



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 03:49 AM JST

PDB ID : 9IOX / pdb_00009iox
EMDB ID : EMD-60748
Title : Cryo-EM structure of a TEF30-associated intermediate PSII core dimer complex, type II, from *Chlamydomonas reinhardtii*
Authors : Wang, Y.; Wang, C.; Li, A.; Liu, Z.
Deposited on : 2024-07-09
Resolution : 3.30 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

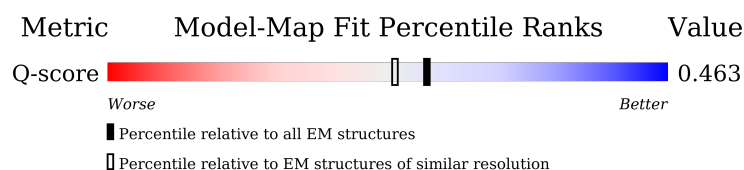
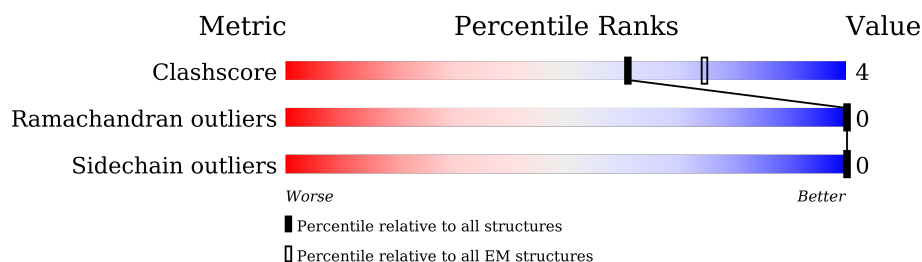
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	327	
1	a	327	
2	B	480	
2	b	480	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	450	
3	c	450	
4	D	351	
4	d	351	
5	E	74	
5	e	74	
6	F	31	
6	f	31	
7	G	195	
7	g	195	
8	H	71	
8	h	71	
9	I	34	
9	i	34	
10	K	37	
10	k	37	
11	L	38	
11	l	38	
12	M	27	
12	m	27	
13	T	28	
13	t	28	
14	V	31	
14	v	31	
15	X	32	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	x	32	69% 91% 9%
16	Z	61	95% 87% 13%
16	z	61	97% 84% 16%

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 41854 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	306	Total	C	N	O	S	0	0
			2388	1568	395	410	15		
1	a	306	Total	C	N	O	S	0	0
			2388	1568	395	410	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	480	Total	C	N	O	S	0	0
			3755	2462	630	651	12		
2	b	480	Total	C	N	O	S	0	0
			3755	2462	630	651	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	441	Total	C	N	O	S	0	0
			3444	2256	574	597	17		
3	c	441	Total	C	N	O	S	0	0
			3444	2256	574	597	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	337	Total	C	N	O	S	0	0
			2686	1777	439	458	12		
4	d	337	Total	C	N	O	S	0	0
			2686	1777	439	458	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	74	Total	C	N	O	0	0
			602	395	99	108		
5	e	74	Total	C	N	O	0	0
			602	395	99	108		

- 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
			251	171	42	37	1		
6	f	31	Total	C	N	O	S	0	0
			251	171	42	37	1		

- Molecule 7 is a protein called PDZ domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	169	Total	C	N	O	S	0	0
			1368	856	245	260	7		
7	g	169	Total	C	N	O	S	0	0
			1368	856	245	260	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	71	Total	C	N	O	S	0	0
			546	366	81	97	2		
8	h	71	Total	C	N	O	S	0	0
			546	366	81	97	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total	C	N	O	S	0	0
			275	189	41	43	2		
9	i	34	Total	C	N	O	S	0	0
			275	189	41	43	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	37	Total	C	N	O	0	0
			297	209	43	45		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
10	k	37	Total	C	N	O	0	0
			297	209	43	45		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	38	Total	C	N	O	S	0	0
			314	210	51	52	1		
11	l	38	Total	C	N	O	S	0	0
			314	210	51	52	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	27	Total	C	N	O	0	0
			210	146	29	35		
12	m	27	Total	C	N	O	0	0
			210	146	29	35		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	28	Total	C	N	O	S	0	0
			231	160	34	36	1		
13	t	28	Total	C	N	O	S	0	0
			231	160	34	36	1		

- Molecule 14 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	V	31	Total	C	N	O	0	0
			216	143	35	38		
14	v	31	Total	C	N	O	0	0
			216	143	35	38		

- Molecule 15 is a protein called Chloroplast photosystem II subunit X.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	X	32	Total	C	N	O	0	0
			214	140	35	39		
15	x	32	Total	C	N	O	0	0
			214	140	35	39		

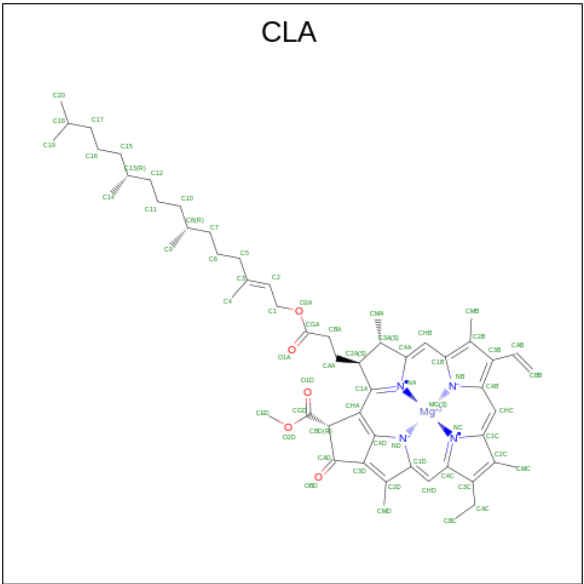
- Molecule 16 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Z	61	Total	C	N	O	S	0	0
			458	314	68	75	1		
16	z	61	Total	C	N	O	S	0	0
			458	314	68	75	1		

- Molecule 17 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 18 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
18	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
18	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

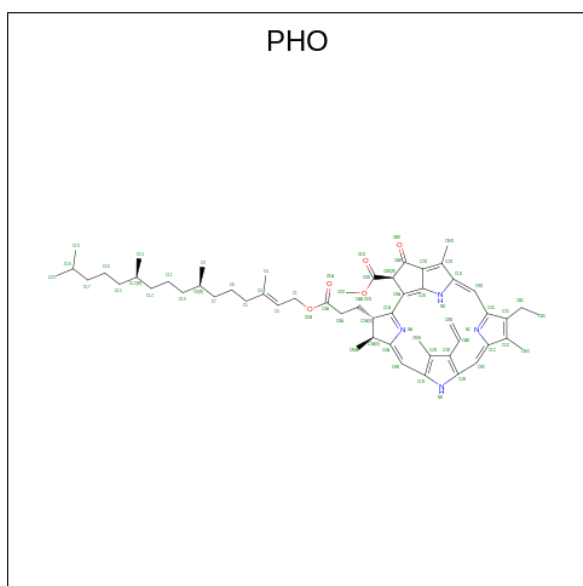
Mol	Chain	Residues	Atoms					AltConf
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

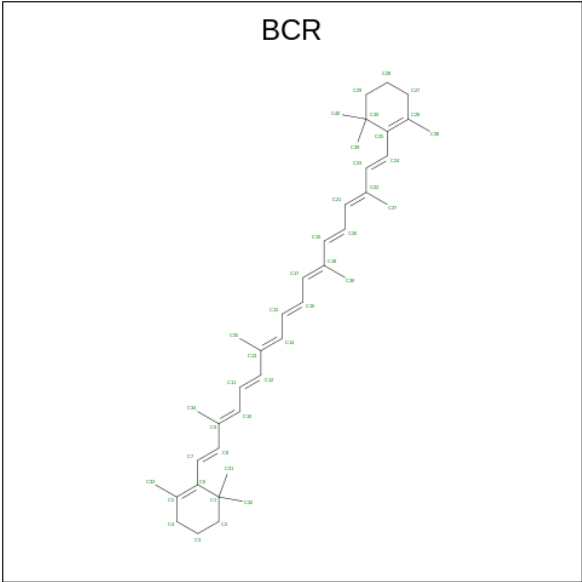
Mol	Chain	Residues	Atoms					AltConf
18	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 19 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 20 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



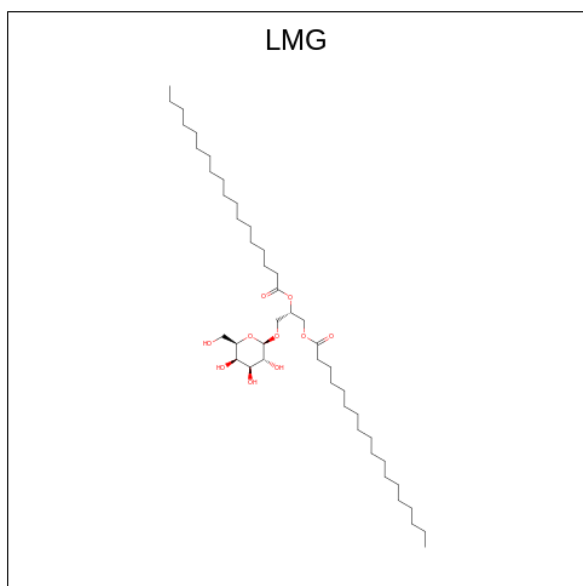
Mol	Chain	Residues	Atoms	AltConf
20	A	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	C	1	Total C 40 40	0
20	C	1	Total C 40 40	0
20	C	1	Total C 40 40	0
20	D	1	Total C 40 40	0
20	K	1	Total C 40 40	0
20	X	1	Total C 40 40	0
20	a	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	b	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
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	k	1	Total C 40 40	0
20	x	1	Total C 40 40	0
20	z	1	Total C 40 40	0

- Molecule 21 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



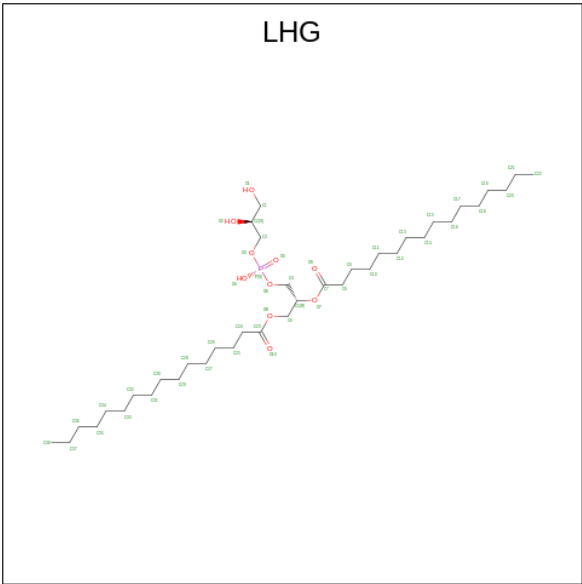
Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total C O 46 36 10	0
21	B	1	Total C O 42 32 10	0
21	C	1	Total C O 51 41 10	0
21	D	1	Total C O 46 36 10	0
21	D	1	Total C O 48 38 10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
21	b	1	Total	C	O	0
			42	32	10	
21	c	1	Total	C	O	0
			46	36	10	
21	c	1	Total	C	O	0
			51	41	10	
21	d	1	Total	C	O	0
			46	36	10	
21	h	1	Total	C	O	0
			48	38	10	

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



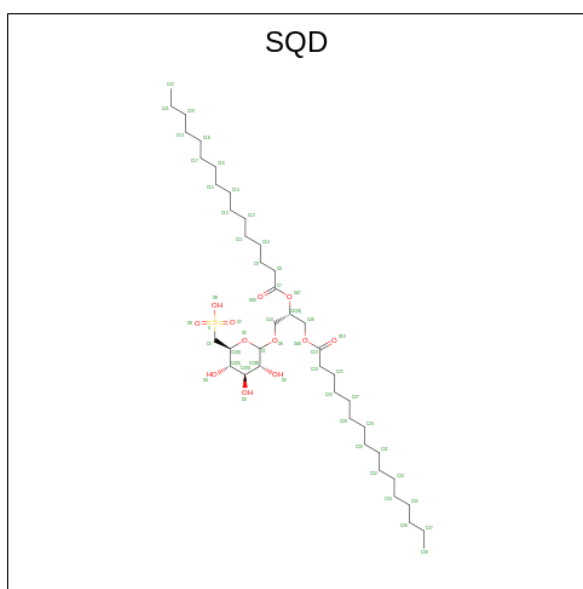
Mol	Chain	Residues	Atoms				AltConf
22	A	1	Total	C	O	P	0
			43	32	10	1	
22	A	1	Total	C	O	P	0
			44	33	10	1	
22	B	1	Total	C	O	P	0
			44	33	10	1	
22	B	1	Total	C	O	P	0
			49	38	10	1	
22	D	1	Total	C	O	P	0
			49	38	10	1	
22	L	1	Total	C	O	P	0
			49	38	10	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
22	X	1	Total	C	O	P	0
			49	38	10	1	
22	a	1	Total	C	O	P	0
			43	32	10	1	
22	a	1	Total	C	O	P	0
			44	33	10	1	
22	b	1	Total	C	O	P	0
			44	33	10	1	
22	b	1	Total	C	O	P	0
			49	38	10	1	
22	d	1	Total	C	O	P	0
			49	38	10	1	
22	l	1	Total	C	O	P	0
			49	38	10	1	
22	x	1	Total	C	O	P	0
			49	38	10	1	

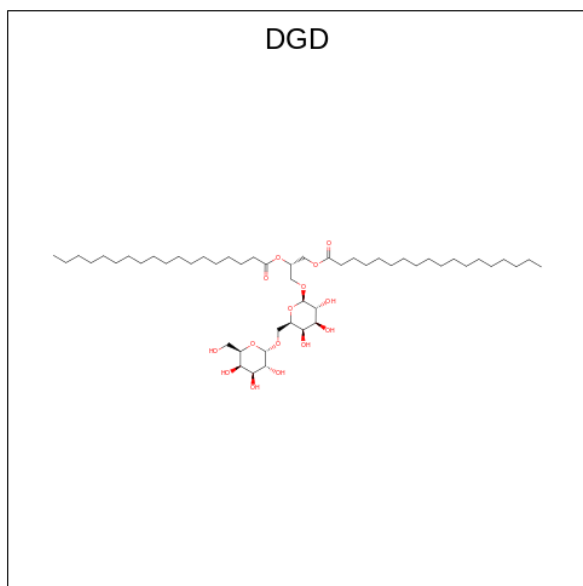
- Molecule 23 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
23	C	1	Total	C	O	S	0
			51	38	12	1	
23	c	1	Total	C	O	S	0
			51	38	12	1	

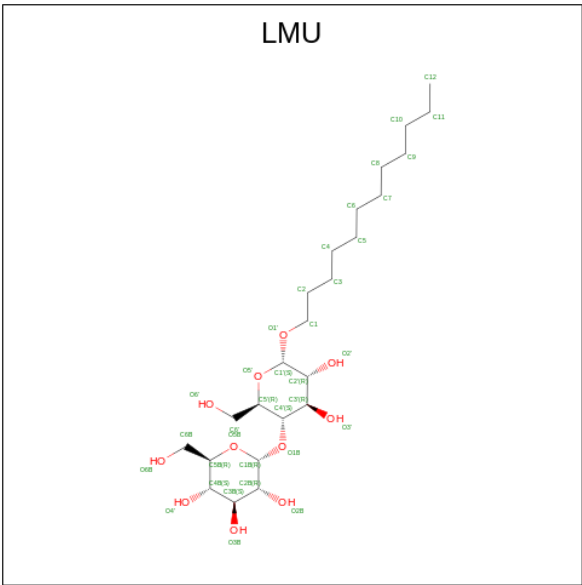
- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:

C₅₁H₉₆O₁₅) (labeled as "Ligand of Interest" by depositor).



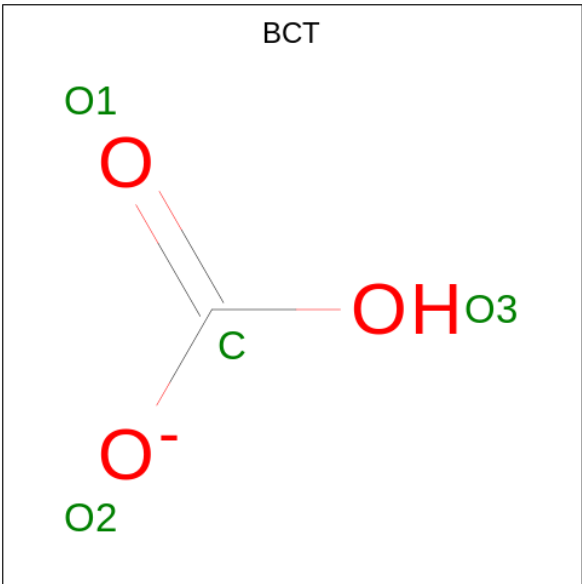
Mol	Chain	Residues	Atoms			AltConf
24	C	1	Total	C	O	0
			53	38	15	
24	C	1	Total	C	O	0
			49	34	15	
24	C	1	Total	C	O	0
			59	44	15	
24	c	1	Total	C	O	0
			53	38	15	
24	c	1	Total	C	O	0
			49	34	15	
24	c	1	Total	C	O	0
			59	44	15	

- Molecule 25 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
25	C	1	Total	C	O	0
			35	24	11	
25	c	1	Total	C	O	0
			35	24	11	

- Molecule 26 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



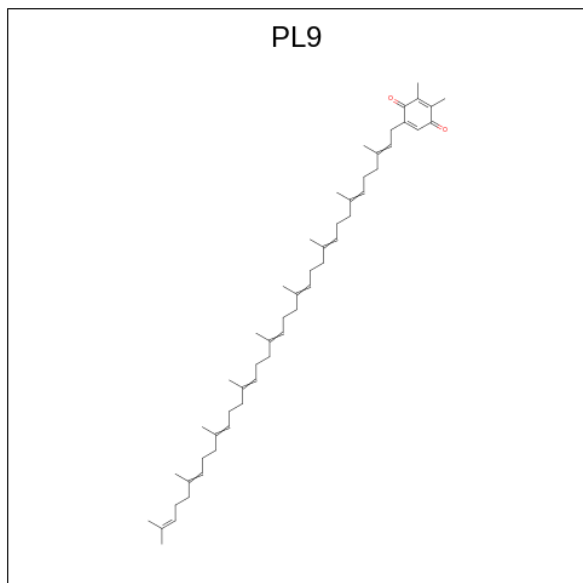
Mol	Chain	Residues	Atoms			AltConf
26	D	1	Total	C	O	0
			4	1	3	

Continued on next page...

Continued from previous page...

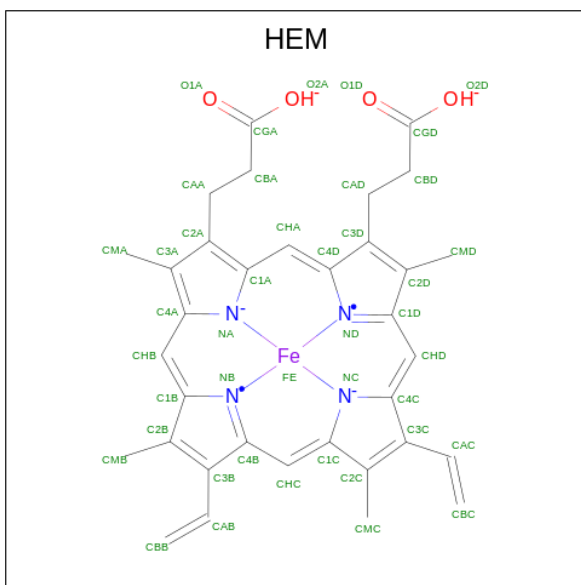
Mol	Chain	Residues	Atoms			AltConf
26	d	1	Total	C	O	0
			4	1	3	

- Molecule 27 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 28 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

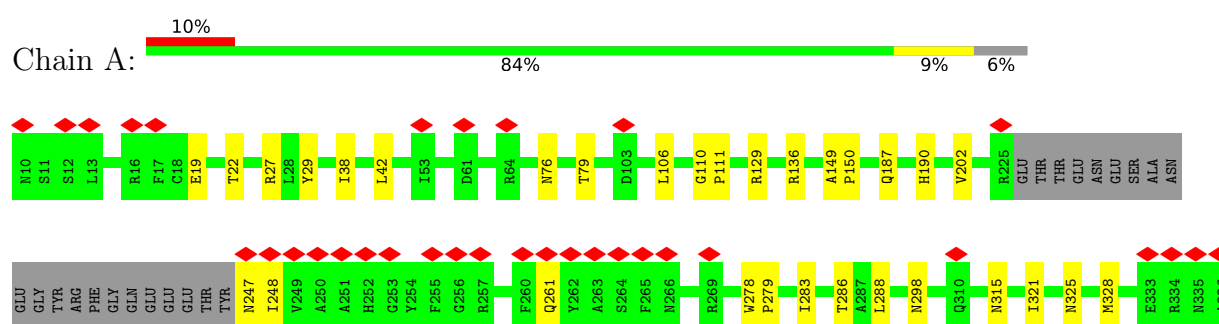


Mol	Chain	Residues	Atoms					AltConf
28	F	1	Total 43	C 34	Fe 1	N 4	O 4	0
28	e	1	Total 43	C 34	Fe 1	N 4	O 4	0

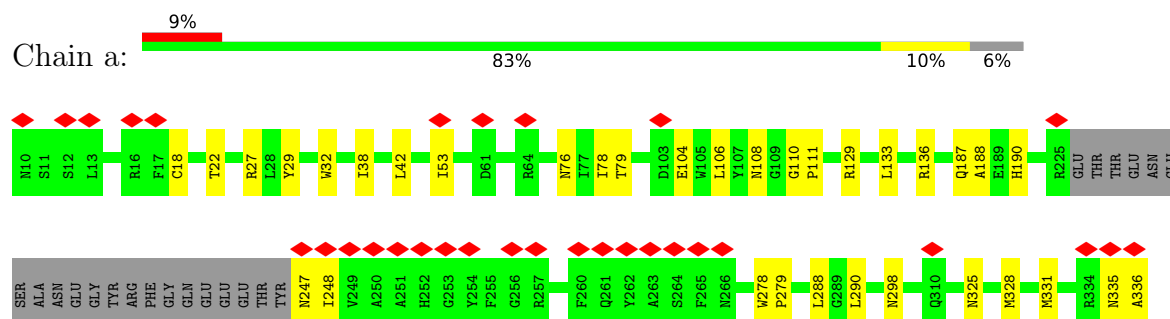
3 Residue-property plots

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

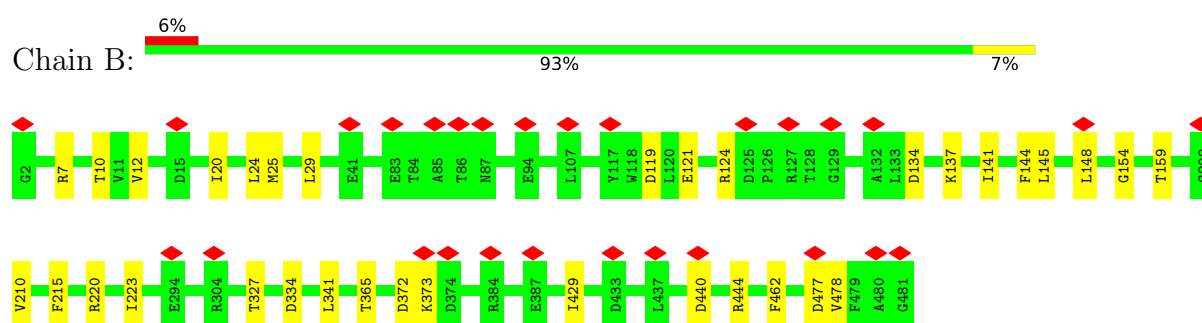
- Molecule 1: Photosystem II protein D1



- Molecule 1: Photosystem II protein D1

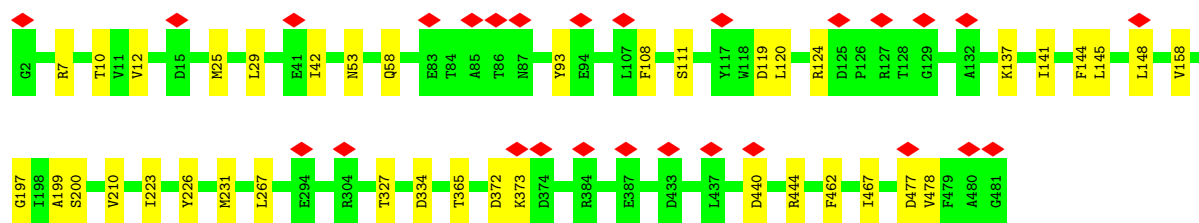


- Molecule 2: Photosystem II CP47 reaction center protein

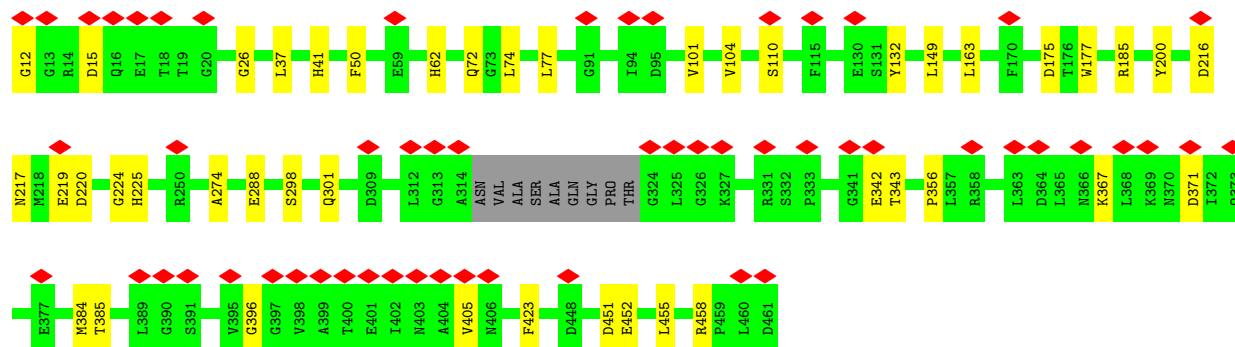
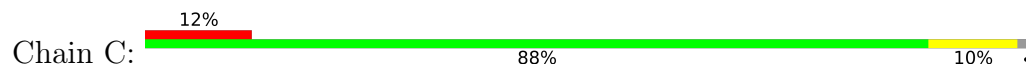


- Molecule 2: Photosystem II CP47 reaction center protein

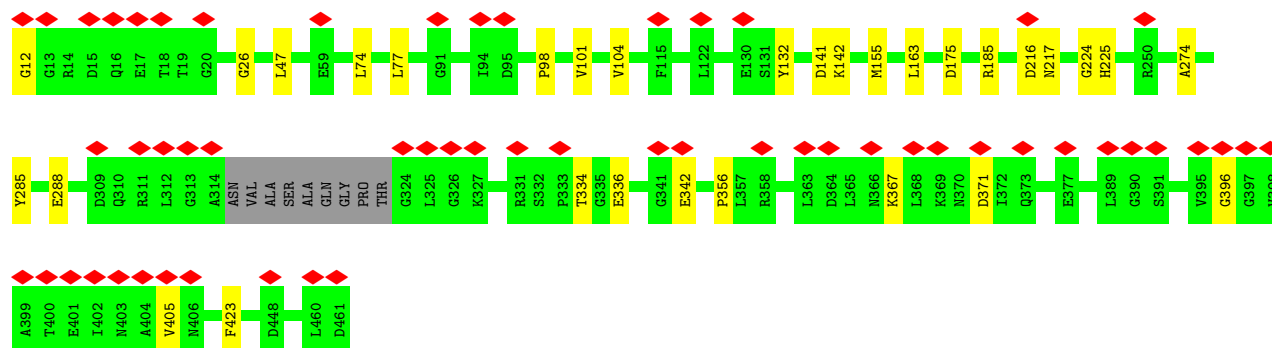
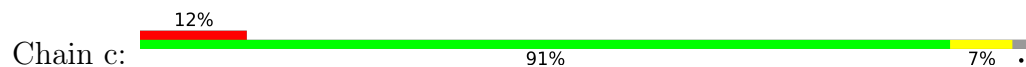




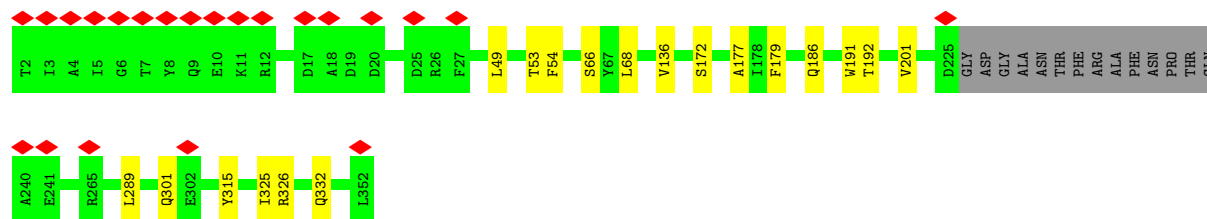
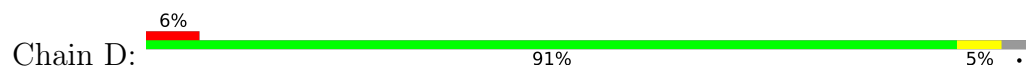
• Molecule 3: Photosystem II CP43 reaction center protein



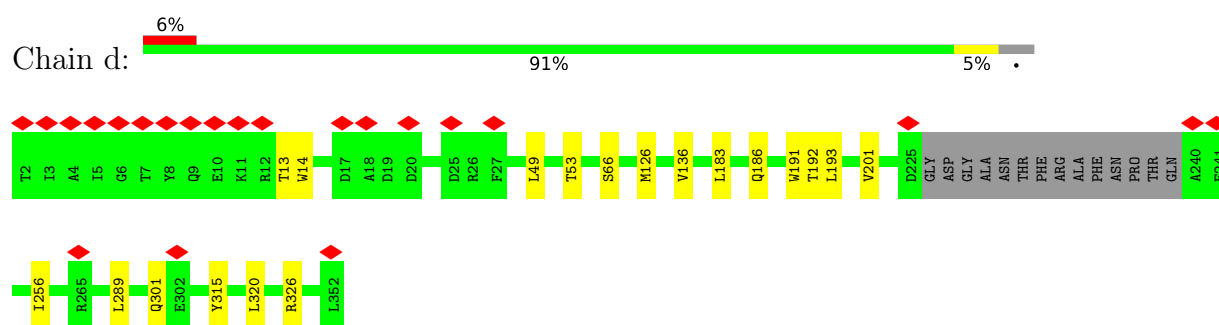
• Molecule 3: Photosystem II CP43 reaction center protein



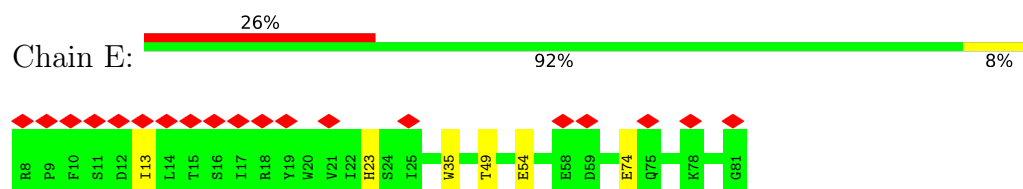
• Molecule 4: Photosystem II D2 protein



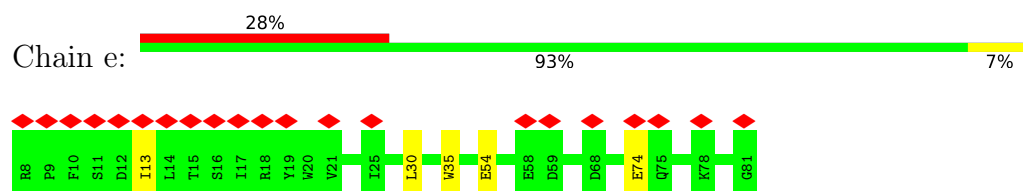
• Molecule 4: Photosystem II D2 protein



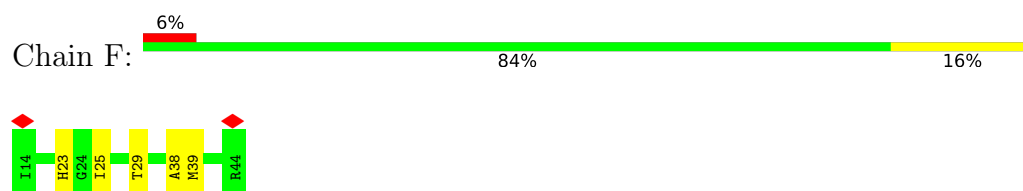
• Molecule 5: Cytochrome b559 subunit alpha



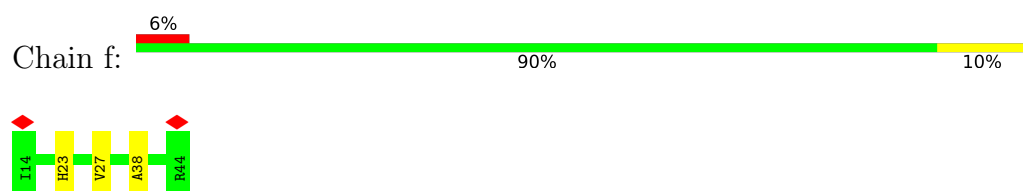
• Molecule 5: Cytochrome b559 subunit alpha



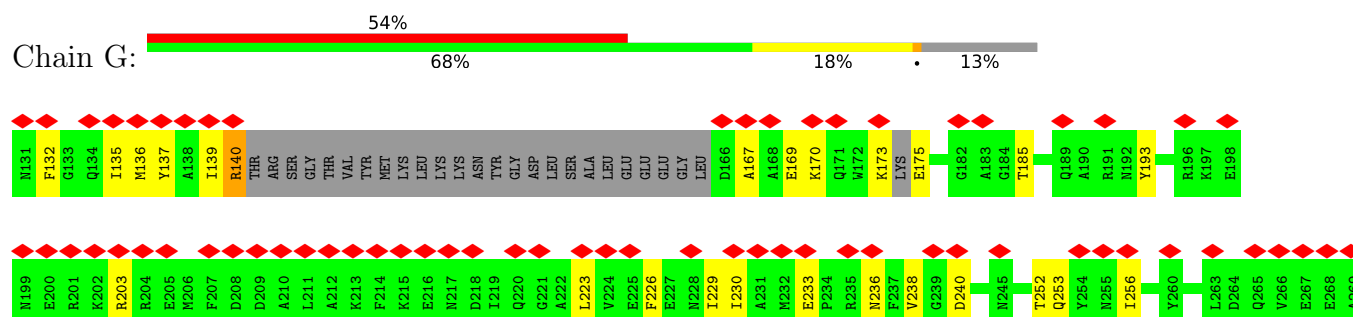
• Molecule 6: Cytochrome b559 subunit beta



• Molecule 6: Cytochrome b559 subunit beta

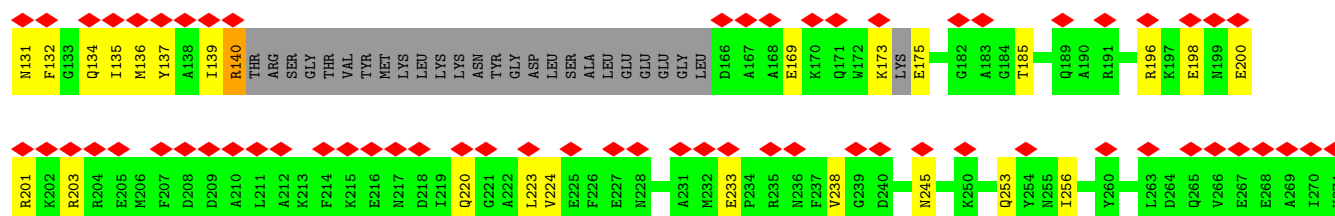


• Molecule 7: PDZ domain-containing protein

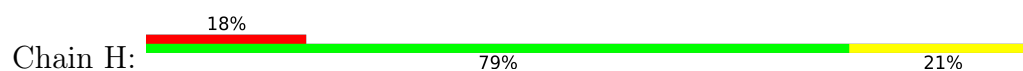




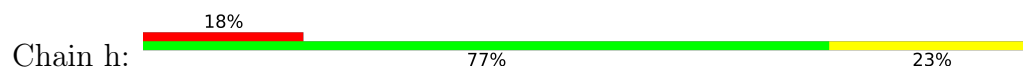
• Molecule 7: PDZ domain-containing protein



• Molecule 8: Photosystem II reaction center protein H



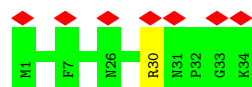
• Molecule 8: Photosystem II reaction center protein H



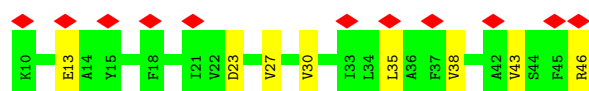
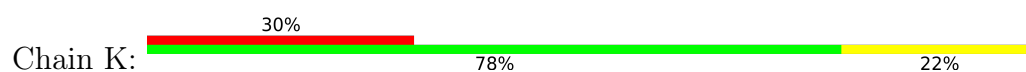
• Molecule 9: Photosystem II reaction center protein I



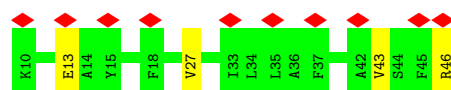
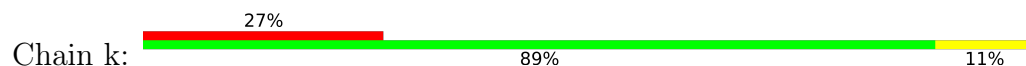
• Molecule 9: Photosystem II reaction center protein I



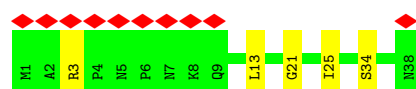
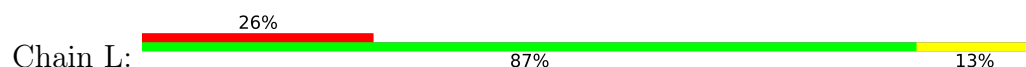
• Molecule 10: Photosystem II reaction center protein K



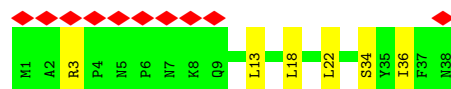
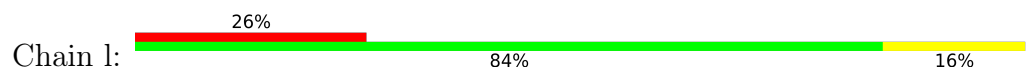
• Molecule 10: Photosystem II reaction center protein K



• Molecule 11: Photosystem II reaction center protein L



• Molecule 11: Photosystem II reaction center protein L



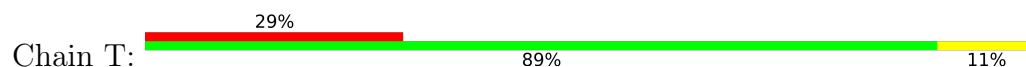
• Molecule 12: Photosystem II reaction center protein M



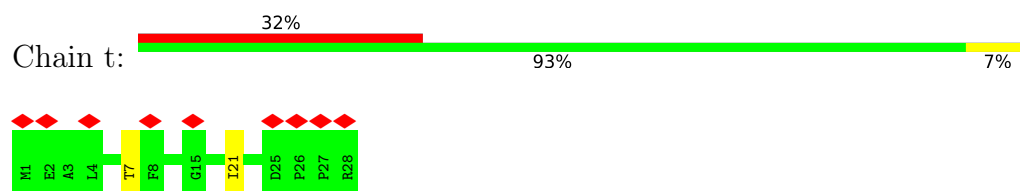
• Molecule 12: Photosystem II reaction center protein M



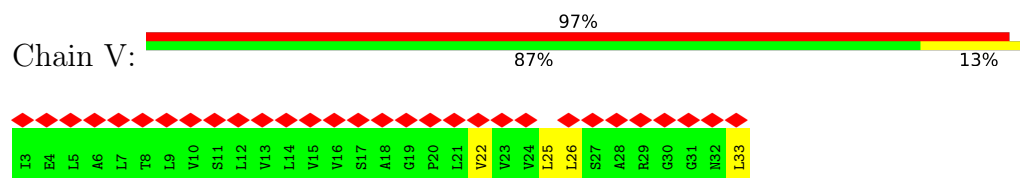
• Molecule 13: Photosystem II reaction center protein T



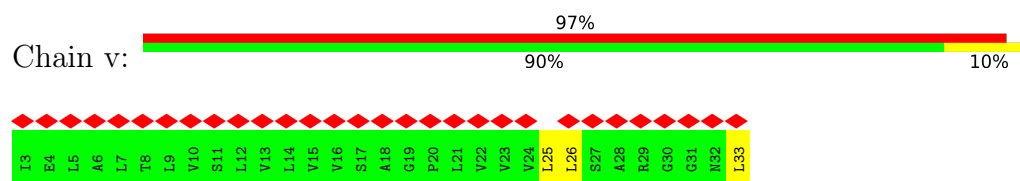
- Molecule 13: Photosystem II reaction center protein T



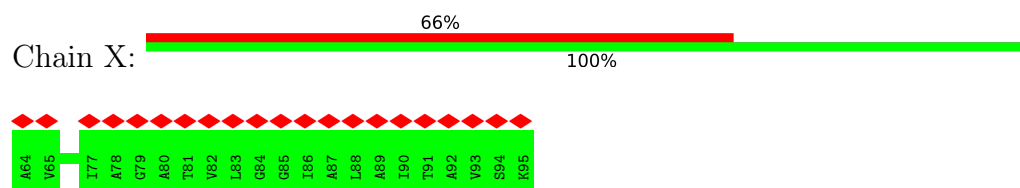
- Molecule 14: Photosystem II reaction center protein Psb30



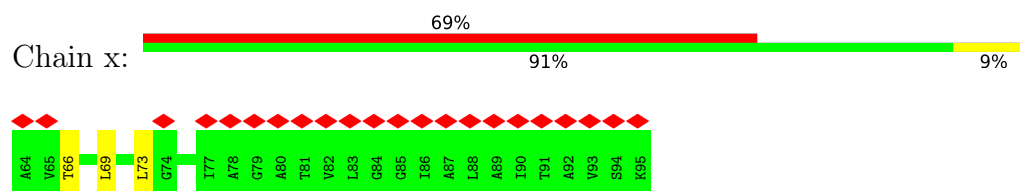
- Molecule 14: Photosystem II reaction center protein Psb30



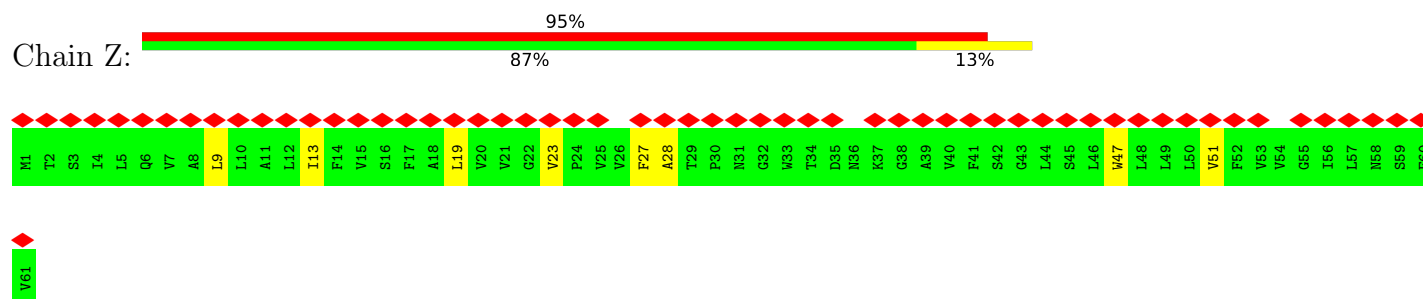
- Molecule 15: Chloroplast photosystem II subunit X



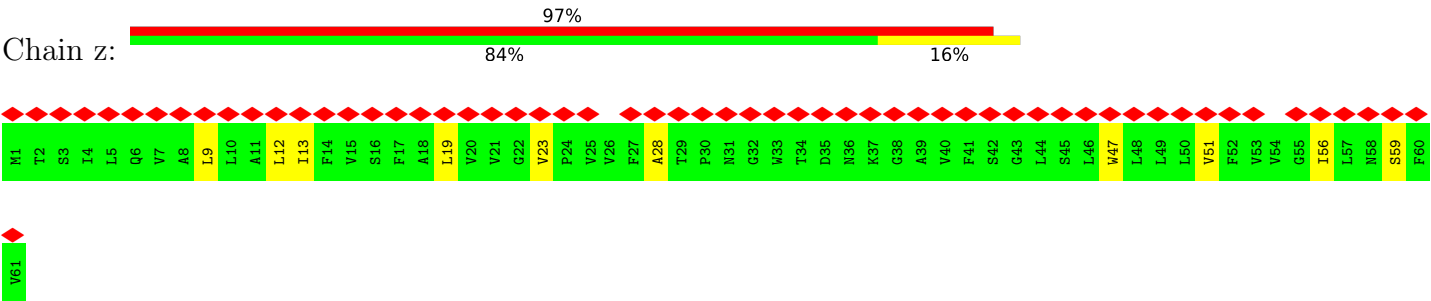
- Molecule 15: Chloroplast photosystem II subunit X



- Molecule 16: Photosystem II reaction center protein Z



- Molecule 16: Photosystem II reaction center protein Z



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33509	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.770	Depositor
Minimum map value	-0.485	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.165	Depositor
Map size ($\text{\AA}$)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.14	0/2463	0.32	0/3358
1	a	0.14	0/2463	0.31	0/3358
2	B	0.12	0/3883	0.28	0/5286
2	b	0.12	0/3883	0.28	0/5286
3	C	0.12	0/3563	0.29	0/4851
3	c	0.12	0/3563	0.28	0/4851
4	D	0.12	0/2777	0.29	0/3787
4	d	0.13	0/2777	0.29	0/3787
5	E	0.18	0/620	0.33	0/846
5	e	0.13	0/620	0.33	0/846
6	F	0.28	0/258	0.40	0/349
6	f	0.16	0/258	0.39	0/349
7	G	0.24	0/1390	0.40	0/1864
7	g	0.24	0/1390	0.44	0/1864
8	H	0.13	0/558	0.29	0/763
8	h	0.14	0/558	0.29	0/763
9	I	0.18	0/283	0.39	0/383
9	i	0.22	0/283	0.38	0/383
10	K	0.16	0/309	0.44	0/425
10	k	0.16	0/309	0.37	0/425
11	L	0.16	0/322	0.30	0/437
11	l	0.16	0/322	0.32	0/437
12	M	0.19	0/214	0.47	0/293
12	m	0.15	0/214	0.39	0/293
13	T	0.19	0/238	0.34	0/322
13	t	0.19	0/238	0.37	0/322
14	V	0.11	0/216	0.26	0/296
14	v	0.13	0/216	0.30	0/296
15	X	0.11	0/215	0.24	0/292
15	x	0.13	0/215	0.25	0/292
16	Z	0.16	0/469	0.37	0/644
16	z	0.15	0/469	0.40	0/644

