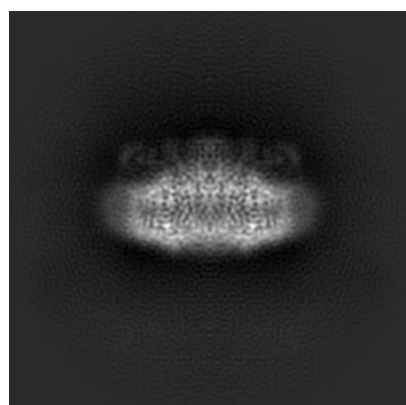
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30511. These allow visual inspection of the internal detail of the map and identification of artifacts.

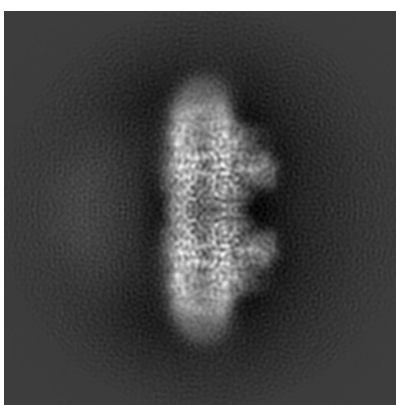
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

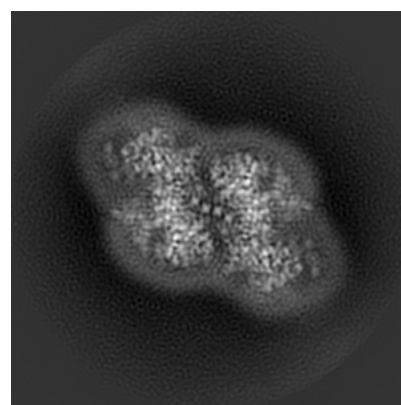
6.1.1 Primary map



X



Y

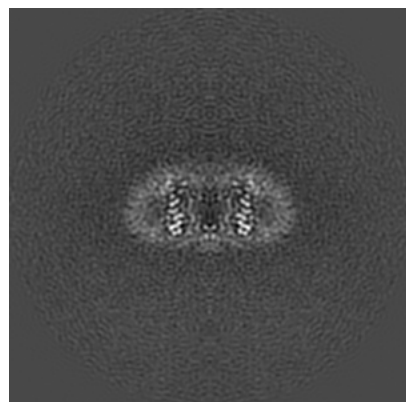


Z

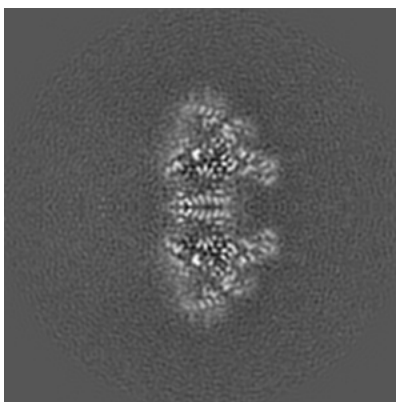
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