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.15	0/35556	0.31	0/48392

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
7	G	0	1
7	g	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	G	140	ARG	Sidechain
7	g	140	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2388	0	2327	27	0
1	a	2388	0	2327	27	0
2	B	3755	0	3642	24	0
2	b	3755	0	3642	27	0
3	C	3444	0	3319	34	0
3	c	3444	0	3319	25	0
4	D	2686	0	2585	19	0
4	d	2686	0	2585	17	0
5	E	602	0	593	6	0
5	e	602	0	593	6	0
6	F	251	0	263	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	f	251	0	263	4	0
7	G	1368	0	1323	30	0
7	g	1368	0	1327	23	0
8	H	546	0	575	12	0
8	h	546	0	575	13	0
9	I	275	0	287	1	0
9	i	275	0	287	1	0
10	K	297	0	308	7	0
10	k	297	0	308	4	0
11	L	314	0	327	4	0
11	l	314	0	327	5	0
12	M	210	0	231	8	0
12	m	210	0	231	6	0
13	T	231	0	240	2	0
13	t	231	0	240	2	0
14	V	216	0	250	4	0
14	v	216	0	250	3	0
15	X	214	0	240	0	0
15	x	214	0	240	2	0
16	Z	458	0	490	10	0
16	z	458	0	490	9	0
17	A	1	0	0	0	0
17	a	1	0	0	0	0
18	A	174	0	170	3	0
18	B	1020	0	1113	7	0
18	C	845	0	936	7	0
18	D	195	0	216	5	0
18	a	174	0	170	1	0
18	b	1020	0	1113	7	0
18	c	845	0	936	7	0
18	d	195	0	216	5	0
19	A	64	0	74	0	0
19	D	64	0	74	0	0
19	a	64	0	74	0	0
19	d	64	0	74	0	0
20	A	80	0	112	5	0
20	B	120	0	168	3	0
20	C	120	0	168	16	0
20	D	40	0	56	2	0
20	K	40	0	56	4	0
20	X	40	0	56	2	0
20	a	40	0	56	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	b	80	0	112	1	0
20	c	80	0	112	9	0
20	d	40	0	56	1	0
20	k	40	0	56	4	0
20	x	40	0	56	4	0
20	z	40	0	56	6	0
21	A	46	0	62	0	0
21	B	42	0	54	0	0
21	C	51	0	72	0	0
21	D	94	0	128	1	0
21	b	42	0	54	0	0
21	c	97	0	134	0	0
21	d	46	0	62	0	0
21	h	48	0	66	1	0
22	A	87	0	117	1	0
22	B	93	0	135	0	0
22	D	49	0	74	0	0
22	L	49	0	74	0	0
22	X	49	0	74	0	0
22	a	87	0	117	1	0
22	b	93	0	135	0	0
22	d	49	0	74	0	0
22	l	49	0	74	1	0
22	x	49	0	74	0	0
23	C	51	0	69	0	0
23	c	51	0	69	0	0
24	C	161	0	196	0	0
24	c	161	0	196	0	0
25	C	35	0	46	0	0
25	c	35	0	46	0	0
26	D	4	0	0	0	0
26	d	4	0	0	0	0
27	D	55	0	80	0	0
27	d	55	0	80	0	0
28	F	43	0	30	6	0
28	e	43	0	30	5	0
All	All	41854	0	42712	370	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (370) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:119:ASP:OD1	2:b:124:ARG:NH1	2.17	0.78
1:a:104:GLU:OE2	1:a:108:ASN:ND2	2.17	0.77
2:B:119:ASP:OD1	2:B:124:ARG:NH1	2.19	0.76
2:B:148:LEU:HD22	2:B:210:VAL:HG22	1.68	0.76
2:B:121:GLU:O	8:H:31:ARG:NH1	2.20	0.75
1:A:42:LEU:HB3	20:A:406:BCR:H353	1.69	0.74
3:C:342:GLU:N	3:C:342:GLU:OE1	2.22	0.72
28:e:101:HEM:HHC	28:e:101:HEM:HBB2	1.70	0.72
3:c:342:GLU:N	3:c:342:GLU:OE1	2.23	0.71
1:a:187:GLN:OE1	1:a:325:ASN:ND2	2.24	0.70
1:a:42:LEU:HB3	20:a:406:BCR:H353	1.74	0.70
21:h:101:LMG:HO4	21:h:101:LMG:HO5	1.38	0.70
7:g:198:GLU:OE1	7:g:201:ARG:NH2	2.25	0.69
1:A:315:ASN:ND2	4:D:332:GLN:OE1	2.25	0.69
7:g:173:LYS:O	7:g:175:GLU:N	2.25	0.69
7:G:173:LYS:O	7:G:175:GLU:N	2.25	0.69
3:C:175:ASP:OD2	3:C:185:ARG:NH1	2.26	0.69
3:c:175:ASP:OD2	3:c:185:ARG:NH1	2.27	0.67
2:B:440:ASP:OD2	2:B:444:ARG:NH2	2.28	0.67
2:b:327:THR:O	2:b:444:ARG:NH1	2.27	0.67
2:b:53:ASN:OD1	2:b:58:GLN:NE2	2.28	0.67
20:k:101:BCR:H321	20:k:101:BCR:HC8	1.76	0.67
2:b:137:LYS:O	2:b:141:ILE:HD12	1.95	0.66
2:b:440:ASP:OD2	2:b:444:ARG:NH2	2.28	0.66
1:A:286:THR:OG1	18:A:402:CLA:O1D	2.05	0.66
2:B:327:THR:O	2:B:444:ARG:NH1	2.28	0.66
10:K:13:GLU:OE2	10:K:13:GLU:N	2.28	0.66
3:C:224:GLY:HA3	20:C:516:BCR:H402	1.78	0.66
28:F:101:HEM:HHC	28:F:101:HEM:HBB2	1.77	0.66
12:m:25:LEU:O	12:m:29:THR:HG23	1.96	0.65
7:G:139:ILE:O	7:G:140:ARG:C	2.39	0.65
3:C:356:PRO:O	3:C:367:LYS:NZ	2.30	0.65
7:g:139:ILE:O	7:g:140:ARG:C	2.39	0.65
3:c:224:GLY:HA3	20:c:516:BCR:H402	1.79	0.64
16:Z:9:LEU:O	16:Z:13:ILE:HD12	1.98	0.64
1:A:29:TYR:O	1:A:129:ARG:NH2	2.30	0.64
20:c:517:BCR:H383	20:c:517:BCR:H23C	1.79	0.64
2:B:137:LYS:O	2:B:141:ILE:HD12	1.96	0.64
20:B:519:BCR:H383	20:B:519:BCR:H23C	1.80	0.64
18:B:509:CLA:OBD	8:H:46:THR:OG1	2.16	0.64
20:A:410:BCR:H383	20:A:410:BCR:H23C	1.80	0.64
2:b:119:ASP:OD2	11:l:3:ARG:NH1	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:K:101:BCR:H321	20:K:101:BCR:HC8	1.80	0.63
18:D:404:CLA:HBC3	18:D:404:CLA:HHD	1.81	0.63
5:e:74:GLU:OE2	5:e:74:GLU:N	2.32	0.63
10:k:13:GLU:OE2	10:k:13:GLU:N	2.28	0.63
16:Z:23:VAL:HG13	16:Z:27:PHE:HE2	1.64	0.63
20:C:517:BCR:H383	20:C:517:BCR:H23C	1.80	0.62
8:H:75:ASP:OD1	8:H:76:ASP:N	2.33	0.62
8:h:75:ASP:OD1	8:h:76:ASP:N	2.33	0.62
4:d:186:GLN:HB2	18:d:404:CLA:HBC1	1.81	0.62
12:M:21:PHE:O	12:M:25:LEU:HD12	2.00	0.62
3:c:163:LEU:HD23	3:c:225:HIS:CD2	2.34	0.61
3:c:274:ALA:HB2	18:c:504:CLA:HMD1	1.83	0.60
20:C:515:BCR:H343	16:Z:51:VAL:HG12	1.83	0.60
4:d:49:LEU:HD13	20:d:406:BCR:C16	2.32	0.60
12:M:25:LEU:O	12:M:29:THR:HG23	2.01	0.60
18:b:509:CLA:OBD	8:h:46:THR:OG1	2.19	0.59
20:C:517:BCR:H312	16:Z:9:LEU:HD11	1.84	0.59
3:c:356:PRO:O	3:c:367:LYS:NZ	2.36	0.59
16:z:47:TRP:O	16:z:51:VAL:HG23	2.02	0.59
1:a:190:HIS:ND1	1:a:298:ASN:OD1	2.36	0.58
2:b:226:TYR:HA	2:b:231:MET:HE3	1.85	0.58
1:A:190:HIS:ND1	1:A:298:ASN:OD1	2.36	0.58
16:z:51:VAL:HG12	20:z:101:BCR:H343	1.86	0.58
20:C:515:BCR:H331	20:C:515:BCR:HC8	1.84	0.58
7:g:306:LEU:O	7:g:310:ASP:N	2.35	0.58
20:z:101:BCR:H331	20:z:101:BCR:HC8	1.86	0.58
7:G:132:PHE:CE1	7:G:136:MET:CG	2.87	0.58
3:c:12:GLY:N	14:v:33:LEU:O	2.37	0.58
8:H:19:GLU:OE1	8:H:19:GLU:N	2.37	0.58
2:b:365:THR:OG1	4:d:326:ARG:NH2	2.37	0.57
8:h:19:GLU:N	8:h:19:GLU:OE1	2.37	0.57
16:z:56:ILE:O	16:z:59:SER:OG	2.19	0.57
5:E:74:GLU:N	5:E:74:GLU:OE1	2.38	0.57
3:C:15:ASP:OD1	10:K:46:ARG:NH1	2.38	0.57
16:Z:23:VAL:HG13	16:Z:27:PHE:CE2	2.38	0.57
5:E:35:TRP:CD2	6:F:38:ALA:HB2	2.40	0.56
14:V:26:LEU:HD11	16:Z:28:ALA:HB3	1.87	0.56
7:G:306:LEU:O	7:G:310:ASP:N	2.36	0.56
3:C:274:ALA:HB2	18:C:503:CLA:HMD1	1.87	0.56
20:C:516:BCR:HC8	20:C:516:BCR:H311	1.88	0.56
7:G:277:MET:HA	7:G:277:MET:HE3	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:283:ASN:ND2	7:G:286:GLN:OE1	2.39	0.56
8:H:35:SER:OG	8:H:36:GLU:OE1	2.21	0.56
22:a:407:LHG:O3	22:a:407:LHG:O1	2.20	0.56
1:a:29:TYR:O	1:a:129:ARG:NH2	2.39	0.56
4:D:186:GLN:HB2	18:D:404:CLA:HBC1	1.88	0.55
8:h:35:SER:OG	8:h:36:GLU:OE1	2.23	0.55
2:B:20:ILE:O	2:B:24:LEU:HD23	2.06	0.55
20:c:516:BCR:HC8	20:c:516:BCR:H311	1.87	0.55
3:C:458:ARG:NH2	7:G:193:TYR:OH	2.40	0.55
7:G:140:ARG:HG3	7:G:140:ARG:O	2.07	0.55
2:B:223:ILE:HA	8:H:40:VAL:HG21	1.89	0.54
1:A:202:VAL:HG23	18:A:402:CLA:HMB3	1.89	0.54
2:B:372:ASP:OD1	2:B:373:LYS:N	2.40	0.54
2:b:372:ASP:OD1	2:b:373:LYS:N	2.40	0.54
2:B:119:ASP:OD2	11:L:3:ARG:NH1	2.41	0.54
3:c:132:TYR:OH	18:c:515:CLA:O1D	2.19	0.54
20:B:518:BCR:H383	20:B:518:BCR:H23C	1.89	0.54
3:c:104:VAL:HG13	20:z:101:BCR:H312	1.90	0.54
4:D:53:THR:O	4:D:66:SER:OG	2.26	0.54
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.43	0.54
1:A:328:MET:SD	4:D:325:ILE:HD11	2.48	0.53
7:G:203:ARG:NH2	7:G:233:GLU:OE1	2.40	0.53
2:b:148:LEU:HD22	2:b:210:VAL:HG22	1.90	0.53
1:A:136:ARG:NH1	7:G:238:VAL:O	2.38	0.53
16:Z:47:TRP:O	16:Z:51:VAL:HG23	2.09	0.53
7:g:137:TYR:O	7:g:140:ARG:HG2	2.08	0.53
20:C:517:BCR:C11	20:K:101:BCR:H333	2.39	0.53
16:z:13:ILE:HD12	16:z:13:ILE:H	1.74	0.53
3:c:26:GLY:HA3	18:c:513:CLA:HMD2	1.89	0.53
3:C:12:GLY:N	14:V:33:LEU:O	2.41	0.53
7:G:277:MET:HE1	7:G:281:PHE:O	2.08	0.53
7:g:136:MET:O	7:g:139:ILE:HG12	2.08	0.53
20:b:518:BCR:H383	20:b:518:BCR:H23C	1.90	0.53
1:A:76:ASN:ND2	11:L:34:SER:OG	2.42	0.53
2:B:334:ASP:N	2:B:334:ASP:OD1	2.42	0.52
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.44	0.52
12:M:21:PHE:CE1	12:M:25:LEU:HD11	2.45	0.52
5:e:54:GLU:OE1	5:e:54:GLU:N	2.42	0.52
5:E:54:GLU:N	5:E:54:GLU:OE1	2.42	0.52
18:d:404:CLA:HBC3	18:d:404:CLA:HHD	1.92	0.52
2:b:334:ASP:OD1	2:b:334:ASP:N	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:VAL:O	2:B:12:VAL:HG12	2.10	0.51
2:b:12:VAL:HG12	2:b:12:VAL:O	2.09	0.51
6:F:25:ILE:O	6:F:29:THR:OG1	2.25	0.51
18:b:502:CLA:H43	8:h:65:LEU:HA	1.92	0.51
4:D:136:VAL:O	4:D:136:VAL:HG12	2.09	0.51
4:D:192:THR:HG23	18:D:404:CLA:HBC2	1.91	0.51
3:C:298:SER:OG	3:C:343:THR:HG22	2.10	0.51
7:g:137:TYR:CZ	7:g:220:GLN:HG2	2.45	0.51
7:g:290:ASP:O	7:g:297:ARG:NH2	2.44	0.51
3:C:452:GLU:OE1	3:C:455:LEU:HD12	2.09	0.51
7:G:137:TYR:HE2	7:G:223:LEU:HD12	1.76	0.51
3:C:396:GLY:N	3:C:405:VAL:O	2.38	0.51
2:b:467:ILE:HD12	4:d:126:MET:HE2	1.92	0.51
7:G:290:ASP:O	7:G:297:ARG:NH2	2.43	0.51
4:d:136:VAL:HG12	4:d:136:VAL:O	2.10	0.51
2:B:144:PHE:O	2:B:148:LEU:HD23	2.11	0.51
2:B:365:THR:OG1	4:D:326:ARG:NH2	2.43	0.51
3:C:224:GLY:CA	20:C:516:BCR:H402	2.41	0.51
1:A:79:THR:HG22	4:D:315:TYR:HB2	1.92	0.51
7:G:132:PHE:CE1	7:G:136:MET:HG3	2.46	0.50
7:G:136:MET:O	7:G:139:ILE:HG12	2.12	0.50
8:H:50:MET:HE2	8:H:50:MET:HA	1.94	0.50
2:b:223:ILE:HA	8:h:40:VAL:HG21	1.93	0.50
4:d:53:THR:O	4:d:66:SER:OG	2.28	0.50
5:e:13:ILE:HD12	28:e:101:HEM:HAD2	1.92	0.50
2:B:7:ARG:O	2:B:10:THR:HG22	2.11	0.50
3:C:104:VAL:HG13	20:C:515:BCR:H312	1.94	0.50
7:G:137:TYR:O	7:G:140:ARG:HG2	2.12	0.50
22:A:408:LHG:O3	22:A:408:LHG:O1	2.24	0.50
13:T:3:ALA:O	13:T:7:THR:HG23	2.12	0.50
1:a:76:ASN:ND2	11:l:34:SER:OG	2.45	0.50
2:b:7:ARG:O	2:b:10:THR:HG22	2.11	0.50
1:A:247:ASN:OD1	1:A:248:ILE:N	2.45	0.50
10:k:43:VAL:HG12	10:k:43:VAL:O	2.11	0.49
3:C:101:VAL:HG23	20:C:515:BCR:H313	1.94	0.49
20:k:101:BCR:H383	20:k:101:BCR:H23C	1.94	0.49
7:G:132:PHE:HE1	7:G:136:MET:HG3	1.76	0.49
1:a:247:ASN:OD1	1:a:248:ILE:N	2.45	0.49
5:e:30:LEU:HD21	6:f:27:VAL:HG13	1.95	0.49
7:g:137:TYR:CD2	7:g:223:LEU:HD22	2.48	0.49
7:g:196:ARG:O	7:g:200:GLU:OE1	2.29	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:334:THR:OG1	3:c:336:GLU:OE1	2.25	0.49
3:c:163:LEU:HD22	18:c:503:CLA:C2D	2.42	0.49
7:g:135:ILE:O	7:g:139:ILE:HG23	2.12	0.49
7:g:137:TYR:CE2	7:g:220:GLN:HG2	2.48	0.49
10:k:27:VAL:HG22	10:k:27:VAL:O	2.13	0.49
3:C:72:GLN:N	3:C:72:GLN:OE1	2.46	0.49
7:g:169:GLU:N	7:g:169:GLU:OE1	2.46	0.49
2:b:141:ILE:O	2:b:145:LEU:HD23	2.12	0.49
1:A:106:LEU:HD21	20:A:406:BCR:H402	1.95	0.48
4:D:49:LEU:HD13	20:D:406:BCR:C15	2.43	0.48
2:b:477:ASP:OD1	2:b:478:VAL:N	2.45	0.48
20:z:101:BCR:H331	20:z:101:BCR:C8	2.42	0.48
20:C:515:BCR:H331	20:C:515:BCR:C8	2.42	0.48
7:G:169:GLU:N	7:G:169:GLU:OE1	2.46	0.48
7:g:203:ARG:NH2	7:g:233:GLU:OE1	2.42	0.48
7:g:132:PHE:O	7:g:135:ILE:HG12	2.13	0.48
10:K:27:VAL:O	10:K:30:VAL:HG12	2.13	0.48
14:v:26:LEU:HD11	16:z:28:ALA:HB3	1.94	0.48
21:D:410:LMG:O5	21:D:410:LMG:O4	2.14	0.48
1:a:79:THR:HG21	4:d:301:GLN:OE1	2.14	0.48
4:d:201:VAL:HG23	18:d:404:CLA:CMB	2.43	0.48
2:B:477:ASP:OD1	2:B:478:VAL:N	2.46	0.48
16:Z:19:LEU:O	16:Z:23:VAL:HG23	2.14	0.48
7:g:245:ASN:OD1	9:i:30:ARG:NH1	2.46	0.48
1:a:136:ARG:NH1	7:g:238:VAL:O	2.46	0.48
3:C:26:GLY:HA3	18:C:512:CLA:HMD2	1.95	0.47
7:G:175:GLU:OE2	7:G:185:THR:N	2.47	0.47
3:c:224:GLY:CA	20:c:516:BCR:H402	2.42	0.47
16:z:9:LEU:O	16:z:13:ILE:HD12	2.14	0.47
1:A:187:GLN:NE2	1:A:325:ASN:OD1	2.47	0.47
4:D:201:VAL:HG23	18:D:404:CLA:C2B	2.44	0.47
1:a:106:LEU:HD21	20:a:406:BCR:H402	1.96	0.47
11:L:13:LEU:HD23	12:M:29:THR:HG21	1.96	0.47
1:a:188:ALA:HB2	1:a:328:MET:HB3	1.96	0.47
3:C:62:HIS:NE2	10:K:23:ASP:OD1	2.45	0.47
5:e:35:TRP:CD2	6:f:38:ALA:HB2	2.49	0.47
7:g:288:ARG:NH2	7:g:310:ASP:OD2	2.47	0.47
4:D:201:VAL:HG23	18:D:404:CLA:CMB	2.45	0.47
1:a:79:THR:HG22	4:d:315:TYR:HB2	1.96	0.47
1:a:110:GLY:N	1:a:111:PRO:HD2	2.30	0.47
1:a:133:LEU:HD23	4:d:256:ILE:HG13	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:502:CLA:H43	8:H:65:LEU:HA	1.97	0.47
1:A:79:THR:HG21	4:D:301:GLN:OE1	2.15	0.46
8:H:26:LEU:HD23	8:H:30:LEU:HD23	1.98	0.46
1:A:27:ARG:NH2	13:T:21:ILE:O	2.49	0.46
3:C:163:LEU:HD23	3:C:225:HIS:CD2	2.51	0.46
5:E:13:ILE:HD12	28:F:101:HEM:HAD2	1.97	0.46
16:z:19:LEU:O	16:z:23:VAL:HG23	2.16	0.46
18:b:501:CLA:HMD1	20:x:102:BCR:H271	1.98	0.46
16:z:12:LEU:HD11	16:z:51:VAL:HG22	1.98	0.46
1:A:110:GLY:N	1:A:111:PRO:HD2	2.30	0.46
4:D:68:LEU:HD13	6:F:39:MET:HE2	1.98	0.46
10:K:43:VAL:O	10:K:43:VAL:HG12	2.17	0.45
3:C:216:ASP:OD1	3:C:217:ASN:N	2.49	0.45
4:d:201:VAL:HG23	18:d:404:CLA:C2B	2.46	0.45
3:C:200:TYR:OH	3:C:220:ASP:OD2	2.24	0.45
8:h:61:LEU:HD23	8:h:64:ILE:HD11	1.98	0.45
4:D:49:LEU:HD13	20:D:406:BCR:C16	2.47	0.45
1:a:106:LEU:HD21	20:a:406:BCR:C40	2.46	0.45
3:c:104:VAL:CG1	20:z:101:BCR:H312	2.46	0.45
20:c:517:BCR:H312	16:z:9:LEU:HD11	1.98	0.45
1:a:335:ASN:OD1	1:a:336:ALA:N	2.45	0.45
2:b:42:ILE:HD11	2:b:93:TYR:HB3	1.98	0.45
7:G:226:PHE:HB3	7:G:256:ILE:HD12	1.99	0.45
22:l:101:LHG:O3	22:l:101:LHG:O1	2.31	0.45
28:e:101:HEM:HBC2	28:e:101:HEM:HMC2	1.99	0.44
2:B:25:MET:O	2:B:29:LEU:HD23	2.17	0.44
18:C:512:CLA:C20	16:Z:23:VAL:HG11	2.47	0.44
20:a:406:BCR:H15C	20:a:406:BCR:H351	1.89	0.44
10:k:43:VAL:HG12	10:k:46:ARG:HG2	1.98	0.44
1:A:106:LEU:HD21	20:A:406:BCR:C40	2.48	0.44
1:A:261:GLN:OE1	1:A:261:GLN:HA	2.17	0.44
3:C:288:GLU:OE1	3:C:288:GLU:N	2.50	0.44
7:G:278:LEU:O	9:I:30:ARG:NE	2.49	0.44
2:B:141:ILE:O	2:B:145:LEU:HD23	2.18	0.44
11:l:13:LEU:HD23	12:m:29:THR:HG21	2.00	0.44
18:B:501:CLA:HMD1	20:X:102:BCR:H271	1.98	0.44
1:A:202:VAL:HG23	18:A:402:CLA:CMB	2.48	0.44
3:C:74:LEU:HD23	3:C:77:LEU:HD12	1.98	0.44
8:H:69:ASN:O	8:H:70:SER:OG	2.33	0.44
2:b:144:PHE:O	2:b:148:LEU:HD23	2.18	0.44
7:G:135:ILE:O	7:G:139:ILE:HG23	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:THR:HG23	7:G:240:ASP:OD2	2.17	0.44
20:C:515:BCR:HC8	20:C:515:BCR:C33	2.48	0.44
14:V:25:LEU:O	14:V:25:LEU:HD23	2.17	0.44
1:a:278:TRP:HB3	1:a:279:PRO:HD3	2.00	0.44
2:b:267:LEU:HD23	2:b:267:LEU:H	1.83	0.43
20:c:517:BCR:C11	20:k:101:BCR:H333	2.47	0.43
7:g:137:TYR:HB2	7:g:224:VAL:HG12	2.00	0.43
1:a:18:CYS:HG	1:a:32:TRP:HZ2	1.62	0.43
20:c:516:BCR:H311	20:c:516:BCR:C8	2.48	0.43
2:B:134:ASP:OD1	2:B:220:ARG:NH2	2.51	0.43
28:e:101:HEM:C1B	6:f:23:HIS:NE2	2.79	0.43
3:C:301:GLN:OE1	3:C:384:MET:HE2	2.19	0.43
2:b:25:MET:O	2:b:29:LEU:HD23	2.18	0.43
4:d:192:THR:HG23	18:d:404:CLA:HBC2	2.00	0.43
2:B:462:PHE:CE2	18:B:513:CLA:HMB2	2.54	0.43
6:F:23:HIS:NE2	28:F:101:HEM:C1B	2.82	0.43
3:c:74:LEU:HD23	3:c:77:LEU:HD12	1.99	0.43
2:B:341:LEU:HD12	2:B:429:ILE:HG22	2.01	0.43
3:C:367:LYS:O	3:C:371:ASP:N	2.51	0.43
12:M:18:PRO:O	12:M:22:LEU:HD23	2.18	0.43
1:A:321:ILE:HD11	4:D:179:PHE:HB2	1.99	0.43
14:V:22:VAL:O	14:V:26:LEU:HD23	2.18	0.43
1:a:53:ILE:CD1	13:t:7:THR:HG22	2.48	0.43
3:c:288:GLU:OE1	3:c:288:GLU:N	2.49	0.43
11:l:18:LEU:O	11:l:22:LEU:HD23	2.19	0.43
3:C:217:ASN:OD1	3:C:219:GLU:HB2	2.19	0.43
10:K:27:VAL:O	10:K:27:VAL:HG12	2.19	0.43
3:c:47:LEU:HD13	18:c:512:CLA:HMD1	2.00	0.43
3:c:367:LYS:O	3:c:371:ASP:N	2.52	0.43
1:A:283:ILE:HA	1:A:286:THR:HG22	2.01	0.42
3:C:132:TYR:OH	18:C:514:CLA:O1D	2.29	0.42
3:C:163:LEU:HD22	18:C:502:CLA:C2D	2.49	0.42
28:F:101:HEM:HBC2	28:F:101:HEM:HMC2	2.01	0.42
2:b:108:PHE:O	2:b:111:SER:OG	2.30	0.42
7:G:132:PHE:CD1	7:G:136:MET:HG2	2.54	0.42
7:G:167:ALA:O	7:G:170:LYS:NZ	2.47	0.42
12:m:11:THR:O	12:m:15:ILE:HG12	2.19	0.42
20:K:101:BCR:H383	20:K:101:BCR:H23C	2.01	0.42
4:d:13:THR:HG22	4:d:14:TRP:N	2.34	0.42
20:z:101:BCR:HC8	20:z:101:BCR:C33	2.48	0.42
18:b:505:CLA:HMA1	18:b:506:CLA:H3A	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:54:ILE:HD13	20:x:102:BCR:H333	2.01	0.42
20:k:101:BCR:H321	20:k:101:BCR:C8	2.46	0.42
12:m:20:SER:O	12:m:24:ILE:HG12	2.20	0.42
15:x:69:LEU:O	15:x:73:LEU:HD23	2.19	0.42
1:A:288:LEU:HD21	3:C:423:PHE:CD2	2.55	0.42
10:K:35:LEU:O	10:K:38:VAL:HG22	2.19	0.42
18:b:507:CLA:H203	11:l:36:ILE:HG13	2.01	0.42
20:C:516:BCR:H311	20:C:516:BCR:C8	2.48	0.42
8:H:17:PHE:N	8:H:19:GLU:OE1	2.53	0.42
3:c:98:PRO:HA	3:c:101:VAL:HG12	2.01	0.42
3:C:177:TRP:NE1	3:C:216:ASP:O	2.53	0.42
12:m:18:PRO:O	12:m:22:LEU:HD23	2.19	0.42
14:v:25:LEU:O	14:v:25:LEU:HD23	2.20	0.42
20:A:410:BCR:H383	20:A:410:BCR:C23	2.50	0.42
20:B:519:BCR:H383	20:B:519:BCR:C23	2.49	0.42
4:D:54:PHE:O	5:E:49:THR:OG1	2.34	0.42
1:a:38:ILE:O	1:a:42:LEU:HD23	2.20	0.42
2:b:197:GLY:O	2:b:200:SER:OG	2.36	0.42
7:g:175:GLU:OE2	7:g:185:THR:N	2.52	0.42
1:A:19:GLU:OE1	1:A:19:GLU:HA	2.20	0.42
3:C:149:LEU:HD11	18:C:507:CLA:CMB	2.50	0.42
2:b:144:PHE:CZ	2:b:148:LEU:HD21	2.54	0.42
20:C:515:BCR:H11C	20:C:515:BCR:H341	1.88	0.42
1:a:290:LEU:HD22	18:a:402:CLA:OBD	2.19	0.42
7:G:226:PHE:O	7:G:229:ILE:HG22	2.20	0.41
12:M:11:THR:O	12:M:15:ILE:HG12	2.20	0.41
12:M:30:ALA:HB1	12:m:30:ALA:HB1	2.02	0.41
1:a:331:MET:HE2	4:d:320:LEU:HB3	2.02	0.41
3:c:216:ASP:OD1	3:c:217:ASN:N	2.53	0.41
3:c:285:TYR:OH	18:c:504:CLA:HED2	2.20	0.41
8:h:17:PHE:N	8:h:19:GLU:OE1	2.53	0.41
2:B:215:PHE:CZ	18:B:509:CLA:HMD1	2.55	0.41
20:C:515:BCR:HC7	20:C:515:BCR:H311	1.85	0.41
7:g:137:TYR:HD2	7:g:223:LEU:HD22	1.85	0.41
20:x:102:BCR:H11C	20:x:102:BCR:H341	1.96	0.41
1:A:38:ILE:O	1:A:42:LEU:HD23	2.20	0.41
2:B:144:PHE:CZ	2:B:148:LEU:HD21	2.55	0.41
8:h:32:PRO:O	8:h:35:SER:OG	2.37	0.41
18:c:507:CLA:H11	20:c:516:BCR:H333	2.03	0.41
8:h:54:ILE:CD1	20:x:102:BCR:H333	2.50	0.41
5:E:23:HIS:NE2	28:F:101:HEM:C4C	2.87	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:K:101:BCR:H321	20:K:101:BCR:C8	2.47	0.41
20:X:102:BCR:H11C	20:X:102:BCR:H341	1.95	0.41
1:a:22:THR:O	1:a:22:THR:HG22	2.20	0.41
7:G:230:ILE:HD11	7:G:252:THR:HG23	2.02	0.41
7:G:253:GLN:HE22	7:G:275:ALA:HB3	1.85	0.41
7:G:288:ARG:NH2	7:G:310:ASP:OD2	2.53	0.41
20:c:517:BCR:H383	20:c:517:BCR:C23	2.48	0.41
3:C:451:ASP:O	7:G:236:ASN:ND2	2.48	0.41
12:M:20:SER:O	12:M:24:ILE:HG12	2.20	0.41
2:B:154:GLY:O	2:B:159:THR:OG1	2.38	0.41
18:B:505:CLA:HMA1	18:B:506:CLA:H3A	2.02	0.41
18:B:513:CLA:HMB3	18:B:513:CLA:HBB1	2.02	0.41
3:C:50:PHE:HB2	3:C:110:SER:OG	2.21	0.41
2:b:119:ASP:C	2:b:120:LEU:HD22	2.45	0.41
2:b:462:PHE:CE2	18:b:513:CLA:HMB2	2.55	0.41
28:e:101:HEM:HBC2	28:e:101:HEM:CMC	2.50	0.41
7:g:131:ASN:O	7:g:134:GLN:HG2	2.21	0.41
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.03	0.41
28:F:101:HEM:HBC2	28:F:101:HEM:CMC	2.50	0.41
1:a:328:MET:HE1	4:d:183:LEU:HD22	2.02	0.41
5:e:35:TRP:CE2	6:f:38:ALA:HB2	2.56	0.41
1:A:278:TRP:HB3	1:A:279:PRO:HD3	2.02	0.40
1:a:78:ILE:HG21	4:d:193:LEU:CD1	2.51	0.40
3:c:396:GLY:N	3:c:405:VAL:O	2.39	0.40
7:g:253:GLN:HA	7:g:256:ILE:HG22	2.02	0.40
1:A:149:ALA:HB3	1:A:150:PRO:CD	2.51	0.40
18:C:512:CLA:H202	16:Z:23:VAL:HG11	2.03	0.40
4:D:68:LEU:CD1	6:F:39:MET:HE2	2.51	0.40
11:L:21:GLY:O	11:L:25:ILE:HG12	2.21	0.40
8:h:73:ILE:O	15:x:66:THR:HG21	2.21	0.40
18:b:513:CLA:HMB3	18:b:513:CLA:HBB1	2.03	0.40
3:c:141:ASP:OD1	3:c:142:LYS:N	2.55	0.40
3:c:155:MET:HE3	3:c:155:MET:HA	2.03	0.40
3:C:37:LEU:HD21	3:C:41:HIS:CE1	2.57	0.40
3:C:384:MET:SD	3:C:385:THR:N	2.94	0.40
20:C:517:BCR:H383	20:C:517:BCR:C23	2.48	0.40
1:a:27:ARG:NH2	13:t:21:ILE:O	2.54	0.40
1:a:288:LEU:HD21	3:c:423:PHE:CD2	2.56	0.40
2:b:158:VAL:HG11	2:b:199:ALA:HA	2.04	0.40
8:h:69:ASN:O	8:h:70:SER:OG	2.32	0.40
8:H:50:MET:HE2	8:H:50:MET:CA	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	302/327 (92%)	289 (96%)	13 (4%)	0	100	100
1	a	302/327 (92%)	289 (96%)	13 (4%)	0	100	100
2	B	478/480 (100%)	467 (98%)	11 (2%)	0	100	100
2	b	478/480 (100%)	464 (97%)	14 (3%)	0	100	100
3	C	437/450 (97%)	428 (98%)	9 (2%)	0	100	100
3	c	437/450 (97%)	428 (98%)	9 (2%)	0	100	100
4	D	333/351 (95%)	319 (96%)	14 (4%)	0	100	100
4	d	333/351 (95%)	323 (97%)	10 (3%)	0	100	100
5	E	72/74 (97%)	68 (94%)	4 (6%)	0	100	100
5	e	72/74 (97%)	68 (94%)	4 (6%)	0	100	100
6	F	29/31 (94%)	29 (100%)	0	0	100	100
6	f	29/31 (94%)	29 (100%)	0	0	100	100
7	G	163/195 (84%)	158 (97%)	5 (3%)	0	100	100
7	g	163/195 (84%)	161 (99%)	2 (1%)	0	100	100
8	H	69/71 (97%)	66 (96%)	3 (4%)	0	100	100
8	h	69/71 (97%)	67 (97%)	2 (3%)	0	100	100
9	I	32/34 (94%)	32 (100%)	0	0	100	100
9	i	32/34 (94%)	32 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
11	l	36/38 (95%)	34 (94%)	2 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	M	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
12	m	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
13	T	26/28 (93%)	24 (92%)	2 (8%)	0	100	100
13	t	26/28 (93%)	24 (92%)	2 (8%)	0	100	100
14	V	29/31 (94%)	29 (100%)	0	0	100	100
14	v	29/31 (94%)	29 (100%)	0	0	100	100
15	X	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
15	x	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
16	Z	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
16	z	59/61 (97%)	59 (100%)	0	0	100	100
All	All	4310/4534 (95%)	4184 (97%)	126 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	248/266 (93%)	248 (100%)	0	100	100
1	a	248/266 (93%)	248 (100%)	0	100	100
2	B	382/382 (100%)	382 (100%)	0	100	100
2	b	382/382 (100%)	382 (100%)	0	100	100
3	C	346/352 (98%)	346 (100%)	0	100	100
3	c	346/352 (98%)	346 (100%)	0	100	100
4	D	270/280 (96%)	270 (100%)	0	100	100
4	d	270/280 (96%)	270 (100%)	0	100	100
5	E	65/65 (100%)	65 (100%)	0	100	100
5	e	65/65 (100%)	65 (100%)	0	100	100
6	F	25/25 (100%)	25 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	f	25/25 (100%)	25 (100%)	0	100	100
7	G	140/162 (86%)	140 (100%)	0	100	100
7	g	140/162 (86%)	140 (100%)	0	100	100
8	H	61/61 (100%)	61 (100%)	0	100	100
8	h	61/61 (100%)	61 (100%)	0	100	100
9	I	31/31 (100%)	31 (100%)	0	100	100
9	i	31/31 (100%)	31 (100%)	0	100	100
10	K	31/31 (100%)	31 (100%)	0	100	100
10	k	31/31 (100%)	31 (100%)	0	100	100
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	23/23 (100%)	23 (100%)	0	100	100
12	m	23/23 (100%)	23 (100%)	0	100	100
13	T	25/25 (100%)	25 (100%)	0	100	100
13	t	25/25 (100%)	25 (100%)	0	100	100
14	V	25/25 (100%)	25 (100%)	0	100	100
14	v	25/25 (100%)	25 (100%)	0	100	100
15	X	22/22 (100%)	22 (100%)	0	100	100
15	x	22/22 (100%)	22 (100%)	0	100	100
16	Z	51/51 (100%)	51 (100%)	0	100	100
16	z	51/51 (100%)	51 (100%)	0	100	100
All	All	3560/3672 (97%)	3560 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	187	GLN
1	A	325	ASN
1	a	76	ASN
1	a	322	ASN
3	c	143	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	d	164	GLN
4	d	292	ASN
7	g	134	GLN
10	k	40	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 136 ligands modelled in this entry, 2 are monoatomic - leaving 134 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	$\# Z > 2$
21	LMG	c	521	-	51,51,55	0.94	2 (3%)	59,59,63	0.92	2 (3%)
18	CLA	B	508	2	69,73,73	1.24	7 (10%)	83,113,113	1.08	5 (6%)
18	CLA	d	405	4	69,73,73	1.25	6 (8%)	83,113,113	1.14	6 (7%)
18	CLA	B	506	2	69,73,73	1.24	6 (8%)	83,113,113	1.10	5 (6%)
24	DGD	C	519	-	50,50,67	0.99	2 (4%)	64,64,81	0.88	2 (3%)
18	CLA	b	515	2	69,73,73	1.25	6 (8%)	83,113,113	1.16	5 (6%)
20	BCR	C	515	-	41,41,41	0.77	0	56,56,56	2.09	20 (35%)
20	BCR	C	517	-	41,41,41	0.73	0	56,56,56	1.93	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	507	-	69,73,73	1.26	7 (10%)	83,113,113	1.11	6 (7%)
22	LHG	d	408	-	48,48,48	0.93	2 (4%)	51,54,54	1.03	3 (5%)
18	CLA	c	505	3	69,73,73	1.25	7 (10%)	83,113,113	1.07	5 (6%)
18	CLA	c	510	3	69,73,73	1.24	7 (10%)	83,113,113	1.10	3 (3%)
18	CLA	b	513	2	69,73,73	1.26	6 (8%)	83,113,113	1.11	4 (4%)
20	BCR	B	519	-	41,41,41	0.75	0	56,56,56	1.93	18 (32%)
18	CLA	c	507	3	69,73,73	1.24	6 (8%)	83,113,113	1.08	5 (6%)
22	LHG	D	408	-	48,48,48	0.93	2 (4%)	51,54,54	1.03	3 (5%)
18	CLA	b	508	2	69,73,73	1.24	7 (10%)	83,113,113	1.04	6 (7%)
18	CLA	B	509	2	69,73,73	1.25	6 (8%)	83,113,113	1.07	5 (6%)
18	CLA	c	512	3	69,73,73	1.26	5 (7%)	83,113,113	1.12	4 (4%)
18	CLA	B	514	2	49,53,73	1.47	5 (10%)	59,89,113	1.29	5 (8%)
22	LHG	A	408	-	42,42,48	1.01	2 (4%)	45,48,54	1.03	2 (4%)
18	CLA	C	503	3	69,73,73	1.25	7 (10%)	83,113,113	1.18	7 (8%)
22	LHG	l	101	-	48,48,48	0.94	2 (4%)	51,54,54	0.92	2 (3%)
23	SQD	C	501	-	50,51,54	1.21	4 (8%)	59,62,65	1.08	5 (8%)
18	CLA	b	514	2	49,53,73	1.47	7 (14%)	59,89,113	1.25	5 (8%)
22	LHG	X	101	-	48,48,48	0.95	2 (4%)	51,54,54	0.95	2 (3%)
22	LHG	b	520	-	43,43,48	1.00	2 (4%)	46,49,54	0.90	2 (4%)
18	CLA	B	503	2	69,73,73	1.25	7 (10%)	83,113,113	1.13	6 (7%)
19	PHO	A	404	-	58,69,69	2.08	10 (17%)	56,99,99	1.56	8 (14%)
18	CLA	B	505	2	69,73,73	1.26	6 (8%)	83,113,113	1.09	5 (6%)
28	HEM	F	101	6,5	50,50,50	1.47	8 (16%)	66,82,82	1.22	5 (7%)
18	CLA	a	402	1	69,73,73	1.25	6 (8%)	83,113,113	1.13	8 (9%)
21	LMG	D	410	-	48,48,55	0.97	2 (4%)	56,56,63	0.95	2 (3%)
18	CLA	b	512	2	69,73,73	1.26	8 (11%)	83,113,113	1.16	4 (4%)
22	LHG	b	521	-	48,48,48	0.94	2 (4%)	51,54,54	0.91	2 (3%)
18	CLA	b	511	2	69,73,73	1.24	7 (10%)	83,113,113	1.14	6 (7%)
22	LHG	a	407	-	42,42,48	1.01	2 (4%)	45,48,54	1.04	2 (4%)
18	CLA	b	503	2	69,73,73	1.25	7 (10%)	83,113,113	1.15	7 (8%)
18	CLA	b	504	2	69,73,73	1.25	6 (8%)	83,113,113	1.12	5 (6%)
18	CLA	B	513	2	69,73,73	1.25	6 (8%)	83,113,113	1.10	5 (6%)
18	CLA	C	513	3	69,73,73	1.25	6 (8%)	83,113,113	1.16	5 (6%)
20	BCR	x	102	-	41,41,41	0.70	0	56,56,56	2.13	24 (42%)
20	BCR	B	517	-	41,41,41	0.81	0	56,56,56	2.13	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	D	401	-	69,73,73	1.26	8 (11%)	83,113,113	1.05	5 (6%)
18	CLA	c	511	3	69,73,73	1.25	6 (8%)	83,113,113	1.11	4 (4%)
20	BCR	c	516	-	41,41,41	0.80	1 (2%)	56,56,56	2.26	21 (37%)
18	CLA	c	503	3	69,73,73	1.24	7 (10%)	83,113,113	1.10	6 (7%)
18	CLA	c	506	-	69,73,73	1.26	6 (8%)	83,113,113	1.07	5 (6%)
22	LHG	L	101	-	48,48,48	0.94	2 (4%)	51,54,54	0.91	2 (3%)
18	CLA	C	512	3	69,73,73	1.26	5 (7%)	83,113,113	1.07	5 (6%)
18	CLA	c	504	3	69,73,73	1.25	7 (10%)	83,113,113	1.19	7 (8%)
20	BCR	b	517	-	41,41,41	0.81	0	56,56,56	2.12	22 (39%)
25	LMU	c	522	-	36,36,36	1.15	2 (5%)	47,47,47	0.84	1 (2%)
20	BCR	d	406	-	41,41,41	0.79	0	56,56,56	2.00	17 (30%)
18	CLA	b	506	2	69,73,73	1.25	7 (10%)	83,113,113	1.10	6 (7%)
20	BCR	a	406	-	41,41,41	0.81	1 (2%)	56,56,56	2.10	21 (37%)
18	CLA	B	511	2	69,73,73	1.24	6 (8%)	83,113,113	1.15	7 (8%)
18	CLA	d	404	4	69,73,73	1.26	7 (10%)	83,113,113	1.12	5 (6%)
21	LMG	h	101	-	48,48,55	0.98	3 (6%)	56,56,63	1.02	3 (5%)
19	PHO	D	402	-	58,69,69	2.08	10 (17%)	56,99,99	1.42	6 (10%)
21	LMG	A	407	-	46,46,55	0.99	2 (4%)	54,54,63	0.99	3 (5%)
18	CLA	B	501	-	69,73,73	1.26	5 (7%)	83,113,113	1.11	6 (7%)
18	CLA	b	510	-	69,73,73	1.24	7 (10%)	83,113,113	1.17	7 (8%)
18	CLA	c	508	3	69,73,73	1.25	6 (8%)	83,113,113	1.13	6 (7%)
18	CLA	B	516	2	69,73,73	1.26	8 (11%)	83,113,113	1.11	4 (4%)
18	CLA	c	509	-	69,73,73	1.24	6 (8%)	83,113,113	1.12	3 (3%)
18	CLA	D	405	4	69,73,73	1.25	6 (8%)	83,113,113	1.13	5 (6%)
18	CLA	b	507	-	69,73,73	1.25	6 (8%)	83,113,113	1.09	6 (7%)
18	CLA	C	507	3	69,73,73	1.25	7 (10%)	83,113,113	1.13	6 (7%)
20	BCR	X	102	-	41,41,41	0.70	0	56,56,56	2.15	25 (44%)
18	CLA	c	514	3	69,73,73	1.25	6 (8%)	83,113,113	1.17	5 (6%)
21	LMG	b	519	-	42,42,55	1.02	2 (4%)	50,50,63	0.96	2 (4%)
18	CLA	b	516	2	69,73,73	1.26	8 (11%)	83,113,113	1.12	5 (6%)
26	BCT	D	403	17	2,3,3	1.25	0	2,3,3	4.19	2 (100%)
20	BCR	A	406	-	41,41,41	0.81	1 (2%)	56,56,56	2.05	20 (35%)
21	LMG	D	409	-	46,46,55	0.99	2 (4%)	54,54,63	0.93	2 (3%)
20	BCR	B	518	-	41,41,41	0.78	0	56,56,56	1.95	18 (32%)
20	BCR	b	518	-	41,41,41	0.79	0	56,56,56	1.95	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	C	506	3	69,73,73	1.24	6 (8%)	83,113,113	1.09	8 (9%)
18	CLA	B	515	2	69,73,73	1.25	5 (7%)	83,113,113	1.17	5 (6%)
18	CLA	A	402	1	69,73,73	1.25	6 (8%)	83,113,113	1.12	9 (10%)
21	LMG	c	502	-	46,46,55	0.99	2 (4%)	54,54,63	1.00	3 (5%)
18	CLA	C	509	3	69,73,73	1.25	8 (11%)	83,113,113	1.10	3 (3%)
20	BCR	K	101	-	41,41,41	0.66	0	56,56,56	2.16	24 (42%)
24	DGD	C	518	-	54,54,67	0.94	2 (3%)	68,68,81	0.94	3 (4%)
22	LHG	B	522	-	48,48,48	0.94	2 (4%)	51,54,54	0.91	2 (3%)
18	CLA	b	505	2	69,73,73	1.26	6 (8%)	83,113,113	1.08	5 (6%)
23	SQD	c	501	-	50,51,54	1.21	4 (8%)	59,62,65	1.14	4 (6%)
18	CLA	A	403	-	53,57,73	1.43	7 (13%)	62,93,113	1.21	4 (6%)
25	LMU	C	522	-	36,36,36	1.15	2 (5%)	47,47,47	0.85	1 (2%)
18	CLA	C	511	3	69,73,73	1.25	6 (8%)	83,113,113	1.11	4 (4%)
20	BCR	C	516	-	41,41,41	0.80	1 (2%)	56,56,56	2.24	22 (39%)
22	LHG	A	409	-	43,43,48	1.00	2 (4%)	46,49,54	0.91	2 (4%)
22	LHG	x	101	-	48,48,48	0.95	2 (4%)	51,54,54	0.95	2 (3%)
18	CLA	b	509	2	69,73,73	1.25	6 (8%)	83,113,113	1.14	9 (10%)
20	BCR	A	410	-	41,41,41	0.75	0	56,56,56	1.93	17 (30%)
18	CLA	C	502	3	69,73,73	1.25	7 (10%)	83,113,113	1.10	7 (8%)
19	PHO	d	402	-	58,69,69	2.08	10 (17%)	56,99,99	1.44	6 (10%)
18	CLA	C	510	3	69,73,73	1.25	6 (8%)	83,113,113	1.09	3 (3%)
21	LMG	B	520	-	42,42,55	1.02	2 (4%)	50,50,63	0.95	2 (4%)
21	LMG	d	409	-	46,46,55	0.99	2 (4%)	54,54,63	0.91	2 (3%)
24	DGD	c	519	-	50,50,67	0.99	2 (4%)	64,64,81	0.86	2 (3%)
18	CLA	c	513	3	69,73,73	1.26	6 (8%)	83,113,113	1.08	5 (6%)
18	CLA	d	401	-	69,73,73	1.26	8 (11%)	83,113,113	1.06	6 (7%)
18	CLA	C	508	-	69,73,73	1.24	6 (8%)	83,113,113	1.14	5 (6%)
18	CLA	b	501	-	69,73,73	1.25	6 (8%)	83,113,113	1.09	5 (6%)
28	HEM	e	101	6,5	50,50,50	1.46	7 (14%)	66,82,82	1.24	6 (9%)
18	CLA	A	405	1	64,68,73	1.30	6 (9%)	77,107,113	1.13	6 (7%)
18	CLA	B	510	-	69,73,73	1.25	6 (8%)	83,113,113	1.19	6 (7%)
20	BCR	k	101	-	41,41,41	0.66	0	56,56,56	2.18	23 (41%)
22	LHG	a	408	-	43,43,48	1.00	2 (4%)	46,49,54	0.92	2 (4%)
18	CLA	C	514	3	69,73,73	1.25	5 (7%)	83,113,113	1.06	5 (6%)
18	CLA	C	504	3	69,73,73	1.26	6 (8%)	83,113,113	1.08	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LHG	B	521	-	43,43,48	1.01	2 (4%)	46,49,54	0.91	2 (4%)
27	PL9	d	407	-	55,55,55	1.01	3 (5%)	68,69,69	1.55	12 (17%)
20	BCR	z	101	-	41,41,41	0.79	0	56,56,56	2.07	21 (37%)
18	CLA	B	504	2	69,73,73	1.25	5 (7%)	83,113,113	1.11	4 (4%)
24	DGD	c	520	-	60,60,67	0.91	2 (3%)	74,74,81	0.87	2 (2%)
19	PHO	a	404	-	58,69,69	2.08	10 (17%)	56,99,99	1.55	8 (14%)
18	CLA	D	404	4	69,73,73	1.25	7 (10%)	83,113,113	1.10	5 (6%)
20	BCR	D	406	-	41,41,41	0.79	0	56,56,56	2.00	18 (32%)
18	CLA	a	403	-	53,57,73	1.41	7 (13%)	62,93,113	1.22	5 (8%)
18	CLA	C	505	-	69,73,73	1.26	7 (10%)	83,113,113	1.07	5 (6%)
24	DGD	c	518	-	54,54,67	0.93	2 (3%)	68,68,81	0.94	3 (4%)
26	BCT	d	403	17	2,3,3	1.25	0	2,3,3	4.18	1 (50%)
27	PL9	D	407	-	55,55,55	1.01	3 (5%)	68,69,69	1.55	12 (17%)
18	CLA	a	405	1	64,68,73	1.30	6 (9%)	77,107,113	1.15	6 (7%)
18	CLA	B	512	2	69,73,73	1.26	7 (10%)	83,113,113	1.16	4 (4%)
24	DGD	C	520	-	60,60,67	0.91	2 (3%)	74,74,81	0.87	2 (2%)
21	LMG	C	521	-	51,51,55	0.94	2 (3%)	59,59,63	0.92	2 (3%)
18	CLA	B	502	2	69,73,73	1.26	6 (8%)	83,113,113	1.11	5 (6%)
18	CLA	b	502	2	69,73,73	1.25	7 (10%)	83,113,113	1.09	5 (6%)
18	CLA	c	515	3	69,73,73	1.25	6 (8%)	83,113,113	1.07	5 (6%)
20	BCR	c	517	-	41,41,41	0.74	0	56,56,56	1.87	16 (28%)

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
21	LMG	c	521	-	-	9/46/66/70	0/1/1/1
18	CLA	B	508	2	-	12/39/115/115	-
18	CLA	d	405	4	-	18/39/115/115	-
18	CLA	B	506	2	-	13/39/115/115	-
24	DGD	C	519	-	-	8/38/78/95	0/2/2/2
18	CLA	b	515	2	-	7/39/115/115	-
20	BCR	C	515	-	-	6/29/63/63	0/2/2/2
20	BCR	C	517	-	-	4/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	507	-	-	13/39/115/115	-
22	LHG	d	408	-	-	6/53/53/53	-
18	CLA	c	505	3	-	17/39/115/115	-
18	CLA	c	510	3	-	9/39/115/115	-
18	CLA	b	513	2	-	12/39/115/115	-
20	BCR	B	519	-	-	4/29/63/63	0/2/2/2
18	CLA	c	507	3	-	17/39/115/115	-
22	LHG	D	408	-	-	6/53/53/53	-
18	CLA	b	508	2	-	10/39/115/115	-
18	CLA	B	509	2	-	18/39/115/115	-
18	CLA	c	512	3	-	15/39/115/115	-
18	CLA	B	514	2	-	2/15/91/115	-
22	LHG	A	408	-	-	13/47/47/53	-
18	CLA	C	503	3	-	11/39/115/115	-
22	LHG	l	101	-	-	12/53/53/53	-
23	SQD	C	501	-	-	13/46/66/69	0/1/1/1
18	CLA	b	514	2	-	2/15/91/115	-
22	LHG	X	101	-	-	16/53/53/53	-
22	LHG	b	520	-	-	7/48/48/53	-
18	CLA	B	503	2	-	12/39/115/115	-
19	PHO	A	404	-	-	11/37/103/103	0/5/6/6
18	CLA	B	505	2	-	15/39/115/115	-
28	HEM	F	101	6,5	-	6/14/54/54	-
18	CLA	a	402	1	-	9/39/115/115	-
21	LMG	D	410	-	-	11/43/63/70	0/1/1/1
18	CLA	b	512	2	-	12/39/115/115	-
22	LHG	b	521	-	-	9/53/53/53	-
18	CLA	b	511	2	-	17/39/115/115	-
22	LHG	a	407	-	-	13/47/47/53	-
18	CLA	b	503	2	-	10/39/115/115	-
18	CLA	b	504	2	-	17/39/115/115	-
18	CLA	B	513	2	-	12/39/115/115	-
18	CLA	C	513	3	-	10/39/115/115	-
20	BCR	x	102	-	-	5/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	BCR	B	517	-	-	4/29/63/63	0/2/2/2
18	CLA	D	401	-	-	10/39/115/115	-
18	CLA	c	511	3	-	16/39/115/115	-
20	BCR	c	516	-	-	3/29/63/63	0/2/2/2
18	CLA	c	503	3	-	15/39/115/115	-
18	CLA	c	506	-	-	10/39/115/115	-
22	LHG	L	101	-	-	14/53/53/53	-
18	CLA	C	512	3	-	13/39/115/115	-
18	CLA	c	504	3	-	11/39/115/115	-
20	BCR	b	517	-	-	4/29/63/63	0/2/2/2
25	LMU	c	522	-	-	7/21/61/61	0/2/2/2
20	BCR	d	406	-	-	4/29/63/63	0/2/2/2
18	CLA	b	506	2	-	14/39/115/115	-
20	BCR	a	406	-	-	4/29/63/63	0/2/2/2
18	CLA	B	511	2	-	17/39/115/115	-
18	CLA	d	404	4	-	9/39/115/115	-
21	LMG	h	101	-	-	11/43/63/70	0/1/1/1
19	PHO	D	402	-	-	9/37/103/103	0/5/6/6
21	LMG	A	407	-	-	5/41/61/70	0/1/1/1
18	CLA	B	501	-	-	17/39/115/115	-
18	CLA	b	510	-	-	10/39/115/115	-
18	CLA	c	508	3	-	18/39/115/115	-
18	CLA	B	516	2	-	11/39/115/115	-
18	CLA	c	509	-	-	10/39/115/115	-
18	CLA	D	405	4	-	17/39/115/115	-
18	CLA	b	507	-	-	13/39/115/115	-
18	CLA	C	507	3	-	18/39/115/115	-
20	BCR	X	102	-	-	5/29/63/63	0/2/2/2
18	CLA	c	514	3	-	10/39/115/115	-
21	LMG	b	519	-	-	4/37/57/70	0/1/1/1
18	CLA	b	516	2	-	9/39/115/115	-
20	BCR	A	406	-	-	4/29/63/63	0/2/2/2
21	LMG	D	409	-	-	8/41/61/70	0/1/1/1
20	BCR	B	518	-	-	4/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	BCR	b	518	-	-	4/29/63/63	0/2/2/2
18	CLA	C	506	3	-	18/39/115/115	-
18	CLA	B	515	2	-	7/39/115/115	-
18	CLA	A	402	1	-	10/39/115/115	-
21	LMG	c	502	-	-	5/41/61/70	0/1/1/1
18	CLA	C	509	3	-	9/39/115/115	-
20	BCR	K	101	-	-	2/29/63/63	0/2/2/2
24	DGD	C	518	-	-	5/42/82/95	0/2/2/2
22	LHG	B	522	-	-	9/53/53/53	-
18	CLA	b	505	2	-	14/39/115/115	-
23	SQD	c	501	-	-	10/46/66/69	0/1/1/1
18	CLA	A	403	-	-	7/20/96/115	-
25	LMU	C	522	-	-	8/21/61/61	0/2/2/2
18	CLA	C	511	3	-	12/39/115/115	-
20	BCR	C	516	-	-	3/29/63/63	0/2/2/2
22	LHG	A	409	-	-	17/48/48/53	-
22	LHG	x	101	-	-	17/53/53/53	-
18	CLA	b	509	2	-	18/39/115/115	-
20	BCR	A	410	-	-	4/29/63/63	0/2/2/2
18	CLA	C	502	3	-	15/39/115/115	-
19	PHO	d	402	-	-	9/37/103/103	0/5/6/6
18	CLA	C	510	3	-	14/39/115/115	-
21	LMG	B	520	-	-	4/37/57/70	0/1/1/1
21	LMG	d	409	-	-	7/41/61/70	0/1/1/1
24	DGD	c	519	-	-	8/38/78/95	0/2/2/2
18	CLA	c	513	3	-	13/39/115/115	-
18	CLA	d	401	-	-	11/39/115/115	-
18	CLA	C	508	-	-	10/39/115/115	-
18	CLA	b	501	-	-	18/39/115/115	-
28	HEM	e	101	6,5	-	6/14/54/54	-
18	CLA	A	405	1	-	4/33/109/115	-
18	CLA	B	510	-	-	10/39/115/115	-
20	BCR	k	101	-	-	2/29/63/63	0/2/2/2
22	LHG	a	408	-	-	17/48/48/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	C	514	3	-	12/39/115/115	-
18	CLA	C	504	3	-	16/39/115/115	-
22	LHG	B	521	-	-	7/48/48/53	-
27	PL9	d	407	-	-	11/53/73/73	0/1/1/1
20	BCR	z	101	-	-	6/29/63/63	0/2/2/2
18	CLA	B	504	2	-	15/39/115/115	-
24	DGD	c	520	-	-	4/48/88/95	0/2/2/2
19	PHO	a	404	-	-	10/37/103/103	0/5/6/6
18	CLA	D	404	4	-	10/39/115/115	-
20	BCR	D	406	-	-	4/29/63/63	0/2/2/2
18	CLA	a	403	-	-	9/20/96/115	-
18	CLA	C	505	-	-	10/39/115/115	-
24	DGD	c	518	-	-	5/42/82/95	0/2/2/2
27	PL9	D	407	-	-	10/53/73/73	0/1/1/1
18	CLA	a	405	1	-	4/33/109/115	-
18	CLA	B	512	2	-	11/39/115/115	-
24	DGD	C	520	-	-	4/48/88/95	0/2/2/2
21	LMG	C	521	-	-	9/46/66/70	0/1/1/1
18	CLA	B	502	2	-	10/39/115/115	-
18	CLA	b	502	2	-	10/39/115/115	-
18	CLA	c	515	3	-	12/39/115/115	-
20	BCR	c	517	-	-	4/29/63/63	0/2/2/2

All (586) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	404	PHO	C1B-C2B	9.61	1.50	1.39
19	a	404	PHO	C1B-C2B	9.60	1.50	1.39
19	d	402	PHO	C1B-C2B	9.56	1.50	1.39
19	D	402	PHO	C1B-C2B	9.55	1.50	1.39
19	d	402	PHO	C3B-C4B	7.75	1.50	1.41
19	D	402	PHO	C3B-C4B	7.71	1.50	1.41
19	A	404	PHO	C3B-C4B	7.66	1.50	1.41
19	a	404	PHO	C3B-C4B	7.63	1.50	1.41
23	C	501	SQD	O8-S	4.62	1.64	1.47
23	c	501	SQD	O8-S	4.61	1.63	1.47
22	a	407	LHG	O8-C23	4.35	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	521	LMG	O8-C28	4.35	1.46	1.33
22	A	408	LHG	O8-C23	4.34	1.46	1.33
22	B	521	LHG	O7-C7	4.33	1.46	1.34
22	X	101	LHG	O8-C23	4.32	1.46	1.33
21	D	409	LMG	O8-C28	4.32	1.46	1.33
24	c	519	DGD	O1G-C1A	4.31	1.45	1.33
21	c	521	LMG	O8-C28	4.31	1.45	1.33
24	C	519	DGD	O1G-C1A	4.31	1.45	1.33
22	a	408	LHG	O8-C23	4.31	1.45	1.33
22	x	101	LHG	O8-C23	4.30	1.45	1.33
21	d	409	LMG	O8-C28	4.29	1.45	1.33
24	c	520	DGD	O1G-C1A	4.29	1.45	1.33
22	A	409	LHG	O8-C23	4.28	1.45	1.33
22	b	520	LHG	O8-C23	4.27	1.45	1.33
22	b	520	LHG	O7-C7	4.27	1.46	1.34
22	B	521	LHG	O8-C23	4.27	1.45	1.33
21	D	410	LMG	O8-C28	4.27	1.45	1.33
21	b	519	LMG	O8-C28	4.27	1.45	1.33
21	A	407	LMG	O8-C28	4.27	1.45	1.33
21	c	502	LMG	O8-C28	4.26	1.45	1.33
21	B	520	LMG	O8-C28	4.26	1.45	1.33
21	h	101	LMG	O8-C28	4.26	1.45	1.33
19	a	404	PHO	C1D-C2D	4.25	1.44	1.39
24	C	520	DGD	O1G-C1A	4.25	1.45	1.33
23	c	501	SQD	O48-C23	4.24	1.45	1.33
22	b	521	LHG	O7-C7	4.23	1.46	1.34
19	A	404	PHO	C1D-C2D	4.22	1.44	1.39
23	C	501	SQD	O48-C23	4.21	1.45	1.33
24	c	518	DGD	O1G-C1A	4.21	1.45	1.33
24	C	518	DGD	O1G-C1A	4.21	1.45	1.33
22	B	522	LHG	O7-C7	4.21	1.46	1.34
22	L	101	LHG	O8-C23	4.21	1.45	1.33
22	l	101	LHG	O8-C23	4.20	1.45	1.33
21	D	410	LMG	O7-C10	4.20	1.46	1.34
22	B	522	LHG	O8-C23	4.20	1.45	1.33
21	d	409	LMG	O7-C10	4.20	1.46	1.34
22	d	408	LHG	O8-C23	4.19	1.45	1.33
24	c	520	DGD	O2G-C1B	4.19	1.46	1.34
22	b	521	LHG	O8-C23	4.19	1.45	1.33
22	D	408	LHG	O8-C23	4.18	1.45	1.33
24	C	520	DGD	O2G-C1B	4.18	1.46	1.34
19	D	402	PHO	C1D-C2D	4.18	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	518	DGD	O2G-C1B	4.17	1.46	1.34
21	D	409	LMG	O7-C10	4.17	1.46	1.34
24	C	518	DGD	O2G-C1B	4.17	1.46	1.34
22	A	409	LHG	O7-C7	4.17	1.46	1.34
22	L	101	LHG	O7-C7	4.16	1.46	1.34
22	x	101	LHG	O7-C7	4.15	1.46	1.34
24	C	519	DGD	O2G-C1B	4.14	1.46	1.34
22	X	101	LHG	O7-C7	4.14	1.46	1.34
22	l	101	LHG	O7-C7	4.14	1.46	1.34
22	a	408	LHG	O7-C7	4.13	1.46	1.34
21	h	101	LMG	O7-C10	4.13	1.46	1.34
21	A	407	LMG	O7-C10	4.12	1.45	1.34
24	c	519	DGD	O2G-C1B	4.12	1.45	1.34
21	B	520	LMG	O7-C10	4.12	1.45	1.34
22	A	408	LHG	O7-C7	4.12	1.45	1.34
19	d	402	PHO	C1D-C2D	4.11	1.44	1.39
22	a	407	LHG	O7-C7	4.11	1.45	1.34
21	c	502	LMG	O7-C10	4.10	1.45	1.34
21	C	521	LMG	O7-C10	4.09	1.45	1.34
22	D	408	LHG	O7-C7	4.08	1.45	1.34
21	c	521	LMG	O7-C10	4.08	1.45	1.34
21	b	519	LMG	O7-C10	4.08	1.45	1.34
23	C	501	SQD	O47-C7	4.05	1.45	1.34
22	d	408	LHG	O7-C7	4.04	1.45	1.34
23	c	501	SQD	O47-C7	4.03	1.45	1.34
18	c	513	CLA	C1D-ND	4.03	1.42	1.37
18	C	512	CLA	C1D-ND	4.03	1.42	1.37
18	B	501	CLA	C1D-ND	3.97	1.42	1.37
18	A	403	CLA	C1D-ND	3.94	1.42	1.37
18	b	516	CLA	C1D-ND	3.93	1.42	1.37
18	B	516	CLA	C1D-ND	3.90	1.42	1.37
18	b	502	CLA	C1D-ND	3.89	1.42	1.37
18	d	401	CLA	C1D-ND	3.88	1.42	1.37
18	b	506	CLA	C1D-ND	3.87	1.42	1.37
18	C	511	CLA	C1D-ND	3.87	1.42	1.37
18	b	501	CLA	C1D-ND	3.87	1.42	1.37
18	b	513	CLA	C1D-ND	3.86	1.42	1.37
18	C	514	CLA	C1D-ND	3.86	1.42	1.37
18	C	508	CLA	C1D-ND	3.85	1.42	1.37
18	C	504	CLA	C1D-ND	3.85	1.42	1.37
18	c	515	CLA	C1D-ND	3.85	1.42	1.37
18	B	514	CLA	C1D-ND	3.85	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	c	512	CLA	C1D-ND	3.85	1.42	1.37
18	B	506	CLA	C1D-ND	3.84	1.42	1.37
18	c	506	CLA	C1D-ND	3.84	1.42	1.37
18	B	515	CLA	C1D-ND	3.84	1.42	1.37
18	c	509	CLA	C1D-ND	3.84	1.42	1.37
18	B	507	CLA	C1D-ND	3.84	1.42	1.37
18	B	502	CLA	C1D-ND	3.84	1.42	1.37
18	c	505	CLA	C1D-ND	3.84	1.42	1.37
18	d	405	CLA	C1D-ND	3.83	1.42	1.37
18	D	405	CLA	C1D-ND	3.83	1.42	1.37
18	c	514	CLA	C1D-ND	3.83	1.42	1.37
18	C	505	CLA	C1D-ND	3.83	1.42	1.37
18	c	507	CLA	C1D-ND	3.83	1.42	1.37
18	C	503	CLA	C1D-ND	3.82	1.42	1.37
18	c	511	CLA	C1D-ND	3.82	1.42	1.37
18	C	513	CLA	C1D-ND	3.82	1.42	1.37
18	B	513	CLA	C1D-ND	3.82	1.42	1.37
18	b	507	CLA	C1D-ND	3.82	1.42	1.37
18	B	508	CLA	C1D-ND	3.81	1.42	1.37
18	D	401	CLA	C1D-ND	3.81	1.42	1.37
18	b	515	CLA	C1D-ND	3.81	1.42	1.37
18	b	514	CLA	C1D-ND	3.80	1.42	1.37
18	B	512	CLA	C1D-ND	3.79	1.42	1.37
18	c	504	CLA	C1D-ND	3.79	1.42	1.37
18	b	512	CLA	C1D-ND	3.78	1.42	1.37
18	C	510	CLA	C1D-ND	3.77	1.42	1.37
18	b	508	CLA	C1D-ND	3.77	1.42	1.37
18	A	402	CLA	C1D-ND	3.77	1.42	1.37
18	B	511	CLA	C1D-ND	3.77	1.42	1.37
18	b	504	CLA	C1D-ND	3.77	1.42	1.37
28	F	101	HEM	FE-ND	3.76	2.06	1.94
18	A	405	CLA	C1D-ND	3.76	1.42	1.37
18	a	405	CLA	C1D-ND	3.75	1.42	1.37
18	a	402	CLA	C1D-ND	3.74	1.42	1.37
18	C	506	CLA	C1D-ND	3.74	1.42	1.37
18	B	505	CLA	C1D-ND	3.73	1.42	1.37
18	c	508	CLA	C1D-ND	3.72	1.42	1.37
18	c	503	CLA	C1D-ND	3.71	1.42	1.37
18	B	510	CLA	C1D-ND	3.70	1.42	1.37
18	b	509	CLA	C1D-ND	3.70	1.42	1.37
18	b	511	CLA	C1D-ND	3.70	1.42	1.37
18	C	502	CLA	C1D-ND	3.70	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	507	CLA	C1D-ND	3.70	1.42	1.37
18	a	403	CLA	C1D-ND	3.70	1.42	1.37
18	c	510	CLA	C1D-ND	3.69	1.42	1.37
18	b	503	CLA	C1D-ND	3.69	1.42	1.37
18	d	404	CLA	C1D-ND	3.69	1.42	1.37
18	B	504	CLA	C1D-ND	3.68	1.42	1.37
28	e	101	HEM	FE-ND	3.67	2.06	1.94
18	B	509	CLA	C1D-ND	3.67	1.42	1.37
28	e	101	HEM	FE-NB	3.66	2.06	1.94
18	b	505	CLA	C1D-ND	3.66	1.42	1.37
18	B	501	CLA	C4B-NB	3.65	1.42	1.37
18	C	509	CLA	C1D-ND	3.65	1.42	1.37
28	F	101	HEM	FE-NB	3.63	2.06	1.94
18	D	404	CLA	C1D-ND	3.63	1.42	1.37
18	B	509	CLA	C4B-NB	3.62	1.42	1.37
18	B	503	CLA	C1D-ND	3.62	1.42	1.37
18	c	512	CLA	C4B-NB	3.61	1.42	1.37
18	D	401	CLA	C4B-NB	3.61	1.42	1.37
18	b	510	CLA	C1D-ND	3.60	1.42	1.37
18	C	505	CLA	C4B-NB	3.58	1.42	1.37
18	b	501	CLA	C4B-NB	3.58	1.42	1.37
18	C	510	CLA	C4B-NB	3.56	1.42	1.37
18	C	512	CLA	C4B-NB	3.55	1.42	1.37
18	b	515	CLA	C4B-NB	3.54	1.42	1.37
18	d	405	CLA	C4B-NB	3.54	1.42	1.37
18	b	509	CLA	C4B-NB	3.54	1.42	1.37
18	d	401	CLA	C4B-NB	3.53	1.42	1.37
18	A	403	CLA	C4B-NB	3.53	1.42	1.37
18	C	513	CLA	C4B-NB	3.53	1.42	1.37
18	b	503	CLA	C4B-NB	3.53	1.42	1.37
18	c	514	CLA	C4B-NB	3.52	1.42	1.37
18	B	507	CLA	C4B-NB	3.52	1.42	1.37
18	c	506	CLA	C4B-NB	3.52	1.42	1.37
18	B	505	CLA	C4B-NB	3.51	1.42	1.37
18	C	504	CLA	C4B-NB	3.51	1.42	1.37
18	c	508	CLA	C4B-NB	3.51	1.42	1.37
18	A	405	CLA	C4B-NB	3.51	1.42	1.37
18	C	514	CLA	C4B-NB	3.50	1.42	1.37
18	c	511	CLA	C4B-NB	3.50	1.42	1.37
18	C	509	CLA	C4B-NB	3.50	1.42	1.37
18	c	507	CLA	C4B-NB	3.50	1.42	1.37
28	F	101	HEM	FE-NA	3.50	2.07	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	507	CLA	C4B-NB	3.50	1.42	1.37
18	c	505	CLA	C4B-NB	3.50	1.42	1.37
18	b	505	CLA	C4B-NB	3.49	1.42	1.37
18	C	511	CLA	C4B-NB	3.49	1.42	1.37
18	b	506	CLA	C4B-NB	3.49	1.42	1.37
18	B	512	CLA	C4B-NB	3.49	1.42	1.37
18	b	513	CLA	C4B-NB	3.48	1.42	1.37
18	d	404	CLA	C4B-NB	3.48	1.42	1.37
18	B	504	CLA	C4B-NB	3.48	1.42	1.37
18	a	405	CLA	C4B-NB	3.48	1.42	1.37
18	C	506	CLA	C4B-NB	3.47	1.42	1.37
18	D	405	CLA	C4B-NB	3.47	1.42	1.37
18	B	503	CLA	C4B-NB	3.47	1.42	1.37
18	b	507	CLA	C4B-NB	3.47	1.42	1.37
18	c	513	CLA	C4B-NB	3.47	1.42	1.37
18	B	506	CLA	C4B-NB	3.46	1.42	1.37
18	B	514	CLA	C4B-NB	3.46	1.42	1.37
18	B	513	CLA	C4B-NB	3.46	1.42	1.37
18	c	515	CLA	C4B-NB	3.46	1.42	1.37
18	B	515	CLA	C4B-NB	3.46	1.42	1.37
18	b	504	CLA	C4B-NB	3.46	1.42	1.37
18	c	510	CLA	C4B-NB	3.46	1.42	1.37
18	b	512	CLA	C4B-NB	3.45	1.42	1.37
18	a	402	CLA	C4B-NB	3.45	1.42	1.37
18	b	516	CLA	C4B-NB	3.43	1.42	1.37
18	a	403	CLA	C4B-NB	3.43	1.42	1.37
18	b	514	CLA	C4B-NB	3.43	1.42	1.37
18	b	511	CLA	C4B-NB	3.43	1.42	1.37
18	B	502	CLA	C4B-NB	3.42	1.42	1.37
18	B	511	CLA	C4B-NB	3.42	1.42	1.37
18	B	516	CLA	C4B-NB	3.42	1.42	1.37
18	D	404	CLA	C4B-NB	3.41	1.42	1.37
19	a	404	PHO	C4D-CHA	3.41	1.45	1.39
18	C	508	CLA	C4B-NB	3.41	1.42	1.37
19	A	404	PHO	C4D-CHA	3.40	1.45	1.39
18	C	502	CLA	C4B-NB	3.39	1.42	1.37
25	c	522	LMU	O5B-C1B	3.39	1.50	1.41
18	A	402	CLA	C4B-NB	3.39	1.41	1.37
28	e	101	HEM	FE-NA	3.37	2.06	1.95
25	C	522	LMU	O5B-C1B	3.37	1.50	1.41
18	b	502	CLA	C4B-NB	3.37	1.41	1.37
18	c	503	CLA	C4B-NB	3.37	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	c	509	CLA	C4B-NB	3.36	1.41	1.37
25	C	522	LMU	O5'-C1'	3.36	1.50	1.41
25	c	522	LMU	O5'-C1'	3.35	1.50	1.41
19	D	402	PHO	C4D-CHA	3.35	1.44	1.39
18	b	510	CLA	C4B-NB	3.34	1.41	1.37
18	B	510	CLA	C4B-NB	3.34	1.41	1.37
18	c	504	CLA	C4B-NB	3.33	1.41	1.37
18	C	503	CLA	C4B-NB	3.33	1.41	1.37
18	b	508	CLA	C4B-NB	3.32	1.41	1.37
19	d	402	PHO	C4D-CHA	3.30	1.44	1.39
18	B	508	CLA	C4B-NB	3.28	1.41	1.37
27	d	407	PL9	C7-C3	-3.26	1.48	1.51
27	D	407	PL9	C7-C3	-3.24	1.48	1.51
18	D	401	CLA	C4D-ND	-3.21	1.33	1.37
18	d	401	CLA	C4D-ND	-3.21	1.33	1.37
18	A	403	CLA	C4D-ND	-3.15	1.33	1.37
18	a	403	CLA	C4D-ND	-3.09	1.33	1.37
18	C	507	CLA	C4D-ND	-3.08	1.33	1.37
18	B	511	CLA	C4D-ND	-3.08	1.33	1.37
18	B	505	CLA	C4D-ND	-3.07	1.33	1.37
18	c	512	CLA	C4D-ND	-3.05	1.33	1.37
18	c	508	CLA	C4D-ND	-3.05	1.33	1.37
18	a	402	CLA	C4D-ND	-3.05	1.33	1.37
18	B	510	CLA	C4D-ND	-3.04	1.33	1.37
18	b	511	CLA	C4D-ND	-3.04	1.33	1.37
18	b	505	CLA	C4D-ND	-3.03	1.33	1.37
18	b	510	CLA	C4D-ND	-3.02	1.33	1.37
18	c	504	CLA	C4D-ND	-3.02	1.33	1.37
18	C	505	CLA	C4D-ND	-3.02	1.33	1.37
18	C	509	CLA	C4D-ND	-3.01	1.33	1.37
18	B	509	CLA	C4D-ND	-3.01	1.33	1.37
28	e	101	HEM	CAB-C3B	3.01	1.55	1.47
18	B	516	CLA	C4D-ND	-3.00	1.33	1.37
18	c	506	CLA	C4D-ND	-3.00	1.33	1.37
18	C	512	CLA	C4D-ND	-3.00	1.33	1.37
18	B	513	CLA	C3B-C4B	3.00	1.49	1.42
18	b	508	CLA	C4D-ND	-2.99	1.33	1.37
18	C	514	CLA	C4D-ND	-2.99	1.33	1.37
18	b	514	CLA	C3B-C4B	2.99	1.49	1.42
18	C	502	CLA	C4D-ND	-2.99	1.33	1.37
18	D	405	CLA	C4D-ND	-2.99	1.33	1.37
18	C	511	CLA	C4D-ND	-2.99	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b	513	CLA	C3B-C4B	2.98	1.49	1.42
18	c	503	CLA	C4D-ND	-2.98	1.33	1.37
18	B	502	CLA	C4D-ND	-2.98	1.33	1.37
18	c	513	CLA	C4D-ND	-2.98	1.33	1.37
18	b	505	CLA	C1B-C2B	2.98	1.50	1.43
18	b	504	CLA	C4D-ND	-2.98	1.33	1.37
18	c	510	CLA	C4D-ND	-2.97	1.33	1.37
18	d	405	CLA	C4D-ND	-2.97	1.33	1.37
18	C	504	CLA	C4D-ND	-2.97	1.33	1.37
28	F	101	HEM	CAB-C3B	2.97	1.55	1.47
18	C	503	CLA	C4D-ND	-2.97	1.33	1.37
18	A	402	CLA	C4D-ND	-2.96	1.33	1.37
18	c	515	CLA	C4D-ND	-2.96	1.33	1.37
18	B	506	CLA	C4D-ND	-2.96	1.33	1.37
18	B	508	CLA	C4D-ND	-2.96	1.33	1.37
18	b	506	CLA	C4D-ND	-2.96	1.33	1.37
27	d	407	PL9	C3-C4	-2.95	1.44	1.49
18	B	503	CLA	C4D-ND	-2.95	1.33	1.37
18	C	510	CLA	C4D-ND	-2.95	1.33	1.37
18	b	516	CLA	C4D-ND	-2.95	1.33	1.37
18	b	508	CLA	C1B-C2B	2.95	1.50	1.43
18	b	503	CLA	C4D-ND	-2.94	1.33	1.37
27	D	407	PL9	C3-C4	-2.94	1.44	1.49
28	e	101	HEM	CAC-C3C	2.94	1.55	1.47
18	B	505	CLA	C1B-C2B	2.94	1.50	1.43
18	C	506	CLA	C3B-C4B	2.93	1.49	1.42
18	D	404	CLA	C4D-ND	-2.93	1.33	1.37
18	B	514	CLA	C3B-C4B	2.93	1.49	1.42
18	a	405	CLA	C4D-ND	-2.93	1.33	1.37
18	B	504	CLA	C4D-ND	-2.92	1.33	1.37
18	B	501	CLA	C3B-C4B	2.92	1.49	1.42
18	B	507	CLA	C4D-ND	-2.92	1.33	1.37
18	b	507	CLA	C4D-ND	-2.92	1.33	1.37
18	c	505	CLA	C4D-ND	-2.92	1.33	1.37
28	e	101	HEM	FE-NC	2.92	2.05	1.95
18	B	514	CLA	C4D-ND	-2.91	1.33	1.37
18	b	509	CLA	C4D-ND	-2.91	1.33	1.37
18	c	507	CLA	C3B-C4B	2.91	1.49	1.42
18	b	512	CLA	C4D-ND	-2.91	1.33	1.37
18	A	405	CLA	C4D-ND	-2.91	1.33	1.37
18	B	512	CLA	C4D-ND	-2.91	1.33	1.37
18	B	513	CLA	C4D-ND	-2.90	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b	514	CLA	C4D-ND	-2.90	1.33	1.37
18	c	511	CLA	C4D-ND	-2.90	1.33	1.37
18	c	509	CLA	C4D-ND	-2.89	1.33	1.37
18	b	502	CLA	C4D-ND	-2.89	1.33	1.37
28	F	101	HEM	CAC-C3C	2.89	1.55	1.47
18	D	401	CLA	C3B-C4B	2.89	1.49	1.42
18	b	501	CLA	C3B-C4B	2.88	1.49	1.42
18	C	514	CLA	C1B-C2B	2.88	1.50	1.43
18	b	510	CLA	C3B-C4B	2.87	1.49	1.42
18	b	501	CLA	C4D-ND	-2.87	1.33	1.37
18	B	508	CLA	C1B-C2B	2.86	1.50	1.43
18	d	404	CLA	C4D-ND	-2.86	1.33	1.37
18	B	515	CLA	C4D-ND	-2.86	1.33	1.37
18	b	515	CLA	C3B-C4B	2.85	1.49	1.42
18	C	504	CLA	C3B-C4B	2.85	1.49	1.42
18	C	502	CLA	C1B-C2B	2.85	1.50	1.43
18	b	507	CLA	C1B-C2B	2.85	1.50	1.43
18	B	501	CLA	C4D-ND	-2.85	1.33	1.37
18	c	503	CLA	C1B-C2B	2.85	1.50	1.43
18	b	512	CLA	C3B-C4B	2.85	1.49	1.42
18	c	515	CLA	C1B-C2B	2.85	1.50	1.43
18	d	401	CLA	C3B-C4B	2.85	1.49	1.42
18	b	507	CLA	C3B-C4B	2.84	1.49	1.42
18	C	506	CLA	C4D-ND	-2.84	1.33	1.37
18	C	508	CLA	C4D-ND	-2.84	1.33	1.37
18	b	516	CLA	C3B-C4B	2.84	1.49	1.42
18	c	506	CLA	C3B-C4B	2.84	1.49	1.42
18	c	513	CLA	C1B-C2B	2.84	1.49	1.43
18	b	515	CLA	C4D-ND	-2.83	1.33	1.37
18	B	507	CLA	C3B-C4B	2.83	1.49	1.42
18	A	402	CLA	C1B-C2B	2.83	1.49	1.43
18	c	514	CLA	C3B-C4B	2.83	1.49	1.42
18	c	511	CLA	C3B-C4B	2.83	1.49	1.42
18	B	512	CLA	C3B-C4B	2.82	1.49	1.42
18	C	512	CLA	C1B-C2B	2.82	1.49	1.43
18	C	511	CLA	C1B-C2B	2.82	1.49	1.43
18	C	505	CLA	C3B-C4B	2.82	1.49	1.42
18	b	511	CLA	C3B-C4B	2.82	1.49	1.42
18	c	505	CLA	C3B-C4B	2.82	1.49	1.42
18	B	515	CLA	C3B-C4B	2.82	1.49	1.42
18	B	502	CLA	C3B-C4B	2.81	1.49	1.42
18	C	510	CLA	C3B-C4B	2.81	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	513	CLA	C1B-C2B	2.81	1.49	1.43
18	b	513	CLA	C4D-ND	-2.81	1.33	1.37
18	b	503	CLA	C3B-C4B	2.81	1.49	1.42
18	b	509	CLA	C3B-C4B	2.81	1.49	1.42
28	F	101	HEM	FE-NC	2.81	2.04	1.95
18	b	509	CLA	C1B-C2B	2.81	1.49	1.43
18	B	510	CLA	C3B-C4B	2.81	1.49	1.42
18	C	509	CLA	C3B-C4B	2.80	1.49	1.42
18	b	502	CLA	C3B-C4B	2.80	1.49	1.42
18	c	510	CLA	C3B-C4B	2.80	1.49	1.42
18	c	507	CLA	C4D-ND	-2.80	1.33	1.37
18	b	513	CLA	C1B-C2B	2.80	1.49	1.43
18	B	506	CLA	C3B-C4B	2.80	1.49	1.42
18	d	404	CLA	C3B-C4B	2.79	1.49	1.42
18	C	513	CLA	C3B-C4B	2.79	1.49	1.42
18	c	514	CLA	C4D-ND	-2.79	1.33	1.37
18	A	405	CLA	C3B-C4B	2.79	1.49	1.42
18	C	508	CLA	C1B-C2B	2.79	1.49	1.43
18	b	504	CLA	C3B-C4B	2.79	1.49	1.42
18	C	513	CLA	C4D-ND	-2.78	1.33	1.37
18	B	511	CLA	C3B-C4B	2.78	1.49	1.42
23	C	501	SQD	C6-S	-2.78	1.67	1.77
18	c	509	CLA	C1B-C2B	2.78	1.49	1.43
18	b	506	CLA	C3B-C4B	2.78	1.49	1.42
18	B	509	CLA	C1B-C2B	2.77	1.49	1.43
23	c	501	SQD	C6-S	-2.77	1.67	1.77
18	b	514	CLA	C1B-C2B	2.77	1.49	1.43
18	B	516	CLA	C3B-C4B	2.77	1.49	1.42
18	c	515	CLA	C3B-C4B	2.77	1.49	1.42
18	B	509	CLA	C3B-C4B	2.77	1.49	1.42
18	a	405	CLA	C3B-C4B	2.76	1.49	1.42
18	B	504	CLA	C3B-C4B	2.75	1.49	1.42
18	D	404	CLA	C3B-C4B	2.75	1.49	1.42
18	C	511	CLA	C3B-C4B	2.75	1.49	1.42
18	A	402	CLA	C3B-C4B	2.74	1.49	1.42
18	c	512	CLA	C3B-C4B	2.74	1.49	1.42
18	C	507	CLA	C3B-C4B	2.74	1.49	1.42
18	B	503	CLA	C3B-C4B	2.73	1.49	1.42
18	C	505	CLA	C1B-C2B	2.73	1.49	1.43
18	C	514	CLA	C3B-C4B	2.72	1.49	1.42
18	C	503	CLA	C3B-C4B	2.72	1.49	1.42
18	C	506	CLA	C1B-C2B	2.72	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	402	CLA	C1B-C2B	2.72	1.49	1.43
18	c	513	CLA	C3B-C4B	2.71	1.49	1.42
18	D	405	CLA	C3B-C4B	2.71	1.49	1.42
18	d	405	CLA	C3B-C4B	2.71	1.49	1.42
18	c	512	CLA	C1B-C2B	2.71	1.49	1.43
18	c	506	CLA	C1B-C2B	2.71	1.49	1.43
18	B	505	CLA	C3B-C4B	2.71	1.49	1.42
18	A	403	CLA	C3B-C4B	2.70	1.49	1.42
18	c	508	CLA	C3B-C4B	2.70	1.49	1.42
18	b	502	CLA	C1B-C2B	2.70	1.49	1.43
18	B	507	CLA	C1B-C2B	2.70	1.49	1.43
18	C	512	CLA	C3B-C4B	2.70	1.49	1.42
18	c	504	CLA	C1B-C2B	2.70	1.49	1.43
18	c	509	CLA	C3B-C4B	2.70	1.49	1.42
18	B	510	CLA	C1B-C2B	2.70	1.49	1.43
18	A	405	CLA	C1B-C2B	2.70	1.49	1.43
18	B	502	CLA	C1B-C2B	2.69	1.49	1.43
18	C	504	CLA	C1B-C2B	2.69	1.49	1.43
18	C	502	CLA	C3B-C4B	2.69	1.49	1.42
18	a	402	CLA	C3B-C4B	2.69	1.49	1.42
18	c	503	CLA	C3B-C4B	2.69	1.49	1.42
18	c	505	CLA	C1B-C2B	2.69	1.49	1.43
18	d	405	CLA	C1B-C2B	2.68	1.49	1.43
18	b	506	CLA	C1B-C2B	2.68	1.49	1.43
18	B	506	CLA	C1B-C2B	2.68	1.49	1.43
18	C	507	CLA	C1B-C2B	2.68	1.49	1.43
18	C	508	CLA	C3B-C4B	2.68	1.49	1.42
18	C	503	CLA	C1B-C2B	2.68	1.49	1.43
18	c	508	CLA	C1B-C2B	2.67	1.49	1.43
18	d	404	CLA	C1B-C2B	2.67	1.49	1.43
18	D	405	CLA	C1B-C2B	2.67	1.49	1.43
18	c	507	CLA	C1B-C2B	2.67	1.49	1.43
18	a	403	CLA	C3B-C4B	2.67	1.49	1.42
18	b	505	CLA	C3B-C4B	2.67	1.49	1.42
18	D	404	CLA	C1B-C2B	2.66	1.49	1.43
18	a	405	CLA	C1B-C2B	2.66	1.49	1.43
18	b	510	CLA	C1B-C2B	2.66	1.49	1.43
18	b	508	CLA	C3B-C4B	2.65	1.49	1.42
18	B	514	CLA	C1B-C2B	2.65	1.49	1.43
18	C	509	CLA	C1B-C2B	2.65	1.49	1.43
18	c	510	CLA	C1B-C2B	2.64	1.49	1.43
18	c	504	CLA	C3B-C4B	2.64	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b	501	CLA	C1B-C2B	2.64	1.49	1.43
18	C	513	CLA	C1B-C2B	2.63	1.49	1.43
18	B	515	CLA	C1B-C2B	2.63	1.49	1.43
18	b	504	CLA	C1B-C2B	2.62	1.49	1.43
18	c	514	CLA	C1B-C2B	2.62	1.49	1.43
18	B	504	CLA	C1B-C2B	2.61	1.49	1.43
18	B	501	CLA	C1B-C2B	2.61	1.49	1.43
18	a	403	CLA	C1B-C2B	2.61	1.49	1.43
18	b	511	CLA	C1B-C2B	2.60	1.49	1.43
18	b	515	CLA	C1B-C2B	2.60	1.49	1.43
18	B	503	CLA	C1B-C2B	2.59	1.49	1.43
18	A	403	CLA	C1B-C2B	2.59	1.49	1.43
18	d	401	CLA	C1B-C2B	2.59	1.49	1.43
18	D	401	CLA	C1B-C2B	2.58	1.49	1.43
18	B	516	CLA	C1B-C2B	2.57	1.49	1.43
18	B	511	CLA	C1B-C2B	2.57	1.49	1.43
18	b	516	CLA	C1B-C2B	2.56	1.49	1.43
19	d	402	PHO	CMC-C2C	-2.54	1.46	1.50
18	b	512	CLA	C1B-C2B	2.53	1.49	1.43
18	B	512	CLA	C1B-C2B	2.52	1.49	1.43
18	c	511	CLA	C1B-C2B	2.51	1.49	1.43
19	D	402	PHO	CMC-C2C	-2.51	1.46	1.50
18	b	503	CLA	C1B-C2B	2.50	1.49	1.43
18	C	510	CLA	C1B-C2B	2.48	1.49	1.43
18	B	508	CLA	C3B-C4B	2.46	1.48	1.42
19	A	404	PHO	CMC-C2C	-2.42	1.46	1.50
19	a	404	PHO	CMC-C2C	-2.42	1.46	1.50
19	D	402	PHO	CMD-C2D	-2.41	1.46	1.51
27	d	407	PL9	C6-C1	-2.40	1.44	1.48
27	D	407	PL9	C6-C1	-2.40	1.44	1.48
19	a	404	PHO	CMD-C2D	-2.39	1.46	1.51
19	d	402	PHO	CMD-C2D	-2.38	1.46	1.51
19	a	404	PHO	CMB-C2B	-2.37	1.46	1.51
19	D	402	PHO	CMB-C2B	-2.37	1.46	1.51
19	A	404	PHO	CMB-C2B	-2.37	1.46	1.51
19	A	404	PHO	CMD-C2D	-2.33	1.46	1.51
19	d	402	PHO	CMB-C2B	-2.32	1.46	1.51
19	d	402	PHO	C4D-ND	-2.29	1.35	1.38
19	a	404	PHO	CAC-C3C	-2.29	1.47	1.51
19	A	404	PHO	CAC-C3C	-2.28	1.47	1.51
18	C	503	CLA	CMD-C2D	-2.25	1.46	1.50
18	c	504	CLA	CMD-C2D	-2.23	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	404	PHO	C4D-ND	-2.23	1.35	1.38
19	a	404	PHO	C4D-ND	-2.22	1.35	1.38
18	D	404	CLA	CMD-C2D	-2.21	1.46	1.50
18	d	404	CLA	CMD-C2D	-2.21	1.46	1.50
19	D	402	PHO	C4D-ND	-2.20	1.35	1.38
19	D	402	PHO	C3D-C4D	2.20	1.44	1.41
18	b	510	CLA	CHC-C1C	2.19	1.43	1.38
18	b	503	CLA	CMB-C2B	-2.19	1.46	1.50
21	h	101	LMG	O1-C1	2.19	1.43	1.40
19	D	402	PHO	CAC-C3C	-2.18	1.47	1.51
20	a	406	BCR	C30-C25	-2.18	1.50	1.53
19	d	402	PHO	CAC-C3C	-2.18	1.47	1.51
18	B	508	CLA	CMD-C2D	-2.18	1.46	1.50
18	B	512	CLA	CMB-C2B	-2.17	1.46	1.50
19	a	404	PHO	C3D-C4D	2.17	1.44	1.41
18	B	503	CLA	CMB-C2B	-2.16	1.46	1.50
19	A	404	PHO	C3D-C4D	2.15	1.44	1.41
19	d	402	PHO	C3D-C4D	2.15	1.44	1.41
18	C	513	CLA	CMD-C2D	-2.14	1.46	1.50
18	a	403	CLA	CMD-C2D	-2.14	1.46	1.50
20	C	516	BCR	C30-C25	-2.14	1.50	1.53
18	b	508	CLA	CMD-C2D	-2.13	1.46	1.50
18	C	502	CLA	CMD-C2D	-2.12	1.46	1.50
18	D	401	CLA	CMD-C2D	-2.12	1.46	1.50
18	D	404	CLA	CHC-C1C	2.12	1.42	1.38
18	B	507	CLA	CHC-C1C	2.11	1.42	1.38
18	c	514	CLA	CMD-C2D	-2.11	1.46	1.50
18	b	516	CLA	CHC-C1C	2.11	1.42	1.38
18	c	510	CLA	CHC-C1C	2.09	1.42	1.38
18	b	503	CLA	CMD-C2D	-2.09	1.46	1.50
18	d	404	CLA	CHC-C1C	2.09	1.42	1.38
20	c	516	BCR	C30-C25	-2.09	1.50	1.53
18	a	402	CLA	CMD-C2D	-2.09	1.46	1.50
18	c	505	CLA	CMD-C2D	-2.09	1.46	1.50
18	a	405	CLA	CMD-C2D	-2.08	1.46	1.50
18	b	508	CLA	CHC-C1C	2.08	1.42	1.38
18	B	503	CLA	CMD-C2D	-2.08	1.46	1.50
18	C	506	CLA	CMD-C2D	-2.08	1.46	1.50
20	A	406	BCR	C30-C25	-2.08	1.50	1.53
18	A	403	CLA	CMD-C2D	-2.08	1.46	1.50
18	B	508	CLA	CMB-C2B	-2.08	1.46	1.50
18	b	512	CLA	CMB-C2B	-2.08	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	c	503	CLA	CMD-C2D	-2.07	1.46	1.50
18	A	402	CLA	CMD-C2D	-2.07	1.46	1.50
18	C	509	CLA	CMD-C2D	-2.07	1.46	1.50
18	c	509	CLA	CMD-C2D	-2.07	1.46	1.50
18	c	507	CLA	CMD-C2D	-2.07	1.46	1.50
18	b	506	CLA	CMD-C2D	-2.06	1.46	1.50
18	b	512	CLA	CHC-C1C	2.06	1.42	1.38
18	B	502	CLA	CHC-C1C	2.06	1.42	1.38
18	B	511	CLA	CMD-C2D	-2.05	1.46	1.50
18	C	505	CLA	CMD-C2D	-2.05	1.46	1.50
18	b	511	CLA	CMD-C2D	-2.05	1.46	1.50
18	d	401	CLA	CMD-C2D	-2.05	1.46	1.50
18	A	405	CLA	CMD-C2D	-2.05	1.46	1.50
18	d	401	CLA	CMB-C2B	-2.05	1.46	1.50
18	b	502	CLA	CHC-C1C	2.05	1.42	1.38
18	C	503	CLA	CMB-C2B	-2.04	1.46	1.50
28	e	101	HEM	CMC-C2C	2.04	1.55	1.50
18	C	510	CLA	CMB-C2B	-2.04	1.46	1.50
18	C	508	CLA	CMD-C2D	-2.04	1.46	1.50
28	F	101	HEM	CMB-C2B	2.04	1.55	1.50
18	C	504	CLA	CMD-C2D	-2.04	1.46	1.50
18	b	509	CLA	CMD-C2D	-2.04	1.46	1.50
18	c	510	CLA	CMD-C2D	-2.04	1.46	1.50
18	B	516	CLA	CMD-C2D	-2.04	1.46	1.50
18	b	514	CLA	CMD-C2D	-2.04	1.46	1.50
18	C	502	CLA	CHC-C1C	2.04	1.42	1.38
18	b	513	CLA	CMD-C2D	-2.04	1.46	1.50
18	c	504	CLA	CMB-C2B	-2.04	1.46	1.50
18	b	502	CLA	CMD-C2D	-2.03	1.46	1.50
18	B	516	CLA	CHC-C1C	2.03	1.42	1.38
18	c	506	CLA	CMD-C2D	-2.03	1.46	1.50
18	A	403	CLA	CMB-C2B	-2.03	1.46	1.50
28	F	101	HEM	CMC-C2C	2.03	1.55	1.50
18	b	516	CLA	CMB-C2B	-2.03	1.46	1.50
18	d	405	CLA	CMD-C2D	-2.03	1.46	1.50
18	C	507	CLA	CMB-C2B	-2.03	1.46	1.50
18	C	509	CLA	CHC-C1C	2.03	1.42	1.38
18	B	506	CLA	CMD-C2D	-2.03	1.46	1.50
18	c	503	CLA	CHC-C1C	2.03	1.42	1.38
18	b	506	CLA	CMB-C2B	-2.03	1.46	1.50
18	b	505	CLA	CMD-C2D	-2.03	1.46	1.50
18	B	516	CLA	CMB-C2B	-2.02	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	505	CLA	CHC-C1C	2.02	1.42	1.38
18	B	513	CLA	CMD-C2D	-2.02	1.46	1.50
18	B	509	CLA	CMD-C2D	-2.02	1.46	1.50
18	b	516	CLA	CMD-C2D	-2.02	1.46	1.50
18	c	513	CLA	CMB-C2B	-2.02	1.46	1.50
18	c	505	CLA	CHC-C1C	2.02	1.42	1.38
18	b	514	CLA	CHC-C1C	2.02	1.42	1.38
18	b	515	CLA	CMD-C2D	-2.02	1.46	1.50
18	b	501	CLA	CMD-C2D	-2.02	1.46	1.50
18	b	512	CLA	CMD-C2D	-2.02	1.46	1.50
18	c	511	CLA	CMB-C2B	-2.02	1.46	1.50
18	D	401	CLA	CHC-C1C	2.02	1.42	1.38
18	b	507	CLA	CHC-C1C	2.02	1.42	1.38
18	C	511	CLA	CMD-C2D	-2.02	1.46	1.50
18	a	403	CLA	CMB-C2B	-2.02	1.46	1.50
18	B	510	CLA	CHC-C1C	2.01	1.42	1.38
18	d	401	CLA	CHC-C1C	2.01	1.42	1.38
18	b	504	CLA	CMD-C2D	-2.01	1.46	1.50
18	B	512	CLA	CHC-C1C	2.01	1.42	1.38
18	D	401	CLA	CMB-C2B	-2.01	1.46	1.50
18	C	507	CLA	CMD-C2D	-2.01	1.46	1.50
18	D	405	CLA	CMB-C2B	-2.01	1.46	1.50
18	C	509	CLA	CMB-C2B	-2.00	1.46	1.50
18	b	511	CLA	CHC-C1C	2.00	1.42	1.38
18	b	510	CLA	CMD-C2D	-2.00	1.46	1.50
18	C	505	CLA	CHC-C1C	2.00	1.42	1.38
18	B	507	CLA	CMD-C2D	-2.00	1.46	1.50
18	c	515	CLA	CMD-C2D	-2.00	1.46	1.50
18	c	508	CLA	CMD-C2D	-2.00	1.46	1.50