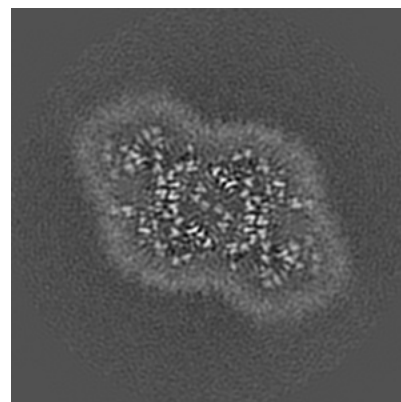
6.2.1 Primary map



X Index: 120



Y Index: 120

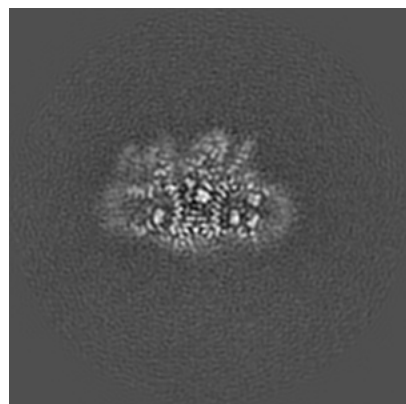


Z Index: 120

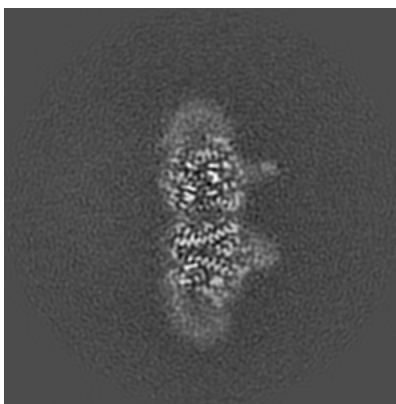
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

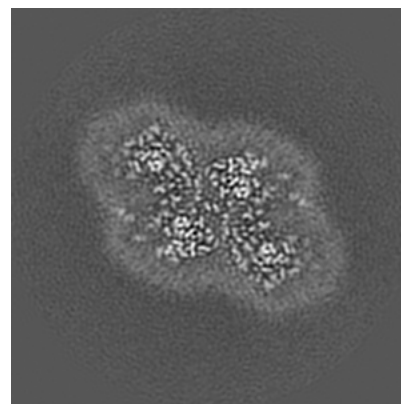
6.3.1 Primary map



X Index: 146



Y Index: 144

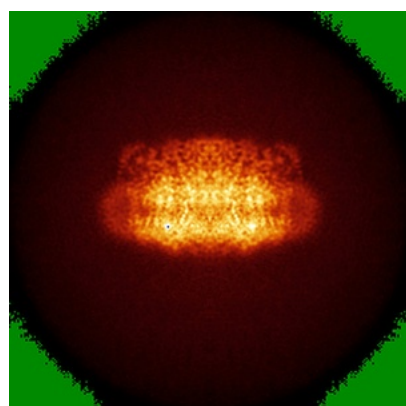


Z Index: 111

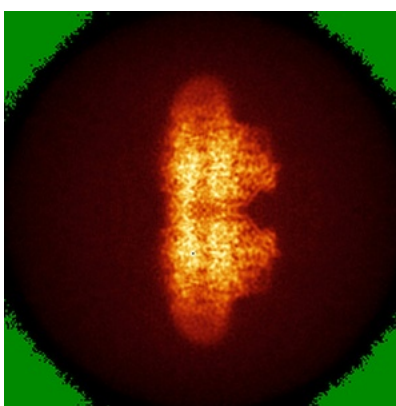
The images above show the largest variance slices of the map in three orthogonal directions.