All (922) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	404	PHO	C4D-CHA-CBD	-6.72	105.48	108.52
19	a	404	PHO	C4D-CHA-CBD	-6.65	105.51	108.52
19	d	402	PHO	C4D-CHA-CBD	-6.35	105.65	108.52
19	D	402	PHO	C4D-CHA-CBD	-6.15	105.73	108.52
20	z	101	BCR	C3-C4-C5	-6.13	103.14	114.08
20	C	515	BCR	C3-C4-C5	-6.01	103.35	114.08
20	C	516	BCR	C3-C4-C5	-5.85	103.63	114.08
20	c	516	BCR	C30-C25-C26	-5.77	114.49	122.61
20	K	101	BCR	C28-C27-C26	-5.76	103.79	114.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	516	BCR	C3-C4-C5	-5.71	103.88	114.08
20	k	101	BCR	C28-C27-C26	-5.71	103.88	114.08
20	C	516	BCR	C30-C25-C26	-5.65	114.65	122.61
26	d	403	BCT	O2-C-O1	5.58	134.02	119.55
26	D	403	BCT	O2-C-O1	5.57	134.00	119.55
20	c	517	BCR	C28-C27-C26	-5.55	104.17	114.08
27	d	407	PL9	C7-C3-C4	5.53	121.37	116.88
27	D	407	PL9	C7-C3-C4	5.44	121.30	116.88
20	C	517	BCR	C28-C27-C26	-5.39	104.45	114.08
18	B	512	CLA	C4A-NA-C1A	5.34	109.11	106.71
18	c	512	CLA	C4A-NA-C1A	5.33	109.10	106.71
18	b	512	CLA	C4A-NA-C1A	5.31	109.09	106.71
18	b	513	CLA	C4A-NA-C1A	5.30	109.09	106.71
20	a	406	BCR	C3-C4-C5	-5.30	104.62	114.08
20	A	406	BCR	C3-C4-C5	-5.29	104.64	114.08
20	k	101	BCR	C3-C4-C5	-5.27	104.66	114.08
18	C	511	CLA	C4A-NA-C1A	5.25	109.07	106.71
18	B	505	CLA	C4A-NA-C1A	5.24	109.06	106.71
18	b	505	CLA	C4A-NA-C1A	5.24	109.06	106.71
20	B	518	BCR	C28-C27-C26	-5.17	104.85	114.08
18	B	510	CLA	C4A-NA-C1A	5.16	109.03	106.71
18	c	504	CLA	C4A-NA-C1A	5.12	109.01	106.71
20	b	518	BCR	C28-C27-C26	-5.12	104.94	114.08
20	B	519	BCR	C28-C27-C26	-5.10	104.97	114.08
20	K	101	BCR	C3-C4-C5	-5.10	104.97	114.08
18	C	503	CLA	C4A-NA-C1A	5.07	108.99	106.71
18	B	513	CLA	C4A-NA-C1A	5.02	108.96	106.71
18	C	508	CLA	C4A-NA-C1A	5.02	108.96	106.71
20	A	410	BCR	C28-C27-C26	-5.01	105.13	114.08
18	b	510	CLA	C4A-NA-C1A	5.01	108.96	106.71
18	B	515	CLA	C4A-NA-C1A	4.94	108.93	106.71
18	b	511	CLA	C4A-NA-C1A	4.94	108.92	106.71
18	b	515	CLA	C4A-NA-C1A	4.92	108.92	106.71
18	c	509	CLA	C4A-NA-C1A	4.91	108.91	106.71
20	A	406	BCR	C38-C26-C25	-4.82	119.11	124.53
18	B	501	CLA	C4A-NA-C1A	4.80	108.86	106.71
18	B	511	CLA	C4A-NA-C1A	4.80	108.86	106.71
20	x	102	BCR	C28-C27-C26	-4.74	105.61	114.08
18	C	509	CLA	C4A-NA-C1A	4.72	108.83	106.71
20	d	406	BCR	C30-C25-C26	-4.71	115.98	122.61
20	D	406	BCR	C30-C25-C26	-4.71	115.98	122.61
20	c	516	BCR	C33-C5-C6	-4.69	119.26	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	c	514	CLA	C4A-NA-C1A	4.68	108.81	106.71
18	C	510	CLA	C4A-NA-C1A	4.68	108.81	106.71
18	c	511	CLA	C4A-NA-C1A	4.67	108.80	106.71
20	z	101	BCR	C30-C25-C26	-4.65	116.06	122.61
20	C	515	BCR	C30-C25-C26	-4.65	116.06	122.61
18	b	507	CLA	C4A-NA-C1A	4.62	108.78	106.71
20	X	102	BCR	C28-C27-C26	-4.62	105.83	114.08
18	C	507	CLA	C4A-NA-C1A	4.62	108.78	106.71
18	B	507	CLA	C4A-NA-C1A	4.62	108.78	106.71
18	c	510	CLA	C4A-NA-C1A	4.61	108.78	106.71
18	b	509	CLA	C4A-NA-C1A	4.60	108.78	106.71
18	d	404	CLA	C4A-NA-C1A	4.59	108.77	106.71
18	c	515	CLA	C4A-NA-C1A	4.57	108.76	106.71
18	b	501	CLA	C4A-NA-C1A	4.57	108.76	106.71
18	B	502	CLA	C4A-NA-C1A	4.56	108.76	106.71
20	C	516	BCR	C33-C5-C6	-4.54	119.43	124.53
18	C	513	CLA	C4A-NA-C1A	4.53	108.74	106.71
18	D	404	CLA	C4A-NA-C1A	4.53	108.74	106.71
18	c	508	CLA	C4A-NA-C1A	4.53	108.74	106.71
20	a	406	BCR	C38-C26-C25	-4.52	119.45	124.53
18	b	514	CLA	C4A-NA-C1A	4.51	108.73	106.71
18	B	514	CLA	C4A-NA-C1A	4.50	108.73	106.71
20	C	517	BCR	C33-C5-C6	-4.45	119.53	124.53
18	D	405	CLA	C4A-NA-C1A	4.44	108.70	106.71
18	a	405	CLA	C4A-NA-C1A	4.41	108.69	106.71
18	c	513	CLA	C4A-NA-C1A	4.41	108.69	106.71
18	d	405	CLA	C4A-NA-C1A	4.41	108.69	106.71
20	a	406	BCR	C30-C25-C26	-4.40	116.41	122.61
18	C	514	CLA	C4A-NA-C1A	4.40	108.68	106.71
18	A	405	CLA	C4A-NA-C1A	4.40	108.68	106.71
18	b	516	CLA	C4A-NA-C1A	4.39	108.68	106.71
18	B	516	CLA	C4A-NA-C1A	4.38	108.68	106.71
20	B	517	BCR	C1-C6-C5	-4.30	116.56	122.61
20	b	517	BCR	C1-C6-C5	-4.29	116.57	122.61
18	C	502	CLA	C4A-NA-C1A	4.28	108.63	106.71
18	C	512	CLA	C4A-NA-C1A	4.24	108.61	106.71
18	b	502	CLA	C4A-NA-C1A	4.24	108.61	106.71
18	c	503	CLA	C4A-NA-C1A	4.24	108.61	106.71
18	C	505	CLA	C4A-NA-C1A	4.23	108.61	106.71
18	C	504	CLA	C4A-NA-C1A	4.18	108.58	106.71
18	B	508	CLA	C4A-NA-C1A	4.17	108.58	106.71
20	X	102	BCR	C3-C4-C5	-4.16	106.65	114.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	c	506	CLA	C4A-NA-C1A	4.15	108.57	106.71
18	c	505	CLA	C4A-NA-C1A	4.15	108.57	106.71
20	B	517	BCR	C30-C25-C26	-4.13	116.80	122.61
20	B	517	BCR	C36-C18-C19	4.12	124.57	118.08
20	b	517	BCR	C36-C18-C19	4.12	124.57	118.08
20	b	517	BCR	C30-C25-C26	-4.12	116.81	122.61
18	a	403	CLA	C4A-NA-C1A	4.11	108.55	106.71
22	d	408	LHG	O7-C7-C8	4.11	120.35	111.50
19	A	404	PHO	C2B-C1B-NB	-4.10	106.69	109.53
19	a	404	PHO	C2B-C1B-NB	-4.09	106.70	109.53
18	B	509	CLA	C4A-NA-C1A	4.08	108.54	106.71
20	x	102	BCR	C3-C4-C5	-4.08	106.80	114.08
22	D	408	LHG	O7-C7-C8	4.07	120.28	111.50
19	d	402	PHO	C2B-C1B-NB	-4.02	106.75	109.53
20	X	102	BCR	C30-C25-C26	-4.01	116.96	122.61
18	B	503	CLA	C4A-NA-C1A	3.99	108.50	106.71
19	D	402	PHO	C2B-C1B-NB	-3.98	106.78	109.53
18	b	503	CLA	C4A-NA-C1A	3.98	108.50	106.71
20	x	102	BCR	C30-C25-C26	-3.96	117.04	122.61
18	a	402	CLA	C4A-NA-C1A	3.94	108.48	106.71
21	c	521	LMG	O7-C10-C11	3.92	119.96	111.50
20	B	518	BCR	C36-C18-C19	3.92	124.26	118.08
20	X	102	BCR	C7-C8-C9	-3.91	120.32	126.23
21	C	521	LMG	O7-C10-C11	3.91	119.94	111.50
24	C	520	DGD	O2G-C1B-C2B	3.91	119.93	111.50
24	c	520	DGD	O2G-C1B-C2B	3.90	119.92	111.50
20	X	102	BCR	C1-C6-C5	-3.90	117.12	122.61
24	C	518	DGD	O2G-C1B-C2B	3.90	119.91	111.50
20	x	102	BCR	C1-C6-C5	-3.89	117.13	122.61
24	c	518	DGD	O2G-C1B-C2B	3.89	119.88	111.50
21	d	409	LMG	O7-C10-C11	3.88	119.86	111.50
20	c	516	BCR	C28-C27-C26	-3.88	107.15	114.08
22	a	407	LHG	O7-C7-C8	3.86	119.82	111.50
20	b	518	BCR	C36-C18-C19	3.85	124.14	118.08
21	c	502	LMG	O7-C10-C11	3.84	119.79	111.50
20	c	516	BCR	C33-C5-C4	3.82	120.95	113.62
21	A	407	LMG	O7-C10-C11	3.82	119.73	111.50
18	A	402	CLA	C4A-NA-C1A	3.81	108.42	106.71
21	b	519	LMG	O7-C10-C11	3.80	119.69	111.50
20	A	406	BCR	C30-C25-C26	-3.79	117.27	122.61
22	A	408	LHG	O7-C7-C8	3.78	119.66	111.50
21	B	520	LMG	O7-C10-C11	3.78	119.65	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	516	BCR	C33-C5-C4	3.78	120.88	113.62
20	x	102	BCR	C7-C8-C9	-3.78	120.53	126.23
20	C	515	BCR	C36-C18-C19	3.76	124.00	118.08
18	b	508	CLA	C4A-NA-C1A	3.75	108.39	106.71
20	C	516	BCR	C28-C27-C26	-3.74	107.39	114.08
18	b	504	CLA	C4A-NA-C1A	3.74	108.39	106.71
20	z	101	BCR	C36-C18-C19	3.73	123.95	118.08
20	K	101	BCR	C30-C25-C26	-3.72	117.37	122.61
20	c	516	BCR	C38-C26-C27	3.72	120.76	113.62
20	a	406	BCR	C38-C26-C27	3.72	120.76	113.62
21	D	409	LMG	O7-C10-C11	3.72	119.51	111.50
21	h	101	LMG	O7-C10-C11	3.71	119.50	111.50
20	D	406	BCR	C1-C6-C5	-3.71	117.39	122.61
18	B	504	CLA	C4A-NA-C1A	3.71	108.37	106.71
20	C	516	BCR	C1-C6-C7	3.70	126.25	115.78
21	D	410	LMG	O7-C10-C11	3.70	119.48	111.50
20	A	410	BCR	C1-C6-C5	-3.70	117.40	122.61
20	C	516	BCR	C38-C26-C27	3.69	120.71	113.62
20	d	406	BCR	C1-C6-C5	-3.69	117.42	122.61
20	k	101	BCR	C37-C22-C23	3.69	123.89	118.08
20	c	516	BCR	C1-C6-C7	3.66	126.12	115.78
23	C	501	SQD	O47-C7-C8	3.65	119.36	111.50
20	c	516	BCR	C38-C26-C25	-3.64	120.44	124.53
18	A	403	CLA	C4A-NA-C1A	3.64	108.34	106.71
20	B	519	BCR	C1-C6-C5	-3.64	117.49	122.61
22	a	408	LHG	O7-C7-C8	3.63	119.33	111.50
20	B	517	BCR	C38-C26-C27	3.62	120.58	113.62
20	c	517	BCR	C33-C5-C6	-3.62	120.47	124.53
18	D	401	CLA	C4A-NA-C1A	3.61	108.33	106.71
20	a	406	BCR	C36-C18-C19	3.61	123.77	118.08
22	A	409	LHG	O7-C7-C8	3.60	119.27	111.50
20	B	517	BCR	C20-C21-C22	-3.60	122.17	127.31
20	b	517	BCR	C38-C26-C27	3.59	120.52	113.62
20	D	406	BCR	C36-C18-C19	3.59	123.73	118.08
27	d	407	PL9	C7-C3-C2	-3.58	118.59	123.30
20	c	516	BCR	C1-C6-C5	-3.58	117.57	122.61
20	b	517	BCR	C20-C21-C22	-3.58	122.20	127.31
20	X	102	BCR	C37-C22-C23	3.58	123.71	118.08
22	x	101	LHG	O7-C7-C8	3.58	119.21	111.50
18	d	401	CLA	C4A-NA-C1A	3.57	108.31	106.71
20	d	406	BCR	C36-C18-C19	3.57	123.70	118.08
20	K	101	BCR	C37-C22-C23	3.57	123.69	118.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	d	406	BCR	C37-C22-C23	3.56	123.69	118.08
20	D	406	BCR	C37-C22-C23	3.56	123.68	118.08
20	C	516	BCR	C38-C26-C25	-3.55	120.54	124.53
23	c	501	SQD	O47-C7-C8	3.55	119.16	111.50
22	X	101	LHG	O7-C7-C8	3.55	119.15	111.50
20	A	406	BCR	C36-C18-C19	3.54	123.66	118.08
27	D	407	PL9	C7-C3-C2	-3.54	118.65	123.30
20	x	102	BCR	C37-C22-C23	3.52	123.62	118.08
20	k	101	BCR	C30-C25-C26	-3.51	117.67	122.61
20	C	516	BCR	C1-C6-C5	-3.50	117.68	122.61
22	b	521	LHG	O7-C7-C8	3.50	119.03	111.50
20	A	410	BCR	C36-C18-C19	3.49	123.58	118.08
22	l	101	LHG	O7-C7-C8	3.46	118.96	111.50
22	B	522	LHG	O7-C7-C8	3.46	118.95	111.50
20	K	101	BCR	C36-C18-C19	3.45	123.52	118.08
20	b	517	BCR	C4-C5-C6	-3.45	117.72	122.73
20	x	102	BCR	C20-C21-C22	-3.45	122.39	127.31
20	X	102	BCR	C36-C18-C19	3.44	123.50	118.08
20	B	517	BCR	C4-C5-C6	-3.44	117.74	122.73
20	z	101	BCR	C11-C10-C9	-3.44	122.41	127.31
18	B	506	CLA	C4A-NA-C1A	3.44	108.25	106.71
18	b	506	CLA	C4A-NA-C1A	3.44	108.25	106.71
20	B	519	BCR	C36-C18-C19	3.43	123.49	118.08
23	c	501	SQD	O7-S-C6	3.43	111.01	106.94
20	b	517	BCR	C37-C22-C23	3.43	123.47	118.08
24	C	519	DGD	O2G-C1B-C2B	3.42	118.88	111.50
20	b	518	BCR	C33-C5-C6	-3.42	120.69	124.53
20	B	517	BCR	C28-C27-C26	-3.42	107.98	114.08
20	B	517	BCR	C37-C22-C23	3.42	123.46	118.08
20	B	518	BCR	C37-C22-C23	3.41	123.44	118.08
20	b	518	BCR	C30-C25-C26	-3.40	117.82	122.61
22	L	101	LHG	O7-C7-C8	3.39	118.82	111.50
20	C	515	BCR	C38-C26-C27	3.39	120.13	113.62
20	c	517	BCR	C29-C30-C25	3.38	115.69	110.48
20	D	406	BCR	C38-C26-C27	3.38	120.11	113.62
20	b	518	BCR	C37-C22-C23	3.37	123.39	118.08
22	b	520	LHG	O7-C7-C8	3.37	118.77	111.50
20	b	517	BCR	C28-C27-C26	-3.37	108.07	114.08
22	B	521	LHG	O7-C7-C8	3.37	118.75	111.50
20	B	517	BCR	C27-C26-C25	-3.36	117.86	122.73
20	z	101	BCR	C38-C26-C27	3.36	120.06	113.62
20	X	102	BCR	C4-C5-C6	-3.36	117.86	122.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	518	BCR	C33-C5-C6	-3.35	120.76	124.53
20	A	406	BCR	C35-C13-C12	3.35	123.36	118.08
20	C	515	BCR	C2-C1-C6	3.35	115.64	110.48
20	x	102	BCR	C36-C18-C19	3.35	123.35	118.08
20	d	406	BCR	C38-C26-C27	3.35	120.05	113.62
20	C	517	BCR	C29-C30-C25	3.34	115.62	110.48
24	c	519	DGD	O1G-C1A-C2A	3.33	120.12	111.38
20	b	517	BCR	C27-C26-C25	-3.33	117.90	122.73
20	k	101	BCR	C27-C26-C25	-3.32	117.91	122.73
20	d	406	BCR	C28-C27-C26	-3.32	108.14	114.08
20	B	518	BCR	C30-C25-C26	-3.32	117.94	122.61
20	b	517	BCR	C33-C5-C4	3.32	119.99	113.62
18	a	405	CLA	O2D-CGD-O1D	-3.32	117.36	123.84
24	C	519	DGD	O1G-C1A-C2A	3.31	120.07	111.38
20	B	517	BCR	C33-C5-C4	3.31	119.97	113.62
20	X	102	BCR	C20-C21-C22	-3.30	122.60	127.31
20	C	517	BCR	C37-C22-C23	3.29	123.27	118.08
20	D	406	BCR	C28-C27-C26	-3.29	108.21	114.08
20	D	406	BCR	C20-C21-C22	-3.29	122.62	127.31
20	z	101	BCR	C2-C1-C6	3.28	115.52	110.48
20	C	515	BCR	C27-C26-C25	-3.28	117.98	122.73
24	c	519	DGD	O2G-C1B-C2B	3.27	118.55	111.50
20	B	517	BCR	C37-C22-C21	-3.27	118.34	122.92
20	a	406	BCR	C35-C13-C12	3.26	123.22	118.08
20	c	517	BCR	C37-C22-C23	3.26	123.21	118.08
20	d	406	BCR	C20-C21-C22	-3.25	122.67	127.31
20	K	101	BCR	C27-C26-C25	-3.25	118.01	122.73
18	a	403	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
20	B	518	BCR	C1-C6-C5	-3.23	118.06	122.61
20	A	406	BCR	C38-C26-C27	3.23	119.83	113.62
20	d	406	BCR	C16-C17-C18	-3.22	122.71	127.31
20	b	518	BCR	C1-C6-C5	-3.22	118.08	122.61
18	A	403	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
20	d	406	BCR	C33-C5-C6	-3.21	120.92	124.53
18	d	404	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
20	c	517	BCR	C1-C6-C5	-3.20	118.11	122.61
23	C	501	SQD	O7-S-C6	3.20	110.74	106.94
20	z	101	BCR	C27-C26-C25	-3.19	118.10	122.73
20	B	519	BCR	C37-C22-C23	3.19	123.10	118.08
18	C	508	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
20	D	406	BCR	C33-C5-C6	-3.18	120.96	124.53
20	x	102	BCR	C4-C5-C6	-3.17	118.13	122.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	410	BCR	C29-C30-C25	3.17	115.36	110.48
20	k	101	BCR	C36-C18-C19	3.17	123.07	118.08
20	D	406	BCR	C16-C17-C18	-3.17	122.78	127.31
20	b	517	BCR	C37-C22-C21	-3.17	118.49	122.92
18	A	405	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
20	A	410	BCR	C37-C22-C23	3.16	123.05	118.08
28	e	101	HEM	C1B-NB-C4B	3.15	108.33	105.07
18	B	514	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
20	D	406	BCR	C27-C26-C25	-3.13	118.18	122.73
20	B	519	BCR	C29-C30-C25	3.13	115.30	110.48
18	b	514	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
18	B	511	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
18	c	509	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
18	c	513	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
20	z	101	BCR	C8-C9-C10	3.11	123.72	118.94
18	D	404	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
18	C	512	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
20	X	102	BCR	C16-C17-C18	-3.10	122.88	127.31
18	b	511	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
20	d	406	BCR	C27-C26-C25	-3.10	118.23	122.73
18	B	515	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
18	b	515	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
20	C	515	BCR	C11-C10-C9	-3.08	122.91	127.31
18	d	401	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
28	F	101	HEM	C1B-NB-C4B	3.08	108.25	105.07
20	A	410	BCR	C3-C4-C5	-3.07	108.60	114.08
20	A	406	BCR	C20-C21-C22	-3.07	122.93	127.31
18	d	405	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
20	x	102	BCR	C16-C17-C18	-3.07	122.93	127.31
20	K	101	BCR	C38-C26-C27	3.07	119.51	113.62
20	A	406	BCR	C16-C17-C18	-3.07	122.94	127.31
18	B	504	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
20	C	515	BCR	C1-C6-C5	-3.06	118.31	122.61
20	a	406	BCR	C20-C21-C22	-3.06	122.95	127.31
20	d	406	BCR	C3-C4-C5	-3.05	108.62	114.08
20	a	406	BCR	C16-C17-C18	-3.05	122.96	127.31
18	D	405	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
27	D	407	PL9	C22-C23-C24	-3.04	120.34	127.66
20	C	517	BCR	C1-C6-C5	-3.04	118.33	122.61
18	b	504	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
20	D	406	BCR	C3-C4-C5	-3.03	108.66	114.08
20	B	519	BCR	C3-C4-C5	-3.03	108.66	114.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	517	BCR	C15-C16-C17	-3.03	117.27	123.47
20	b	517	BCR	C15-C16-C17	-3.02	117.29	123.47
20	A	410	BCR	C33-C5-C6	-3.02	121.14	124.53
18	D	401	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
20	C	515	BCR	C32-C1-C6	-3.01	105.41	110.30
20	B	519	BCR	C16-C17-C18	-3.00	123.03	127.31
20	B	519	BCR	C33-C5-C6	-2.99	121.17	124.53
27	d	407	PL9	C22-C23-C24	-2.99	120.45	127.66
20	B	518	BCR	C29-C30-C25	2.99	115.09	110.48
20	c	516	BCR	C36-C18-C19	2.98	122.77	118.08
20	A	410	BCR	C16-C17-C18	-2.96	123.08	127.31
20	k	101	BCR	C1-C6-C7	2.96	124.16	115.78
18	b	506	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
18	B	506	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
20	C	517	BCR	C36-C18-C19	2.95	122.73	118.08
18	B	503	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
20	k	101	BCR	C38-C26-C27	2.95	119.28	113.62
20	C	515	BCR	C8-C9-C10	2.95	123.47	118.94
18	c	503	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
20	C	516	BCR	C27-C26-C25	-2.92	118.49	122.73
27	D	407	PL9	C40-C39-C41	2.92	120.18	115.27
20	K	101	BCR	C1-C6-C7	2.91	124.02	115.78
20	b	518	BCR	C33-C5-C4	2.91	119.21	113.62
18	b	503	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
18	c	507	CLA	C4A-NA-C1A	2.91	108.01	106.71
18	C	502	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
20	B	517	BCR	C3-C4-C5	-2.90	108.89	114.08
20	c	516	BCR	C27-C26-C25	-2.90	118.52	122.73
18	c	507	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
20	c	516	BCR	C37-C22-C23	2.90	122.64	118.08
27	d	407	PL9	C40-C39-C41	2.90	120.14	115.27
20	C	517	BCR	C33-C5-C4	2.90	119.18	113.62
20	z	101	BCR	C28-C27-C26	-2.89	108.91	114.08
18	C	506	CLA	C4A-NA-C1A	2.89	108.01	106.71
20	C	515	BCR	C28-C27-C26	-2.89	108.92	114.08
18	B	507	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
19	a	404	PHO	O1D-CGD-CBD	2.89	129.55	124.74
20	b	517	BCR	C3-C4-C5	-2.89	108.92	114.08
18	b	507	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
20	k	101	BCR	C29-C30-C25	2.89	114.93	110.48
20	b	518	BCR	C20-C21-C22	-2.89	123.19	127.31
18	b	516	CLA	O2D-CGD-O1D	-2.89	118.20	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	c	510	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
20	B	519	BCR	C33-C5-C4	2.88	119.15	113.62
18	b	502	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
18	c	508	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
20	C	516	BCR	C37-C22-C23	2.87	122.60	118.08
20	B	518	BCR	C33-C5-C4	2.87	119.13	113.62
18	b	512	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
19	A	404	PHO	O1D-CGD-CBD	2.87	129.52	124.74
18	B	512	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
18	c	506	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
18	C	505	CLA	O2D-CGD-O1D	-2.87	118.24	123.84
20	c	517	BCR	C36-C18-C19	2.86	122.58	118.08
18	C	509	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
18	B	502	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
20	b	518	BCR	C29-C30-C25	2.85	114.87	110.48
20	a	406	BCR	C37-C22-C23	2.85	122.57	118.08
18	C	506	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
28	e	101	HEM	C4D-ND-C1D	2.85	108.01	105.07
18	B	516	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
20	A	406	BCR	C37-C22-C23	2.84	122.56	118.08
20	A	410	BCR	C33-C5-C4	2.84	119.08	113.62
20	B	518	BCR	C20-C21-C22	-2.84	123.25	127.31
20	A	406	BCR	C4-C5-C6	-2.84	118.60	122.73
18	c	512	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
18	B	508	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
18	C	514	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
20	X	102	BCR	C11-C10-C9	-2.84	123.26	127.31
18	C	507	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
18	C	513	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
22	a	407	LHG	O8-C23-C24	2.83	120.79	111.91
22	A	408	LHG	O8-C23-C24	2.83	120.78	111.91
20	a	406	BCR	C28-C27-C26	-2.83	109.03	114.08
20	C	516	BCR	C36-C18-C19	2.83	122.53	118.08
18	c	514	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
22	l	101	LHG	O8-C23-C24	2.82	120.77	111.91
18	C	511	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
18	C	503	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
20	k	101	BCR	C31-C1-C6	-2.81	105.73	110.30
19	A	404	PHO	C1-C2-C3	-2.81	121.18	126.04
18	B	509	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
18	c	515	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
18	c	504	CLA	O2D-CGD-O1D	-2.80	118.36	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	D	402	PHO	O2D-CGD-O1D	-2.80	118.36	123.84
28	F	101	HEM	C3B-C2B-C1B	2.80	108.56	106.49
22	L	101	LHG	O8-C23-C24	2.80	120.70	111.91
18	B	508	CLA	CHC-C4B-NB	2.80	127.22	124.26
18	c	511	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
20	B	518	BCR	C36-C18-C17	-2.79	119.01	122.92
20	b	518	BCR	C36-C18-C17	-2.79	119.01	122.92
20	A	410	BCR	C20-C21-C22	-2.79	123.33	127.31
18	C	510	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
20	K	101	BCR	C2-C1-C6	2.78	114.76	110.48
18	b	508	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
19	d	402	PHO	O2D-CGD-O1D	-2.78	118.41	123.84
18	a	402	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
20	x	102	BCR	C11-C10-C9	-2.77	123.35	127.31
18	A	402	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
18	B	513	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
18	b	509	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
18	c	505	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
20	a	406	BCR	C4-C5-C6	-2.77	118.72	122.73
20	k	101	BCR	C23-C22-C21	-2.77	114.70	118.94
20	d	406	BCR	C33-C5-C4	2.76	118.93	113.62
20	B	519	BCR	C20-C21-C22	-2.76	123.37	127.31
18	b	515	CLA	CHB-C4A-NA	2.76	128.32	124.51
20	D	406	BCR	C36-C18-C17	-2.76	119.06	122.92
20	B	517	BCR	C7-C8-C9	-2.76	122.07	126.23
20	d	406	BCR	C36-C18-C17	-2.75	119.07	122.92
18	B	510	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
28	e	101	HEM	C3B-C2B-C1B	2.74	108.52	106.49
20	A	410	BCR	C30-C25-C26	-2.74	118.75	122.61
20	K	101	BCR	C29-C30-C25	2.74	114.70	110.48
20	b	517	BCR	C7-C8-C9	-2.74	122.09	126.23
18	B	510	CLA	CHD-C1D-ND	-2.74	121.94	124.45
20	B	517	BCR	C38-C26-C25	-2.74	121.45	124.53
20	a	406	BCR	C2-C1-C6	2.74	114.70	110.48
19	a	404	PHO	C1-C2-C3	-2.74	121.31	126.04
20	A	406	BCR	C2-C1-C6	2.74	114.70	110.48
18	b	510	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
21	A	407	LMG	O8-C28-C29	2.74	120.50	111.91
28	e	101	HEM	C4A-NA-C1A	2.74	108.03	105.35
20	z	101	BCR	C16-C17-C18	-2.73	123.41	127.31
20	b	517	BCR	C38-C26-C25	-2.73	121.46	124.53
20	C	515	BCR	C16-C17-C18	-2.73	123.42	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	k	101	BCR	C2-C1-C6	2.73	114.68	110.48
20	D	406	BCR	C33-C5-C4	2.73	118.85	113.62
18	B	515	CLA	CHB-C4A-NA	2.72	128.28	124.51
18	b	501	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
18	C	504	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
18	b	513	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
18	B	501	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
20	c	517	BCR	C7-C8-C9	-2.71	122.14	126.23
19	A	404	PHO	O2D-CGD-O1D	-2.71	118.54	123.84
22	X	101	LHG	O8-C23-C24	2.71	120.41	111.91
20	c	517	BCR	C20-C21-C22	-2.71	123.45	127.31
28	F	101	HEM	C4D-ND-C1D	2.70	107.86	105.07
20	a	406	BCR	C36-C18-C17	-2.70	119.14	122.92
20	b	518	BCR	C7-C8-C9	-2.70	122.16	126.23
20	K	101	BCR	C7-C8-C9	-2.70	122.16	126.23
18	B	516	CLA	CHB-C4A-NA	2.70	128.24	124.51
21	c	502	LMG	O8-C28-C29	2.69	120.36	111.91
20	D	406	BCR	C37-C22-C21	-2.69	119.16	122.92
18	C	512	CLA	CHD-C1D-ND	-2.69	121.98	124.45
20	D	406	BCR	C38-C26-C25	-2.69	121.51	124.53
22	x	101	LHG	O8-C23-C24	2.69	120.34	111.91
20	A	406	BCR	C1-C6-C5	-2.69	118.83	122.61
20	k	101	BCR	C16-C17-C18	-2.69	123.48	127.31
19	a	404	PHO	O2D-CGD-O1D	-2.68	118.60	123.84
20	d	406	BCR	C37-C22-C21	-2.68	119.17	122.92
18	b	516	CLA	CHB-C4A-NA	2.68	128.22	124.51
20	x	102	BCR	C38-C26-C27	2.68	118.76	113.62
20	d	406	BCR	C38-C26-C25	-2.67	121.53	124.53
20	C	517	BCR	C20-C21-C22	-2.67	123.50	127.31
19	a	404	PHO	C1C-C2C-C3C	-2.67	106.39	108.61
24	c	518	DGD	O1G-C1A-C2A	2.67	120.28	111.91
20	B	517	BCR	C16-C17-C18	-2.67	123.51	127.31
19	A	404	PHO	C1C-C2C-C3C	-2.67	106.39	108.61
22	B	521	LHG	O8-C23-C24	2.66	120.27	111.91
20	B	518	BCR	C7-C8-C9	-2.66	122.22	126.23
20	b	517	BCR	C16-C17-C18	-2.65	123.52	127.31
18	c	513	CLA	CHD-C1D-ND	-2.65	122.02	124.45
20	B	518	BCR	C37-C22-C21	-2.65	119.21	122.92
24	C	518	DGD	O1G-C1A-C2A	2.65	120.21	111.91
20	A	406	BCR	C36-C18-C17	-2.65	119.22	122.92
20	B	518	BCR	C15-C16-C17	-2.65	118.05	123.47
18	b	510	CLA	CHD-C1D-ND	-2.64	122.02	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	F	101	HEM	C4A-NA-C1A	2.64	107.94	105.35
20	C	515	BCR	C4-C5-C6	-2.64	118.90	122.73
28	F	101	HEM	C4C-NC-C1C	2.64	107.93	105.35
20	a	406	BCR	C7-C8-C9	-2.63	122.26	126.23
18	B	504	CLA	CHB-C4A-NA	2.63	128.15	124.51
20	b	518	BCR	C37-C22-C21	-2.63	119.24	122.92
20	c	517	BCR	C15-C16-C17	-2.63	118.09	123.47
20	d	406	BCR	C16-C15-C14	-2.63	118.09	123.47
23	c	501	SQD	O9-S-C6	2.63	110.06	106.94
20	B	519	BCR	C30-C25-C26	-2.63	118.91	122.61
19	d	402	PHO	O1D-CGD-CBD	2.62	129.11	124.74
20	K	101	BCR	C16-C17-C18	-2.62	123.57	127.31
18	b	504	CLA	CHB-C4A-NA	2.62	128.13	124.51
20	B	518	BCR	C16-C17-C18	-2.61	123.58	127.31
20	b	518	BCR	C15-C16-C17	-2.61	118.13	123.47
20	A	406	BCR	C7-C8-C9	-2.61	122.29	126.23
28	e	101	HEM	C4C-NC-C1C	2.61	107.90	105.35
22	b	520	LHG	O8-C23-C24	2.60	120.08	111.91
20	a	406	BCR	C1-C6-C5	-2.60	118.95	122.61
20	k	101	BCR	C8-C9-C10	-2.59	114.97	118.94
21	B	520	LMG	O8-C28-C29	2.59	120.03	111.91
18	b	511	CLA	CHD-C1D-ND	-2.59	122.08	124.45
20	K	101	BCR	C8-C9-C10	-2.58	114.98	118.94
20	k	101	BCR	C7-C8-C9	-2.58	122.34	126.23
21	b	519	LMG	O8-C28-C29	2.58	120.00	111.91
18	c	514	CLA	CHB-C4A-NA	2.57	128.07	124.51
20	B	517	BCR	C15-C14-C13	-2.57	123.64	127.31
20	D	406	BCR	C16-C15-C14	-2.56	118.23	123.47
20	x	102	BCR	C15-C14-C13	-2.56	123.66	127.31
22	D	408	LHG	O8-C23-C24	2.56	119.94	111.91
20	B	518	BCR	C3-C4-C5	-2.56	109.51	114.08
18	d	405	CLA	C4-C3-C5	2.55	119.57	115.27
20	b	518	BCR	C3-C4-C5	-2.55	109.52	114.08
18	B	514	CLA	CHD-C1D-ND	-2.55	122.11	124.45
20	C	517	BCR	C8-C9-C10	-2.55	115.03	118.94
18	C	508	CLA	CHB-C4A-NA	2.55	128.04	124.51
20	X	102	BCR	C38-C26-C27	2.55	118.51	113.62
20	B	517	BCR	C11-C10-C9	-2.55	123.68	127.31
18	b	509	CLA	CHB-C4A-NA	2.54	128.03	124.51
20	z	101	BCR	C38-C26-C25	-2.54	121.67	124.53
20	b	518	BCR	C16-C17-C18	-2.54	123.69	127.31
21	c	521	LMG	O8-C28-C29	2.54	119.88	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	516	BCR	C15-C16-C17	-2.54	118.27	123.47
20	c	517	BCR	C33-C5-C4	2.54	118.49	113.62
22	a	408	LHG	O8-C23-C24	2.54	119.86	111.91
20	z	101	BCR	C36-C18-C17	-2.53	119.37	122.92
22	d	408	LHG	O8-C23-C24	2.53	119.85	111.91
18	B	505	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
22	A	409	LHG	O8-C23-C24	2.53	119.84	111.91
18	C	513	CLA	CHB-C4A-NA	2.53	128.00	124.51
20	C	517	BCR	C7-C8-C9	-2.52	122.42	126.23
20	C	516	BCR	C15-C16-C17	-2.52	118.31	123.47
20	b	518	BCR	C38-C26-C27	2.52	118.46	113.62
21	C	521	LMG	O8-C28-C29	2.52	119.81	111.91
23	C	501	SQD	O48-C23-C24	2.52	119.81	111.91
18	B	511	CLA	CHD-C1D-ND	-2.51	122.14	124.45
20	b	517	BCR	C15-C14-C13	-2.51	123.72	127.31
23	c	501	SQD	O48-C23-C24	2.51	119.79	111.91
20	x	102	BCR	C27-C26-C25	-2.51	119.09	122.73
20	C	517	BCR	C3-C4-C5	-2.51	109.60	114.08
19	a	404	PHO	CMB-C2B-C3B	2.51	129.37	124.68
20	X	102	BCR	C15-C14-C13	-2.50	123.74	127.31
20	b	517	BCR	C11-C10-C9	-2.50	123.75	127.31
22	B	522	LHG	O8-C23-C24	2.49	119.73	111.91
20	C	515	BCR	C38-C26-C25	-2.49	121.73	124.53
20	c	517	BCR	C30-C25-C26	-2.49	119.11	122.61
20	C	517	BCR	C30-C25-C26	-2.49	119.11	122.61
27	d	407	PL9	C20-C19-C21	2.49	119.45	115.27
18	c	509	CLA	CHB-C4A-NA	2.49	127.95	124.51
20	A	406	BCR	C15-C14-C13	-2.48	123.77	127.31
18	c	515	CLA	CHD-C1D-ND	-2.48	122.17	124.45
20	B	518	BCR	C38-C26-C27	2.48	118.38	113.62
20	A	406	BCR	C28-C27-C26	-2.48	109.65	114.08
20	K	101	BCR	C23-C22-C21	-2.48	115.14	118.94
19	A	404	PHO	CMB-C2B-C3B	2.47	129.30	124.68
20	z	101	BCR	C24-C23-C22	-2.46	122.51	126.23
20	C	515	BCR	C36-C18-C17	-2.46	119.48	122.92
20	x	102	BCR	C37-C22-C21	-2.46	119.48	122.92
22	b	521	LHG	O8-C23-C24	2.46	119.62	111.91
18	b	514	CLA	CHD-C1D-ND	-2.46	122.20	124.45
19	D	402	PHO	O1D-CGD-CBD	2.45	128.82	124.74
21	h	101	LMG	O8-C28-C29	2.45	119.59	111.91
18	c	515	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
18	b	508	CLA	CHB-C4A-NA	2.44	127.89	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	c	511	CLA	CHB-C4A-NA	2.44	127.88	124.51
20	X	102	BCR	C37-C22-C21	-2.43	119.51	122.92
20	C	515	BCR	C24-C23-C22	-2.43	122.56	126.23
18	B	511	CLA	CHB-C4A-NA	2.43	127.87	124.51
18	C	511	CLA	CHB-C4A-NA	2.43	127.87	124.51
19	D	402	PHO	C1C-C2C-C3C	-2.42	106.59	108.61
20	K	101	BCR	C15-C16-C17	-2.42	118.51	123.47
20	A	406	BCR	C24-C23-C22	-2.42	122.58	126.23
18	C	514	CLA	CHD-C1D-ND	-2.42	122.23	124.45
18	C	502	CLA	CHB-C4A-NA	2.41	127.85	124.51
19	D	402	PHO	CMB-C2B-C3B	2.41	129.19	124.68
18	c	503	CLA	CHB-C4A-NA	2.41	127.85	124.51
20	z	101	BCR	C1-C6-C5	-2.41	119.22	122.61
19	d	402	PHO	CMB-C2B-C3B	2.41	129.19	124.68
27	D	407	PL9	C20-C19-C21	2.40	119.31	115.27
20	B	519	BCR	C7-C8-C9	-2.40	122.61	126.23
18	C	514	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
18	b	507	CLA	CHB-C4A-NA	2.39	127.82	124.51
21	D	410	LMG	O8-C28-C29	2.39	119.41	111.91
20	A	410	BCR	C36-C18-C17	-2.39	119.58	122.92
18	a	402	CLA	CHD-C1D-ND	-2.39	122.26	124.45
18	B	514	CLA	CHB-C4A-NA	2.38	127.81	124.51
18	b	514	CLA	CHB-C4A-NA	2.38	127.81	124.51
18	c	512	CLA	CHB-C4A-NA	2.38	127.81	124.51
20	X	102	BCR	C16-C15-C14	-2.38	118.60	123.47
18	D	404	CLA	CHC-C4B-NB	2.38	126.77	124.26
18	b	513	CLA	CHB-C4A-NA	2.37	127.80	124.51
18	b	510	CLA	C3B-C4B-NB	-2.36	108.32	110.52
20	C	517	BCR	C16-C17-C18	-2.36	123.94	127.31
18	B	510	CLA	CHB-C4A-NA	2.36	127.78	124.51
20	b	518	BCR	C38-C26-C25	-2.36	121.87	124.53
20	a	406	BCR	C15-C14-C13	-2.36	123.94	127.31
18	B	503	CLA	CHB-C4A-NA	2.36	127.78	124.51
20	B	519	BCR	C11-C10-C9	-2.36	123.94	127.31
19	d	402	PHO	C1C-C2C-C3C	-2.36	106.65	108.61
21	D	409	LMG	O8-C28-C29	2.35	119.30	111.91
20	C	516	BCR	C20-C21-C22	-2.35	123.95	127.31
20	X	102	BCR	C27-C26-C25	-2.35	119.31	122.73
18	b	505	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
20	k	101	BCR	C15-C16-C17	-2.35	118.66	123.47
18	B	505	CLA	CHD-C1D-ND	-2.35	122.29	124.45
20	c	517	BCR	C3-C4-C5	-2.35	109.88	114.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	c	513	CLA	CHB-C4A-NA	2.35	127.76	124.51
20	B	517	BCR	C36-C18-C17	-2.35	119.64	122.92
20	C	517	BCR	C15-C16-C17	-2.35	118.67	123.47
18	b	505	CLA	CHB-C4A-NA	2.35	127.75	124.51
18	b	508	CLA	CHC-C4B-NB	2.34	126.74	124.26
18	C	509	CLA	CHB-C4A-NA	2.34	127.75	124.51
21	d	409	LMG	O8-C28-C29	2.34	119.25	111.91
18	B	501	CLA	CHB-C4A-NA	2.34	127.75	124.51
18	B	502	CLA	CHB-C4A-NA	2.34	127.75	124.51
18	B	509	CLA	CHB-C4A-NA	2.34	127.75	124.51
18	C	507	CLA	CHD-C1D-ND	-2.34	122.31	124.45
18	A	402	CLA	CHB-C4A-NA	2.34	127.74	124.51
20	x	102	BCR	C38-C26-C25	-2.33	121.91	124.53
18	c	510	CLA	CHB-C4A-NA	2.33	127.74	124.51
20	c	516	BCR	C20-C21-C22	-2.33	123.98	127.31
18	d	404	CLA	CHC-C4B-NB	2.33	126.73	124.26
18	C	503	CLA	CHB-C4A-NA	2.33	127.74	124.51
18	c	504	CLA	CHB-C4A-NA	2.33	127.74	124.51
18	b	511	CLA	CHB-C4A-NA	2.33	127.73	124.51
18	B	507	CLA	CHB-C4A-NA	2.33	127.73	124.51
18	a	402	CLA	CHB-C4A-NA	2.33	127.73	124.51
18	C	507	CLA	CHB-C4A-NA	2.33	127.73	124.51
20	K	101	BCR	C12-C13-C14	-2.33	115.37	118.94
20	b	517	BCR	C36-C18-C17	-2.33	119.67	122.92
18	C	512	CLA	CHB-C4A-NA	2.31	127.71	124.51
20	X	102	BCR	C38-C26-C25	-2.31	121.93	124.53
20	B	518	BCR	C27-C26-C25	-2.31	119.37	122.73
27	D	407	PL9	C27-C28-C29	-2.31	122.09	127.66
18	B	512	CLA	CHD-C1D-ND	-2.31	122.33	124.45
20	C	516	BCR	C7-C6-C5	-2.31	115.87	121.46
18	C	504	CLA	CHB-C4A-NA	2.31	127.70	124.51
18	c	508	CLA	CHB-C4A-NA	2.31	127.70	124.51
20	A	410	BCR	C11-C10-C9	-2.31	124.02	127.31
18	b	505	CLA	CHD-C1D-ND	-2.31	122.33	124.45
20	X	102	BCR	C2-C1-C6	2.31	114.03	110.48
27	d	407	PL9	C27-C28-C29	-2.31	122.11	127.66
18	B	505	CLA	CHB-C4A-NA	2.31	127.70	124.51
18	c	512	CLA	CHD-C1D-ND	-2.31	122.33	124.45
18	b	503	CLA	CHB-C4A-NA	2.31	127.70	124.51
20	x	102	BCR	C16-C15-C14	-2.30	118.75	123.47
18	C	503	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
20	z	101	BCR	C2-C3-C4	-2.30	106.24	111.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	x	102	BCR	C34-C9-C8	2.30	121.70	118.08
18	b	507	CLA	CHD-C1D-ND	-2.30	122.34	124.45
18	c	505	CLA	CHB-C4A-NA	2.30	127.69	124.51
18	b	501	CLA	CHB-C4A-NA	2.30	127.69	124.51
20	B	519	BCR	C34-C9-C8	2.29	121.69	118.08
18	B	513	CLA	CHB-C4A-NA	2.29	127.68	124.51
18	C	502	CLA	C3B-C4B-NB	-2.29	108.39	110.52
20	X	102	BCR	C34-C9-C8	2.29	121.69	118.08
24	C	520	DGD	O1G-C1A-C2A	2.29	119.09	111.91
24	c	520	DGD	O1G-C1A-C2A	2.29	119.09	111.91
20	A	410	BCR	C34-C9-C8	2.29	121.68	118.08
20	b	518	BCR	C27-C26-C25	-2.29	119.41	122.73
18	b	502	CLA	CHB-C4A-NA	2.29	127.67	124.51
20	C	515	BCR	C15-C16-C17	-2.29	118.79	123.47
20	B	519	BCR	C36-C18-C17	-2.29	119.72	122.92
20	D	406	BCR	C7-C8-C9	-2.29	122.78	126.23
20	c	516	BCR	C34-C9-C8	2.29	121.68	118.08
18	c	504	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
18	B	506	CLA	CHB-C4A-NA	2.28	127.67	124.51
18	b	510	CLA	CHB-C4A-NA	2.28	127.67	124.51
18	c	515	CLA	CHB-C4A-NA	2.28	127.67	124.51
20	A	410	BCR	C7-C8-C9	-2.28	122.79	126.23
18	B	507	CLA	C3B-C4B-NB	-2.28	108.40	110.52
18	b	506	CLA	CHB-C4A-NA	2.28	127.66	124.51
20	c	517	BCR	C15-C14-C13	-2.28	124.06	127.31
20	k	101	BCR	C1-C6-C5	-2.28	119.41	122.61
18	A	402	CLA	CHD-C1D-ND	-2.28	122.36	124.45
18	B	507	CLA	CHD-C1D-ND	-2.28	122.36	124.45
18	B	512	CLA	CHB-C4A-NA	2.28	127.66	124.51
18	c	503	CLA	CHD-C1D-ND	-2.28	122.36	124.45
18	c	514	CLA	CHD-C1D-ND	-2.28	122.36	124.45
18	C	506	CLA	C1-C2-C3	-2.27	122.11	126.04
18	C	513	CLA	CHD-C1D-ND	-2.27	122.36	124.45
18	c	508	CLA	CHD-C1D-ND	-2.27	122.36	124.45
18	b	512	CLA	CHD-C1D-ND	-2.27	122.37	124.45
21	c	502	LMG	C8-O7-C10	-2.27	112.21	117.79
20	B	518	BCR	C38-C26-C25	-2.27	121.98	124.53
20	c	517	BCR	C27-C26-C25	-2.26	119.44	122.73
18	b	503	CLA	CHB-C1B-NB	2.26	126.64	124.26
20	z	101	BCR	C15-C16-C17	-2.25	118.86	123.47
18	B	502	CLA	CHD-C1D-ND	-2.25	122.38	124.45
18	b	512	CLA	CHB-C4A-NA	2.25	127.62	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	d	406	BCR	C7-C8-C9	-2.25	122.84	126.23
21	A	407	LMG	C8-O7-C10	-2.25	112.26	117.79
18	C	504	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
20	z	101	BCR	C4-C5-C6	-2.24	119.48	122.73
18	C	507	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
18	B	501	CLA	CHD-C1D-ND	-2.24	122.40	124.45
18	C	514	CLA	CHB-C4A-NA	2.23	127.60	124.51
18	a	402	CLA	C7-C6-C5	-2.23	107.29	113.36
18	b	503	CLA	C3B-C4B-NB	-2.23	108.44	110.52
20	K	101	BCR	C19-C18-C17	-2.23	115.52	118.94
18	c	503	CLA	C3B-C4B-NB	-2.23	108.45	110.52
20	a	406	BCR	C27-C26-C25	-2.23	119.50	122.73
18	d	405	CLA	CHB-C4A-NA	2.22	127.59	124.51
20	a	406	BCR	C24-C23-C22	-2.22	122.87	126.23
20	C	517	BCR	C24-C23-C22	-2.22	122.88	126.23
18	B	508	CLA	CHB-C4A-NA	2.22	127.58	124.51
20	c	516	BCR	C7-C6-C5	-2.22	116.09	121.46
18	b	503	CLA	CHD-C1D-ND	-2.22	122.42	124.45
18	c	506	CLA	CHD-C1D-ND	-2.22	122.42	124.45
23	C	501	SQD	O8-S-C6	2.22	109.27	105.74
18	A	402	CLA	C7-C6-C5	-2.22	107.34	113.36
18	D	405	CLA	CHB-C4A-NA	2.22	127.58	124.51
18	C	503	CLA	C1-C2-C3	-2.21	122.22	126.04
18	C	505	CLA	CHD-C1D-ND	-2.21	122.42	124.45
18	c	505	CLA	CHD-C1D-ND	-2.21	122.42	124.45
20	k	101	BCR	C21-C20-C19	-2.21	116.33	123.22
18	c	507	CLA	CHD-C1D-ND	-2.21	122.43	124.45
18	b	511	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
18	C	502	CLA	CHC-C4B-NB	2.21	126.59	124.26
18	B	511	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
18	c	508	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
20	x	102	BCR	C35-C13-C12	2.20	121.55	118.08
20	C	516	BCR	C23-C24-C25	-2.20	121.02	127.20
20	X	102	BCR	C35-C13-C12	2.20	121.54	118.08
18	c	505	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
18	b	501	CLA	CHD-C1D-ND	-2.20	122.43	124.45
18	a	405	CLA	O2D-CGD-CBD	2.20	115.17	111.27
20	B	517	BCR	C24-C23-C22	-2.19	122.92	126.23
20	C	516	BCR	C34-C9-C8	2.19	121.53	118.08
20	c	516	BCR	C23-C24-C25	-2.19	121.04	127.20
18	d	405	CLA	CHD-C1D-ND	-2.19	122.44	124.45
18	b	509	CLA	O2A-CGA-O1A	-2.19	118.07	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	c	504	CLA	CHC-C4B-NB	2.18	126.57	124.26
20	b	517	BCR	C24-C23-C22	-2.18	122.94	126.23
18	C	511	CLA	CHD-C1D-ND	-2.18	122.45	124.45
20	c	516	BCR	C30-C25-C24	2.18	121.95	115.78
22	d	408	LHG	C5-O7-C7	-2.18	112.42	117.79
18	c	504	CLA	C1-C2-C3	-2.18	122.28	126.04
18	B	511	CLA	O2D-CGD-CBD	2.18	115.14	111.27
18	A	405	CLA	CHB-C4A-NA	2.18	127.52	124.51
18	C	504	CLA	CHD-C1D-ND	-2.18	122.45	124.45
27	D	407	PL9	O1-C4-C3	-2.17	118.33	120.72
18	a	403	CLA	CHD-C1D-ND	-2.17	122.46	124.45
18	b	508	CLA	CHD-C1D-ND	-2.17	122.46	124.45
18	a	405	CLA	CHB-C4A-NA	2.17	127.52	124.51
20	C	516	BCR	C4-C5-C6	-2.17	119.58	122.73
27	D	407	PL9	C31-C32-C33	-2.17	104.75	111.88
20	z	101	BCR	C32-C1-C6	-2.17	106.78	110.30
27	D	407	PL9	O2-C1-C6	2.17	124.35	120.59
25	C	522	LMU	C1B-O1B-C4'	-2.17	112.60	117.96
20	C	517	BCR	C27-C26-C25	-2.16	119.59	122.73
18	A	403	CLA	O2D-CGD-CBD	2.16	115.11	111.27
20	K	101	BCR	C7-C6-C5	-2.16	116.22	121.46
18	C	503	CLA	CHD-C1D-ND	-2.16	122.47	124.45
18	b	508	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
20	k	101	BCR	C19-C18-C17	-2.16	115.62	118.94
18	B	510	CLA	C3B-C4B-NB	-2.16	108.51	110.52
20	c	516	BCR	C39-C30-C25	-2.16	106.80	110.30
19	a	404	PHO	O2A-CGA-O1A	-2.16	118.14	123.59
27	d	407	PL9	O1-C4-C3	-2.16	118.34	120.72
27	d	407	PL9	C36-C34-C33	-2.15	116.76	121.12
20	C	516	BCR	C39-C30-C25	-2.15	106.81	110.30
18	C	506	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
20	B	519	BCR	C16-C15-C14	-2.15	119.07	123.47
20	B	519	BCR	C4-C5-C6	-2.14	119.62	122.73
19	A	404	PHO	O2A-CGA-O1A	-2.14	118.18	123.59
18	d	404	CLA	C3B-C4B-NB	-2.14	108.53	110.52
27	d	407	PL9	O2-C1-C6	2.14	124.30	120.59
18	D	404	CLA	CHB-C4A-NA	2.14	127.47	124.51
20	K	101	BCR	C21-C20-C19	-2.14	116.53	123.22
18	b	502	CLA	C3B-C4B-NB	-2.14	108.53	110.52
18	a	403	CLA	CHB-C4A-NA	2.14	127.47	124.51
20	C	515	BCR	C15-C14-C13	-2.14	124.26	127.31
20	c	517	BCR	C24-C23-C22	-2.14	123.00	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	b	507	CLA	C3B-C4B-NB	-2.14	108.53	110.52
18	D	405	CLA	CHD-C1D-ND	-2.14	122.49	124.45
18	c	503	CLA	CHC-C4B-NB	2.14	126.52	124.26
18	b	509	CLA	CHD-C1D-ND	-2.14	122.49	124.45
22	D	408	LHG	C5-O7-C7	-2.13	112.53	117.79
27	D	407	PL9	O2-C1-C2	-2.13	116.89	121.78
18	B	503	CLA	C3B-C4B-NB	-2.13	108.53	110.52
20	C	516	BCR	C24-C23-C22	-2.13	123.01	126.23
20	x	102	BCR	C24-C23-C22	-2.13	123.01	126.23
20	K	101	BCR	C16-C15-C14	-2.13	119.10	123.47
18	b	509	CLA	C1-C2-C3	-2.13	122.36	126.04
20	A	410	BCR	C16-C15-C14	-2.13	119.11	123.47
18	b	509	CLA	CAA-C2A-C1A	-2.13	104.99	111.97
18	A	402	CLA	CAC-C3C-C4C	2.13	127.58	124.81
20	c	516	BCR	C16-C17-C18	-2.13	124.27	127.31
27	D	407	PL9	C36-C34-C33	-2.13	116.81	121.12
18	b	502	CLA	CHD-C1D-ND	-2.13	122.50	124.45
20	C	516	BCR	C30-C25-C24	2.13	121.80	115.78
20	C	517	BCR	C10-C11-C12	-2.13	116.57	123.22
18	c	504	CLA	CHD-C1D-ND	-2.13	122.50	124.45
18	B	502	CLA	C3B-C4B-NB	-2.12	108.54	110.52
18	B	501	CLA	C3B-C4B-NB	-2.12	108.55	110.52
18	B	508	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
27	d	407	PL9	O2-C1-C2	-2.12	116.92	121.78
27	d	407	PL9	C31-C32-C33	-2.12	104.91	111.88
20	X	102	BCR	C31-C1-C6	-2.12	106.86	110.30
20	c	516	BCR	C4-C5-C6	-2.12	119.66	122.73
18	B	503	CLA	CHD-C1D-ND	-2.12	122.51	124.45
18	B	505	CLA	CHC-C4B-NB	2.11	126.49	124.26
25	c	522	LMU	C1B-O1B-C4'	-2.11	112.74	117.96
18	d	401	CLA	CHD-C1D-ND	-2.11	122.52	124.45
18	c	507	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
18	C	502	CLA	CHD-C1D-ND	-2.11	122.52	124.45
20	k	101	BCR	C12-C13-C14	-2.10	115.71	118.94
18	A	405	CLA	C1-C2-C3	-2.10	122.41	126.04
20	K	101	BCR	C20-C21-C22	-2.10	124.31	127.31
18	b	505	CLA	CHC-C4B-NB	2.10	126.48	124.26
20	c	517	BCR	C10-C11-C12	-2.10	116.67	123.22
18	B	509	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
27	D	407	PL9	C7-C8-C9	-2.10	123.30	126.79
21	h	101	LMG	O1-C1-C2	2.10	111.58	108.30
18	b	516	CLA	O2A-CGA-O1A	-2.10	118.30	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	a	405	CLA	C1-C2-C3	-2.10	122.42	126.04
18	B	515	CLA	CHD-C1D-ND	-2.10	122.53	124.45
18	d	401	CLA	CHB-C4A-NA	2.09	127.41	124.51
20	X	102	BCR	C24-C23-C22	-2.09	123.07	126.23
18	B	506	CLA	CHD-C1D-ND	-2.09	122.53	124.45
18	C	503	CLA	CHC-C4B-NB	2.09	126.47	124.26
20	A	406	BCR	C33-C5-C4	2.09	117.63	113.62
18	C	510	CLA	CHD-C1D-ND	-2.09	122.53	124.45
18	A	405	CLA	O2D-CGD-CBD	2.09	114.97	111.27
18	d	401	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
18	b	510	CLA	C1-C2-C3	-2.08	122.44	126.04
18	c	511	CLA	CHD-C1D-ND	-2.08	122.54	124.45
20	A	410	BCR	C4-C5-C6	-2.08	119.71	122.73
20	k	101	BCR	C7-C6-C5	-2.08	116.42	121.46
20	x	102	BCR	C8-C9-C10	-2.08	115.75	118.94
18	a	402	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
20	b	517	BCR	C19-C18-C17	-2.08	115.75	118.94
20	z	101	BCR	C15-C14-C13	-2.08	124.35	127.31
18	A	402	CLA	O2A-CGA-O1A	-2.08	118.36	123.59
18	b	506	CLA	CHD-C1D-ND	-2.07	122.55	124.45
18	d	404	CLA	CHB-C4A-NA	2.07	127.38	124.51
18	c	507	CLA	CHB-C4A-NA	2.07	127.38	124.51
20	X	102	BCR	C36-C18-C17	-2.07	120.02	122.92
20	x	102	BCR	C36-C18-C17	-2.07	120.02	122.92
18	C	507	CLA	C3B-C4B-NB	-2.07	108.59	110.52
18	c	513	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
18	a	402	CLA	CAC-C3C-C4C	2.07	127.50	124.81
18	A	402	CLA	CHC-C4B-NB	2.07	126.45	124.26
20	K	101	BCR	C1-C6-C5	-2.07	119.70	122.61
18	b	513	CLA	CHD-C1D-ND	-2.07	122.55	124.45
20	a	406	BCR	C33-C5-C4	2.07	117.59	113.62
27	d	407	PL9	C7-C8-C9	-2.07	123.35	126.79
18	B	515	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
18	D	401	CLA	CHD-C1D-ND	-2.06	122.56	124.45
18	D	404	CLA	C3B-C4B-NB	-2.06	108.60	110.52
18	B	516	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
18	b	515	CLA	CHD-C1D-ND	-2.06	122.56	124.45
18	D	405	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
20	C	515	BCR	C20-C21-C22	-2.06	124.37	127.31
24	C	518	DGD	O6D-C5D-C6D	2.06	110.83	106.67
18	b	506	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
18	B	514	CLA	O2A-CGA-O1A	-2.06	118.17	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	X	102	BCR	C15-C16-C17	-2.06	119.26	123.47
20	B	517	BCR	C19-C18-C17	-2.06	115.78	118.94
18	a	403	CLA	O2D-CGD-CBD	2.06	114.92	111.27
18	b	503	CLA	CHC-C4B-NB	2.06	126.43	124.26
18	b	507	CLA	O2A-CGA-O1A	-2.06	118.41	123.59
20	k	101	BCR	C16-C15-C14	-2.06	119.26	123.47
18	C	506	CLA	CHB-C4A-NA	2.05	127.35	124.51
18	B	506	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
18	C	512	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
18	D	401	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
24	c	518	DGD	O6D-C5D-C6D	2.05	110.81	106.67
18	C	506	CLA	C3B-C4B-NB	-2.05	108.61	110.52
18	B	503	CLA	CHC-C4B-NB	2.05	126.42	124.26
18	b	514	CLA	O2A-CGA-O1A	-2.04	118.21	123.30
20	x	102	BCR	C15-C16-C17	-2.04	119.29	123.47
18	C	505	CLA	CHB-C4A-NA	2.04	127.33	124.51
18	b	504	CLA	CHD-C1D-ND	-2.04	122.58	124.45
20	k	101	BCR	C20-C21-C22	-2.04	124.40	127.31
20	B	517	BCR	C33-C5-C6	-2.04	122.24	124.53
20	b	517	BCR	C33-C5-C6	-2.04	122.24	124.53
18	a	402	CLA	C3B-C4B-NB	-2.04	108.62	110.52
18	b	511	CLA	O2D-CGD-CBD	2.04	114.89	111.27
18	D	401	CLA	CHB-C4A-NA	2.04	127.33	124.51
18	a	405	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
18	C	506	CLA	CHD-C1D-ND	-2.03	122.58	124.45
18	B	507	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
18	b	515	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
18	A	402	CLA	C3B-C4B-NB	-2.03	108.63	110.52
18	c	506	CLA	CHB-C4A-NA	2.03	127.32	124.51
20	C	515	BCR	C37-C22-C23	2.03	121.28	118.08
18	A	405	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
20	a	406	BCR	C16-C15-C14	-2.03	119.31	123.47
20	z	101	BCR	C37-C22-C23	2.03	121.27	118.08
18	B	509	CLA	CHD-C1D-ND	-2.03	122.59	124.45
18	c	514	CLA	C1-C2-C3	-2.03	122.54	126.04
20	A	406	BCR	C37-C22-C21	-2.03	120.08	122.92
18	B	511	CLA	C3B-C4B-NB	-2.03	108.64	110.52
18	C	513	CLA	C1-C2-C3	-2.03	122.54	126.04
18	C	508	CLA	O2D-CGD-CBD	2.03	114.87	111.27
20	K	101	BCR	C10-C11-C12	-2.02	116.90	123.22
18	C	505	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
18	d	405	CLA	C6-C5-C3	2.02	118.76	113.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	510	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
18	b	504	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
18	c	506	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
18	C	502	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
18	B	504	CLA	CHD-C1D-ND	-2.02	122.60	124.45
18	B	513	CLA	CHD-C1D-ND	-2.02	122.60	124.45
20	x	102	BCR	C2-C1-C6	2.02	113.59	110.48
18	b	516	CLA	C3B-C4B-NB	-2.02	108.64	110.52
20	D	406	BCR	C12-C13-C14	-2.02	115.84	118.94
28	e	101	HEM	C3D-C4D-ND	-2.02	107.92	110.17
20	X	102	BCR	C8-C9-C10	-2.01	115.85	118.94
18	A	403	CLA	CHB-C4A-NA	2.01	127.30	124.51
18	d	401	CLA	O2D-CGD-CBD	2.01	114.85	111.27
23	C	501	SQD	O9-S-C6	2.01	109.33	106.94
20	C	516	BCR	C7-C8-C9	-2.01	123.19	126.23
26	D	403	BCT	O3-C-O1	-2.01	114.33	119.55
18	c	508	CLA	C3B-C4B-NB	-2.01	108.65	110.52
18	b	510	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
18	C	506	CLA	CHB-C1B-NB	2.01	126.39	124.26
18	b	501	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
18	C	508	CLA	C1-C2-C3	-2.01	122.57	126.04
20	a	406	BCR	C37-C22-C21	-2.01	120.11	122.92
20	z	101	BCR	C20-C21-C22	-2.01	124.44	127.31
20	K	101	BCR	C38-C26-C25	-2.01	122.27	124.53
18	B	513	CLA	C1-C2-C3	-2.01	122.57	126.04
18	b	509	CLA	C3B-C4B-NB	-2.01	108.65	110.52
18	B	501	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
18	b	506	CLA	C3B-C4B-NB	-2.00	108.66	110.52
18	b	509	CLA	CHC-C4B-NB	2.00	126.38	124.26
20	B	519	BCR	C27-C26-C25	-2.00	119.83	122.73
20	A	406	BCR	C16-C15-C14	-2.00	119.38	123.47

There are no chirality outliers.