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

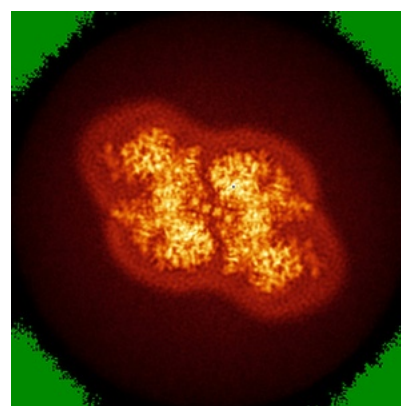
6.4.1 Primary map



X



Y

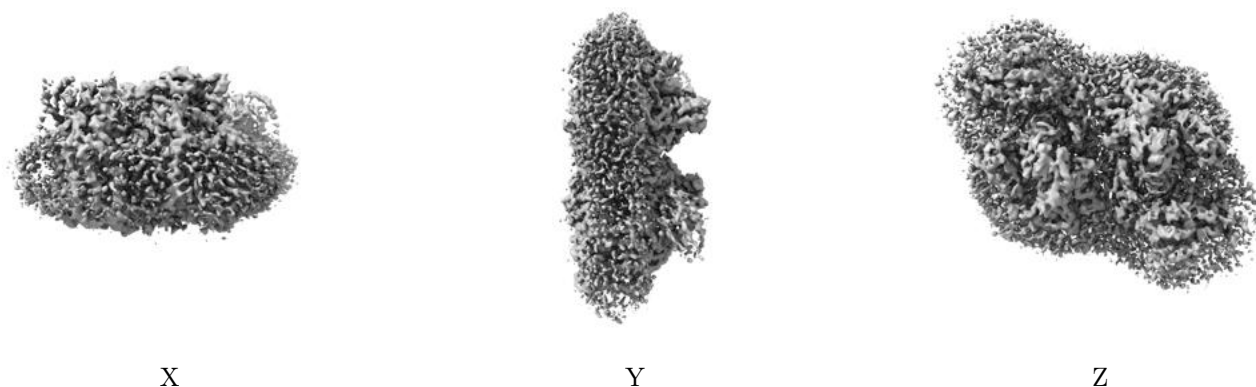


Z

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

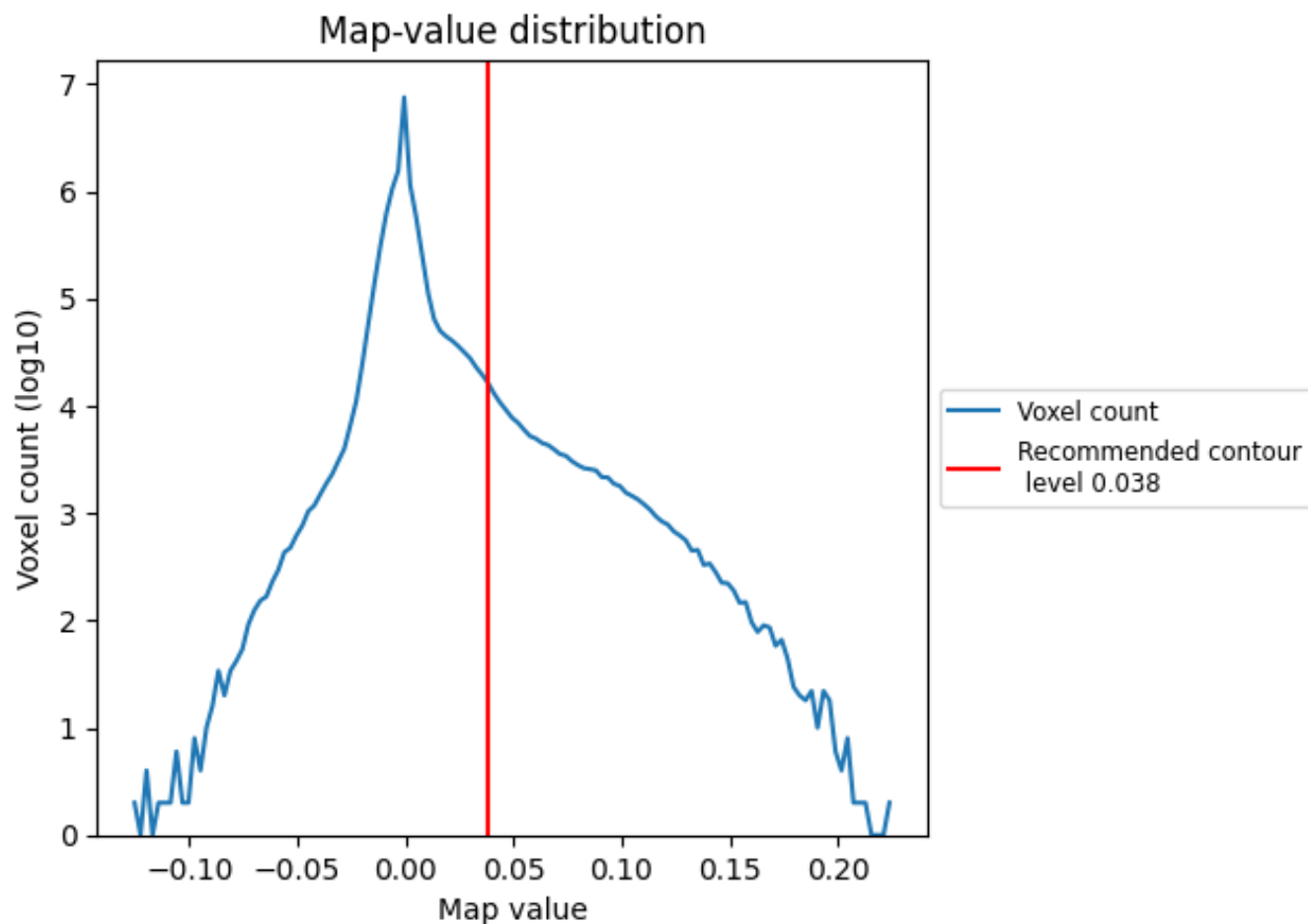
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