All (1307) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	B	501	CLA	C1A-C2A-CAA-CBA
18	B	501	CLA	CHA-CBD-CGD-O1D
18	B	501	CLA	CHA-CBD-CGD-O2D
18	B	501	CLA	CAD-CBD-CGD-O1D
18	B	501	CLA	CAD-CBD-CGD-O2D
18	B	503	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	B	503	CLA	C3A-C2A-CAA-CBA
18	B	504	CLA	C1A-C2A-CAA-CBA
18	B	504	CLA	CHA-CBD-CGD-O1D
18	B	504	CLA	CHA-CBD-CGD-O2D
18	B	504	CLA	CAD-CBD-CGD-O1D
18	B	506	CLA	C1A-C2A-CAA-CBA
18	B	506	CLA	C3A-C2A-CAA-CBA
18	B	506	CLA	CHA-CBD-CGD-O1D
18	B	506	CLA	CHA-CBD-CGD-O2D
18	B	507	CLA	C1A-C2A-CAA-CBA
18	B	509	CLA	CHA-CBD-CGD-O1D
18	B	509	CLA	CHA-CBD-CGD-O2D
18	B	509	CLA	CAD-CBD-CGD-O1D
18	B	509	CLA	CBD-CGD-O2D-CED
18	B	512	CLA	O2A-C1-C2-C3
18	B	515	CLA	CBD-CGD-O2D-CED
18	B	516	CLA	C2B-C3B-CAB-CBB
18	B	516	CLA	C4B-C3B-CAB-CBB
18	C	502	CLA	C3A-C2A-CAA-CBA
18	C	504	CLA	CHA-CBD-CGD-O1D
18	C	504	CLA	CHA-CBD-CGD-O2D
18	C	504	CLA	CAD-CBD-CGD-O1D
18	C	504	CLA	CAD-CBD-CGD-O2D
18	C	505	CLA	CHA-CBD-CGD-O1D
18	C	505	CLA	CHA-CBD-CGD-O2D
18	C	505	CLA	C11-C12-C13-C14
18	C	506	CLA	C1A-C2A-CAA-CBA
18	C	506	CLA	CHA-CBD-CGD-O1D
18	C	506	CLA	CHA-CBD-CGD-O2D
18	C	507	CLA	C1A-C2A-CAA-CBA
18	C	507	CLA	C3A-C2A-CAA-CBA
18	C	509	CLA	C2A-CAA-CBA-CGA
18	C	512	CLA	CHA-CBD-CGD-O1D
18	C	512	CLA	CHA-CBD-CGD-O2D
18	C	512	CLA	CAD-CBD-CGD-O1D
18	C	512	CLA	CAD-CBD-CGD-O2D
18	C	513	CLA	C1A-C2A-CAA-CBA
18	C	513	CLA	C3A-C2A-CAA-CBA
18	C	514	CLA	CBD-CGD-O2D-CED
18	D	401	CLA	C1A-C2A-CAA-CBA
18	D	405	CLA	CHA-CBD-CGD-O1D
18	D	405	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	D	405	CLA	CAD-CBD-CGD-O1D
18	b	501	CLA	CHA-CBD-CGD-O1D
18	b	501	CLA	CHA-CBD-CGD-O2D
18	b	501	CLA	CAD-CBD-CGD-O1D
18	b	501	CLA	CAD-CBD-CGD-O2D
18	b	503	CLA	C1A-C2A-CAA-CBA
18	b	503	CLA	C3A-C2A-CAA-CBA
18	b	504	CLA	C1A-C2A-CAA-CBA
18	b	504	CLA	CHA-CBD-CGD-O1D
18	b	504	CLA	CHA-CBD-CGD-O2D
18	b	504	CLA	CAD-CBD-CGD-O1D
18	b	506	CLA	C1A-C2A-CAA-CBA
18	b	506	CLA	C3A-C2A-CAA-CBA
18	b	506	CLA	C2A-CAA-CBA-CGA
18	b	506	CLA	CHA-CBD-CGD-O1D
18	b	506	CLA	CHA-CBD-CGD-O2D
18	b	507	CLA	C1A-C2A-CAA-CBA
18	b	509	CLA	CHA-CBD-CGD-O1D
18	b	509	CLA	CHA-CBD-CGD-O2D
18	b	509	CLA	CAD-CBD-CGD-O1D
18	b	511	CLA	C2A-CAA-CBA-CGA
18	b	512	CLA	O2A-C1-C2-C3
18	b	515	CLA	CBD-CGD-O2D-CED
18	c	503	CLA	C3A-C2A-CAA-CBA
18	c	505	CLA	CHA-CBD-CGD-O1D
18	c	505	CLA	CHA-CBD-CGD-O2D
18	c	505	CLA	CAD-CBD-CGD-O1D
18	c	505	CLA	CAD-CBD-CGD-O2D
18	c	506	CLA	CHA-CBD-CGD-O1D
18	c	506	CLA	CHA-CBD-CGD-O2D
18	c	506	CLA	C11-C12-C13-C14
18	c	507	CLA	C1A-C2A-CAA-CBA
18	c	507	CLA	CHA-CBD-CGD-O1D
18	c	507	CLA	CHA-CBD-CGD-O2D
18	c	508	CLA	C1A-C2A-CAA-CBA
18	c	508	CLA	C3A-C2A-CAA-CBA
18	c	510	CLA	C2A-CAA-CBA-CGA
18	c	513	CLA	CHA-CBD-CGD-O1D
18	c	513	CLA	CHA-CBD-CGD-O2D
18	c	513	CLA	CAD-CBD-CGD-O1D
18	c	513	CLA	CAD-CBD-CGD-O2D
18	c	514	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	c	514	CLA	C3A-C2A-CAA-CBA
18	c	515	CLA	CBD-CGD-O2D-CED
18	d	401	CLA	C1A-C2A-CAA-CBA
18	d	405	CLA	CHA-CBD-CGD-O1D
18	d	405	CLA	CHA-CBD-CGD-O2D
18	d	405	CLA	CAD-CBD-CGD-O1D
18	d	405	CLA	C2-C3-C5-C6
18	d	405	CLA	C4-C3-C5-C6
19	D	402	PHO	CHA-CBD-CGD-O2D
19	a	404	PHO	O1A-CGA-O2A-C1
20	A	406	BCR	C5-C6-C7-C8
20	A	406	BCR	C23-C24-C25-C26
20	A	410	BCR	C1-C6-C7-C8
20	A	410	BCR	C5-C6-C7-C8
20	B	517	BCR	C1-C6-C7-C8
20	B	517	BCR	C5-C6-C7-C8
20	B	517	BCR	C23-C24-C25-C26
20	B	517	BCR	C23-C24-C25-C30
20	B	518	BCR	C5-C6-C7-C8
20	B	518	BCR	C23-C24-C25-C26
20	B	519	BCR	C1-C6-C7-C8
20	B	519	BCR	C5-C6-C7-C8
20	C	515	BCR	C23-C24-C25-C26
20	C	515	BCR	C23-C24-C25-C30
20	D	406	BCR	C1-C6-C7-C8
20	D	406	BCR	C5-C6-C7-C8
20	D	406	BCR	C23-C24-C25-C26
20	D	406	BCR	C23-C24-C25-C30
20	K	101	BCR	C23-C24-C25-C26
20	X	102	BCR	C1-C6-C7-C8
20	X	102	BCR	C5-C6-C7-C8
20	X	102	BCR	C23-C24-C25-C26
20	a	406	BCR	C5-C6-C7-C8
20	a	406	BCR	C23-C24-C25-C26
20	b	517	BCR	C1-C6-C7-C8
20	b	517	BCR	C5-C6-C7-C8
20	b	517	BCR	C23-C24-C25-C26
20	b	517	BCR	C23-C24-C25-C30
20	b	518	BCR	C5-C6-C7-C8
20	b	518	BCR	C23-C24-C25-C26
20	c	517	BCR	C5-C6-C7-C8
20	d	406	BCR	C1-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	d	406	BCR	C5-C6-C7-C8
20	d	406	BCR	C23-C24-C25-C26
20	d	406	BCR	C23-C24-C25-C30
20	k	101	BCR	C23-C24-C25-C26
20	x	102	BCR	C1-C6-C7-C8
20	x	102	BCR	C5-C6-C7-C8
20	x	102	BCR	C23-C24-C25-C26
20	z	101	BCR	C23-C24-C25-C26
20	z	101	BCR	C23-C24-C25-C30
21	A	407	LMG	O6-C1-O1-C7
21	D	410	LMG	O7-C8-C9-O8
21	c	502	LMG	O6-C1-O1-C7
21	h	101	LMG	O7-C8-C9-O8
22	A	409	LHG	C3-O3-P-O4
22	A	409	LHG	C3-O3-P-O5
22	A	409	LHG	C4-O6-P-O5
22	B	521	LHG	C3-O3-P-O6
22	B	521	LHG	C4-O6-P-O4
22	B	522	LHG	C3-O3-P-O6
22	B	522	LHG	C4-O6-P-O4
22	D	408	LHG	C4-O6-P-O3
22	L	101	LHG	C3-O3-P-O6
22	X	101	LHG	C3-O3-P-O4
22	X	101	LHG	C4-O6-P-O4
22	a	407	LHG	C3-O3-P-O6
22	a	408	LHG	C3-O3-P-O4
22	a	408	LHG	C3-O3-P-O5
22	a	408	LHG	C4-O6-P-O5
22	b	520	LHG	C3-O3-P-O6
22	b	520	LHG	C4-O6-P-O4
22	b	521	LHG	C3-O3-P-O6
22	b	521	LHG	C4-O6-P-O4
22	l	101	LHG	C3-O3-P-O6
22	x	101	LHG	C3-O3-P-O4
22	x	101	LHG	C4-O6-P-O4
23	C	501	SQD	C5-C6-S-O7
25	C	522	LMU	C2-C1-O1'-C1'
25	c	522	LMU	C2-C1-O1'-C1'
27	D	407	PL9	C27-C28-C29-C31
27	D	407	PL9	C47-C48-C49-C51
27	d	407	PL9	C27-C28-C29-C31
18	A	402	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	B	507	CLA	O1D-CGD-O2D-CED
18	C	503	CLA	O1D-CGD-O2D-CED
18	a	402	CLA	O1D-CGD-O2D-CED
18	b	507	CLA	O1D-CGD-O2D-CED
18	c	504	CLA	O1D-CGD-O2D-CED
18	B	515	CLA	O1D-CGD-O2D-CED
18	C	507	CLA	O1D-CGD-O2D-CED
18	b	515	CLA	O1D-CGD-O2D-CED
18	c	508	CLA	O1D-CGD-O2D-CED
18	A	402	CLA	CBD-CGD-O2D-CED
18	B	506	CLA	CBD-CGD-O2D-CED
18	B	507	CLA	CBD-CGD-O2D-CED
18	C	503	CLA	CBD-CGD-O2D-CED
18	C	504	CLA	CBD-CGD-O2D-CED
18	C	507	CLA	CBD-CGD-O2D-CED
18	a	402	CLA	CBD-CGD-O2D-CED
18	b	506	CLA	CBD-CGD-O2D-CED
18	b	507	CLA	CBD-CGD-O2D-CED
18	b	509	CLA	CBD-CGD-O2D-CED
18	c	504	CLA	CBD-CGD-O2D-CED
18	c	505	CLA	CBD-CGD-O2D-CED
18	c	508	CLA	CBD-CGD-O2D-CED
18	B	505	CLA	O1A-CGA-O2A-C1
18	B	507	CLA	O1A-CGA-O2A-C1
18	b	505	CLA	O1A-CGA-O2A-C1
18	b	507	CLA	O1A-CGA-O2A-C1
18	B	509	CLA	O1D-CGD-O2D-CED
18	C	514	CLA	O1D-CGD-O2D-CED
18	b	507	CLA	CBA-CGA-O2A-C1
19	A	404	PHO	CBA-CGA-O2A-C1
18	B	501	CLA	CBD-CGD-O2D-CED
18	B	504	CLA	CBD-CGD-O2D-CED
18	B	505	CLA	CBD-CGD-O2D-CED
18	C	510	CLA	CBD-CGD-O2D-CED
18	C	512	CLA	CBD-CGD-O2D-CED
18	b	501	CLA	CBD-CGD-O2D-CED
18	b	504	CLA	CBD-CGD-O2D-CED
18	b	505	CLA	CBD-CGD-O2D-CED
18	c	511	CLA	CBD-CGD-O2D-CED
18	c	513	CLA	CBD-CGD-O2D-CED
18	B	508	CLA	O1A-CGA-O2A-C1
18	B	511	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	C	507	CLA	O1A-CGA-O2A-C1
18	b	508	CLA	O1A-CGA-O2A-C1
18	b	511	CLA	O1A-CGA-O2A-C1
18	c	508	CLA	O1A-CGA-O2A-C1
19	A	404	PHO	O1A-CGA-O2A-C1
18	c	515	CLA	O1D-CGD-O2D-CED
18	B	503	CLA	CBD-CGD-O2D-CED
18	b	503	CLA	CBD-CGD-O2D-CED
18	B	503	CLA	C3-C5-C6-C7
18	C	513	CLA	C3-C5-C6-C7
18	b	503	CLA	C3-C5-C6-C7
18	b	508	CLA	C3-C5-C6-C7
18	c	514	CLA	C3-C5-C6-C7
19	D	402	PHO	C3-C5-C6-C7
19	d	402	PHO	C3-C5-C6-C7
18	B	505	CLA	CBA-CGA-O2A-C1
18	B	507	CLA	CBA-CGA-O2A-C1
18	C	506	CLA	CBA-CGA-O2A-C1
18	C	509	CLA	CBA-CGA-O2A-C1
18	b	505	CLA	CBA-CGA-O2A-C1
18	c	510	CLA	CBA-CGA-O2A-C1
19	a	404	PHO	CBA-CGA-O2A-C1
27	d	407	PL9	C47-C48-C49-C51
18	D	405	CLA	C4-C3-C5-C6
18	B	511	CLA	CBD-CGD-O2D-CED
18	B	506	CLA	C2A-CAA-CBA-CGA
18	B	509	CLA	C2A-CAA-CBA-CGA
18	B	511	CLA	C2A-CAA-CBA-CGA
18	C	503	CLA	C2A-CAA-CBA-CGA
18	B	506	CLA	O1A-CGA-O2A-C1
18	b	509	CLA	O1D-CGD-O2D-CED
18	B	508	CLA	C3-C5-C6-C7
18	B	502	CLA	CBA-CGA-O2A-C1
18	B	508	CLA	CBA-CGA-O2A-C1
18	B	511	CLA	CBA-CGA-O2A-C1
18	C	507	CLA	CBA-CGA-O2A-C1
18	b	502	CLA	CBA-CGA-O2A-C1
18	b	508	CLA	CBA-CGA-O2A-C1
18	b	511	CLA	CBA-CGA-O2A-C1
18	c	507	CLA	CBA-CGA-O2A-C1
18	c	508	CLA	CBA-CGA-O2A-C1
18	b	511	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	c	505	CLA	O1D-CGD-O2D-CED
18	C	506	CLA	O1A-CGA-O2A-C1
18	C	509	CLA	O1A-CGA-O2A-C1
18	b	506	CLA	O1A-CGA-O2A-C1
18	c	510	CLA	O1A-CGA-O2A-C1
18	B	506	CLA	O1D-CGD-O2D-CED
18	b	506	CLA	O1D-CGD-O2D-CED
18	B	516	CLA	CBD-CGD-O2D-CED
18	D	405	CLA	CBD-CGD-O2D-CED
18	C	514	CLA	C3-C5-C6-C7
18	c	515	CLA	C3-C5-C6-C7
18	B	506	CLA	CBA-CGA-O2A-C1
18	D	401	CLA	CBA-CGA-O2A-C1
18	c	505	CLA	CBA-CGA-O2A-C1
18	d	401	CLA	CBA-CGA-O2A-C1
18	B	502	CLA	O1A-CGA-O2A-C1
18	b	502	CLA	O1A-CGA-O2A-C1
24	C	518	DGD	C4E-C5E-C6E-O5E
18	C	504	CLA	O1D-CGD-O2D-CED
18	d	405	CLA	CBD-CGD-O2D-CED
24	c	518	DGD	O6E-C5E-C6E-O5E
18	c	505	CLA	O1A-CGA-O2A-C1
18	C	504	CLA	CBA-CGA-O2A-C1
18	b	506	CLA	CBA-CGA-O2A-C1
24	C	518	DGD	O6E-C5E-C6E-O5E
18	c	507	CLA	O1A-CGA-O2A-C1
18	b	504	CLA	C2A-CAA-CBA-CGA
18	b	509	CLA	C2A-CAA-CBA-CGA
18	C	510	CLA	O1D-CGD-O2D-CED
18	c	511	CLA	O1D-CGD-O2D-CED
18	C	504	CLA	O1A-CGA-O2A-C1
18	D	401	CLA	O1A-CGA-O2A-C1
18	d	401	CLA	O1A-CGA-O2A-C1
18	b	505	CLA	O1D-CGD-O2D-CED
18	A	402	CLA	CBA-CGA-O2A-C1
18	C	505	CLA	CBA-CGA-O2A-C1
18	C	510	CLA	CBA-CGA-O2A-C1
18	C	514	CLA	CBA-CGA-O2A-C1
18	a	402	CLA	CBA-CGA-O2A-C1
18	c	506	CLA	CBA-CGA-O2A-C1
18	c	515	CLA	CBA-CGA-O2A-C1
18	c	503	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	B	501	CLA	O1D-CGD-O2D-CED
18	b	501	CLA	O1D-CGD-O2D-CED
18	a	402	CLA	O1A-CGA-O2A-C1
18	D	405	CLA	C2-C3-C5-C6
18	B	509	CLA	C6-C7-C8-C9
18	B	511	CLA	C11-C12-C13-C14
18	B	515	CLA	C6-C7-C8-C9
18	C	514	CLA	C14-C13-C15-C16
18	D	405	CLA	C6-C7-C8-C9
18	b	509	CLA	C6-C7-C8-C9
18	b	511	CLA	C11-C12-C13-C14
18	c	515	CLA	C14-C13-C15-C16
18	d	405	CLA	C6-C7-C8-C9
18	B	505	CLA	O1D-CGD-O2D-CED
18	B	504	CLA	C2A-CAA-CBA-CGA
18	c	504	CLA	C2A-CAA-CBA-CGA
20	C	515	BCR	C7-C8-C9-C34
20	z	101	BCR	C7-C8-C9-C34
20	C	515	BCR	C7-C8-C9-C10
20	z	101	BCR	C7-C8-C9-C10
18	A	402	CLA	O1A-CGA-O2A-C1
18	C	505	CLA	O1A-CGA-O2A-C1
18	c	506	CLA	O1A-CGA-O2A-C1
18	B	504	CLA	O1D-CGD-O2D-CED
18	b	504	CLA	O1D-CGD-O2D-CED
18	c	511	CLA	CBA-CGA-O2A-C1
19	D	402	PHO	CBA-CGA-O2A-C1
18	b	504	CLA	C10-C11-C12-C13
18	B	504	CLA	C10-C11-C12-C13
18	B	515	CLA	C8-C10-C11-C12
18	C	507	CLA	C15-C16-C17-C18
27	D	407	PL9	C47-C48-C49-C50
21	D	409	LMG	C10-C11-C12-C13
18	B	502	CLA	CBD-CGD-O2D-CED
18	c	508	CLA	C15-C16-C17-C18
18	c	513	CLA	O1D-CGD-O2D-CED
24	c	518	DGD	C4E-C5E-C6E-O5E
18	b	515	CLA	C8-C10-C11-C12
18	d	405	CLA	C10-C11-C12-C13
21	d	409	LMG	C10-C11-C12-C13
18	C	502	CLA	CBD-CGD-O2D-CED
18	A	402	CLA	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	C	504	CLA	C6-C7-C8-C10
18	C	512	CLA	C3-C5-C6-C7
18	C	510	CLA	O1A-CGA-O2A-C1
18	C	514	CLA	O1A-CGA-O2A-C1
18	c	512	CLA	C2A-CAA-CBA-CGA
18	B	503	CLA	O1D-CGD-O2D-CED
18	C	512	CLA	O1D-CGD-O2D-CED
21	D	410	LMG	C4-C5-C6-O5
18	b	502	CLA	CBD-CGD-O2D-CED
18	B	507	CLA	C5-C6-C7-C8
18	C	512	CLA	C8-C10-C11-C12
27	D	407	PL9	C24-C26-C27-C28
27	d	407	PL9	C24-C26-C27-C28
27	d	407	PL9	C47-C48-C49-C50
18	B	511	CLA	C5-C6-C7-C8
18	C	507	CLA	C5-C6-C7-C8
18	b	511	CLA	C5-C6-C7-C8
18	c	513	CLA	C8-C10-C11-C12
18	c	514	CLA	C10-C11-C12-C13
18	c	512	CLA	CBA-CGA-O2A-C1
19	d	402	PHO	CBA-CGA-O2A-C1
18	c	515	CLA	O1A-CGA-O2A-C1
18	C	508	CLA	C8-C10-C11-C12
18	C	513	CLA	C10-C11-C12-C13
18	b	507	CLA	C5-C6-C7-C8
18	c	508	CLA	C5-C6-C7-C8
18	B	511	CLA	O1D-CGD-O2D-CED
18	c	511	CLA	O1A-CGA-O2A-C1
18	C	512	CLA	C13-C15-C16-C17
22	A	408	LHG	C4-O6-P-O3
22	A	409	LHG	C3-O3-P-O6
22	A	409	LHG	C4-O6-P-O3
22	B	521	LHG	C4-O6-P-O3
22	B	522	LHG	C4-O6-P-O3
22	X	101	LHG	C3-O3-P-O6
22	X	101	LHG	C4-O6-P-O3
22	a	407	LHG	C4-O6-P-O3
22	a	408	LHG	C3-O3-P-O6
22	a	408	LHG	C4-O6-P-O3
22	b	520	LHG	C4-O6-P-O3
22	b	521	LHG	C4-O6-P-O3
22	x	101	LHG	C3-O3-P-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	x	101	LHG	C4-O6-P-O3
18	B	513	CLA	C3-C5-C6-C7
18	C	511	CLA	CBA-CGA-O2A-C1
18	b	509	CLA	CBA-CGA-O2A-C1
18	b	510	CLA	CBA-CGA-O2A-C1
18	b	503	CLA	O1D-CGD-O2D-CED
18	c	513	CLA	C13-C15-C16-C17
18	b	511	CLA	O1D-CGD-O2D-CED
25	c	522	LMU	O5B-C5B-C6B-O6B
25	C	522	LMU	O5B-C5B-C6B-O6B
18	B	510	CLA	CBA-CGA-O2A-C1
18	B	501	CLA	C13-C15-C16-C17
18	c	513	CLA	C3-C5-C6-C7
18	d	405	CLA	CBA-CGA-O2A-C1
18	b	501	CLA	C13-C15-C16-C17
18	b	513	CLA	C3-C5-C6-C7
18	C	511	CLA	O1A-CGA-O2A-C1
19	D	402	PHO	O1A-CGA-O2A-C1
18	B	509	CLA	C16-C17-C18-C20
18	B	511	CLA	C16-C17-C18-C19
18	C	503	CLA	C16-C17-C18-C20
18	b	509	CLA	C16-C17-C18-C20
18	b	511	CLA	C16-C17-C18-C19
18	C	506	CLA	C4-C3-C5-C6
18	c	507	CLA	C4-C3-C5-C6
18	c	512	CLA	C4-C3-C5-C6
27	d	407	PL9	C45-C44-C46-C47
18	C	506	CLA	C2-C3-C5-C6
18	C	510	CLA	C14-C13-C15-C16
18	b	515	CLA	C6-C7-C8-C9
18	b	509	CLA	O1A-CGA-O2A-C1
18	c	512	CLA	O1A-CGA-O2A-C1
19	d	402	PHO	O1A-CGA-O2A-C1
22	A	409	LHG	C31-C32-C33-C34
22	a	408	LHG	C31-C32-C33-C34
25	C	522	LMU	C4-C5-C6-C7
18	b	502	CLA	C3-C5-C6-C7
18	c	509	CLA	C8-C10-C11-C12
25	c	522	LMU	C4-C5-C6-C7
21	c	521	LMG	C37-C38-C39-C40
18	C	502	CLA	C4B-C3B-CAB-CBB
18	b	516	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	c	503	CLA	C4B-C3B-CAB-CBB
18	B	501	CLA	C16-C17-C18-C19
18	B	501	CLA	C16-C17-C18-C20
18	b	501	CLA	C16-C17-C18-C19
18	b	501	CLA	C16-C17-C18-C20
18	B	502	CLA	C10-C11-C12-C13
25	C	522	LMU	C3-C4-C5-C6
21	C	521	LMG	C37-C38-C39-C40
25	c	522	LMU	C3-C4-C5-C6
25	c	522	LMU	O5B-C1B-O1B-C4'
18	b	510	CLA	O1A-CGA-O2A-C1
18	D	405	CLA	O1D-CGD-O2D-CED
18	B	507	CLA	C3A-C2A-CAA-CBA
18	C	504	CLA	C3A-C2A-CAA-CBA
18	C	508	CLA	C3A-C2A-CAA-CBA
18	D	404	CLA	C3A-C2A-CAA-CBA
18	b	507	CLA	C3A-C2A-CAA-CBA
18	c	505	CLA	C3A-C2A-CAA-CBA
18	c	509	CLA	C3A-C2A-CAA-CBA
18	d	404	CLA	C3A-C2A-CAA-CBA
22	B	521	LHG	C30-C31-C32-C33
18	B	509	CLA	C16-C17-C18-C19
18	C	503	CLA	C16-C17-C18-C19
18	b	509	CLA	C16-C17-C18-C19
22	A	409	LHG	C12-C13-C14-C15
22	a	408	LHG	C12-C13-C14-C15
22	b	520	LHG	C30-C31-C32-C33
18	B	516	CLA	O1D-CGD-O2D-CED
18	A	402	CLA	O2A-C1-C2-C3
18	a	402	CLA	O2A-C1-C2-C3
18	c	507	CLA	O2A-C1-C2-C3
18	B	502	CLA	C3-C5-C6-C7
18	B	510	CLA	O1A-CGA-O2A-C1
18	C	511	CLA	C4-C3-C5-C6
19	A	404	PHO	C4-C3-C5-C6
19	a	404	PHO	C4-C3-C5-C6
18	c	507	CLA	C2-C3-C5-C6
18	c	512	CLA	C2-C3-C5-C6
19	a	404	PHO	C2-C3-C5-C6
27	d	407	PL9	C28-C29-C31-C32
22	A	408	LHG	C8-C7-O7-C5
22	X	101	LHG	C8-C7-O7-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	a	407	LHG	C8-C7-O7-C5
22	x	101	LHG	C8-C7-O7-C5
18	D	404	CLA	C4C-C3C-CAC-CBC
18	d	405	CLA	O1A-CGA-O2A-C1
18	B	511	CLA	C16-C17-C18-C20
18	C	502	CLA	C2B-C3B-CAB-CBB
18	b	516	CLA	C2B-C3B-CAB-CBB
18	c	503	CLA	C2B-C3B-CAB-CBB
18	B	509	CLA	CBA-CGA-O2A-C1
25	C	522	LMU	O5B-C1B-O1B-C4'
22	A	408	LHG	O9-C7-O7-C5
22	a	407	LHG	O9-C7-O7-C5
22	B	521	LHG	C11-C10-C9-C8
22	b	520	LHG	C11-C10-C9-C8
24	C	518	DGD	C4B-C5B-C6B-C7B
18	b	507	CLA	C13-C15-C16-C17
20	A	406	BCR	C1-C6-C7-C8
20	A	406	BCR	C23-C24-C25-C30
20	A	410	BCR	C23-C24-C25-C26
20	A	410	BCR	C23-C24-C25-C30
20	B	518	BCR	C1-C6-C7-C8
20	B	518	BCR	C23-C24-C25-C30
20	B	519	BCR	C23-C24-C25-C26
20	B	519	BCR	C23-C24-C25-C30
20	C	515	BCR	C1-C6-C7-C8
20	C	515	BCR	C5-C6-C7-C8
20	C	516	BCR	C23-C24-C25-C26
20	C	516	BCR	C23-C24-C25-C30
20	C	517	BCR	C1-C6-C7-C8
20	C	517	BCR	C5-C6-C7-C8
20	C	517	BCR	C23-C24-C25-C26
20	K	101	BCR	C23-C24-C25-C30
20	X	102	BCR	C23-C24-C25-C30
20	a	406	BCR	C1-C6-C7-C8
20	a	406	BCR	C23-C24-C25-C30
20	b	518	BCR	C1-C6-C7-C8
20	b	518	BCR	C23-C24-C25-C30
20	c	516	BCR	C23-C24-C25-C26
20	c	516	BCR	C23-C24-C25-C30
20	c	517	BCR	C1-C6-C7-C8
20	c	517	BCR	C23-C24-C25-C26
20	k	101	BCR	C23-C24-C25-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	x	102	BCR	C23-C24-C25-C30
20	z	101	BCR	C1-C6-C7-C8
20	z	101	BCR	C5-C6-C7-C8
18	D	405	CLA	CBA-CGA-O2A-C1
18	b	502	CLA	C10-C11-C12-C13
21	B	520	LMG	C11-C10-O7-C8
22	L	101	LHG	C8-C7-O7-C5
22	l	101	LHG	C8-C7-O7-C5
21	D	409	LMG	C29-C30-C31-C32
18	C	510	CLA	C12-C13-C15-C16
18	C	511	CLA	C2-C3-C5-C6
18	C	514	CLA	C6-C7-C8-C10
18	D	405	CLA	C6-C7-C8-C10
18	a	402	CLA	C12-C13-C15-C16
18	c	511	CLA	C12-C13-C15-C16
19	A	404	PHO	C2-C3-C5-C6
27	D	407	PL9	C28-C29-C31-C32
18	B	509	CLA	O1A-CGA-O2A-C1
21	A	407	LMG	C14-C15-C16-C17
21	c	502	LMG	C14-C15-C16-C17
18	C	510	CLA	C8-C10-C11-C12
18	b	511	CLA	C16-C17-C18-C20
18	d	405	CLA	O1D-CGD-O2D-CED
22	X	101	LHG	O9-C7-O7-C5
22	x	101	LHG	O9-C7-O7-C5
21	d	409	LMG	C29-C30-C31-C32
21	h	101	LMG	C15-C16-C17-C18
18	C	511	CLA	C2A-CAA-CBA-CGA
18	B	512	CLA	C15-C16-C17-C18
18	c	503	CLA	C13-C15-C16-C17
21	D	410	LMG	O6-C5-C6-O5
21	D	410	LMG	C15-C16-C17-C18
24	c	518	DGD	C4B-C5B-C6B-C7B
18	c	504	CLA	CBA-CGA-O2A-C1
18	c	504	CLA	C16-C17-C18-C20
18	b	502	CLA	C5-C6-C7-C8
18	c	511	CLA	C8-C10-C11-C12
21	b	519	LMG	C11-C10-O7-C8
21	c	502	LMG	C11-C10-O7-C8
18	B	507	CLA	C13-C15-C16-C17
18	C	514	CLA	C10-C11-C12-C13
18	b	512	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	d	405	CLA	C16-C17-C18-C19
18	C	507	CLA	C10-C11-C12-C13
18	c	515	CLA	C10-C11-C12-C13
18	A	402	CLA	C14-C13-C15-C16
18	B	507	CLA	C6-C7-C8-C9
18	C	504	CLA	C6-C7-C8-C9
18	C	512	CLA	C11-C10-C8-C9
18	a	402	CLA	C14-C13-C15-C16
18	c	511	CLA	C14-C13-C15-C16
18	c	513	CLA	C11-C10-C8-C9
18	c	515	CLA	C6-C7-C8-C9
18	c	508	CLA	C10-C11-C12-C13
18	D	405	CLA	O1A-CGA-O2A-C1
18	B	514	CLA	C1A-C2A-CAA-CBA
18	C	502	CLA	C1A-C2A-CAA-CBA
18	C	504	CLA	C1A-C2A-CAA-CBA
18	C	508	CLA	C1A-C2A-CAA-CBA
18	D	404	CLA	C1A-C2A-CAA-CBA
18	b	501	CLA	C1A-C2A-CAA-CBA
18	b	514	CLA	C1A-C2A-CAA-CBA
18	c	503	CLA	C1A-C2A-CAA-CBA
18	c	505	CLA	C1A-C2A-CAA-CBA
18	c	509	CLA	C1A-C2A-CAA-CBA
18	d	404	CLA	C1A-C2A-CAA-CBA
21	B	520	LMG	O9-C10-O7-C8
21	b	519	LMG	O9-C10-O7-C8
22	L	101	LHG	O9-C7-O7-C5
22	l	101	LHG	O9-C7-O7-C5
21	C	521	LMG	C11-C10-O7-C8
21	c	521	LMG	C11-C10-O7-C8
22	A	408	LHG	C3-O3-P-O6
18	c	503	CLA	O1D-CGD-O2D-CED
22	a	408	LHG	C28-C29-C30-C31
18	c	504	CLA	C16-C17-C18-C19
21	c	521	LMG	O6-C5-C6-O5
22	X	101	LHG	C25-C26-C27-C28
22	x	101	LHG	C25-C26-C27-C28
18	C	502	CLA	C13-C15-C16-C17
21	C	521	LMG	O6-C5-C6-O5
27	D	407	PL9	C45-C44-C46-C47
18	B	502	CLA	C5-C6-C7-C8
21	h	101	LMG	C7-C8-C9-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	A	409	LHG	C28-C29-C30-C31
18	B	502	CLA	O1D-CGD-O2D-CED
21	D	409	LMG	C28-C29-C30-C31
22	l	101	LHG	C14-C15-C16-C17
27	D	407	PL9	C27-C28-C29-C30
27	d	407	PL9	C27-C28-C29-C30
21	A	407	LMG	C11-C10-O7-C8
21	B	520	LMG	O6-C5-C6-O5
21	D	409	LMG	O6-C5-C6-O5
21	b	519	LMG	O6-C5-C6-O5
21	d	409	LMG	O6-C5-C6-O5
22	d	408	LHG	C32-C33-C34-C35
18	C	502	CLA	O1D-CGD-O2D-CED
18	C	502	CLA	CBA-CGA-O2A-C1
18	C	503	CLA	CBA-CGA-O2A-C1
18	a	403	CLA	CBA-CGA-O2A-C1
18	d	405	CLA	C16-C17-C18-C20
18	b	502	CLA	O1D-CGD-O2D-CED
18	B	509	CLA	C13-C15-C16-C17
18	c	504	CLA	O1A-CGA-O2A-C1
24	c	520	DGD	C2A-C3A-C4A-C5A
24	C	520	DGD	C2A-C3A-C4A-C5A
21	C	521	LMG	O9-C10-O7-C8
21	c	502	LMG	O9-C10-O7-C8
21	c	521	LMG	O9-C10-O7-C8
19	D	402	PHO	CHA-CBD-CGD-O1D
19	d	402	PHO	CHA-CBD-CGD-O1D
19	d	402	PHO	CHA-CBD-CGD-O2D
22	L	101	LHG	C14-C15-C16-C17
18	B	507	CLA	C6-C7-C8-C10
18	B	509	CLA	C12-C13-C15-C16
18	B	511	CLA	C11-C12-C13-C15
18	B	512	CLA	C12-C13-C15-C16
18	C	503	CLA	C12-C13-C15-C16
18	C	505	CLA	C11-C12-C13-C15
18	C	512	CLA	C11-C10-C8-C7
18	D	404	CLA	C12-C13-C15-C16
18	b	507	CLA	C6-C7-C8-C10
18	b	509	CLA	C12-C13-C15-C16
18	b	512	CLA	C12-C13-C15-C16
18	c	504	CLA	C12-C13-C15-C16
18	c	505	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	c	506	CLA	C11-C12-C13-C15
18	c	513	CLA	C11-C10-C8-C7
18	c	515	CLA	C6-C7-C8-C10
18	d	405	CLA	C6-C7-C8-C10
18	B	509	CLA	C14-C13-C15-C16
18	B	512	CLA	C11-C10-C8-C9
18	B	512	CLA	C14-C13-C15-C16
18	C	503	CLA	C14-C13-C15-C16
18	C	506	CLA	C14-C13-C15-C16
18	C	514	CLA	C6-C7-C8-C9
18	b	507	CLA	C6-C7-C8-C9
18	b	509	CLA	C14-C13-C15-C16
18	b	512	CLA	C11-C10-C8-C9
18	b	512	CLA	C14-C13-C15-C16
18	c	504	CLA	C14-C13-C15-C16
18	c	505	CLA	C6-C7-C8-C9
18	d	405	CLA	C14-C13-C15-C16
18	A	403	CLA	CBA-CGA-O2A-C1
18	c	510	CLA	C16-C17-C18-C20
21	d	409	LMG	C28-C29-C30-C31
22	B	522	LHG	C24-C23-O8-C6
22	b	521	LHG	C24-C23-O8-C6
18	B	506	CLA	C5-C6-C7-C8
18	b	509	CLA	C13-C15-C16-C17
22	D	408	LHG	C32-C33-C34-C35
18	B	508	CLA	C4B-C3B-CAB-CBB
18	C	507	CLA	C4B-C3B-CAB-CBB
18	C	512	CLA	C4B-C3B-CAB-CBB
18	D	405	CLA	C4B-C3B-CAB-CBB
18	c	508	CLA	C4B-C3B-CAB-CBB
18	c	513	CLA	C4B-C3B-CAB-CBB
18	C	509	CLA	C16-C17-C18-C20
18	C	508	CLA	CBA-CGA-O2A-C1
18	c	509	CLA	CBA-CGA-O2A-C1
18	B	501	CLA	C3A-C2A-CAA-CBA
18	C	506	CLA	C3A-C2A-CAA-CBA
18	D	401	CLA	C3A-C2A-CAA-CBA
18	b	501	CLA	C3A-C2A-CAA-CBA
18	c	507	CLA	C3A-C2A-CAA-CBA
18	d	401	CLA	C3A-C2A-CAA-CBA
18	B	513	CLA	CBA-CGA-O2A-C1
18	b	510	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	c	503	CLA	C8-C10-C11-C12
21	A	407	LMG	O9-C10-O7-C8
18	B	510	CLA	C8-C10-C11-C12
19	A	404	PHO	C3-C5-C6-C7
19	a	404	PHO	C3-C5-C6-C7
18	c	510	CLA	C16-C17-C18-C19
22	d	408	LHG	C4-O6-P-O3
18	C	503	CLA	O1A-CGA-O2A-C1
22	A	408	LHG	O6-C4-C5-O7
22	a	407	LHG	O6-C4-C5-O7
18	C	502	CLA	O1A-CGA-O2A-C1
18	B	508	CLA	C2B-C3B-CAB-CBB
18	C	507	CLA	C2B-C3B-CAB-CBB
18	c	508	CLA	C2B-C3B-CAB-CBB
23	C	501	SQD	O6-C44-C45-O47
24	C	519	DGD	O1G-C1G-C2G-O2G
24	c	519	DGD	O1G-C1G-C2G-O2G
18	D	404	CLA	C2C-C3C-CAC-CBC
21	c	521	LMG	C10-C11-C12-C13
18	C	509	CLA	C16-C17-C18-C19
18	b	504	CLA	C8-C10-C11-C12
27	D	407	PL9	C39-C41-C42-C43
27	d	407	PL9	C34-C36-C37-C38
18	B	508	CLA	C11-C12-C13-C14
18	B	513	CLA	C11-C10-C8-C9
18	C	503	CLA	C11-C10-C8-C9
18	b	508	CLA	C11-C12-C13-C14
18	c	507	CLA	C14-C13-C15-C16
18	c	512	CLA	C11-C12-C13-C14
18	d	401	CLA	C14-C13-C15-C16
18	a	403	CLA	O1A-CGA-O2A-C1
20	C	517	BCR	C23-C24-C25-C30
20	c	517	BCR	C23-C24-C25-C30
18	c	511	CLA	C15-C16-C17-C18
21	C	521	LMG	C28-C29-C30-C31
21	h	101	LMG	C11-C10-O7-C8
24	c	519	DGD	C9B-CAB-CBB-CCB
18	c	506	CLA	C10-C11-C12-C13
18	A	403	CLA	O1A-CGA-O2A-C1
18	B	513	CLA	C5-C6-C7-C8
18	B	508	CLA	C11-C12-C13-C15
18	B	509	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	B	512	CLA	C11-C10-C8-C7
18	B	513	CLA	C11-C10-C8-C7
18	C	502	CLA	C11-C12-C13-C15
18	C	506	CLA	C12-C13-C15-C16
18	C	507	CLA	C12-C13-C15-C16
18	C	510	CLA	C6-C7-C8-C10
18	C	513	CLA	C11-C10-C8-C7
18	D	401	CLA	C12-C13-C15-C16
18	b	508	CLA	C11-C12-C13-C15
18	b	509	CLA	C6-C7-C8-C10
18	b	512	CLA	C6-C7-C8-C10
18	b	512	CLA	C11-C10-C8-C7
18	c	507	CLA	C12-C13-C15-C16
18	c	508	CLA	C12-C13-C15-C16
18	c	511	CLA	C6-C7-C8-C10
18	d	401	CLA	C12-C13-C15-C16
18	d	405	CLA	C12-C13-C15-C16
19	A	404	PHO	C11-C12-C13-C15
19	D	402	PHO	C11-C10-C8-C7
19	a	404	PHO	C11-C12-C13-C15
19	d	402	PHO	C11-C10-C8-C7
22	b	521	LHG	O10-C23-O8-C6
18	b	506	CLA	C5-C6-C7-C8
18	C	506	CLA	C16-C17-C18-C20
24	C	519	DGD	C9B-CAB-CBB-CCB
18	b	501	CLA	CBA-CGA-O2A-C1
24	C	519	DGD	CBB-CCB-CDB-CEB
18	C	505	CLA	C10-C11-C12-C13
18	b	504	CLA	C13-C15-C16-C17
18	a	405	CLA	C2A-CAA-CBA-CGA
22	b	521	LHG	C8-C7-O7-C5
23	C	501	SQD	C8-C7-O47-C45
24	c	519	DGD	CBB-CCB-CDB-CEB
18	B	501	CLA	CBA-CGA-O2A-C1
18	d	404	CLA	C4C-C3C-CAC-CBC
18	B	504	CLA	C13-C15-C16-C17
19	A	404	PHO	C5-C6-C7-C8
18	B	504	CLA	CAD-CBD-CGD-O2D
18	B	509	CLA	CAD-CBD-CGD-O2D
18	C	507	CLA	CAD-CBD-CGD-O2D
18	b	504	CLA	CAD-CBD-CGD-O2D
18	b	509	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	c	508	CLA	CAD-CBD-CGD-O2D
19	a	404	PHO	C5-C6-C7-C8
21	C	521	LMG	C10-C11-C12-C13
23	C	501	SQD	C24-C23-O48-C46
23	c	501	SQD	C24-C23-O48-C46
27	d	407	PL9	C39-C41-C42-C43
21	D	410	LMG	C7-C8-C9-O8
18	C	508	CLA	O1A-CGA-O2A-C1
22	B	522	LHG	C8-C7-O7-C5
24	c	518	DGD	C2B-C1B-O2G-C2G
18	B	504	CLA	C8-C10-C11-C12
18	C	510	CLA	C15-C16-C17-C18
28	e	101	HEM	C4D-C3D-CAD-CBD
28	F	101	HEM	C4B-C3B-CAB-CBB
28	e	101	HEM	C4B-C3B-CAB-CBB
18	B	502	CLA	C2A-CAA-CBA-CGA
18	C	504	CLA	C8-C10-C11-C12
22	B	522	LHG	O9-C7-O7-C5
22	b	521	LHG	O9-C7-O7-C5
18	A	405	CLA	CHA-CBD-CGD-O1D
18	A	405	CLA	CHA-CBD-CGD-O2D
18	B	505	CLA	CHA-CBD-CGD-O1D
18	B	513	CLA	CHA-CBD-CGD-O1D
18	B	513	CLA	CHA-CBD-CGD-O2D
18	B	516	CLA	CHA-CBD-CGD-O1D
18	B	516	CLA	CHA-CBD-CGD-O2D
18	C	502	CLA	CHA-CBD-CGD-O1D
18	C	502	CLA	CHA-CBD-CGD-O2D
18	C	509	CLA	CHA-CBD-CGD-O1D
18	C	509	CLA	CHA-CBD-CGD-O2D
18	C	510	CLA	CHA-CBD-CGD-O1D
18	C	510	CLA	CHA-CBD-CGD-O2D
18	C	513	CLA	CHA-CBD-CGD-O1D
18	C	513	CLA	CHA-CBD-CGD-O2D
18	a	405	CLA	CHA-CBD-CGD-O1D
18	a	405	CLA	CHA-CBD-CGD-O2D
18	b	505	CLA	CHA-CBD-CGD-O1D
18	b	505	CLA	CHA-CBD-CGD-O2D
18	b	516	CLA	CHA-CBD-CGD-O1D
18	b	516	CLA	CHA-CBD-CGD-O2D
18	c	503	CLA	CHA-CBD-CGD-O1D
18	c	503	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	c	509	CLA	CHA-CBD-CGD-O1D
18	c	509	CLA	CHA-CBD-CGD-O2D
18	c	510	CLA	CHA-CBD-CGD-O1D
18	c	510	CLA	CHA-CBD-CGD-O2D
18	c	511	CLA	CHA-CBD-CGD-O1D
18	c	511	CLA	CHA-CBD-CGD-O2D
18	c	514	CLA	CHA-CBD-CGD-O1D
18	B	501	CLA	O1A-CGA-O2A-C1
18	B	513	CLA	O1A-CGA-O2A-C1
18	b	501	CLA	O1A-CGA-O2A-C1
18	c	509	CLA	O1A-CGA-O2A-C1
22	B	522	LHG	O10-C23-O8-C6
18	D	405	CLA	C13-C15-C16-C17
23	c	501	SQD	O6-C44-C45-O47
21	C	521	LMG	C30-C31-C32-C33
27	d	407	PL9	C43-C44-C46-C47
21	h	101	LMG	O9-C10-O7-C8
23	C	501	SQD	O49-C7-O47-C45
24	C	518	DGD	O1B-C1B-O2G-C2G
24	c	518	DGD	O1B-C1B-O2G-C2G
18	B	511	CLA	C8-C10-C11-C12
18	C	511	CLA	C11-C12-C13-C14
18	D	401	CLA	C14-C13-C15-C16
18	b	513	CLA	C11-C10-C8-C9
18	c	503	CLA	C11-C12-C13-C14
19	A	404	PHO	C11-C12-C13-C14
19	D	402	PHO	C11-C10-C8-C9
19	a	404	PHO	C11-C12-C13-C14
19	d	402	PHO	C11-C10-C8-C9
23	C	501	SQD	C5-C6-S-O8
18	A	405	CLA	C2A-CAA-CBA-CGA
18	d	405	CLA	C13-C15-C16-C17
18	b	504	CLA	C2C-C3C-CAC-CBC
18	b	511	CLA	C8-C10-C11-C12
24	C	518	DGD	C2B-C1B-O2G-C2G
24	c	519	DGD	C2B-C1B-O2G-C2G
22	x	101	LHG	C11-C12-C13-C14
18	C	502	CLA	C8-C10-C11-C12
22	l	101	LHG	C12-C13-C14-C15
18	d	401	CLA	C4B-C3B-CAB-CBB
22	A	408	LHG	C3-O3-P-O4
22	A	408	LHG	C4-O6-P-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	A	409	LHG	C4-O6-P-O4
22	B	521	LHG	C3-O3-P-O4
22	B	522	LHG	C3-O3-P-O4
22	D	408	LHG	C4-O6-P-O4
22	L	101	LHG	C3-O3-P-O4
22	a	407	LHG	C3-O3-P-O4
22	a	407	LHG	C4-O6-P-O5
22	a	408	LHG	C4-O6-P-O4
22	b	520	LHG	C3-O3-P-O4
22	b	521	LHG	C3-O3-P-O4
22	l	101	LHG	C3-O3-P-O4
18	c	507	CLA	C16-C17-C18-C20
18	b	513	CLA	CBA-CGA-O2A-C1
23	C	501	SQD	O10-C23-O48-C46
18	b	513	CLA	O1A-CGA-O2A-C1
18	B	505	CLA	CAD-CBD-CGD-O1D
18	B	506	CLA	CAD-CBD-CGD-O1D
18	B	514	CLA	CAD-CBD-CGD-O1D
18	B	516	CLA	CAD-CBD-CGD-O1D
18	C	502	CLA	CAD-CBD-CGD-O1D
18	C	505	CLA	CAD-CBD-CGD-O1D
18	C	506	CLA	CAD-CBD-CGD-O1D
18	b	505	CLA	CAD-CBD-CGD-O1D
18	b	506	CLA	CAD-CBD-CGD-O1D
18	b	514	CLA	CAD-CBD-CGD-O1D
18	b	516	CLA	CAD-CBD-CGD-O1D
18	c	503	CLA	CAD-CBD-CGD-O1D
18	c	506	CLA	CAD-CBD-CGD-O1D
18	c	507	CLA	CAD-CBD-CGD-O1D
18	d	404	CLA	CAD-CBD-CGD-O1D
23	C	501	SQD	C5-C6-S-O9
18	B	504	CLA	C2C-C3C-CAC-CBC
18	c	503	CLA	CBA-CGA-O2A-C1
23	c	501	SQD	O10-C23-O48-C46
22	X	101	LHG	C11-C12-C13-C14
18	B	510	CLA	C12-C13-C15-C16
18	B	511	CLA	C6-C7-C8-C10
18	B	512	CLA	C6-C7-C8-C10
18	C	505	CLA	C12-C13-C15-C16
18	C	506	CLA	C11-C12-C13-C15
18	C	511	CLA	C11-C10-C8-C7
18	b	510	CLA	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	b	511	CLA	C6-C7-C8-C10
18	b	511	CLA	C11-C12-C13-C15
18	c	503	CLA	C11-C12-C13-C15
18	c	505	CLA	C11-C10-C8-C7
18	c	506	CLA	C12-C13-C15-C16
18	c	507	CLA	C11-C12-C13-C15
18	c	512	CLA	C11-C10-C8-C7
18	c	514	CLA	C11-C10-C8-C7
18	b	510	CLA	C15-C16-C17-C18
21	D	410	LMG	C11-C10-O7-C8
24	C	519	DGD	C2B-C1B-O2G-C2G
18	b	502	CLA	C2A-CAA-CBA-CGA
18	B	513	CLA	C16-C17-C18-C20
18	b	513	CLA	C16-C17-C18-C20
19	A	404	PHO	C8-C10-C11-C12
22	A	409	LHG	C14-C15-C16-C17
22	a	408	LHG	C14-C15-C16-C17
18	C	506	CLA	O2A-C1-C2-C3
18	C	506	CLA	C16-C17-C18-C19
18	B	510	CLA	C15-C16-C17-C18
18	C	506	CLA	C10-C11-C12-C13
27	d	407	PL9	C30-C29-C31-C32
18	B	501	CLA	C11-C12-C13-C14
18	B	510	CLA	C14-C13-C15-C16
18	C	502	CLA	C11-C12-C13-C14
18	C	507	CLA	C14-C13-C15-C16
18	C	510	CLA	C6-C7-C8-C9
18	D	405	CLA	C14-C13-C15-C16
18	b	501	CLA	C11-C12-C13-C14
18	b	504	CLA	C6-C7-C8-C9
18	b	510	CLA	C14-C13-C15-C16
18	c	508	CLA	C14-C13-C15-C16
18	c	511	CLA	C6-C7-C8-C9
18	c	514	CLA	C11-C10-C8-C9
18	c	503	CLA	O1A-CGA-O2A-C1
21	D	410	LMG	C38-C39-C40-C41
18	c	505	CLA	C8-C10-C11-C12
18	C	512	CLA	C2B-C3B-CAB-CBB
18	D	405	CLA	C2B-C3B-CAB-CBB
18	c	513	CLA	C2B-C3B-CAB-CBB
18	d	401	CLA	C2B-C3B-CAB-CBB
24	c	519	DGD	O1B-C1B-O2G-C2G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	b	513	CLA	C5-C6-C7-C8
22	L	101	LHG	C11-C12-C13-C14
18	c	512	CLA	C16-C17-C18-C19
28	e	101	HEM	C2D-C3D-CAD-CBD
21	D	410	LMG	C35-C36-C37-C38
22	a	407	LHG	C33-C34-C35-C36
21	D	410	LMG	O9-C10-O7-C8
18	b	501	CLA	C2-C1-O2A-CGA
18	c	512	CLA	C2-C1-O2A-CGA
18	c	507	CLA	C10-C11-C12-C13
22	A	408	LHG	C33-C34-C35-C36
18	C	511	CLA	C16-C17-C18-C19
24	C	519	DGD	O1B-C1B-O2G-C2G
18	b	516	CLA	C13-C15-C16-C17
22	A	408	LHG	C34-C35-C36-C37
22	l	101	LHG	C11-C12-C13-C14
18	b	509	CLA	C5-C6-C7-C8
18	c	508	CLA	C8-C10-C11-C12
23	c	501	SQD	O47-C45-C46-O48
22	D	408	LHG	C3-O3-P-O6
22	L	101	LHG	C4-O6-P-O3
22	d	408	LHG	C3-O3-P-O6
22	l	101	LHG	C4-O6-P-O3
19	a	404	PHO	C8-C10-C11-C12
22	B	522	LHG	C4-C5-C6-O8
22	b	521	LHG	C4-C5-C6-O8
18	b	513	CLA	C11-C10-C8-C7
18	d	404	CLA	C12-C13-C15-C16
22	X	101	LHG	O10-C23-O8-C6
22	A	409	LHG	C24-C25-C26-C27
18	B	512	CLA	C6-C7-C8-C9
18	C	513	CLA	C11-C10-C8-C9
18	b	512	CLA	C6-C7-C8-C9
18	c	504	CLA	C11-C10-C8-C9
18	c	512	CLA	C11-C10-C8-C9
22	X	101	LHG	C24-C23-O8-C6
18	B	513	CLA	C16-C17-C18-C19
18	b	513	CLA	C16-C17-C18-C19
22	a	407	LHG	C34-C35-C36-C37
21	B	520	LMG	C30-C31-C32-C33
24	C	520	DGD	C7B-C8B-C9B-CAB
18	B	516	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	h	101	LMG	C38-C39-C40-C41
24	c	520	DGD	C7B-C8B-C9B-CAB
18	B	509	CLA	C5-C6-C7-C8
21	c	521	LMG	C30-C31-C32-C33
18	c	507	CLA	C16-C17-C18-C19
21	D	409	LMG	C29-C28-O8-C9
21	d	409	LMG	C29-C28-O8-C9
22	x	101	LHG	C24-C23-O8-C6
18	C	507	CLA	C8-C10-C11-C12
18	B	503	CLA	C4B-C3B-CAB-CBB
18	D	404	CLA	C4B-C3B-CAB-CBB
27	D	407	PL9	C34-C36-C37-C38
22	x	101	LHG	O10-C23-O8-C6
21	h	101	LMG	C35-C36-C37-C38
22	X	101	LHG	C27-C28-C29-C30
18	B	503	CLA	C15-C16-C17-C18
21	b	519	LMG	C30-C31-C32-C33
18	A	403	CLA	C3A-C2A-CAA-CBA
18	B	504	CLA	C3A-C2A-CAA-CBA
18	a	403	CLA	C3A-C2A-CAA-CBA
18	b	504	CLA	C3A-C2A-CAA-CBA
22	A	409	LHG	O9-C7-O7-C5
22	a	408	LHG	O9-C7-O7-C5
18	a	403	CLA	O2A-C1-C2-C3
22	x	101	LHG	C27-C28-C29-C30
27	D	407	PL9	C30-C29-C31-C32
18	B	508	CLA	C6-C7-C8-C9
18	B	511	CLA	C6-C7-C8-C9
18	C	508	CLA	C6-C7-C8-C9
18	b	508	CLA	C6-C7-C8-C9
18	b	511	CLA	C6-C7-C8-C9
18	c	505	CLA	C11-C10-C8-C9
18	c	509	CLA	C6-C7-C8-C9
23	c	501	SQD	C44-C45-C46-O48
21	d	409	LMG	O10-C28-O8-C9
18	B	515	CLA	O2A-C1-C2-C3
18	B	516	CLA	O2A-C1-C2-C3
18	b	515	CLA	O2A-C1-C2-C3
24	c	519	DGD	C1B-C2B-C3B-C4B
18	A	405	CLA	C6-C7-C8-C10
18	C	504	CLA	C11-C10-C8-C7
18	a	405	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	D	409	LMG	O10-C28-O8-C9
22	A	409	LHG	C11-C10-C9-C8
22	a	408	LHG	C24-C25-C26-C27
22	a	408	LHG	C11-C10-C9-C8
18	A	403	CLA	O2A-C1-C2-C3
18	b	503	CLA	C15-C16-C17-C18
18	B	503	CLA	C2B-C3B-CAB-CBB
18	C	508	CLA	C2B-C3B-CAB-CBB
18	D	404	CLA	C2B-C3B-CAB-CBB
18	c	509	CLA	C2B-C3B-CAB-CBB
22	A	408	LHG	C32-C33-C34-C35
22	a	407	LHG	C32-C33-C34-C35
21	A	407	LMG	O1-C7-C8-O7
21	c	502	LMG	O1-C7-C8-O7
21	h	101	LMG	C39-C40-C41-C42
18	A	402	CLA	C4C-C3C-CAC-CBC
18	C	511	CLA	C2-C1-O2A-CGA
18	C	511	CLA	C11-C10-C8-C9
22	L	101	LHG	C12-C13-C14-C15
18	B	505	CLA	C8-C10-C11-C12
18	b	501	CLA	CAA-CBA-CGA-O2A
24	C	519	DGD	O1G-C1G-C2G-C3G
24	C	519	DGD	C8B-C9B-CAB-CBB
25	c	522	LMU	C1-C2-C3-C4
22	A	409	LHG	O10-C23-O8-C6
18	c	512	CLA	C16-C17-C18-C20
18	B	501	CLA	CAA-CBA-CGA-O2A
18	B	507	CLA	C16-C17-C18-C20
18	b	507	CLA	C16-C17-C18-C20
22	a	408	LHG	C7-C8-C9-C10
18	D	401	CLA	C2A-CAA-CBA-CGA
18	C	508	CLA	C4B-C3B-CAB-CBB
18	b	512	CLA	C4B-C3B-CAB-CBB
18	c	509	CLA	C4B-C3B-CAB-CBB
18	d	404	CLA	C4B-C3B-CAB-CBB
22	a	407	LHG	O6-C4-C5-C6
18	B	515	CLA	C12-C13-C15-C16
18	b	515	CLA	C12-C13-C15-C16
19	d	402	PHO	C11-C12-C13-C15
22	A	409	LHG	C24-C23-O8-C6
19	A	404	PHO	C10-C11-C12-C13
19	a	404	PHO	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	D	410	LMG	C39-C40-C41-C42
18	A	402	CLA	C15-C16-C17-C18
18	c	505	CLA	CAA-CBA-CGA-O2A
22	L	101	LHG	C17-C18-C19-C20
24	c	519	DGD	C8B-C9B-CAB-CBB
18	B	511	CLA	CAA-CBA-CGA-O2A
18	d	401	CLA	C2A-CAA-CBA-CGA
18	C	511	CLA	C16-C17-C18-C20
18	b	516	CLA	C16-C17-C18-C20
21	h	101	LMG	C19-C20-C21-C22
21	h	101	LMG	C29-C30-C31-C32
22	a	408	LHG	C24-C23-O8-C6
18	b	508	CLA	C16-C17-C18-C20
18	b	511	CLA	CAA-CBA-CGA-O2A
18	a	402	CLA	C4C-C3C-CAC-CBC
18	B	505	CLA	C6-C7-C8-C9
18	B	513	CLA	C14-C13-C15-C16
18	C	504	CLA	C11-C10-C8-C9
18	C	506	CLA	C11-C12-C13-C14
18	b	505	CLA	C6-C7-C8-C9
18	b	505	CLA	C11-C12-C13-C14
18	b	513	CLA	C14-C13-C15-C16
18	c	505	CLA	C11-C12-C13-C14
18	c	506	CLA	C14-C13-C15-C16
18	c	507	CLA	C11-C12-C13-C14
18	B	510	CLA	C3A-C2A-CAA-CBA
18	b	510	CLA	C3A-C2A-CAA-CBA
18	c	511	CLA	C3A-C2A-CAA-CBA
28	F	101	HEM	C4D-C3D-CAD-CBD
18	b	513	CLA	C10-C11-C12-C13
22	a	408	LHG	O10-C23-O8-C6
18	c	511	CLA	CAA-CBA-CGA-O2A
18	B	511	CLA	CAD-CBD-CGD-O2D
18	B	512	CLA	CAD-CBD-CGD-O2D
18	C	503	CLA	CAD-CBD-CGD-O2D
18	D	405	CLA	CAD-CBD-CGD-O2D
18	b	511	CLA	CAD-CBD-CGD-O2D
18	b	512	CLA	CAD-CBD-CGD-O2D
18	c	504	CLA	CAD-CBD-CGD-O2D
18	d	405	CLA	CAD-CBD-CGD-O2D
18	a	402	CLA	C15-C16-C17-C18
18	b	505	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	D	409	LMG	O9-C10-O7-C8
23	c	501	SQD	O49-C7-O47-C45
18	C	504	CLA	CAA-CBA-CGA-O2A
18	d	404	CLA	C2C-C3C-CAC-CBC
21	D	410	LMG	C29-C30-C31-C32
20	X	102	BCR	C7-C8-C9-C10
21	D	409	LMG	C17-C18-C19-C20
22	l	101	LHG	C13-C14-C15-C16
24	c	519	DGD	O1G-C1G-C2G-C3G
25	C	522	LMU	C6-C7-C8-C9
18	b	508	CLA	C13-C15-C16-C17
18	C	507	CLA	O2A-C1-C2-C3
18	C	513	CLA	O2A-C1-C2-C3
18	D	401	CLA	O2A-C1-C2-C3
18	D	404	CLA	O2A-C1-C2-C3
18	b	516	CLA	O2A-C1-C2-C3
18	c	508	CLA	O2A-C1-C2-C3
18	c	514	CLA	O2A-C1-C2-C3
18	d	401	CLA	O2A-C1-C2-C3
18	b	508	CLA	C2A-CAA-CBA-CGA
18	B	507	CLA	CAA-CBA-CGA-O2A
18	b	507	CLA	CAA-CBA-CGA-O2A
21	d	409	LMG	C17-C18-C19-C20
22	A	409	LHG	C7-C8-C9-C10
18	B	505	CLA	CHA-CBD-CGD-O2D
18	B	515	CLA	CHA-CBD-CGD-O1D
18	C	508	CLA	CHA-CBD-CGD-O1D
18	C	508	CLA	CHA-CBD-CGD-O2D
18	a	403	CLA	CHA-CBD-CGD-O1D
18	a	403	CLA	CHA-CBD-CGD-O2D
18	b	512	CLA	CHA-CBD-CGD-O1D
18	b	513	CLA	CHA-CBD-CGD-O1D
18	b	513	CLA	CHA-CBD-CGD-O2D
18	b	515	CLA	CHA-CBD-CGD-O1D
18	c	512	CLA	CHA-CBD-CGD-O1D
18	c	512	CLA	CHA-CBD-CGD-O2D
18	c	514	CLA	CHA-CBD-CGD-O2D
18	c	515	CLA	CHA-CBD-CGD-O1D
22	A	408	LHG	O6-C4-C5-C6
18	B	516	CLA	C16-C17-C18-C20
22	L	101	LHG	O8-C23-C24-C25
23	C	501	SQD	O47-C45-C46-O48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	C	522	LMU	C1-C2-C3-C4
18	B	508	CLA	C13-C15-C16-C17
18	d	401	CLA	C8-C10-C11-C12
19	A	404	PHO	CHA-CBD-CGD-O1D
22	A	409	LHG	C8-C7-O7-C5
22	a	408	LHG	C8-C7-O7-C5
21	c	521	LMG	O8-C28-C29-C30
25	c	522	LMU	C6-C7-C8-C9
18	b	501	CLA	C11-C10-C8-C7
18	b	510	CLA	C11-C10-C8-C7
18	B	508	CLA	C16-C17-C18-C20
22	X	101	LHG	C12-C13-C14-C15
18	B	502	CLA	CAA-CBA-CGA-O2A
22	a	407	LHG	O8-C23-C24-C25
18	B	510	CLA	C11-C10-C8-C9
18	C	505	CLA	C14-C13-C15-C16
18	C	506	CLA	C6-C7-C8-C9
18	b	510	CLA	C11-C10-C8-C9
28	e	101	HEM	CAA-CBA-CGA-O2A
18	b	511	CLA	CAA-CBA-CGA-O1A
23	C	501	SQD	C4-C5-C6-S
23	c	501	SQD	C4-C5-C6-S
18	b	508	CLA	C16-C17-C18-C19
23	c	501	SQD	C8-C7-O47-C45
22	A	408	LHG	O8-C23-C24-C25
22	x	101	LHG	O8-C23-C24-C25
22	x	101	LHG	C12-C13-C14-C15
28	F	101	HEM	CAA-CBA-CGA-O2A
18	B	511	CLA	CAA-CBA-CGA-O1A
18	b	516	CLA	C16-C17-C18-C19
24	c	520	DGD	C7A-C8A-C9A-CAA
28	F	101	HEM	C2D-C3D-CAD-CBD
18	b	502	CLA	CAA-CBA-CGA-O2A
25	C	522	LMU	C2B-C1B-O1B-C4'
20	x	102	BCR	C7-C8-C9-C10
18	A	402	CLA	C13-C15-C16-C17
23	C	501	SQD	C10-C11-C12-C13
23	c	501	SQD	C9-C10-C11-C12
24	C	520	DGD	C7A-C8A-C9A-CAA
18	A	403	CLA	C1A-C2A-CAA-CBA
18	B	505	CLA	C1A-C2A-CAA-CBA
18	B	510	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	a	403	CLA	C1A-C2A-CAA-CBA
18	b	505	CLA	C1A-C2A-CAA-CBA
18	b	510	CLA	C1A-C2A-CAA-CBA
18	c	511	CLA	C1A-C2A-CAA-CBA
18	b	506	CLA	C16-C17-C18-C19
22	D	408	LHG	O9-C7-O7-C5
22	L	101	LHG	C13-C14-C15-C16
22	x	101	LHG	C24-C25-C26-C27
24	C	520	DGD	C5A-C6A-C7A-C8A
22	L	101	LHG	C33-C34-C35-C36
23	C	501	SQD	O6-C44-C45-C46
18	B	508	CLA	C2A-CAA-CBA-CGA
18	b	505	CLA	C2A-CAA-CBA-CGA
22	X	101	LHG	C24-C25-C26-C27
22	B	521	LHG	C35-C36-C37-C38
24	c	520	DGD	C5A-C6A-C7A-C8A
18	C	510	CLA	CAA-CBA-CGA-O2A
22	X	101	LHG	O8-C23-C24-C25
22	l	101	LHG	O8-C23-C24-C25
18	D	401	CLA	C4B-C3B-CAB-CBB
22	D	408	LHG	C3-O3-P-O5
22	L	101	LHG	C4-O6-P-O5
22	d	408	LHG	C4-O6-P-O4
22	l	101	LHG	C4-O6-P-O5
22	b	520	LHG	C35-C36-C37-C38
20	C	516	BCR	C5-C6-C7-C8
20	c	516	BCR	C5-C6-C7-C8
18	B	502	CLA	CAA-CBA-CGA-O1A
18	c	511	CLA	CAA-CBA-CGA-O1A
22	X	101	LHG	C30-C31-C32-C33
22	x	101	LHG	C30-C31-C32-C33
21	h	101	LMG	C4-C5-C6-O5
18	B	508	CLA	C16-C17-C18-C19
18	B	516	CLA	C16-C17-C18-C19
23	c	501	SQD	C10-C11-C12-C13
18	B	505	CLA	C2A-CAA-CBA-CGA
18	B	512	CLA	C2A-CAA-CBA-CGA
18	c	515	CLA	C2A-CAA-CBA-CGA
18	B	503	CLA	C8-C10-C11-C12
24	C	519	DGD	C1B-C2B-C3B-C4B
22	A	408	LHG	O10-C23-C24-C25
18	B	506	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	B	503	CLA	CAD-CBD-CGD-O1D
18	C	514	CLA	CAD-CBD-CGD-O1D
18	D	404	CLA	CAD-CBD-CGD-O1D
18	b	503	CLA	CAD-CBD-CGD-O1D
18	c	515	CLA	CAD-CBD-CGD-O1D
18	B	501	CLA	C11-C10-C8-C9
18	B	503	CLA	C11-C12-C13-C14
18	B	505	CLA	C11-C12-C13-C14
18	B	511	CLA	C11-C10-C8-C9
18	b	501	CLA	C11-C10-C8-C9
18	b	503	CLA	C11-C12-C13-C14
18	b	511	CLA	C11-C10-C8-C9
28	e	101	HEM	CAA-CBA-CGA-O1A
18	B	513	CLA	C10-C11-C12-C13
18	A	403	CLA	CAA-CBA-CGA-O2A
18	C	507	CLA	CAA-CBA-CGA-O2A
18	C	511	CLA	CAA-CBA-CGA-O2A
18	a	403	CLA	CAA-CBA-CGA-O2A
18	b	504	CLA	CAA-CBA-CGA-O2A
18	b	509	CLA	CAA-CBA-CGA-O2A
18	c	508	CLA	CAA-CBA-CGA-O2A
18	c	510	CLA	CAA-CBA-CGA-O2A
22	l	101	LHG	C33-C34-C35-C36
18	b	504	CLA	C4C-C3C-CAC-CBC
19	d	402	PHO	C8-C10-C11-C12
23	C	501	SQD	C9-C10-C11-C12
18	B	504	CLA	CBA-CGA-O2A-C1
18	C	509	CLA	CAA-CBA-CGA-O2A
18	C	514	CLA	CAA-CBA-CGA-O2A
18	b	505	CLA	CAA-CBA-CGA-O2A
18	c	512	CLA	CAA-CBA-CGA-O2A
18	c	514	CLA	C13-C15-C16-C17
18	b	507	CLA	CAA-CBA-CGA-O1A
21	c	521	LMG	O10-C28-C29-C30
18	B	501	CLA	C11-C10-C8-C7
18	B	503	CLA	C11-C12-C13-C15
18	B	505	CLA	C11-C12-C13-C15
18	B	506	CLA	C11-C12-C13-C15
18	B	510	CLA	C11-C10-C8-C7
18	D	405	CLA	C12-C13-C15-C16
18	b	503	CLA	C11-C12-C13-C15
18	b	504	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	b	505	CLA	C11-C12-C13-C15
18	b	506	CLA	C11-C12-C13-C15
18	b	506	CLA	C12-C13-C15-C16
19	D	402	PHO	C11-C12-C13-C15
18	B	507	CLA	CAA-CBA-CGA-O1A
18	b	502	CLA	CAA-CBA-CGA-O1A
22	a	407	LHG	O10-C23-C24-C25
28	F	101	HEM	CAA-CBA-CGA-O1A
18	B	505	CLA	CAA-CBA-CGA-O2A
18	D	404	CLA	CAA-CBA-CGA-O2A
18	b	512	CLA	CAA-CBA-CGA-O2A
21	C	521	LMG	O8-C28-C29-C30
22	d	408	LHG	C9-C10-C11-C12
18	c	508	CLA	CAA-CBA-CGA-O1A
22	x	101	LHG	O10-C23-C24-C25
18	B	509	CLA	CAA-CBA-CGA-O2A
18	B	512	CLA	CAA-CBA-CGA-O2A
18	d	404	CLA	CAA-CBA-CGA-O2A
18	C	513	CLA	C13-C15-C16-C17
18	C	514	CLA	C8-C10-C11-C12
22	d	408	LHG	O9-C7-O7-C5
18	C	510	CLA	CAA-CBA-CGA-O1A
18	c	510	CLA	CAA-CBA-CGA-O1A
21	C	521	LMG	O10-C28-C29-C30
19	D	402	PHO	C8-C10-C11-C12
22	L	101	LHG	O10-C23-C24-C25
22	X	101	LHG	O10-C23-C24-C25
18	B	504	CLA	C4C-C3C-CAC-CBC
18	D	401	CLA	C8-C10-C11-C12
18	b	503	CLA	C8-C10-C11-C12
22	x	101	LHG	C23-C24-C25-C26
18	A	403	CLA	CAA-CBA-CGA-O1A
18	B	505	CLA	CAA-CBA-CGA-O1A
18	C	507	CLA	CAA-CBA-CGA-O1A
18	C	509	CLA	CAA-CBA-CGA-O1A
18	a	403	CLA	CAA-CBA-CGA-O1A
18	c	512	CLA	CAA-CBA-CGA-O1A
18	d	404	CLA	CAA-CBA-CGA-O1A
28	F	101	HEM	C1A-C2A-CAA-CBA
28	e	101	HEM	C1A-C2A-CAA-CBA
21	c	521	LMG	C13-C14-C15-C16