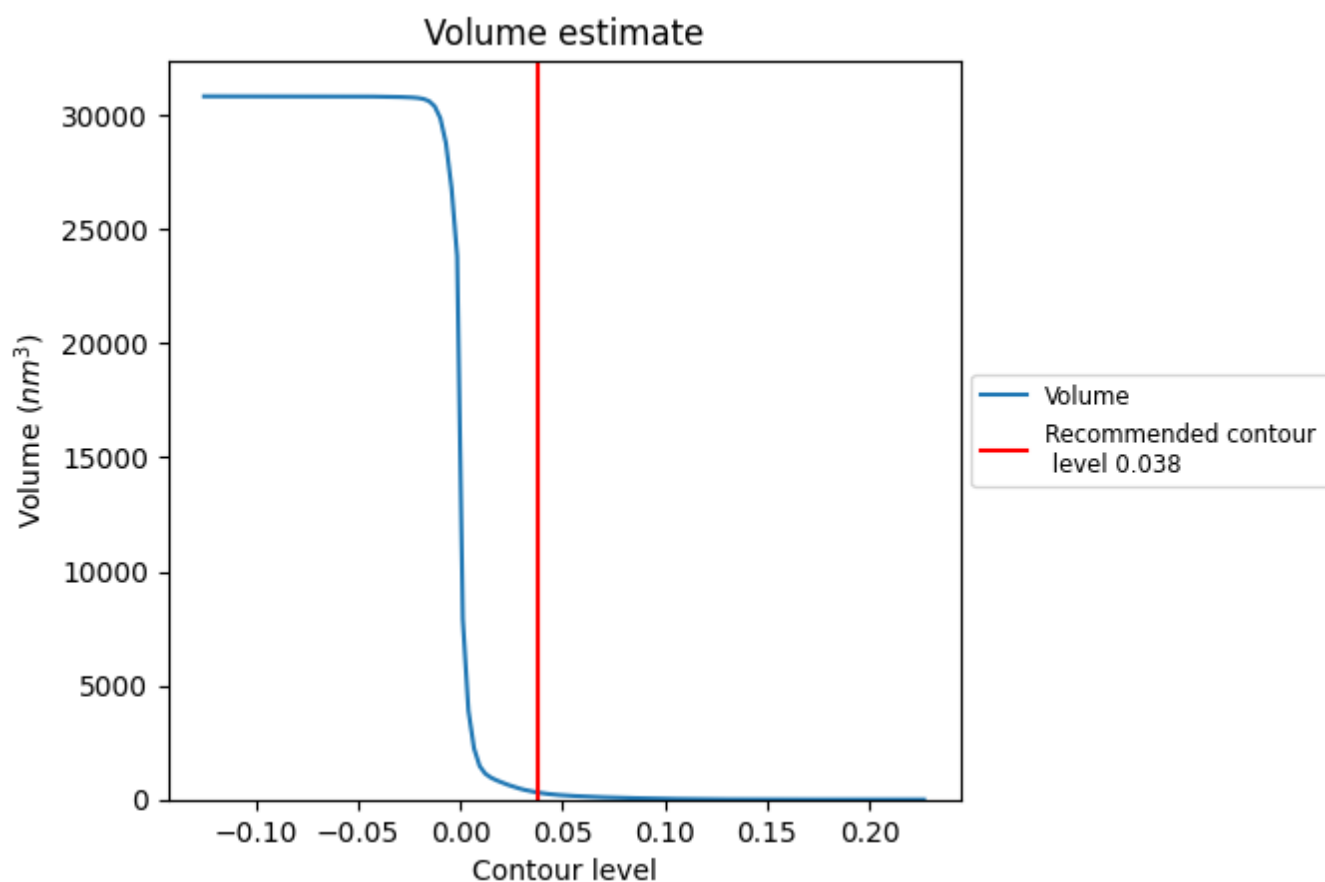
This section contains the results of statistical analysis of the map.