There are no ring outliers.

53 monomers are involved in 114 short contacts:

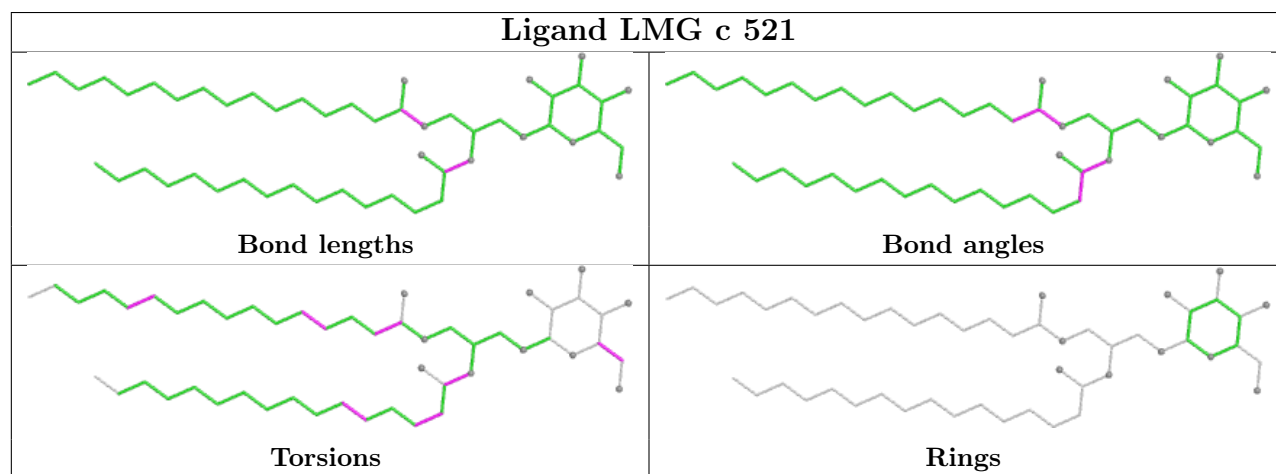
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	506	CLA	1	0
20	C	515	BCR	8	0
20	C	517	BCR	4	0
18	b	513	CLA	2	0
20	B	519	BCR	2	0
18	c	507	CLA	1	0
18	B	509	CLA	2	0
18	c	512	CLA	1	0
22	A	408	LHG	1	0
18	C	503	CLA	1	0
22	l	101	LHG	1	0
18	B	505	CLA	1	0
28	F	101	HEM	6	0
18	a	402	CLA	1	0
21	D	410	LMG	1	0
22	a	407	LHG	1	0
18	B	513	CLA	2	0
20	x	102	BCR	4	0
20	c	516	BCR	5	0
18	c	503	CLA	1	0
18	C	512	CLA	3	0
18	c	504	CLA	2	0
20	d	406	BCR	1	0
18	b	506	CLA	1	0
20	a	406	BCR	4	0
18	d	404	CLA	5	0
21	h	101	LMG	1	0
18	B	501	CLA	1	0
18	b	507	CLA	1	0
18	C	507	CLA	1	0
20	X	102	BCR	2	0
20	A	406	BCR	3	0
20	B	518	BCR	1	0
20	b	518	BCR	1	0
18	A	402	CLA	3	0
20	K	101	BCR	4	0
18	b	505	CLA	1	0
20	C	516	BCR	4	0
18	b	509	CLA	1	0
20	A	410	BCR	2	0
18	C	502	CLA	1	0
18	c	513	CLA	1	0

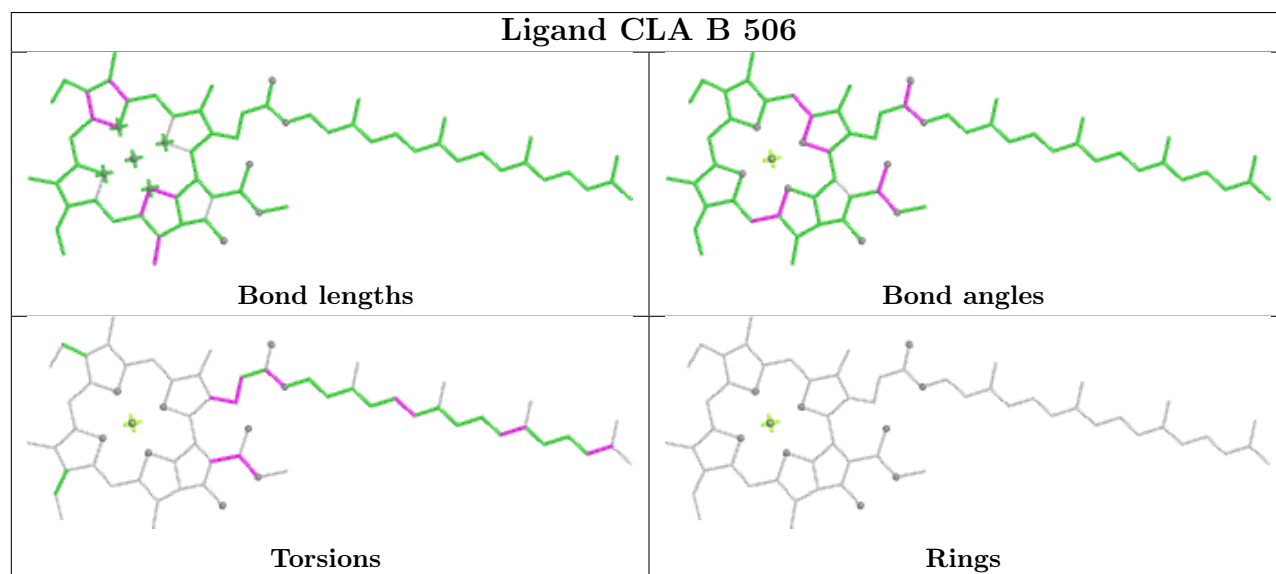
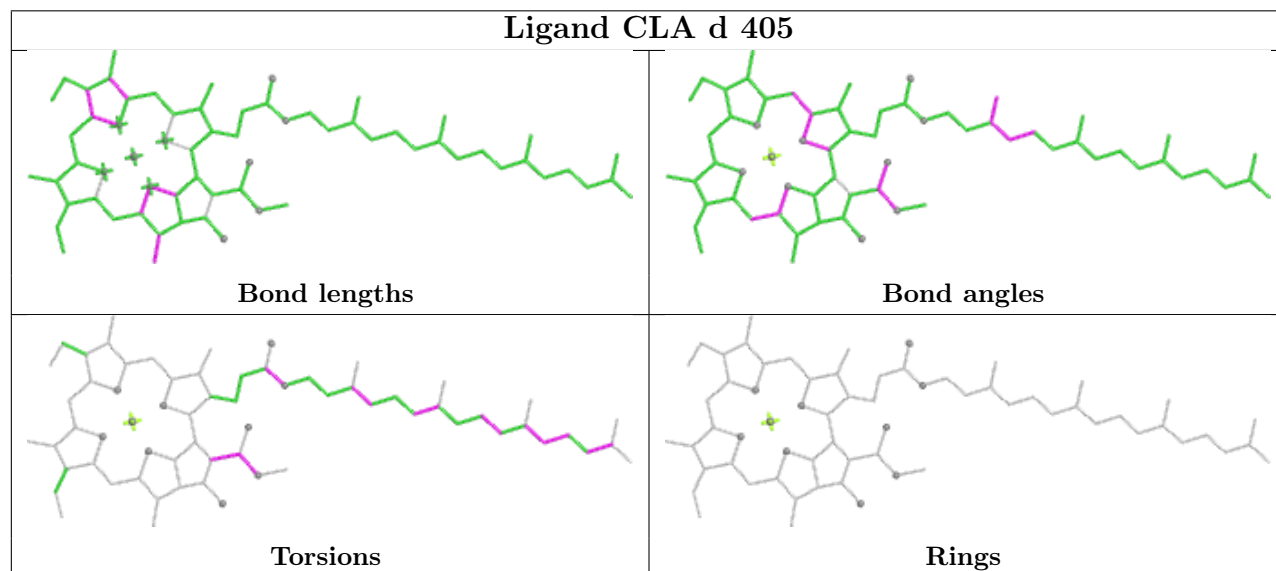
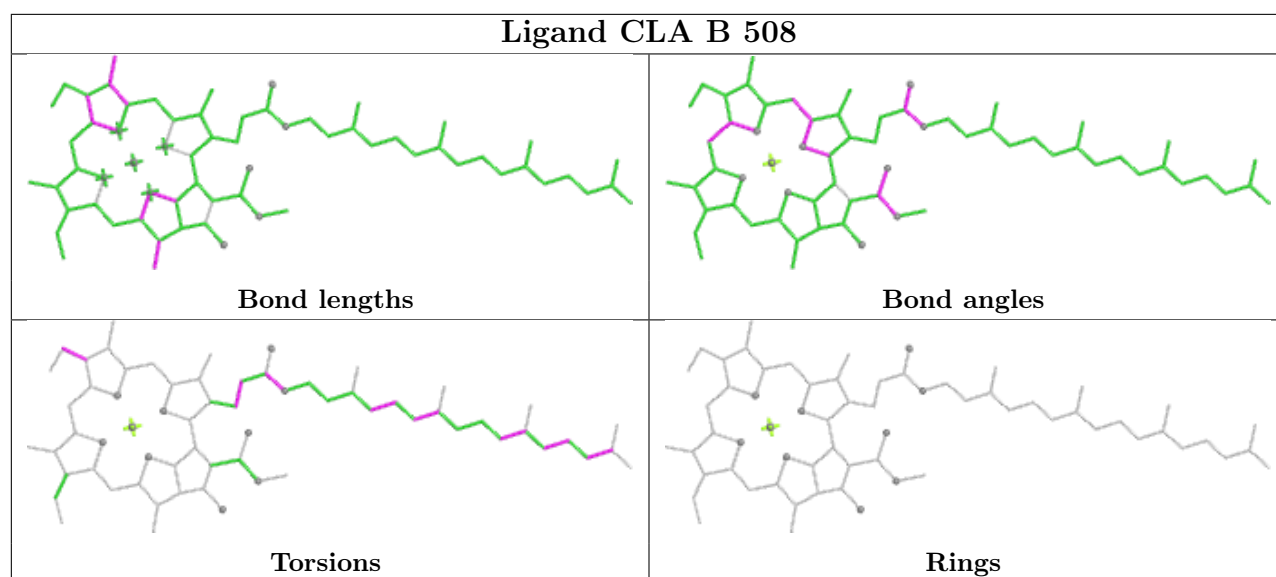
Continued on next page...

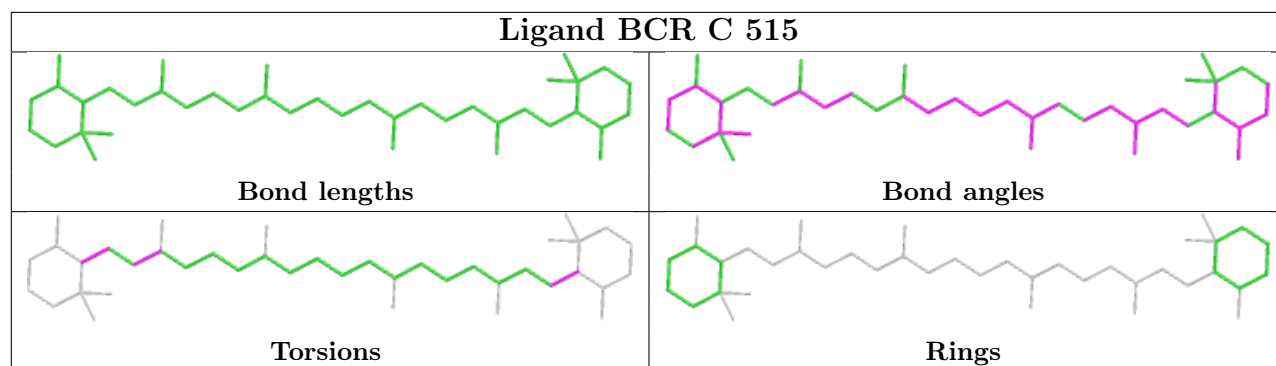
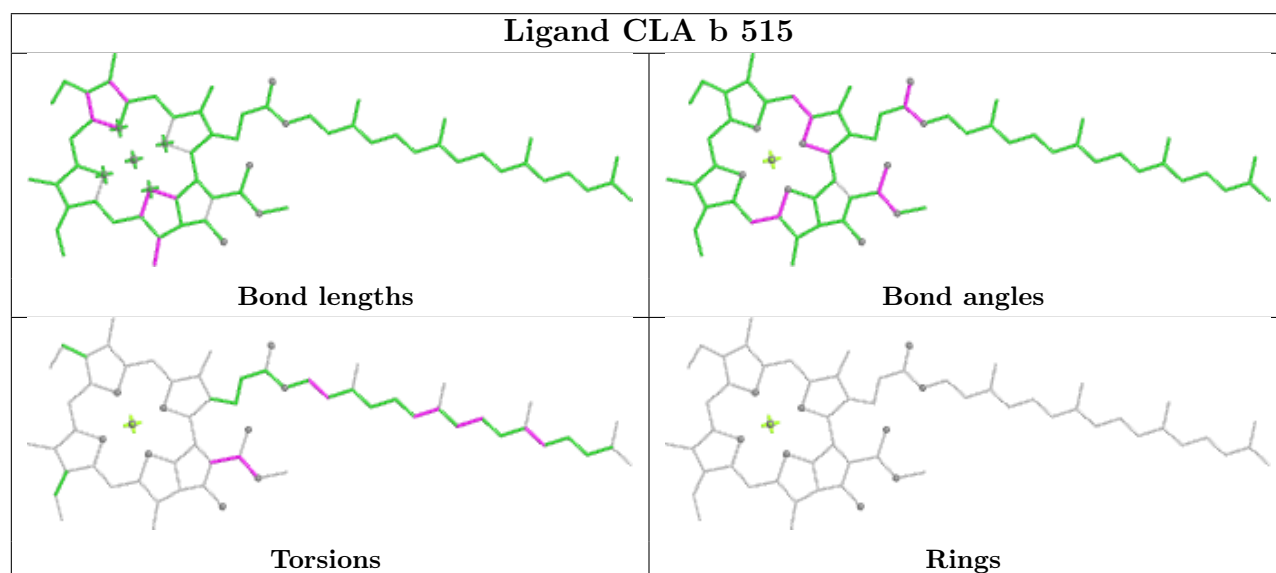
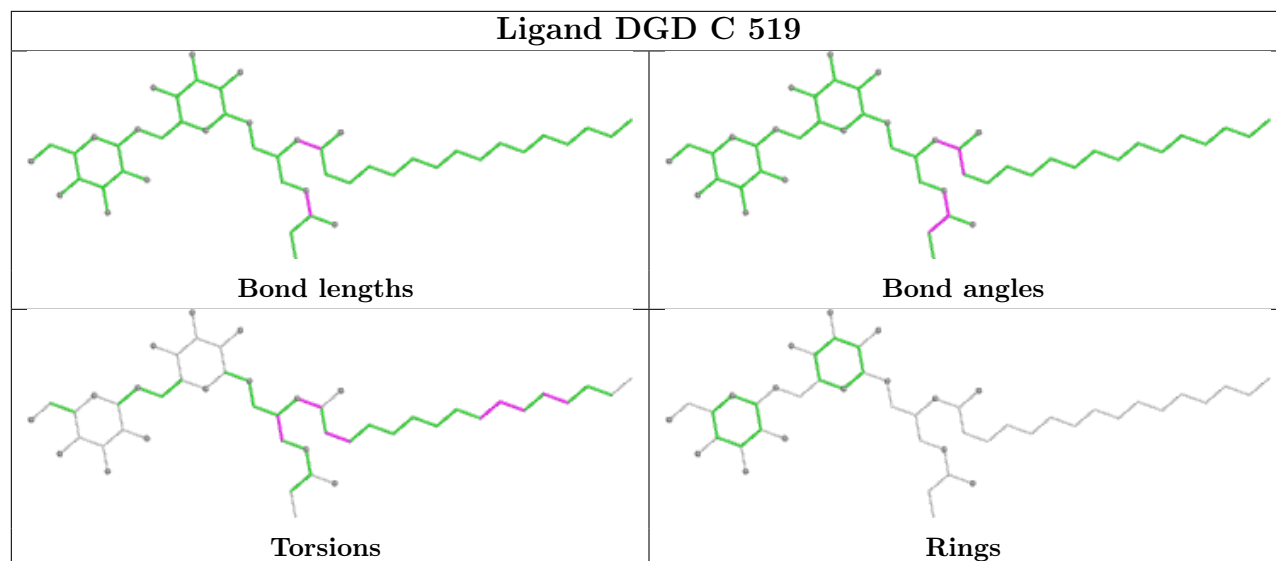
Continued from previous page...

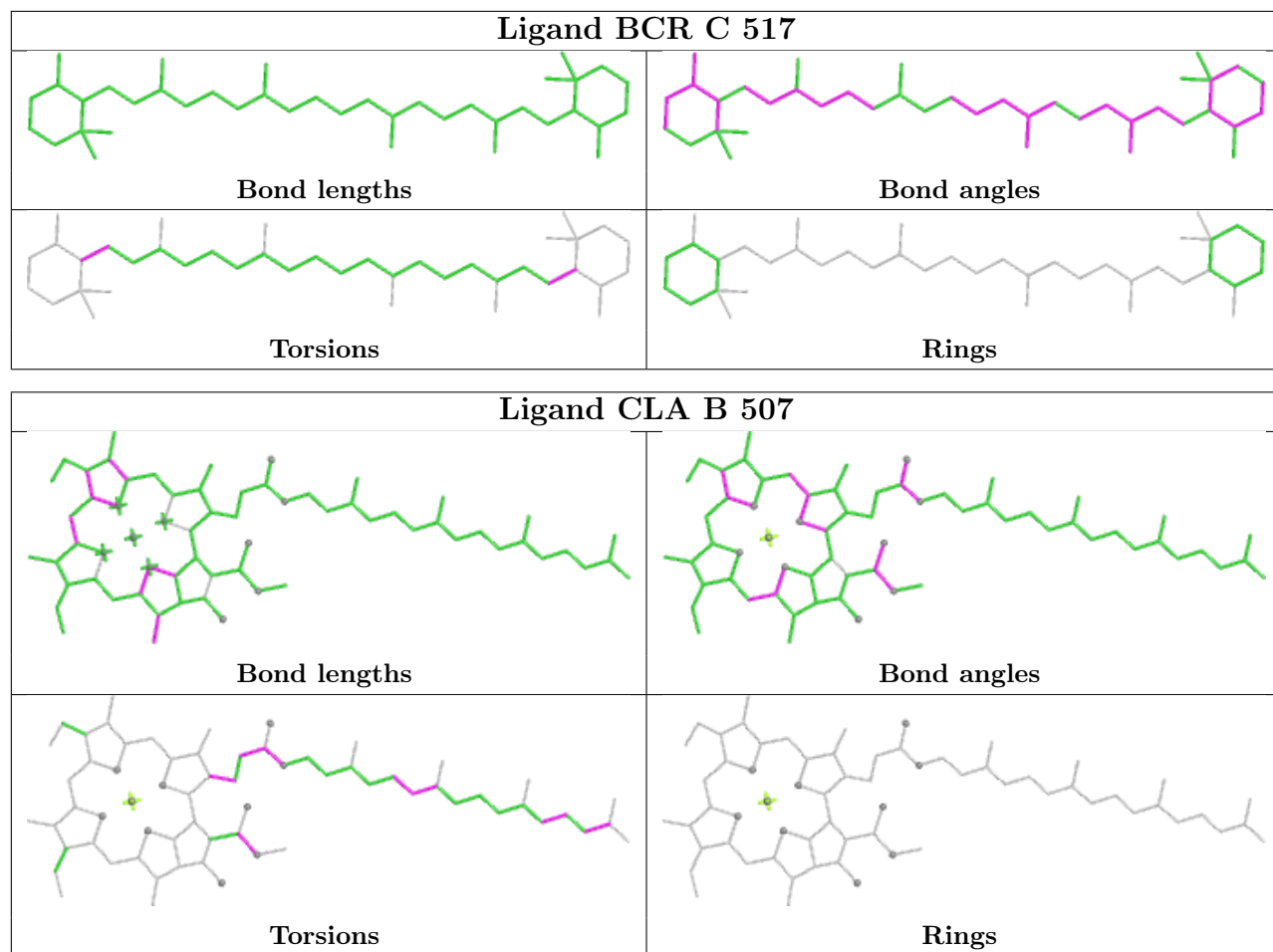
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	b	501	CLA	1	0
28	e	101	HEM	5	0
20	k	101	BCR	4	0
18	C	514	CLA	1	0
20	z	101	BCR	6	0
18	D	404	CLA	5	0
20	D	406	BCR	2	0
18	B	502	CLA	1	0
18	b	502	CLA	1	0
18	c	515	CLA	1	0
20	c	517	BCR	4	0

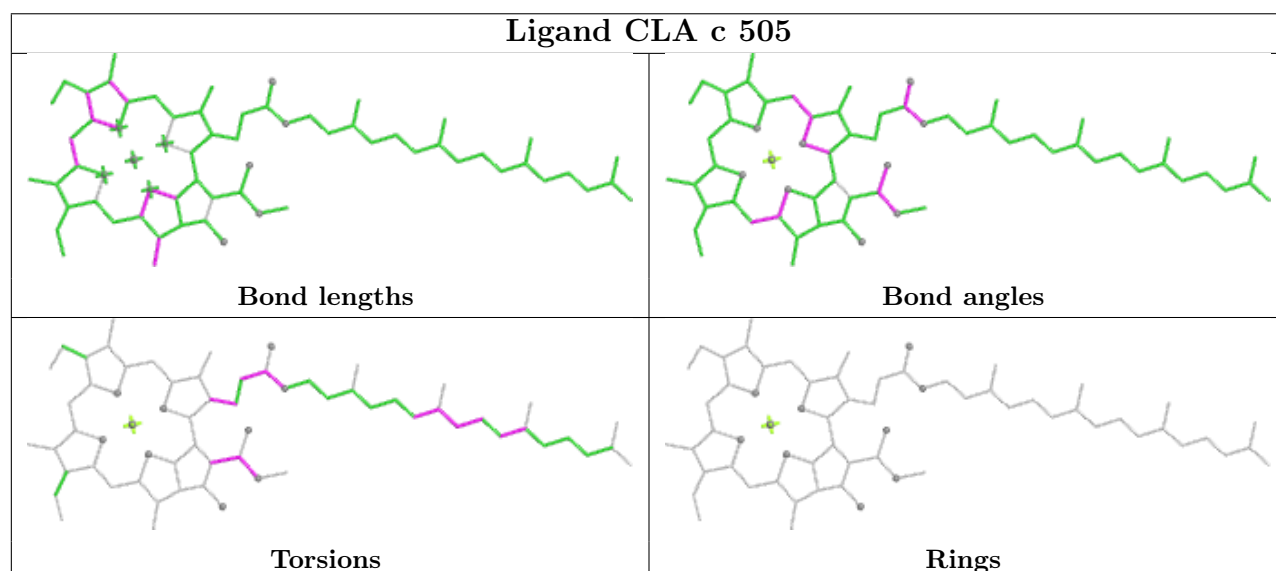
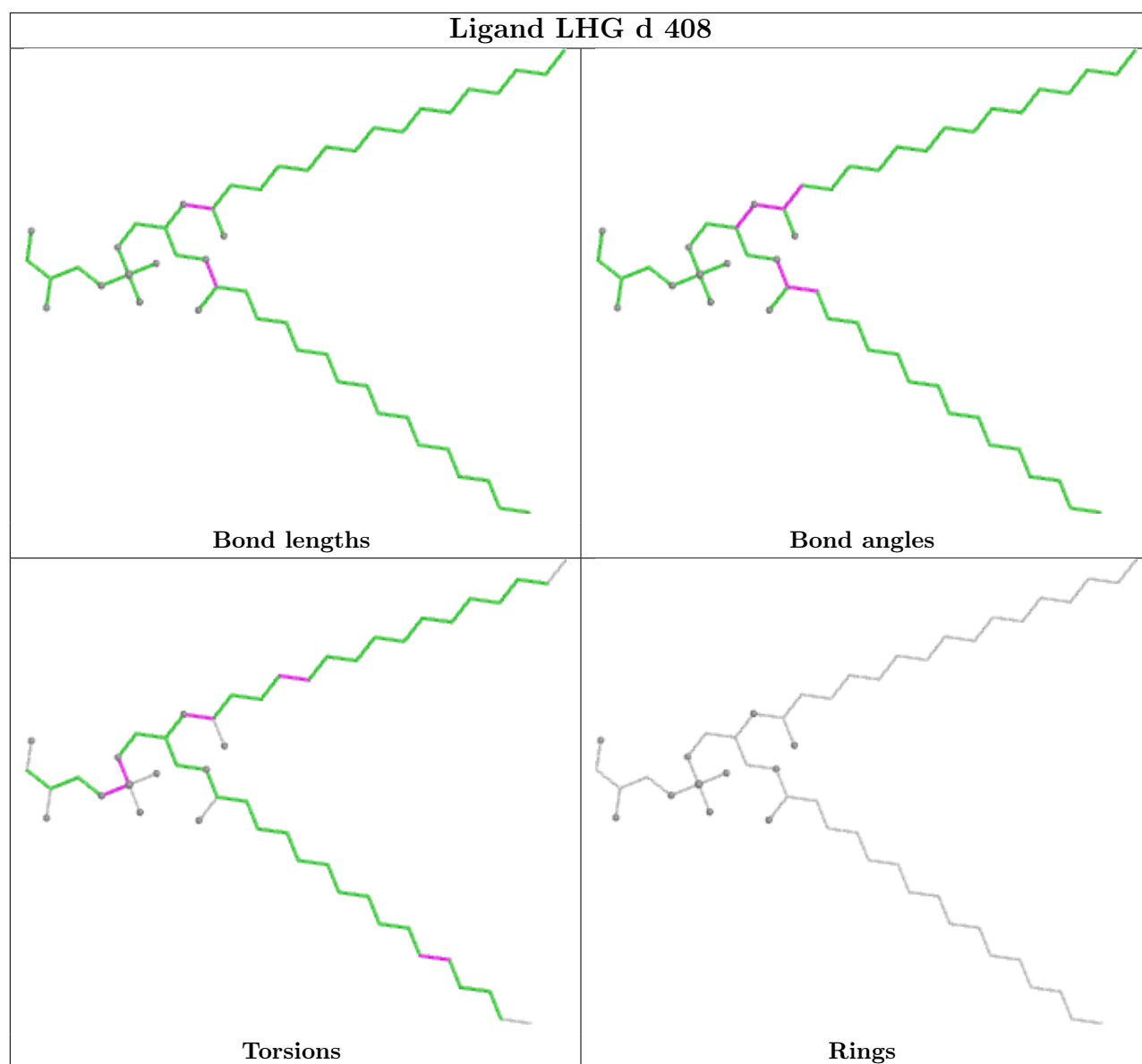
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

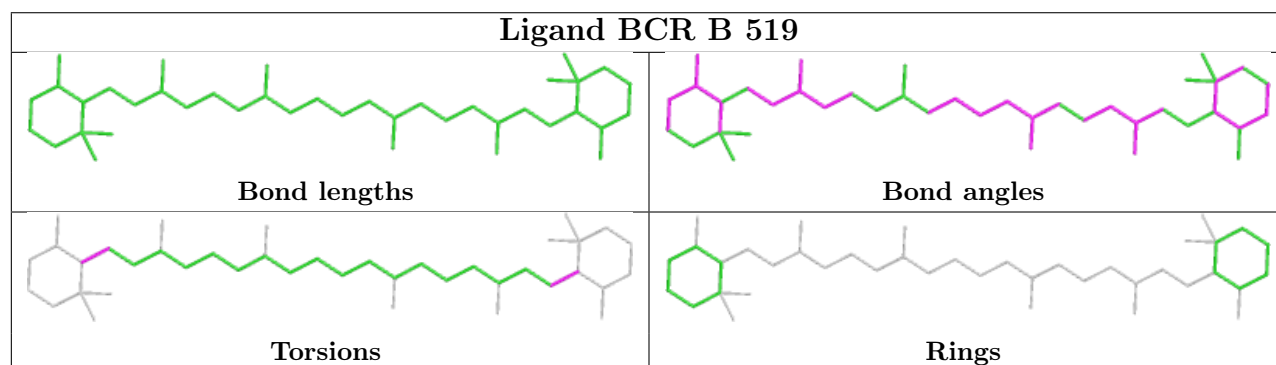
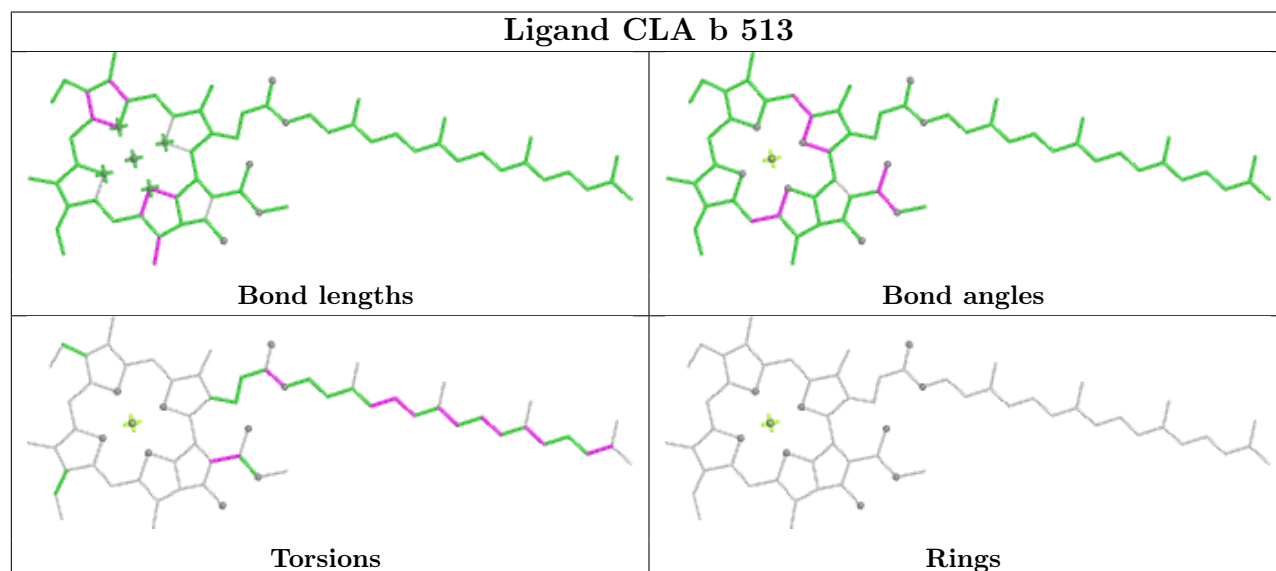
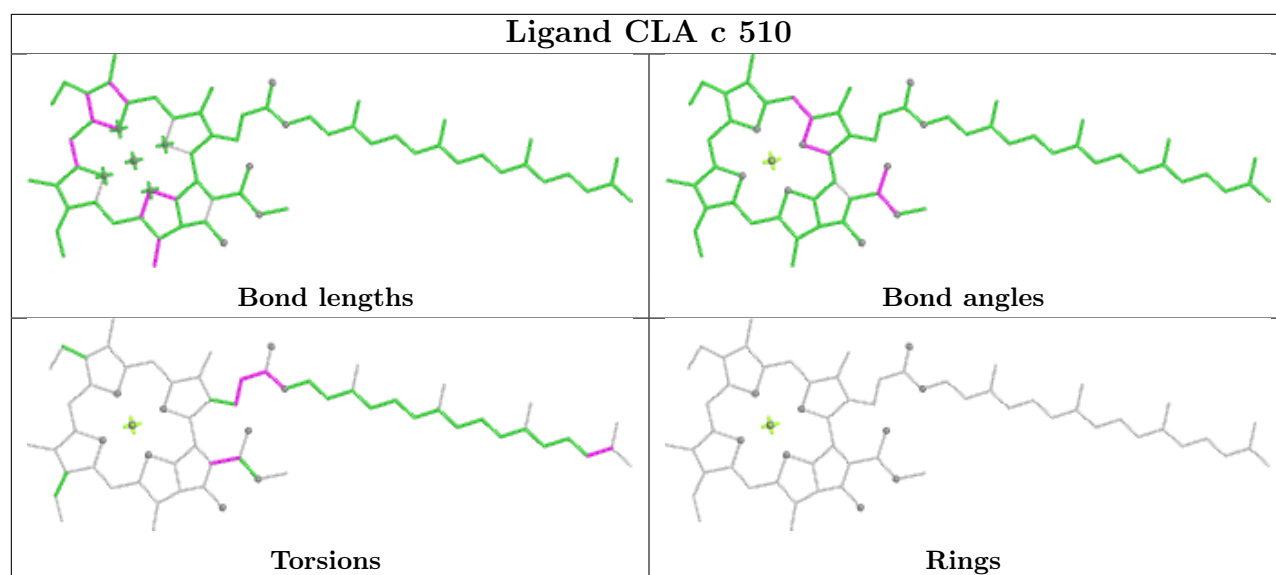