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.

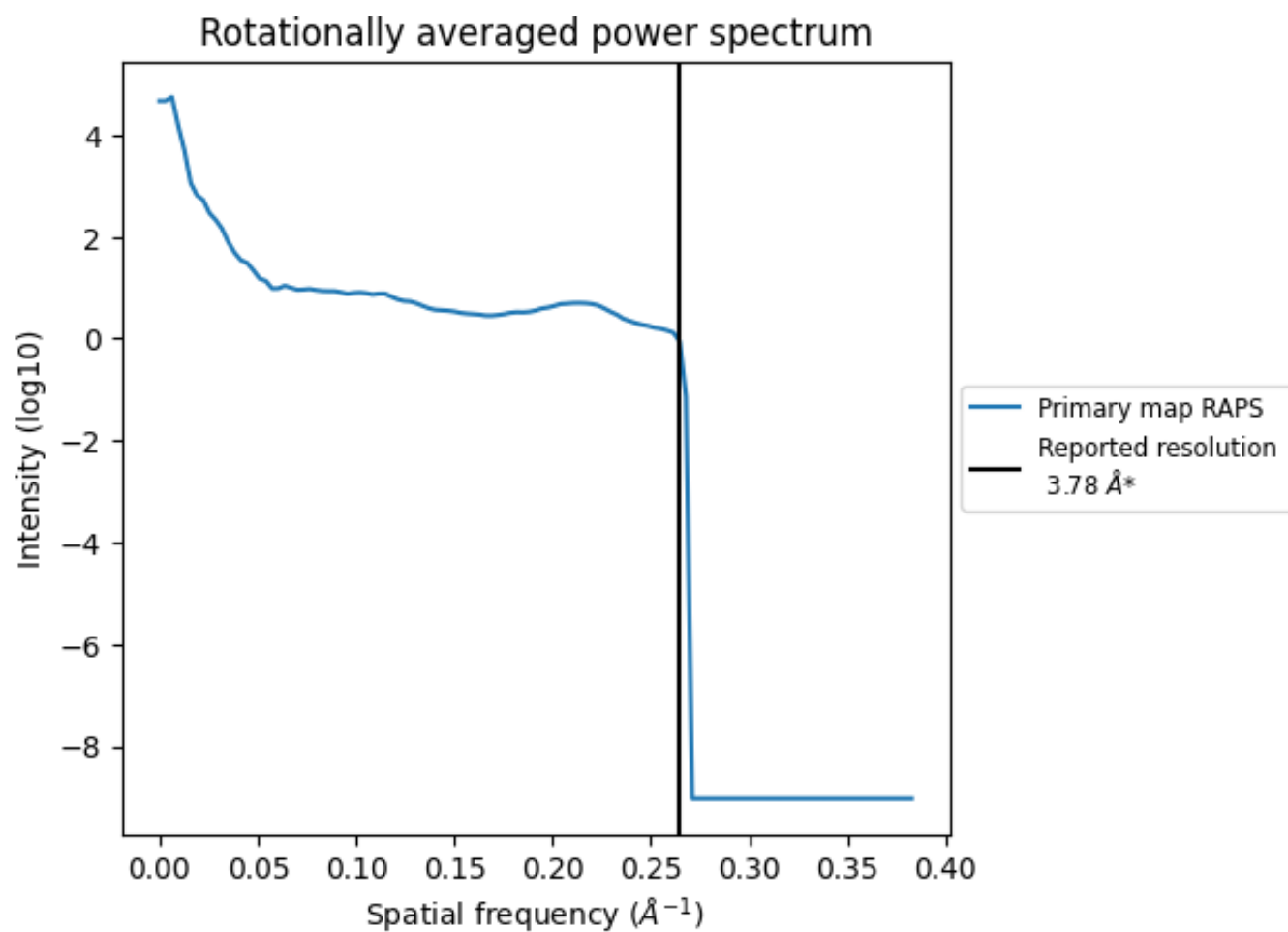
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 307 nm³; this corresponds to an approximate mass of 277 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 0.265 Å⁻¹

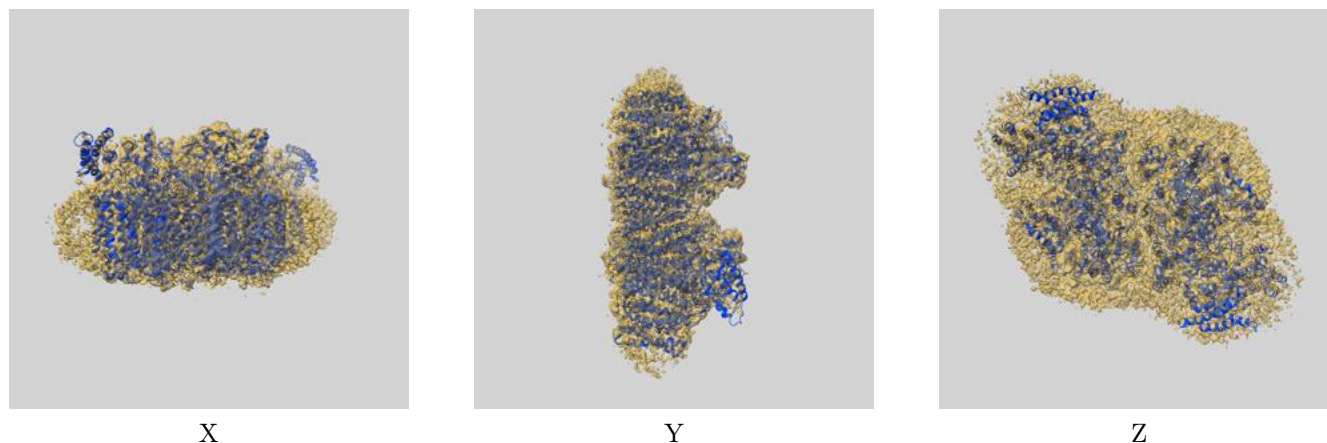
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

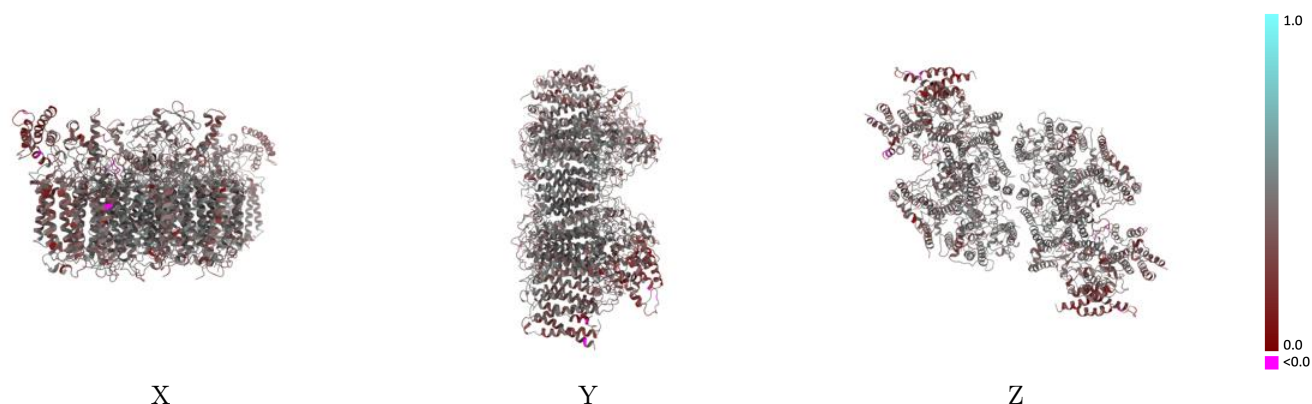
This section contains information regarding the fit between EMDB map EMD-30511 and PDB model 7CZL. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