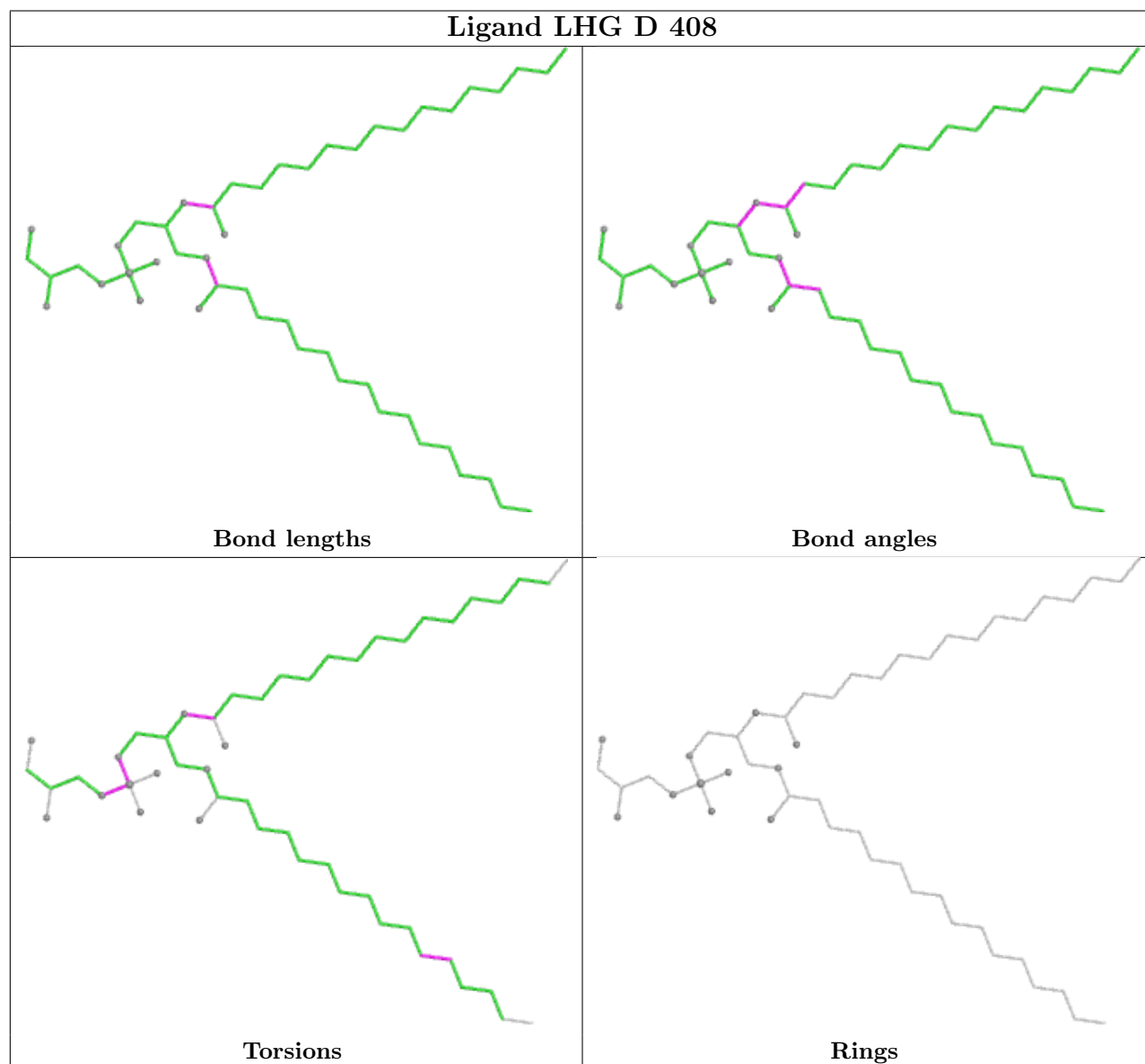
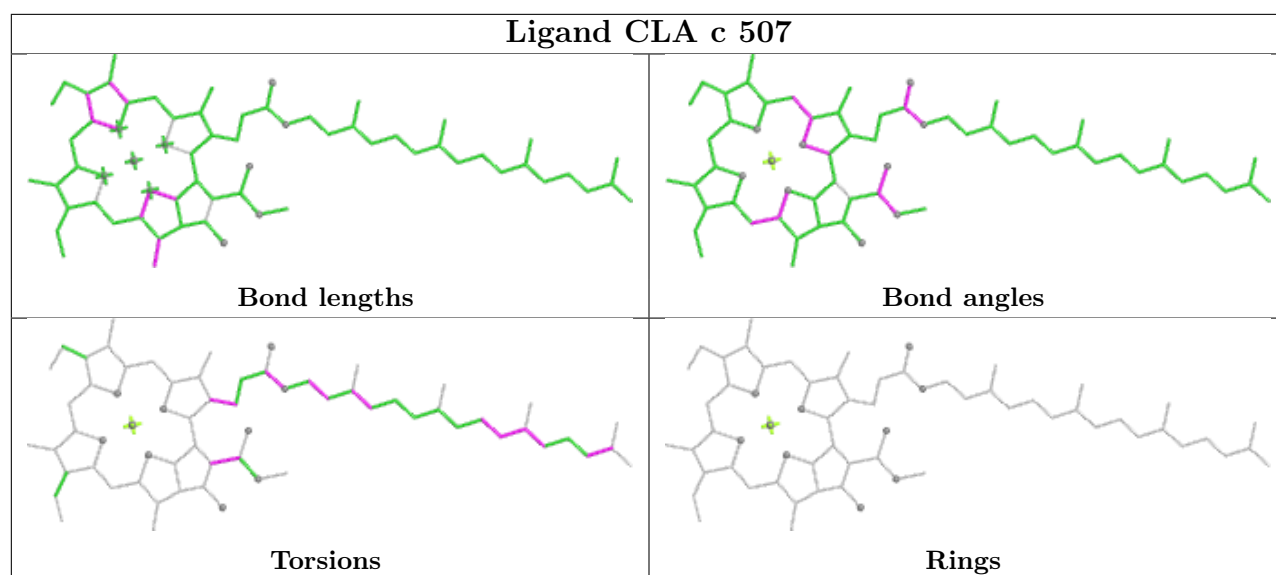


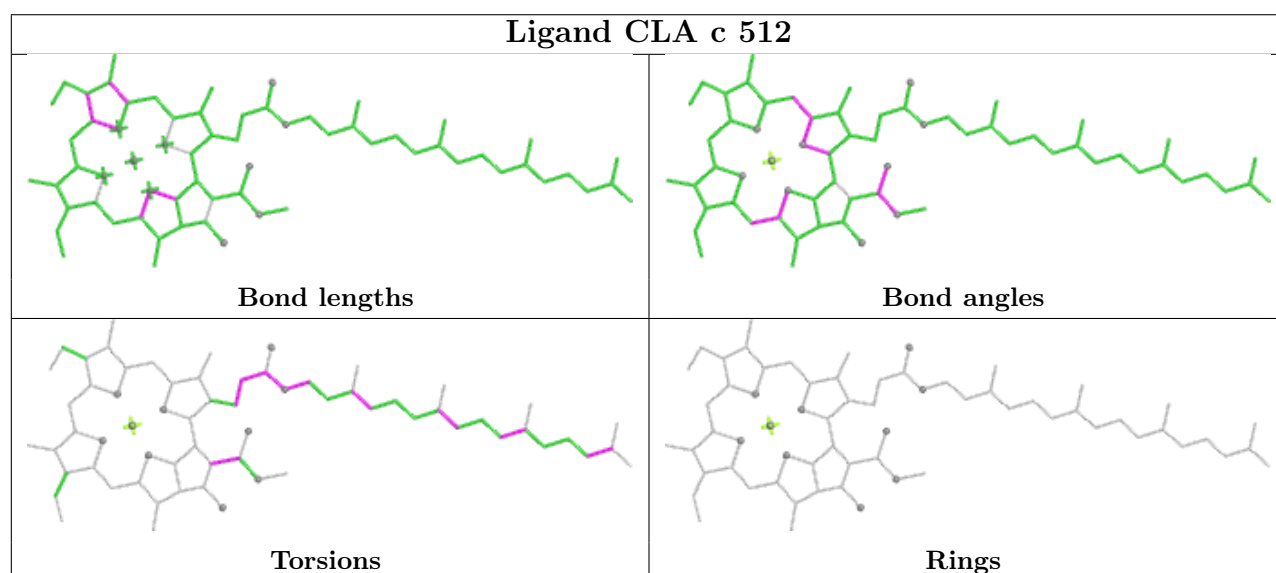
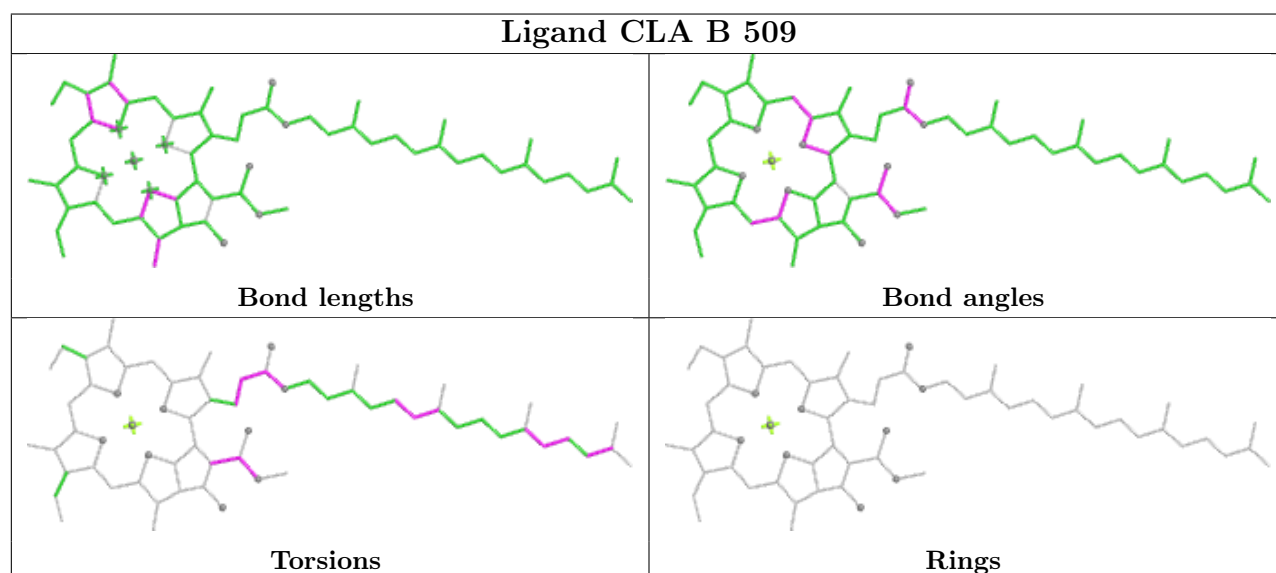
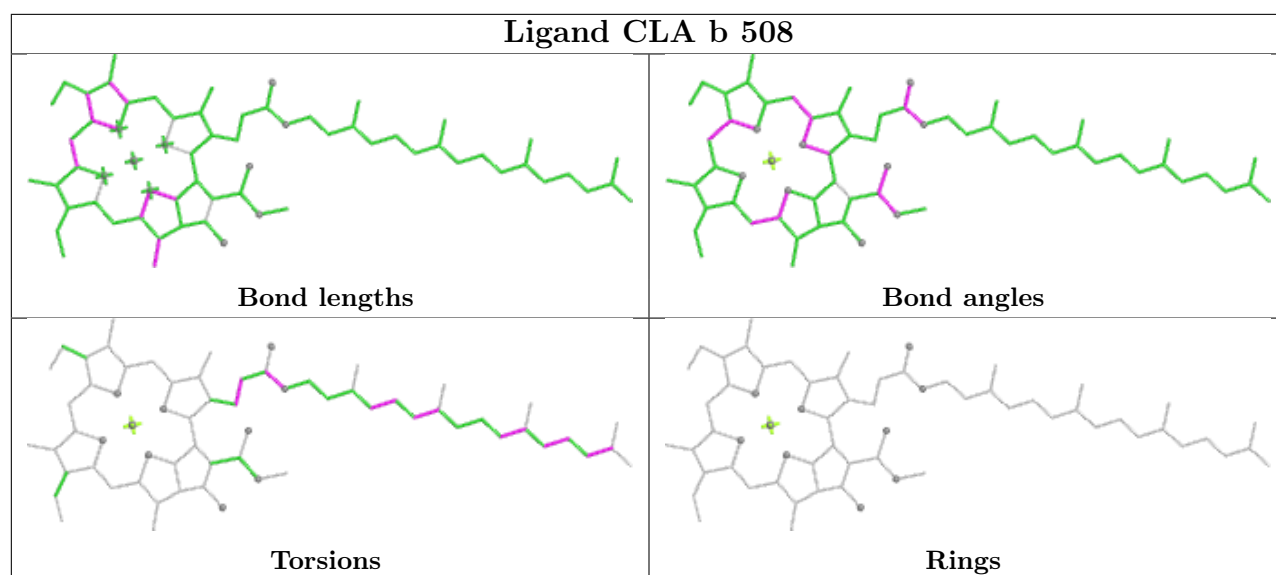


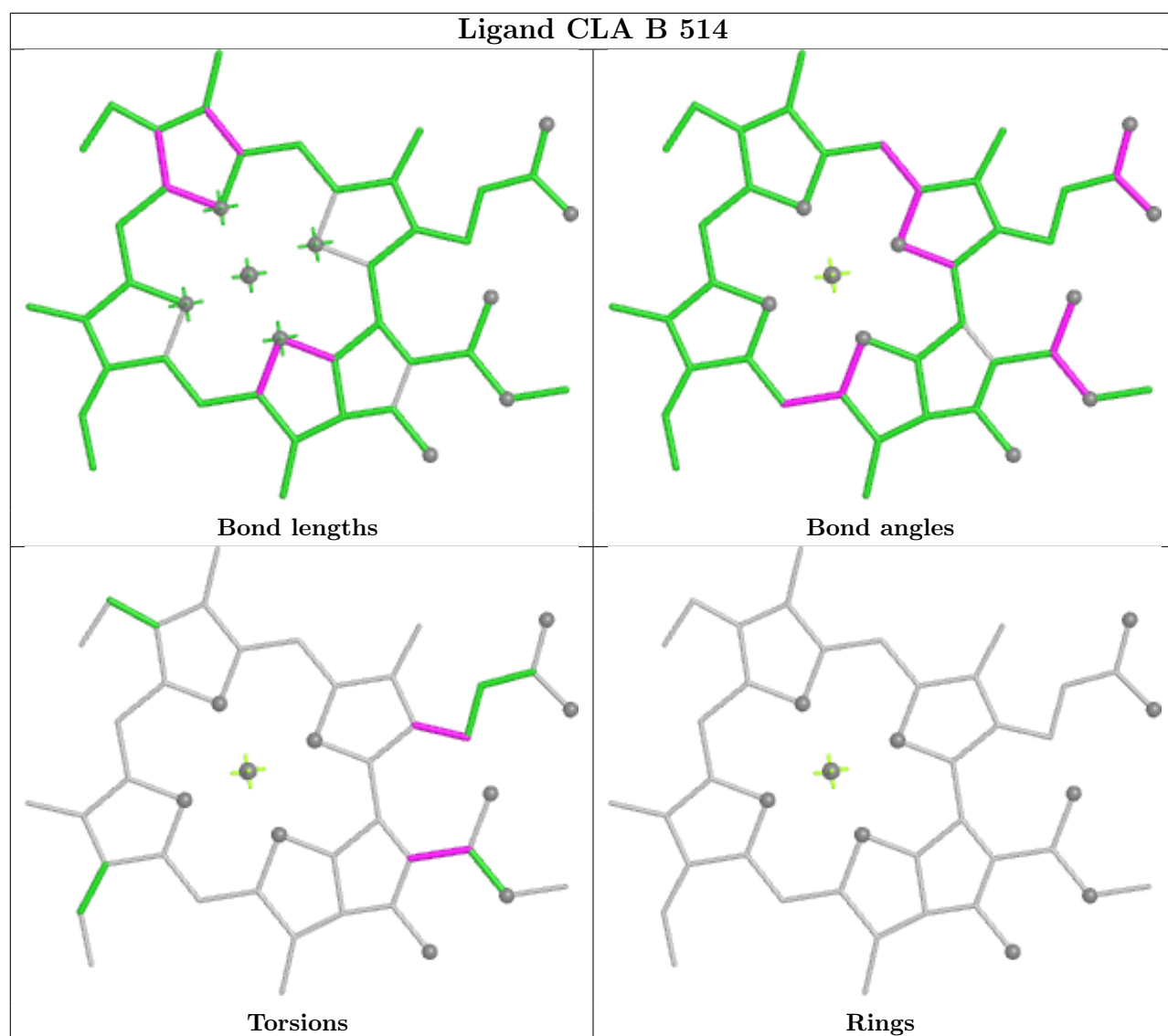


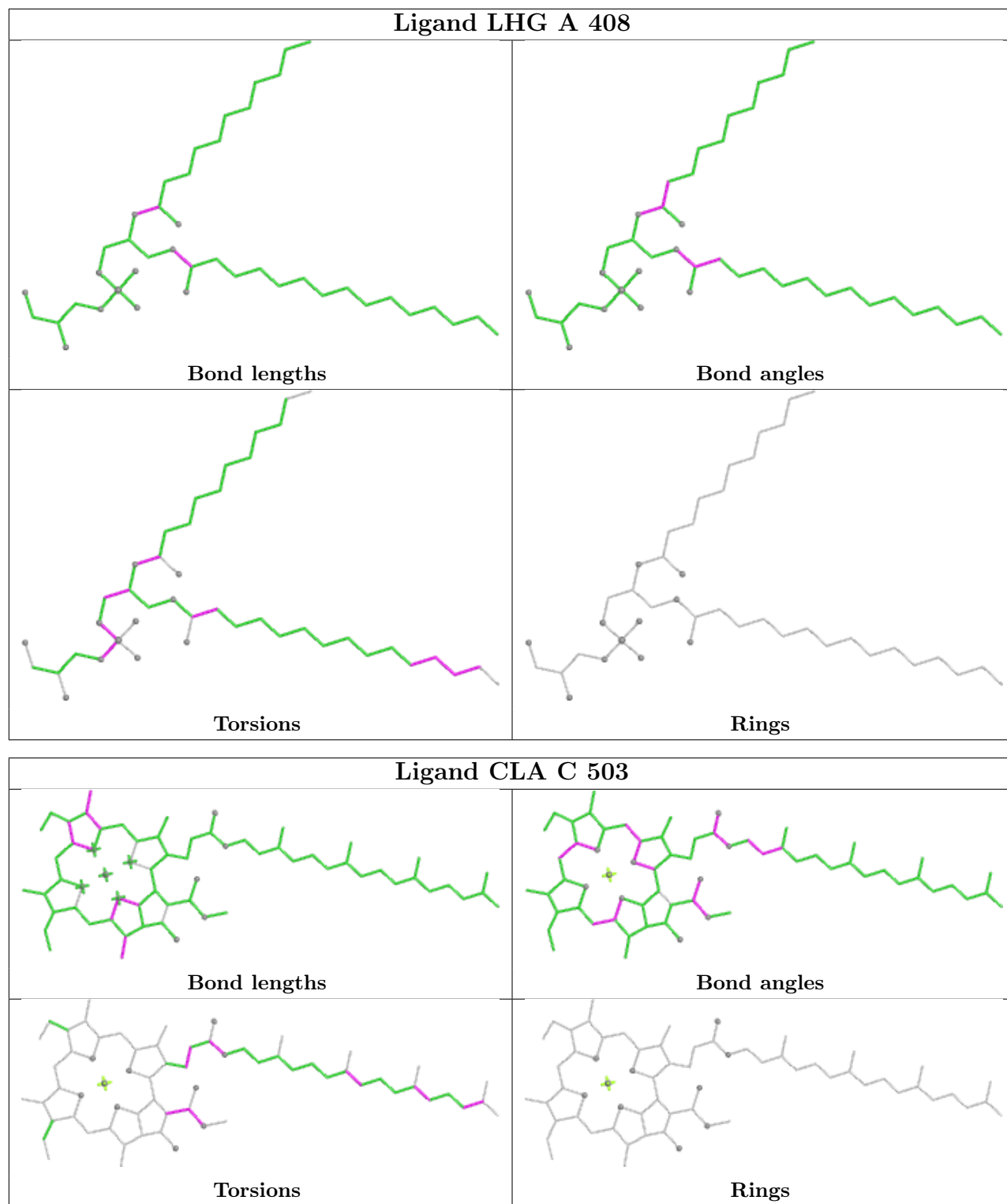


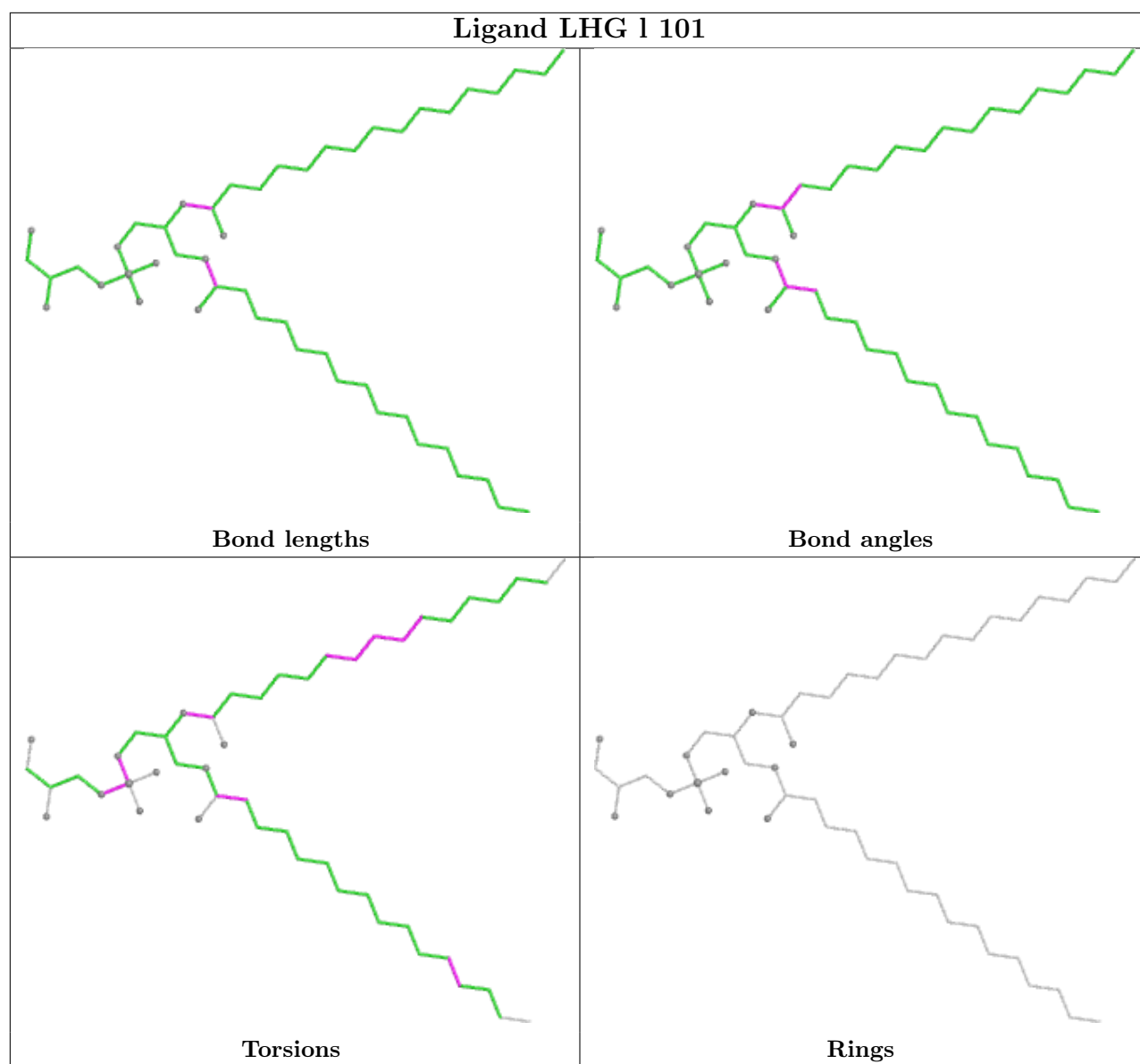


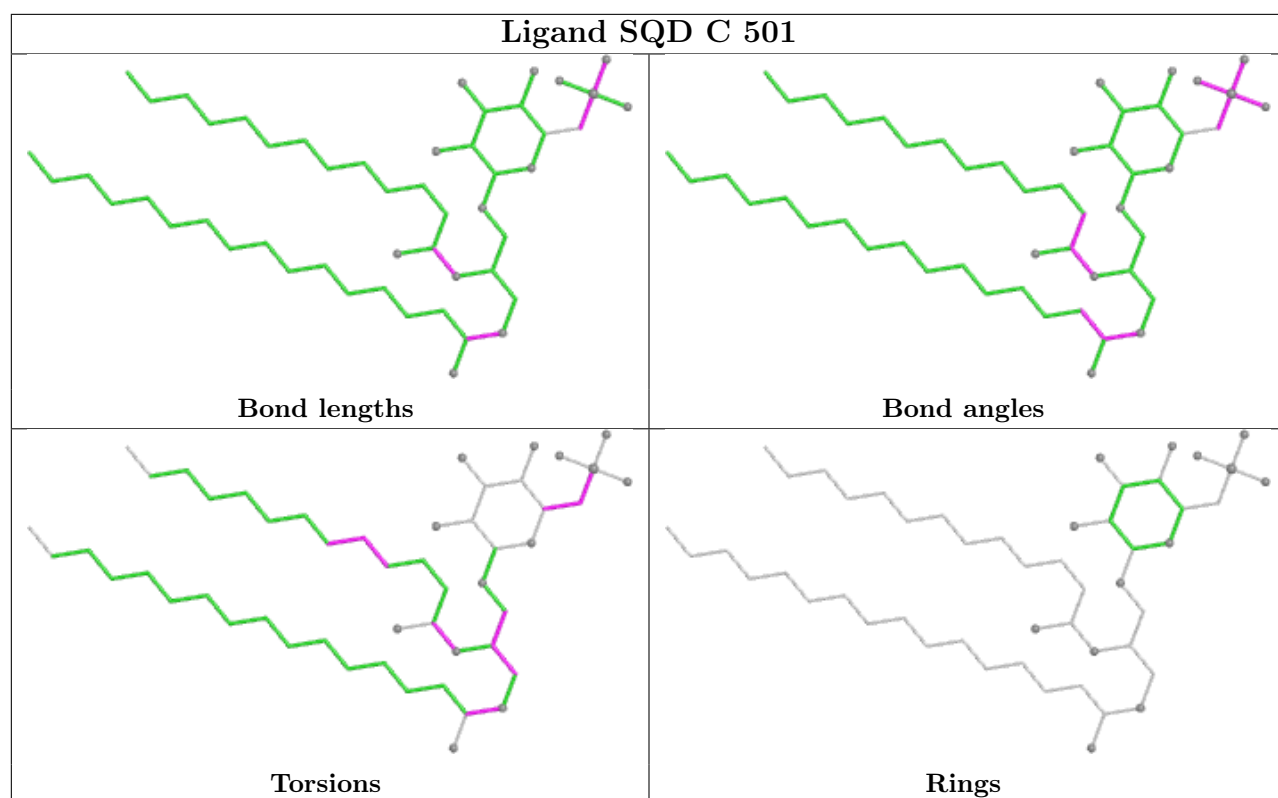


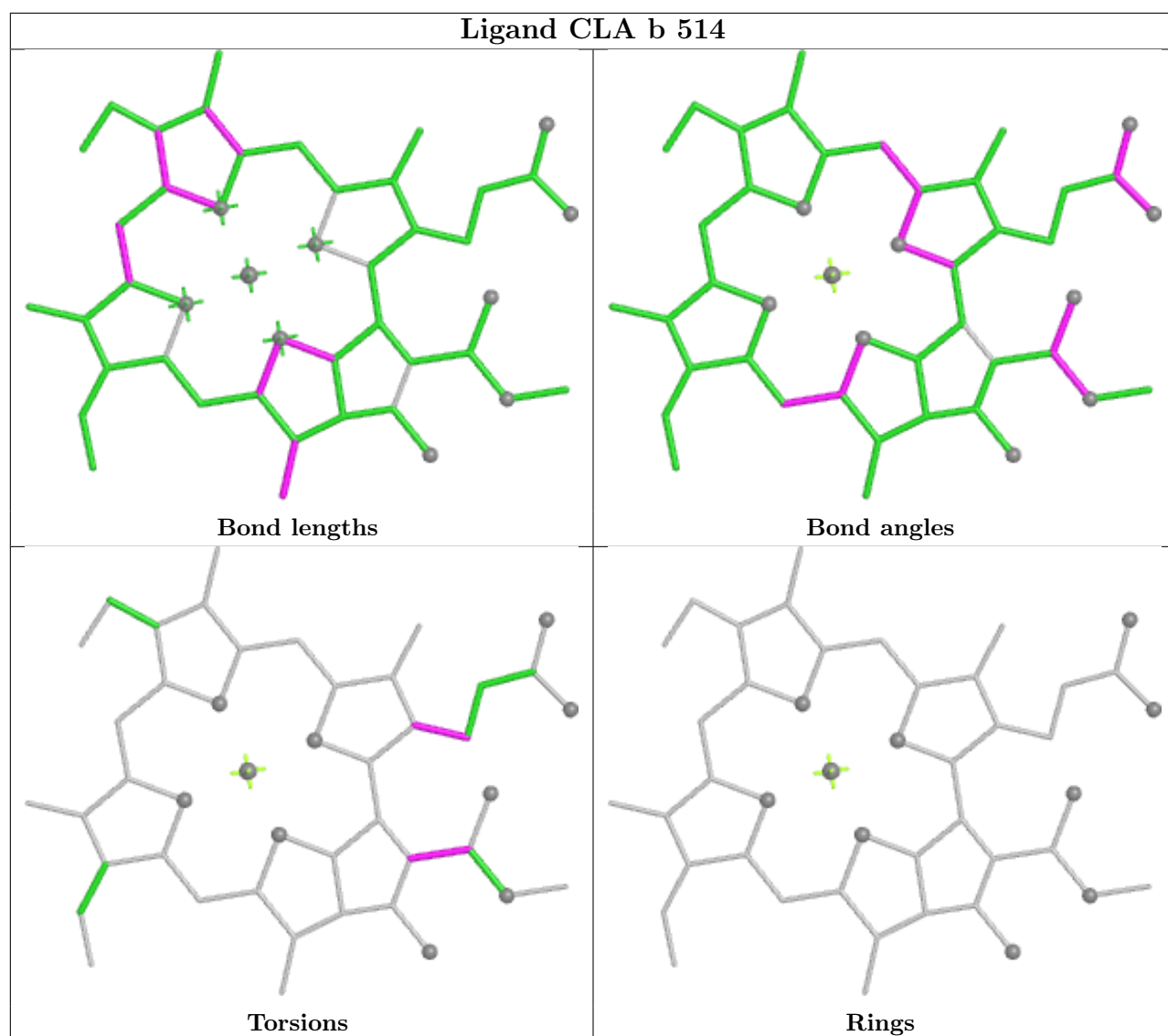


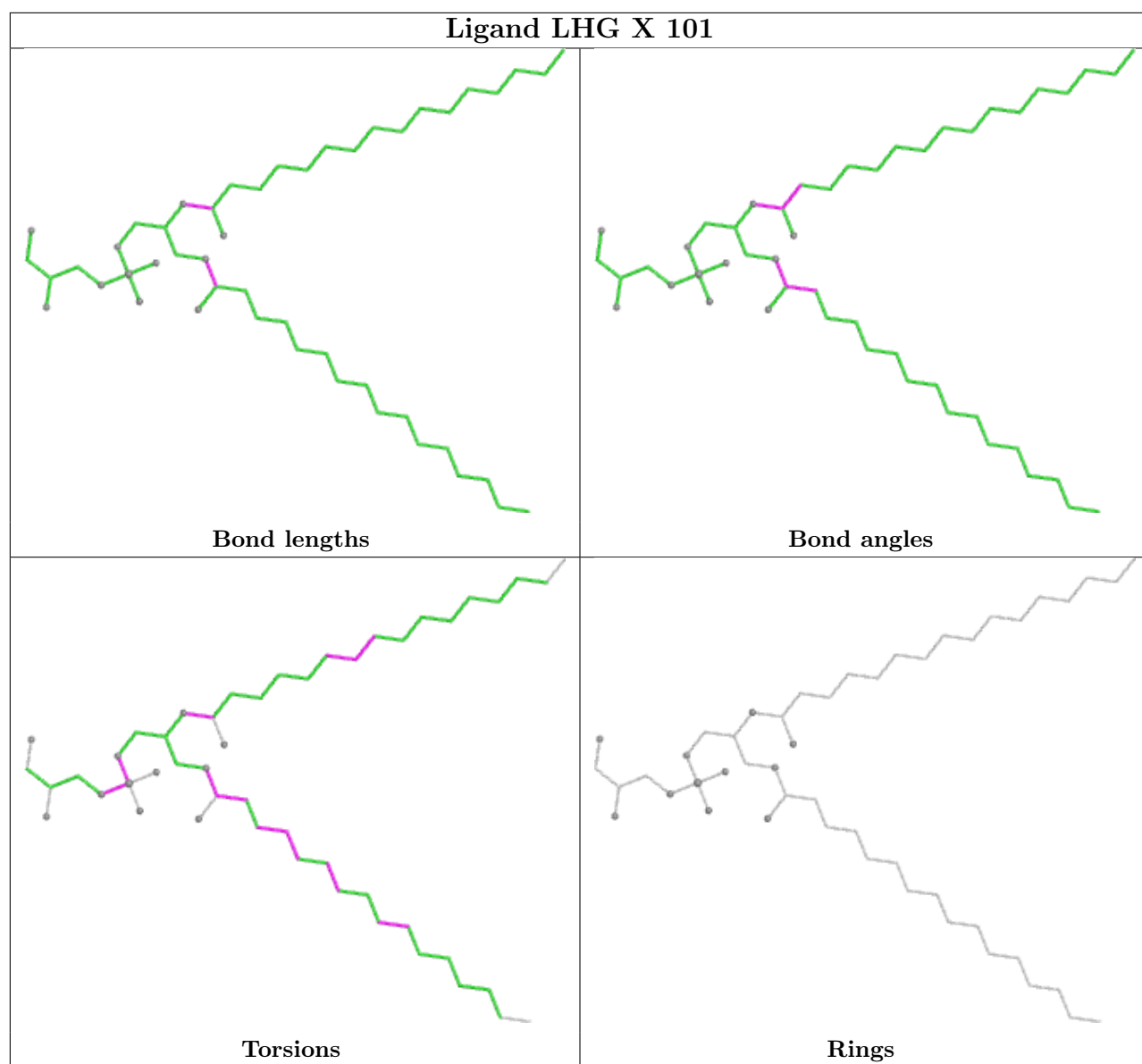


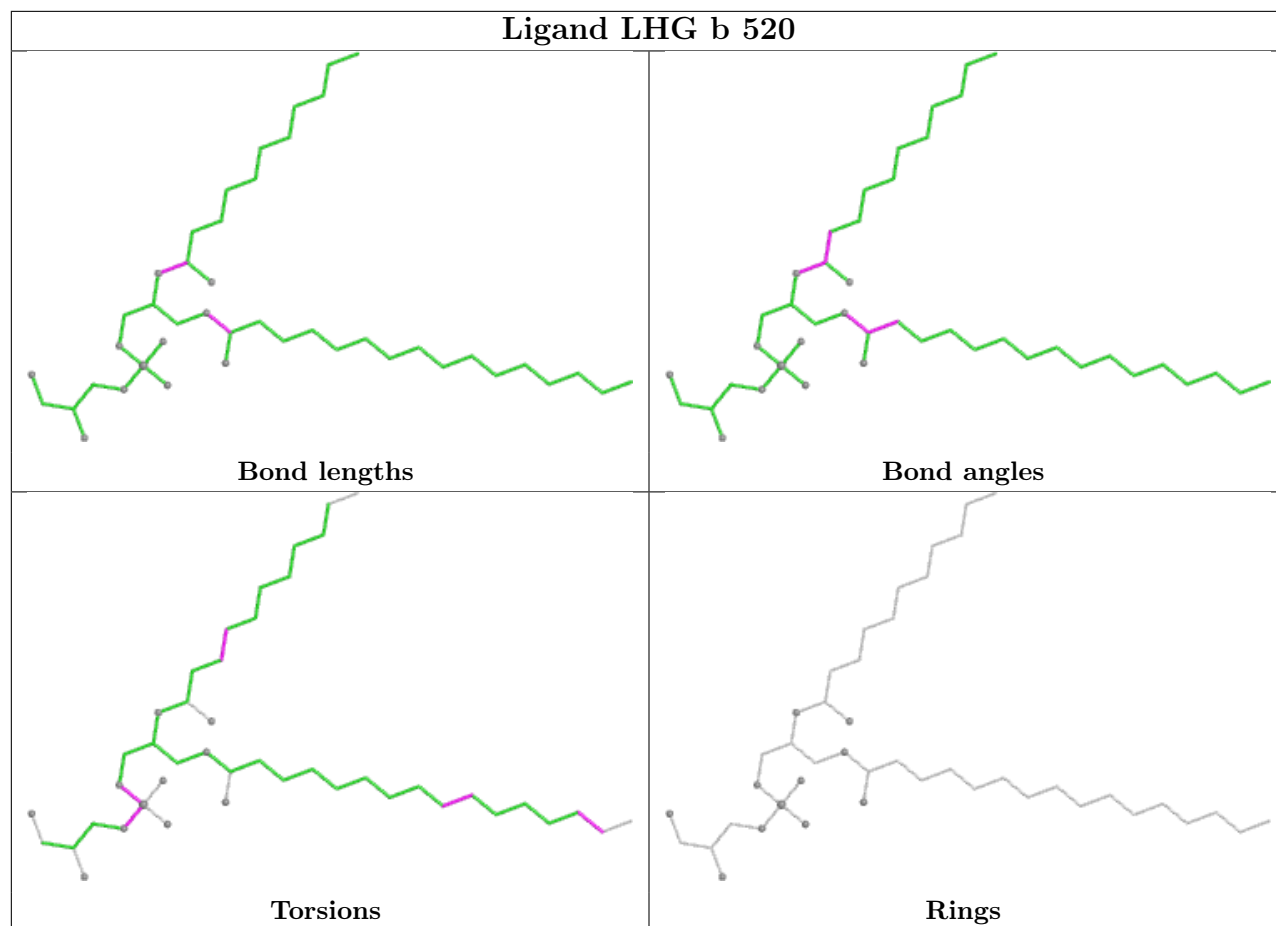
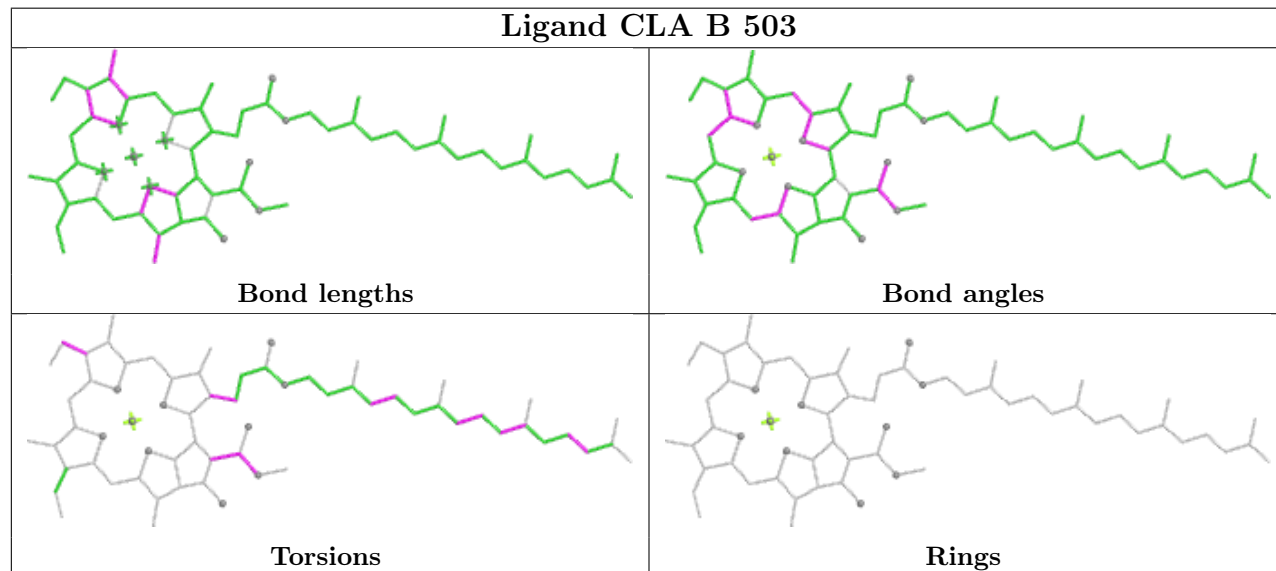


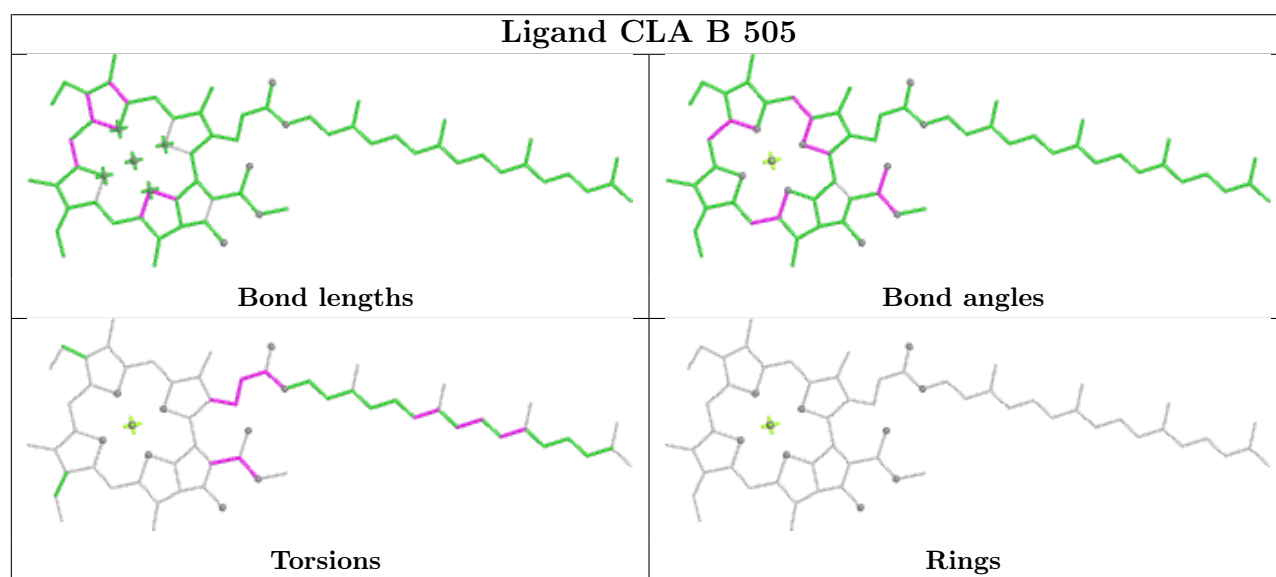
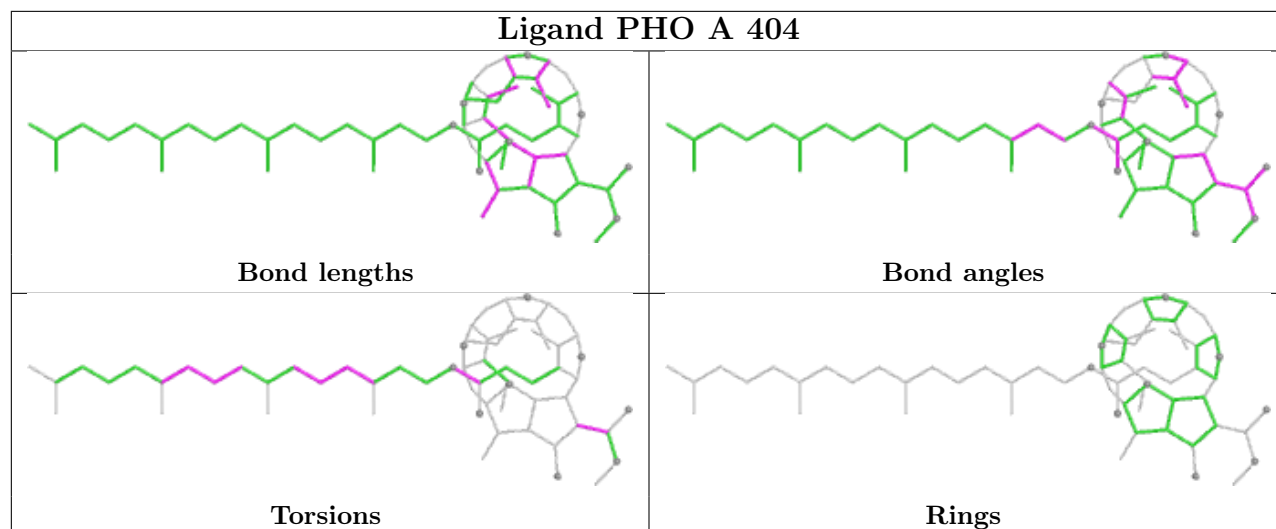


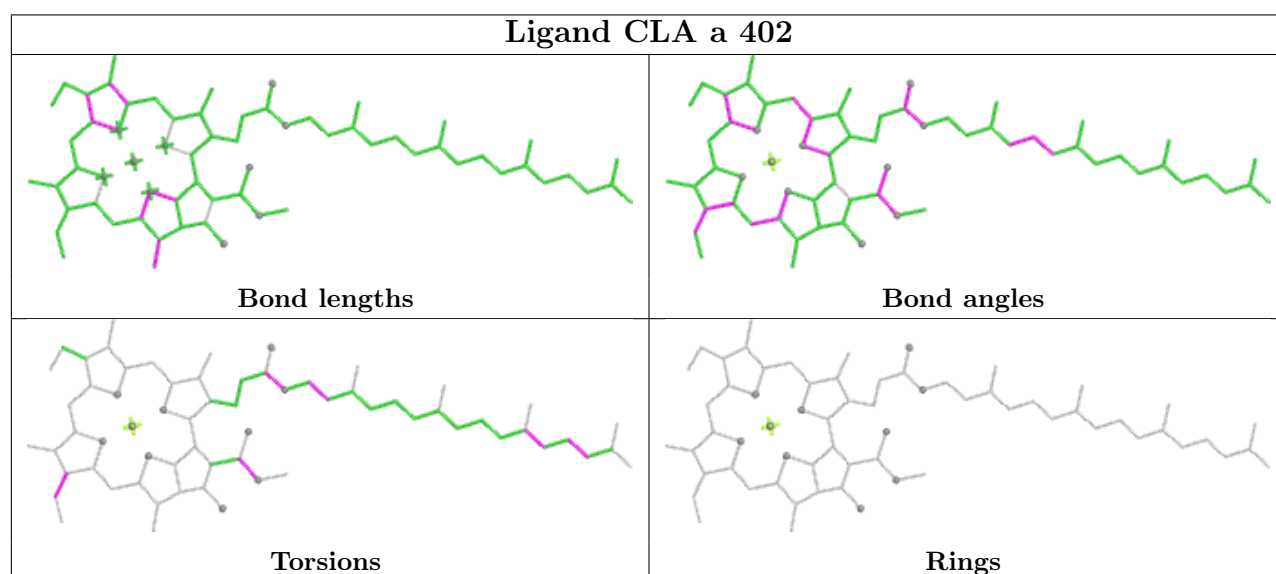
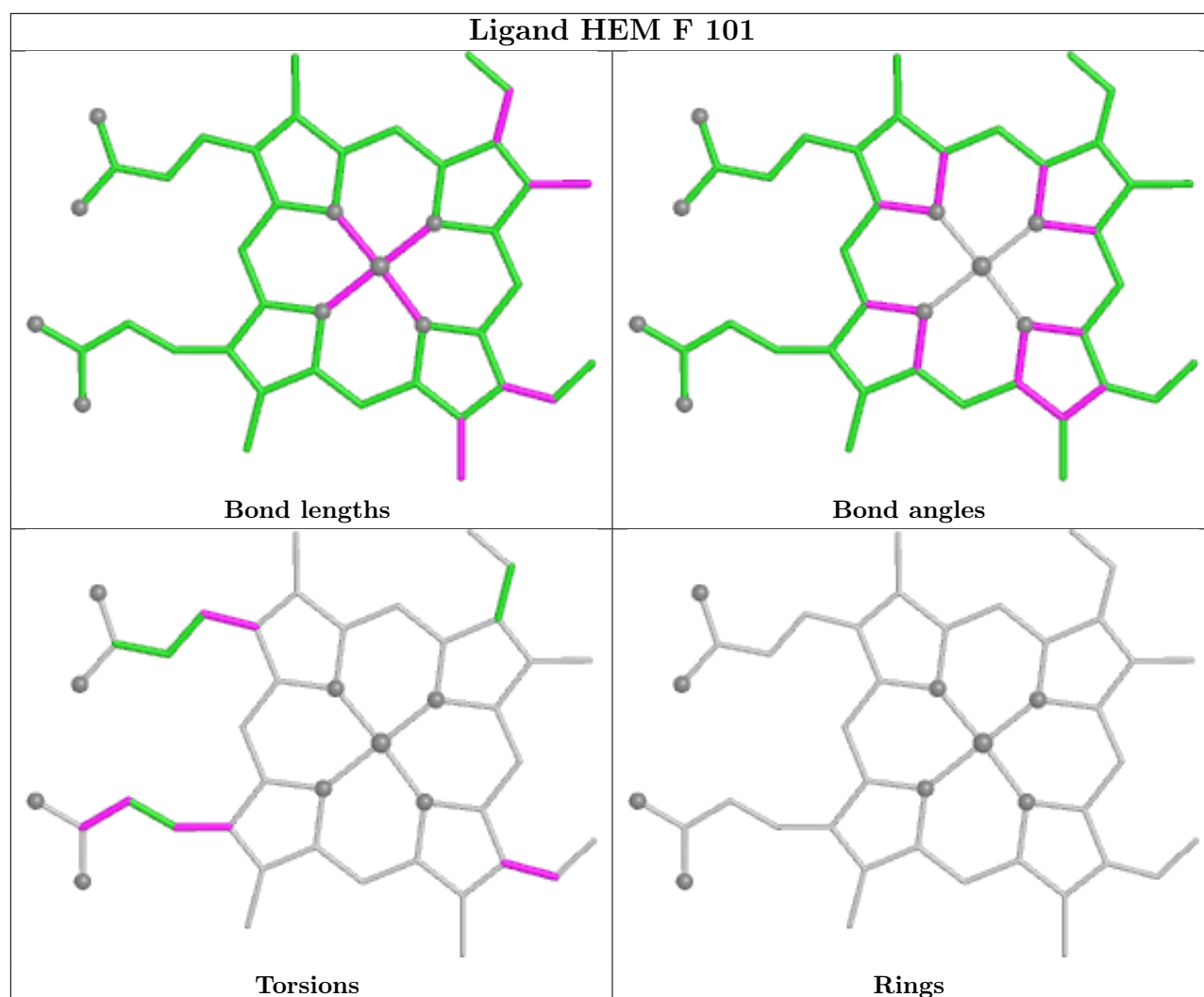