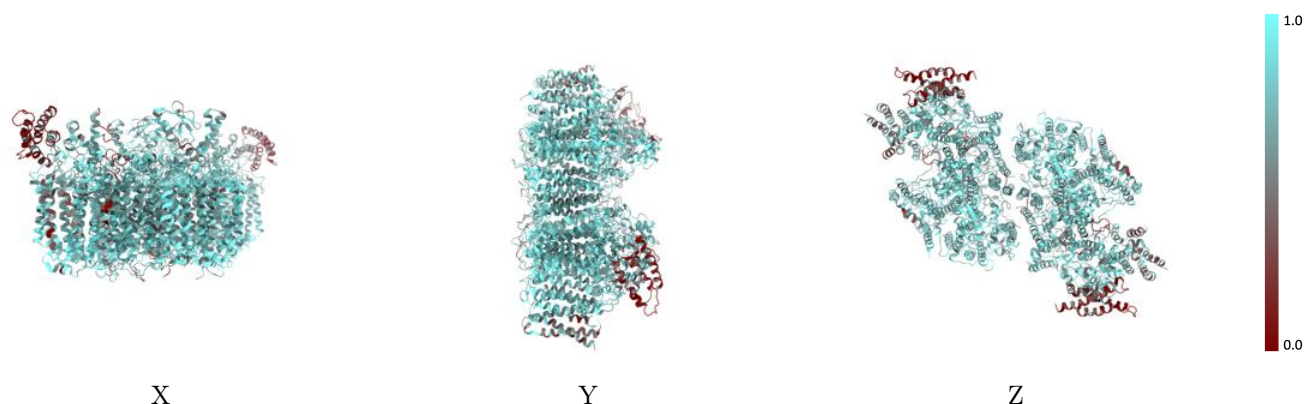
The images above show the 3D surface view of the map at the recommended contour level 0.038 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



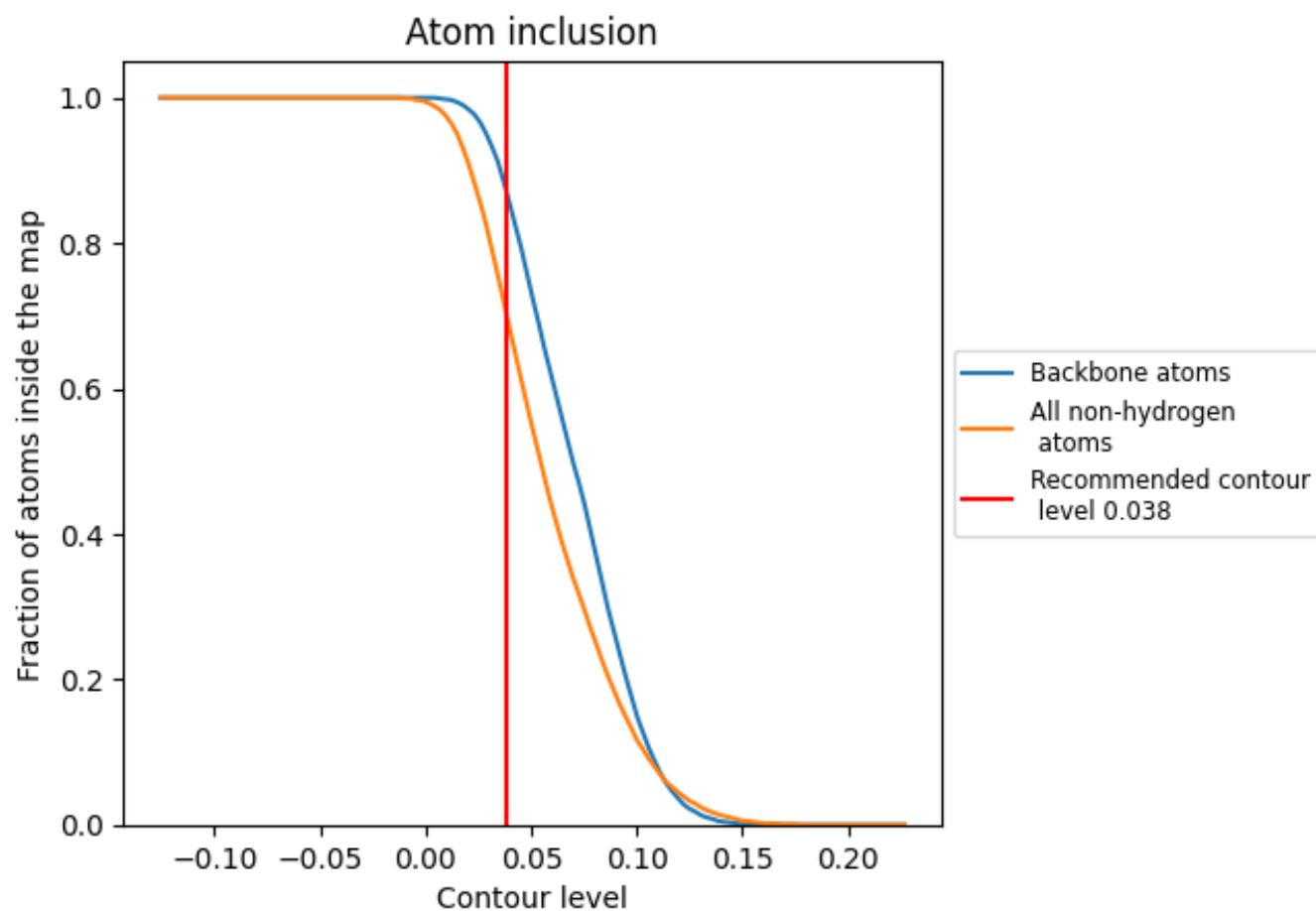
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.038).



































































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 71% 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 (0.038) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7080	 0.4220
A	 0.7340	 0.4410
B	 0.7710	 0.4490
C	 0.6990	 0.4080
D	 0.7710	 0.4490
E	 0.6800	 0.3720
F	 0.7410	 0.3800
H	 0.7950	 0.4370
I	 0.7650	 0.4150
K	 0.6700	 0.3670
L	 0.6960	 0.4470
M	 0.6060	 0.4270
N	 0.2210	 0.2790
T	 0.6080	 0.4550
X	 0.7360	 0.3700
Y	 0.4900	 0.3980
Z	 0.5290	 0.3190
a	 0.7330	 0.4390
b	 0.7760	 0.4500
c	 0.7080	 0.4070
d	 0.7670	 0.4470
e	 0.6860	 0.3680
f	 0.7410	 0.3550
h	 0.7780	 0.4320
i	 0.7680	 0.4200
k	 0.6530	 0.4010
l	 0.6610	 0.4700
m	 0.5950	 0.4350
n	 0.2060	 0.2740
t	 0.6630	 0.4710
x	 0.7640	 0.3980
y	 0.5020	 0.3350
z	 0.5150	 0.3210