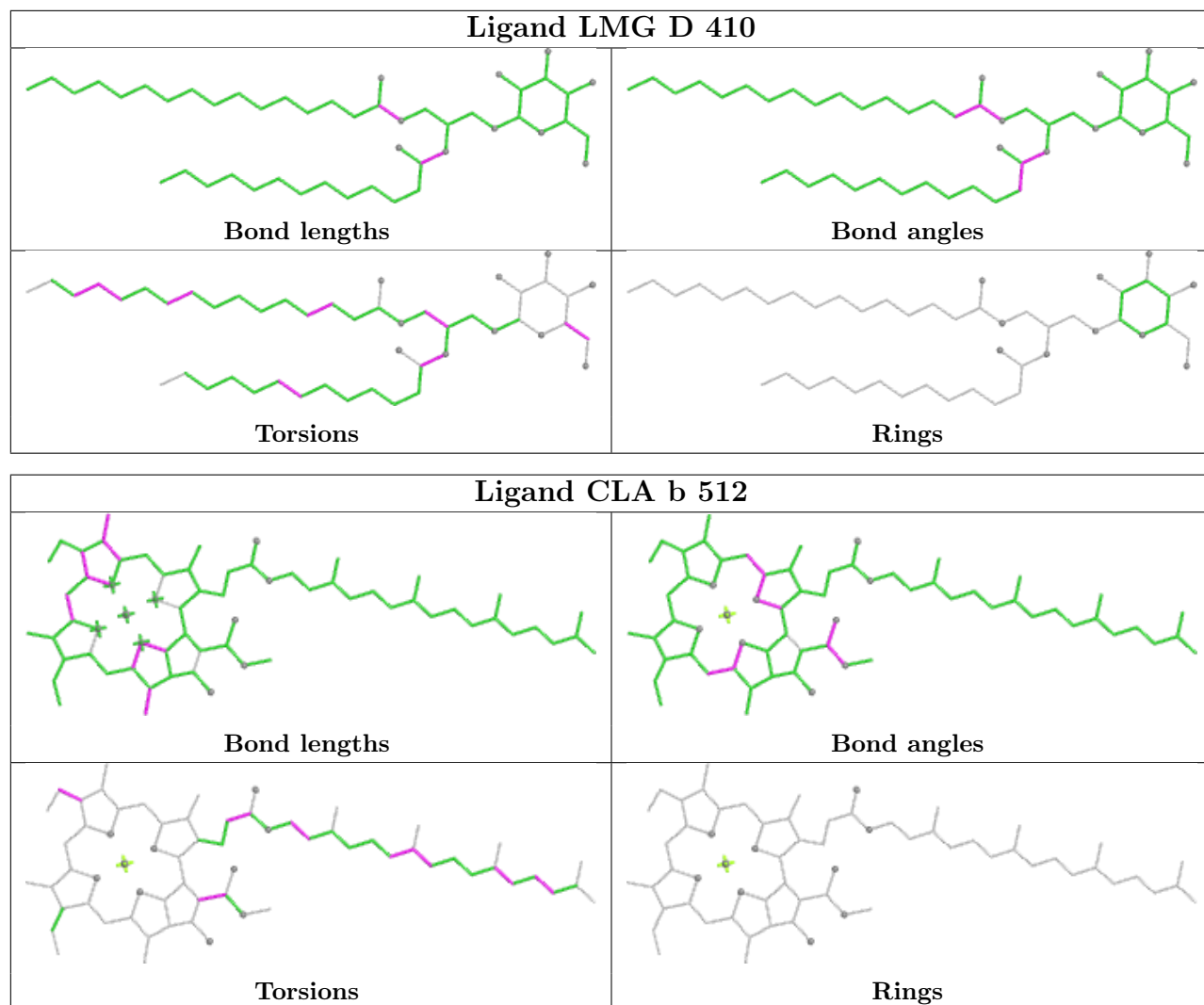


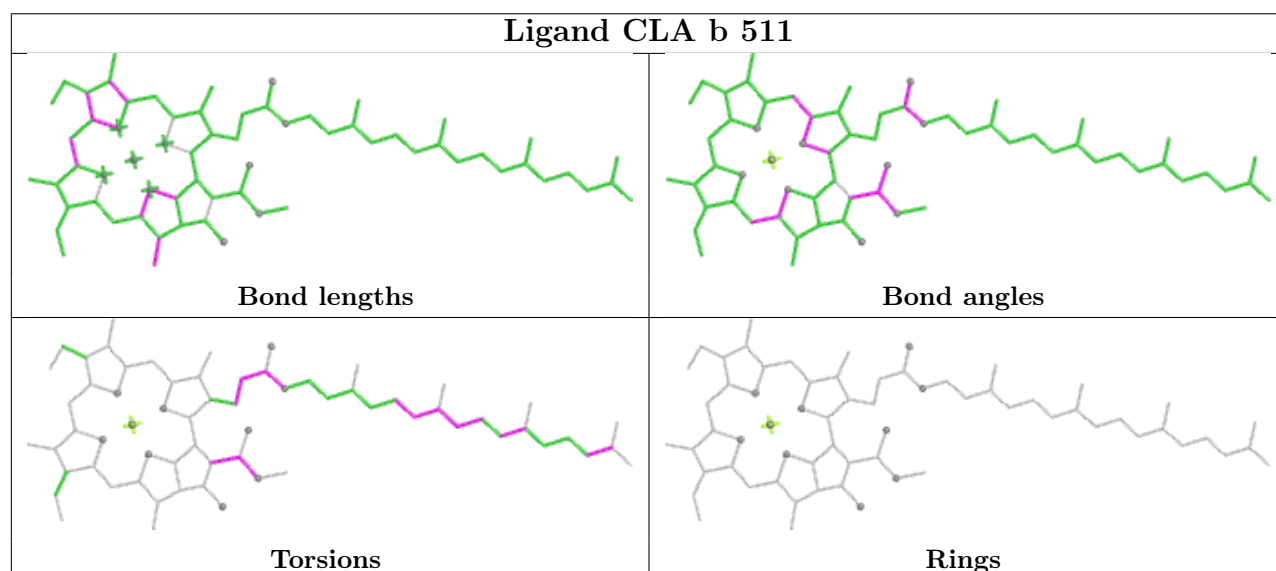
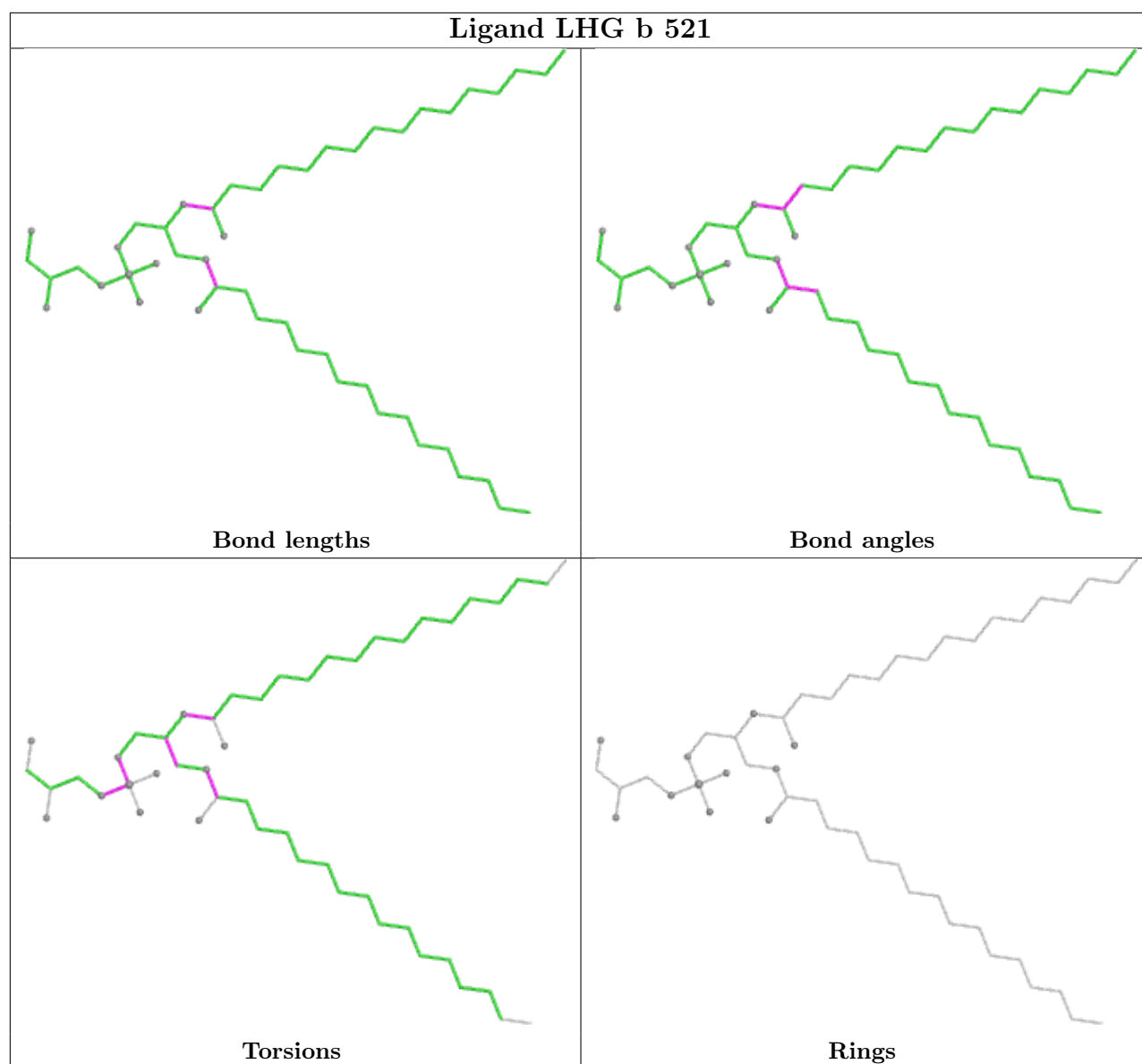


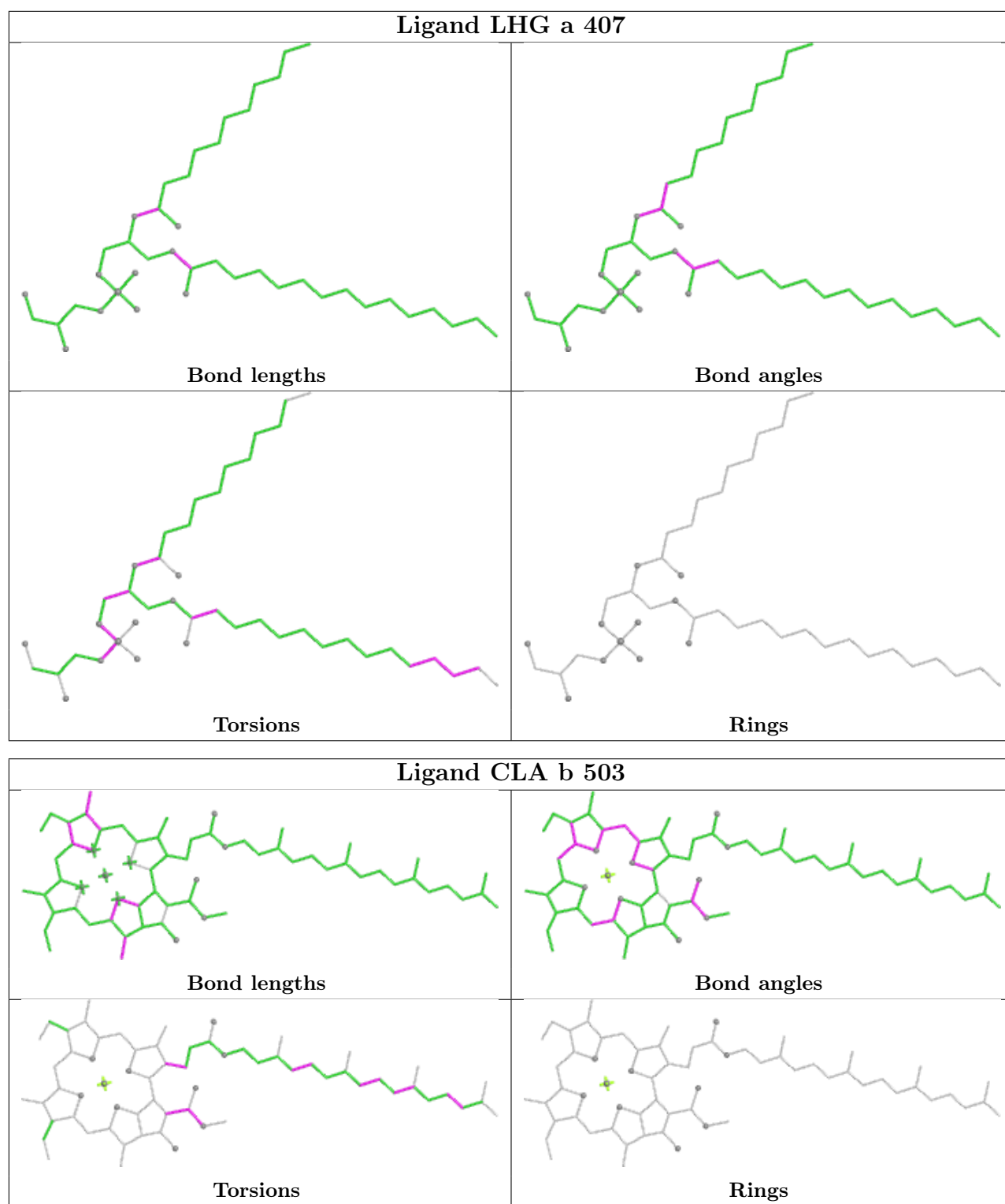
Ligand LHG b 520**Ligand CLA B 503**

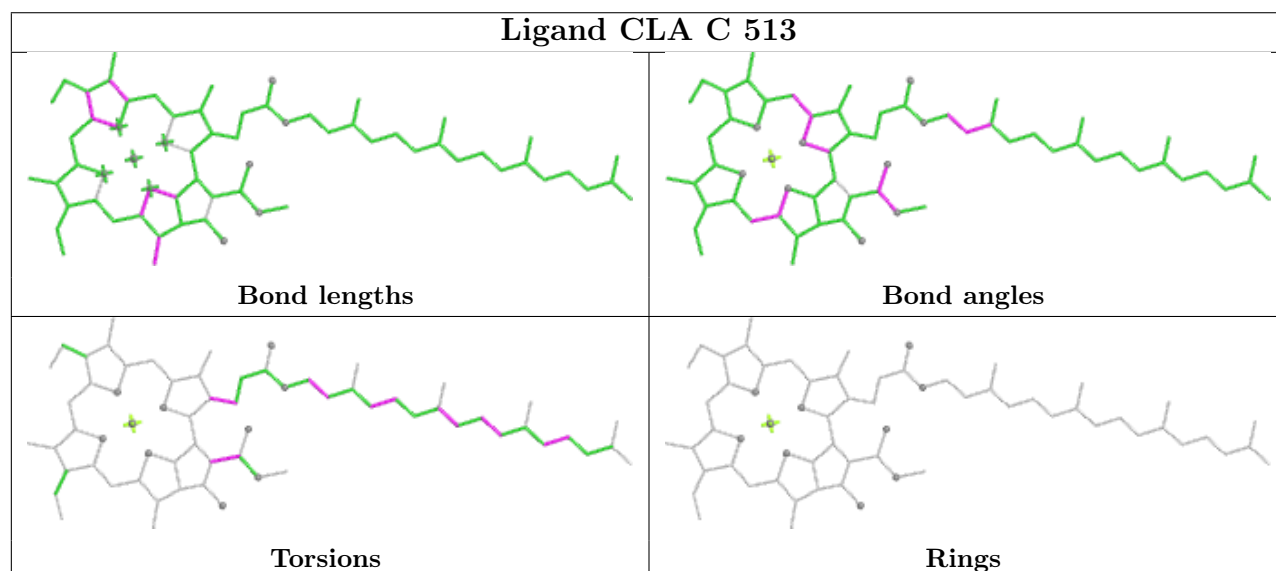
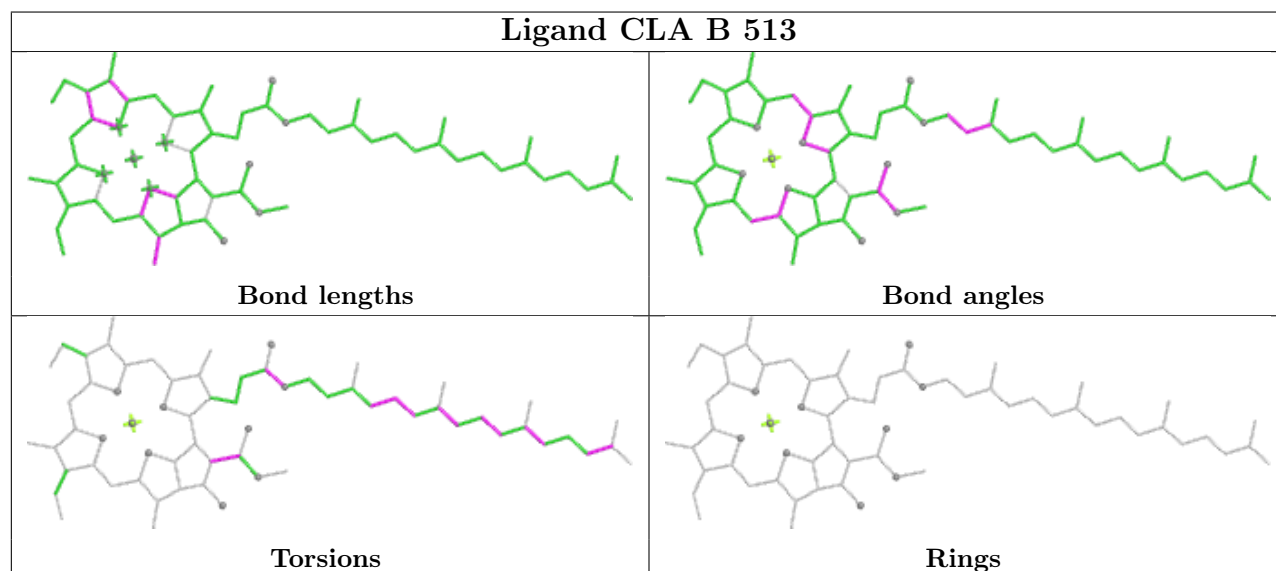
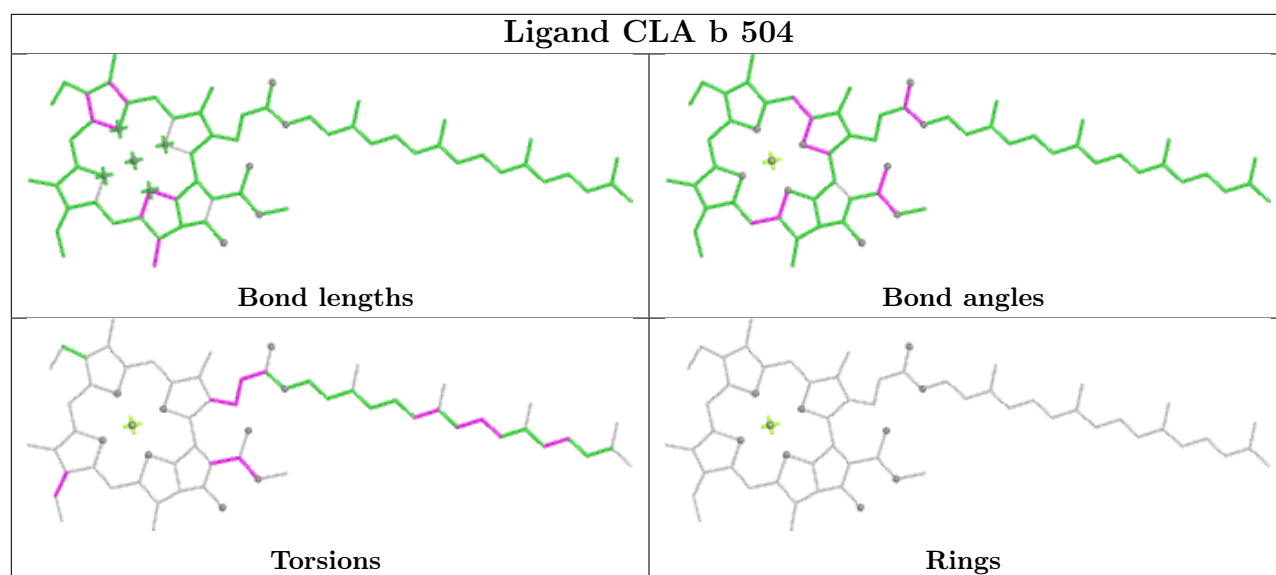


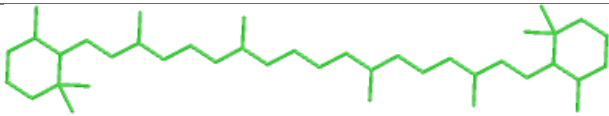
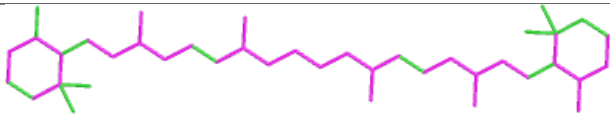
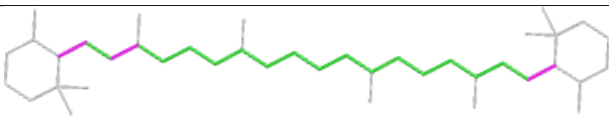
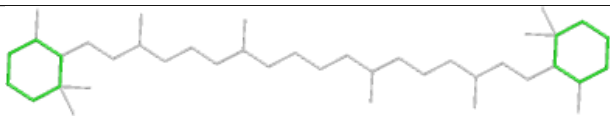


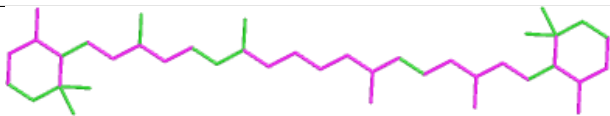
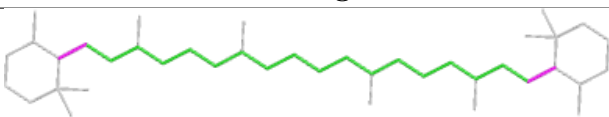
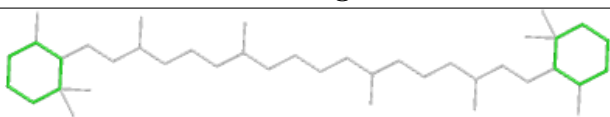


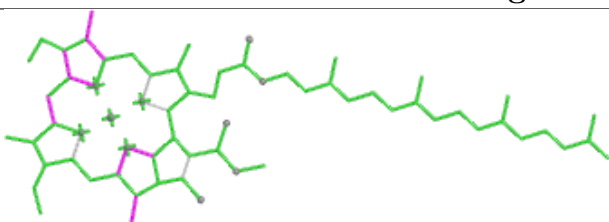
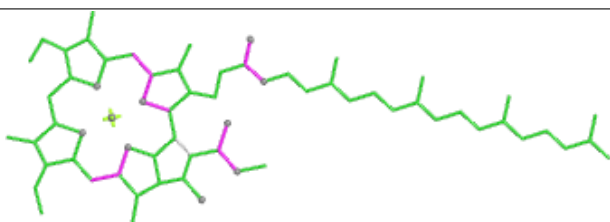
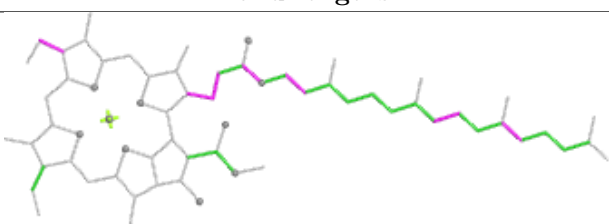
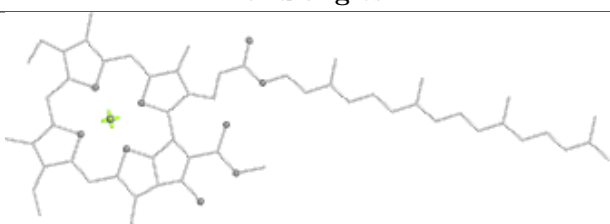


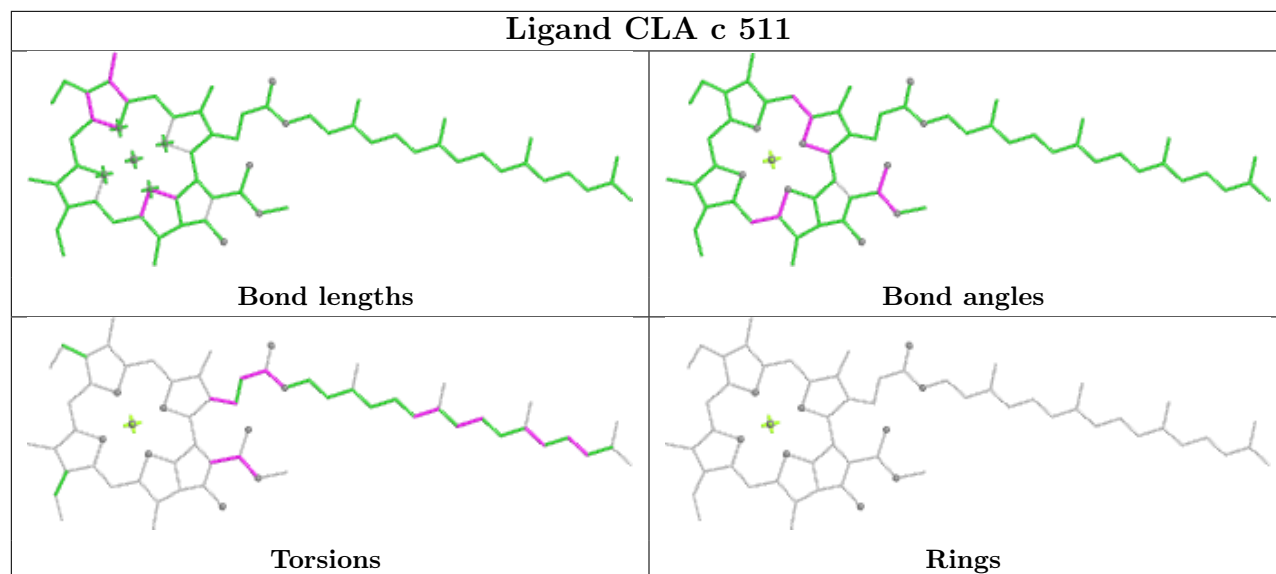
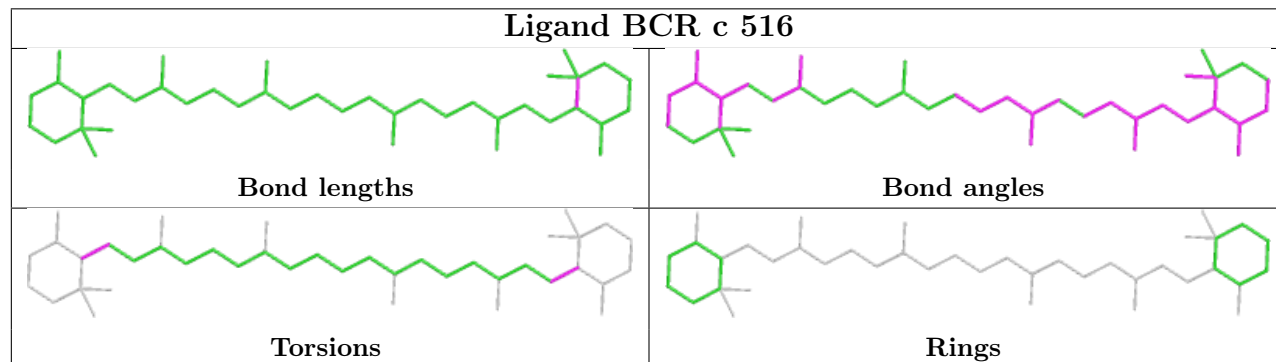
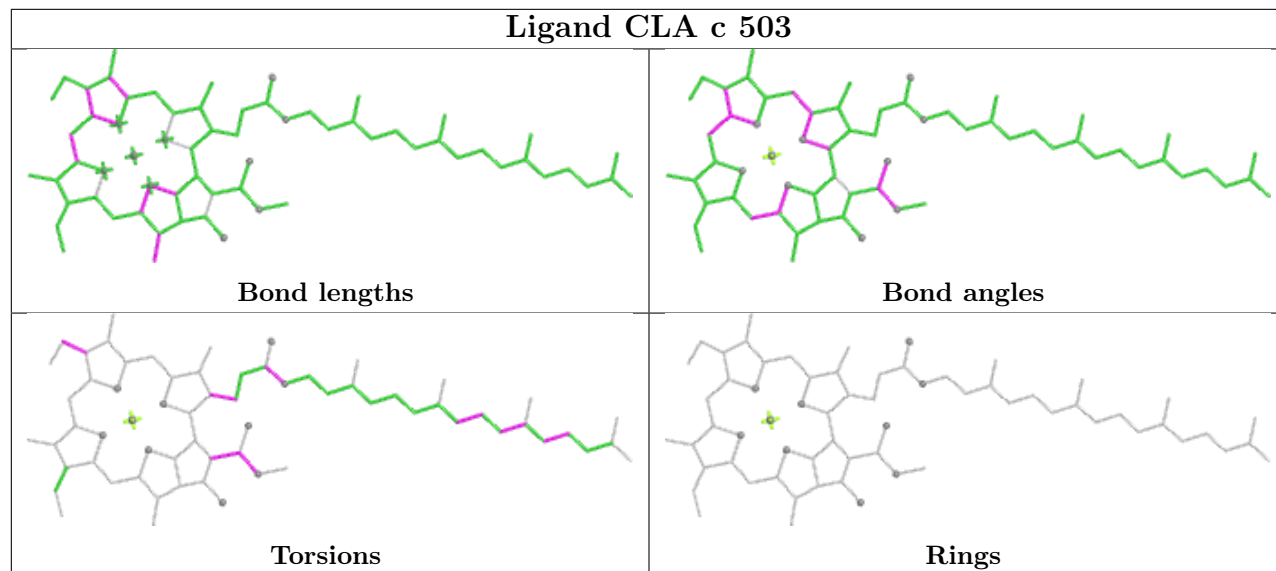


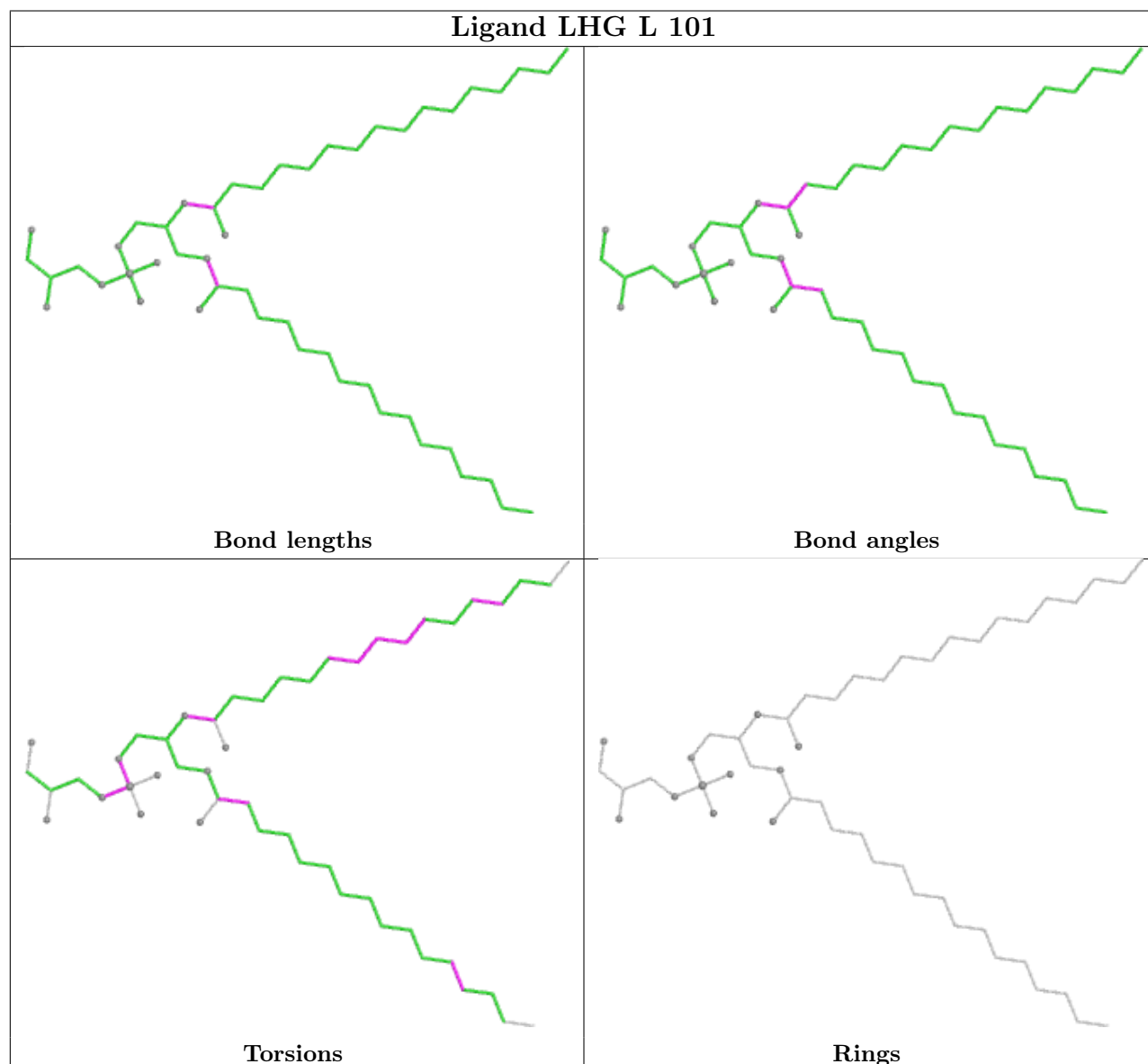
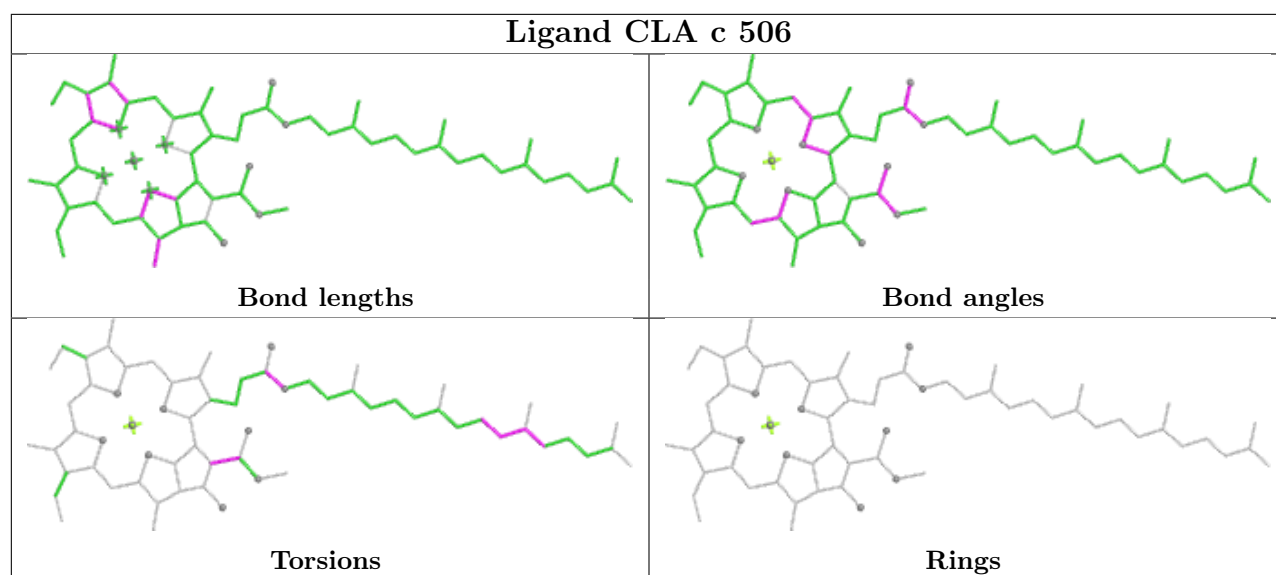


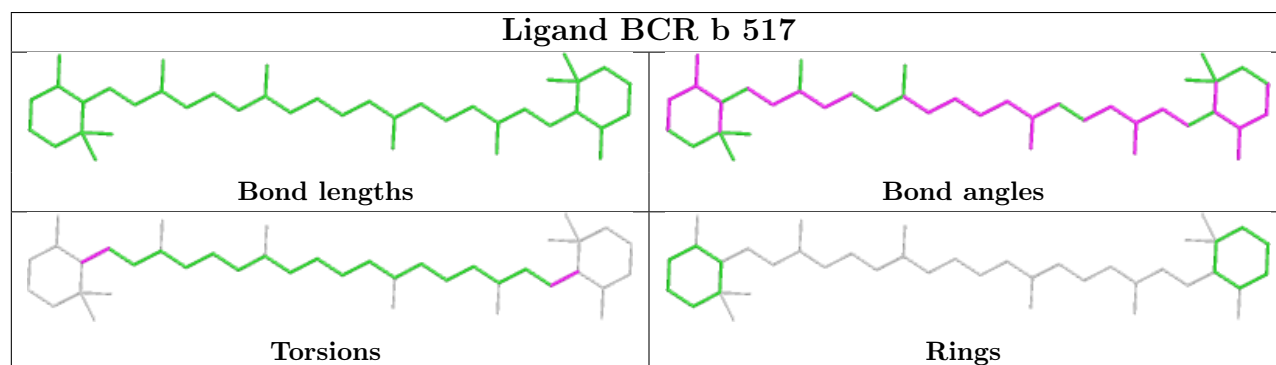
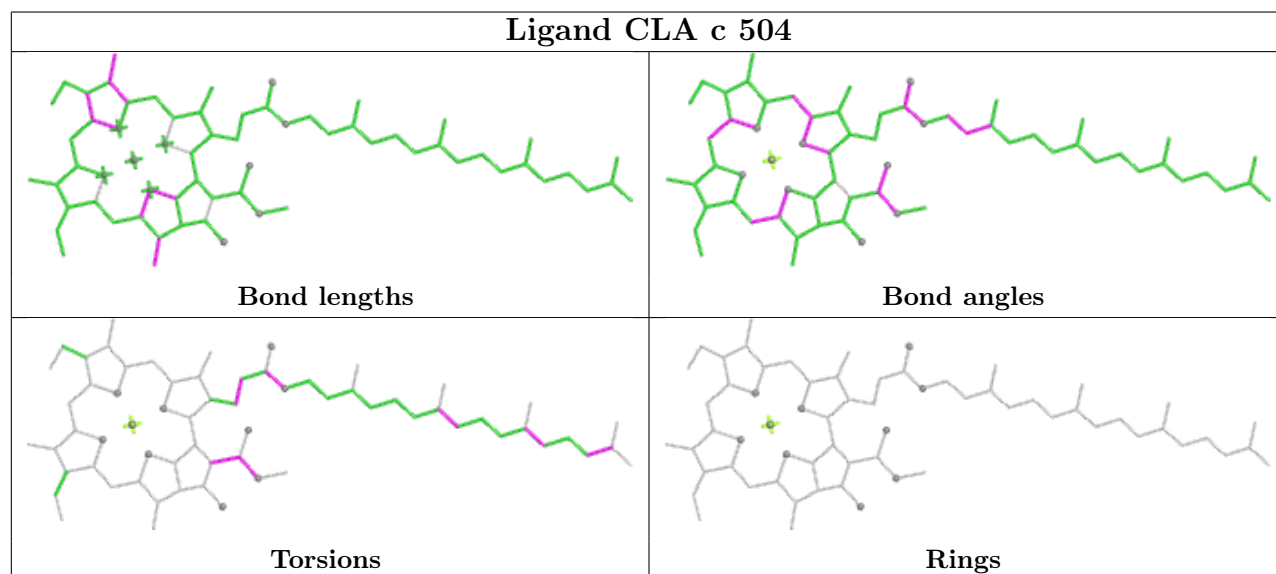
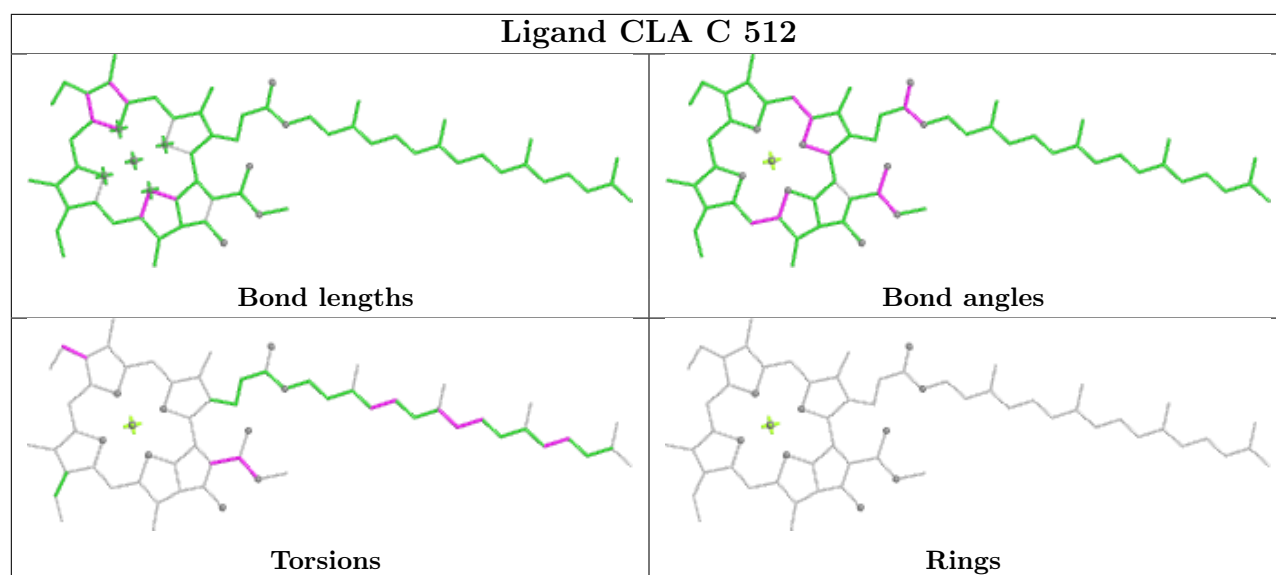
Ligand BCR x 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

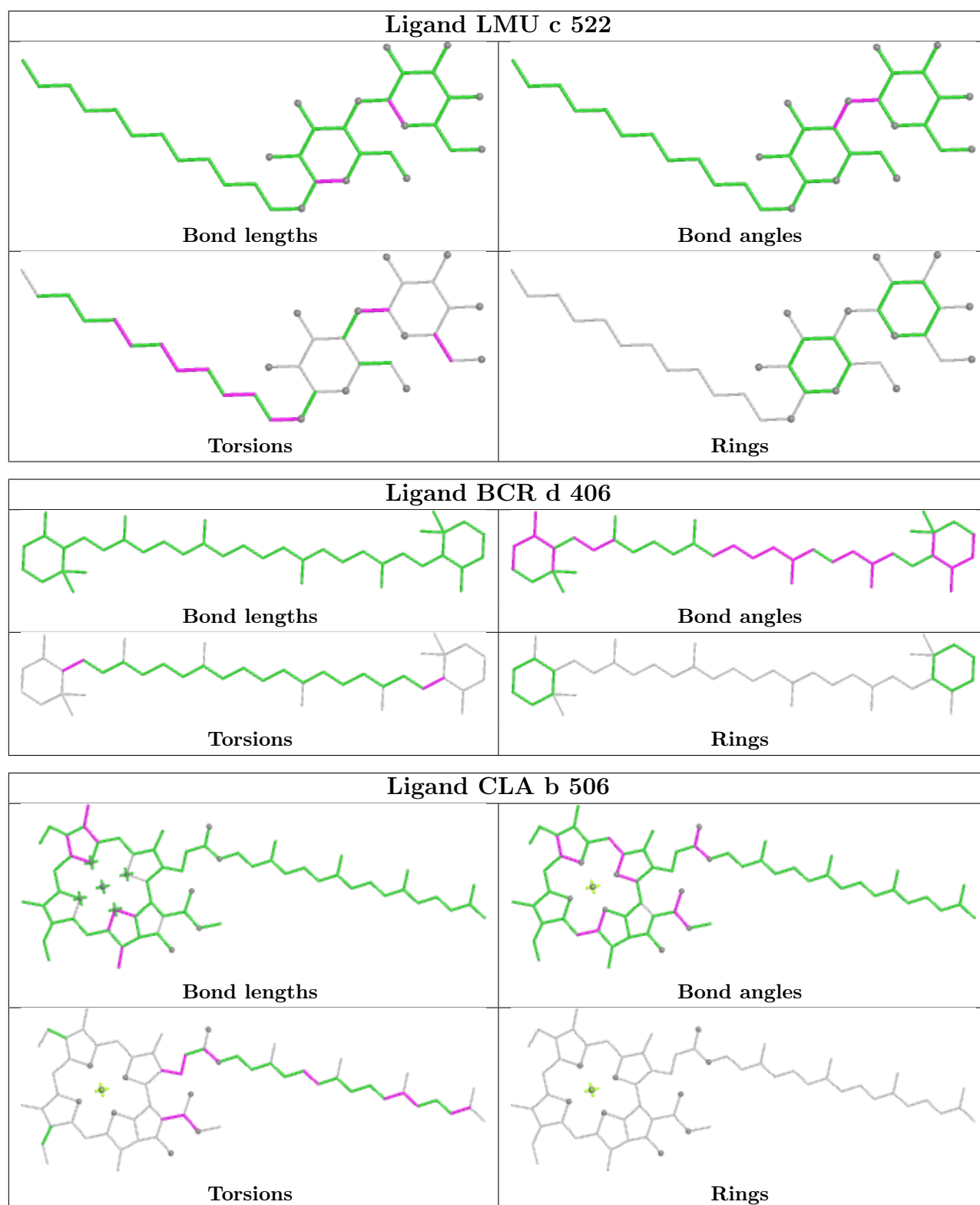
Ligand BCR B 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

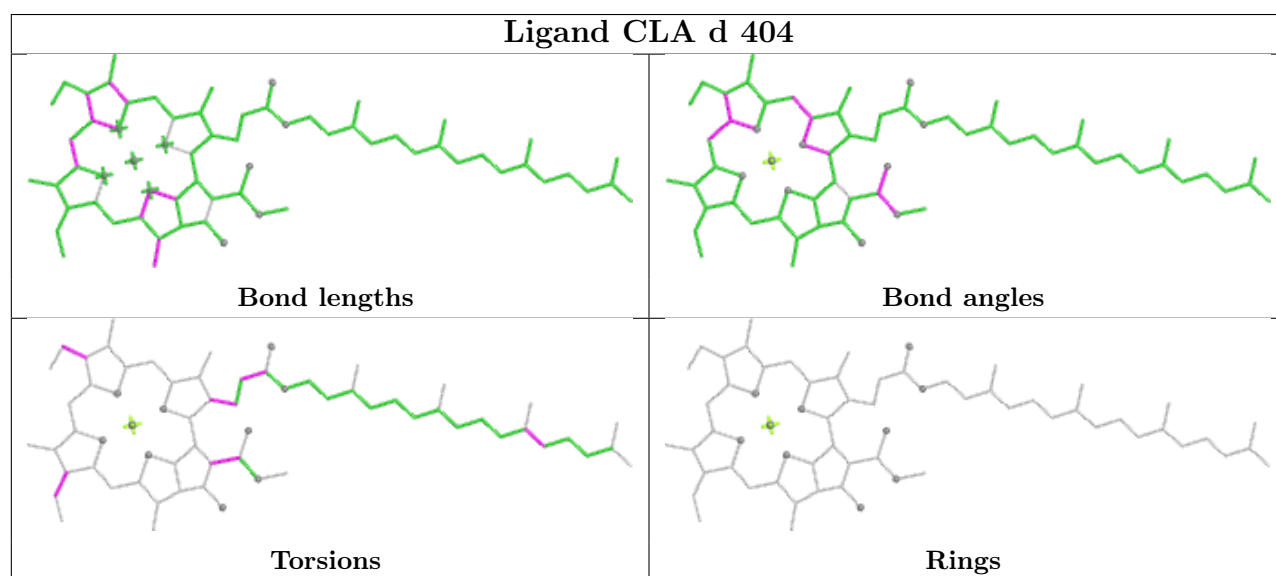
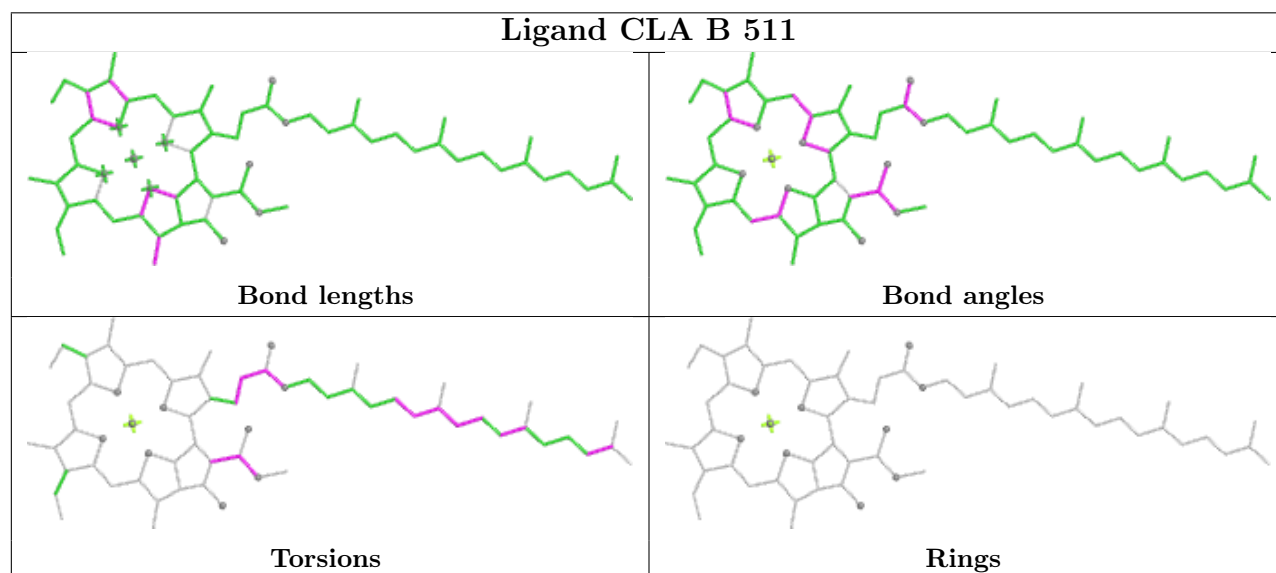
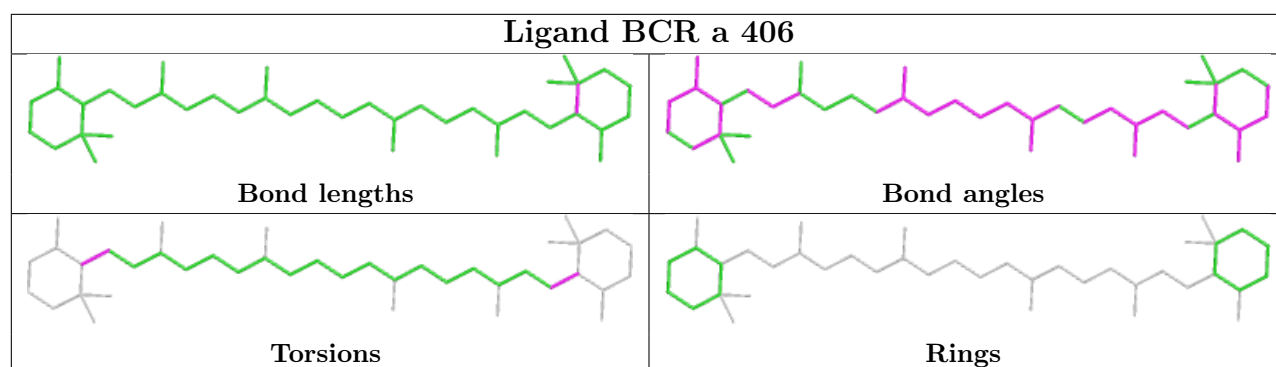
Ligand CLA D 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

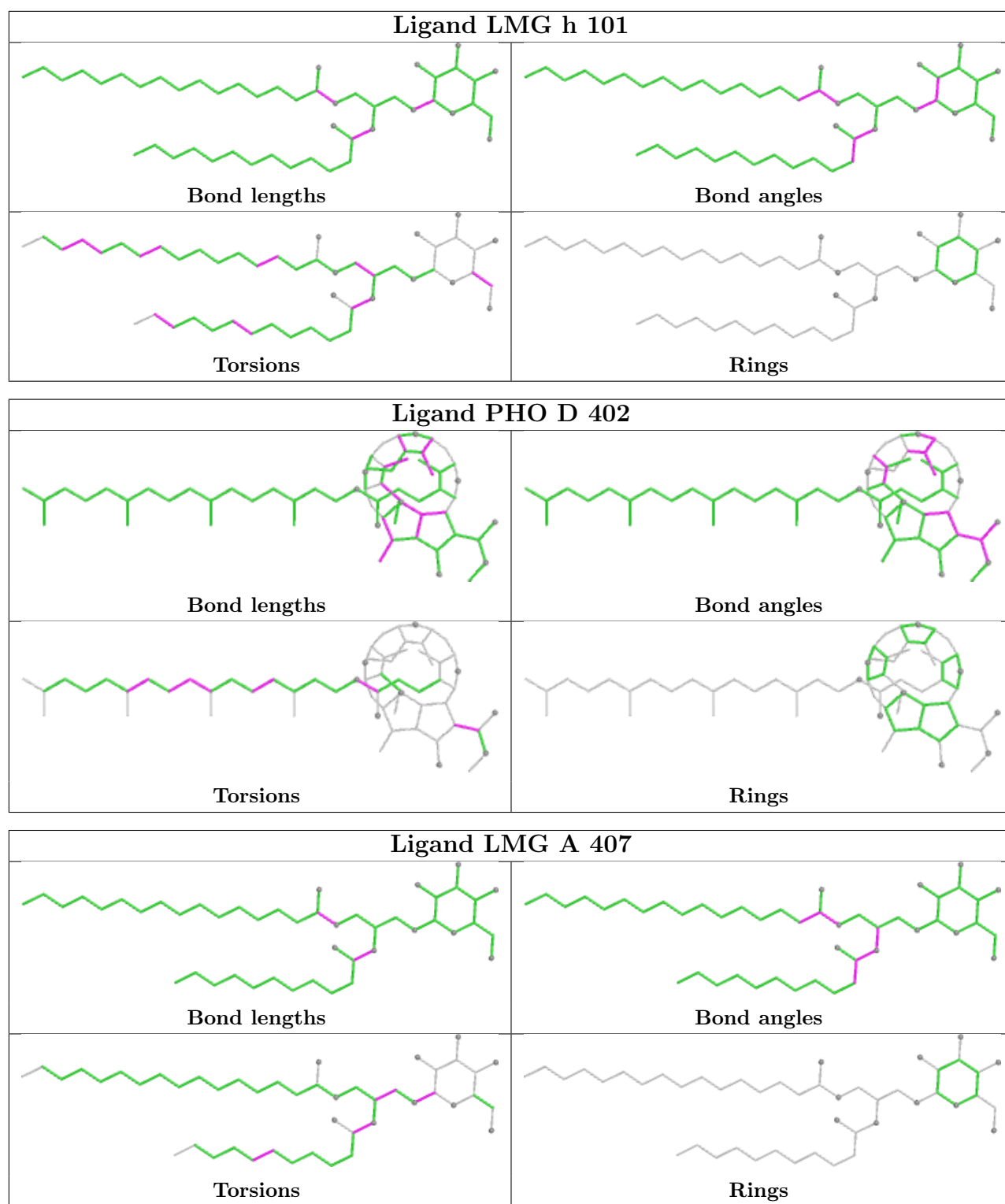
Ligand CLA c 511**Ligand BCR c 516****Ligand CLA c 503**

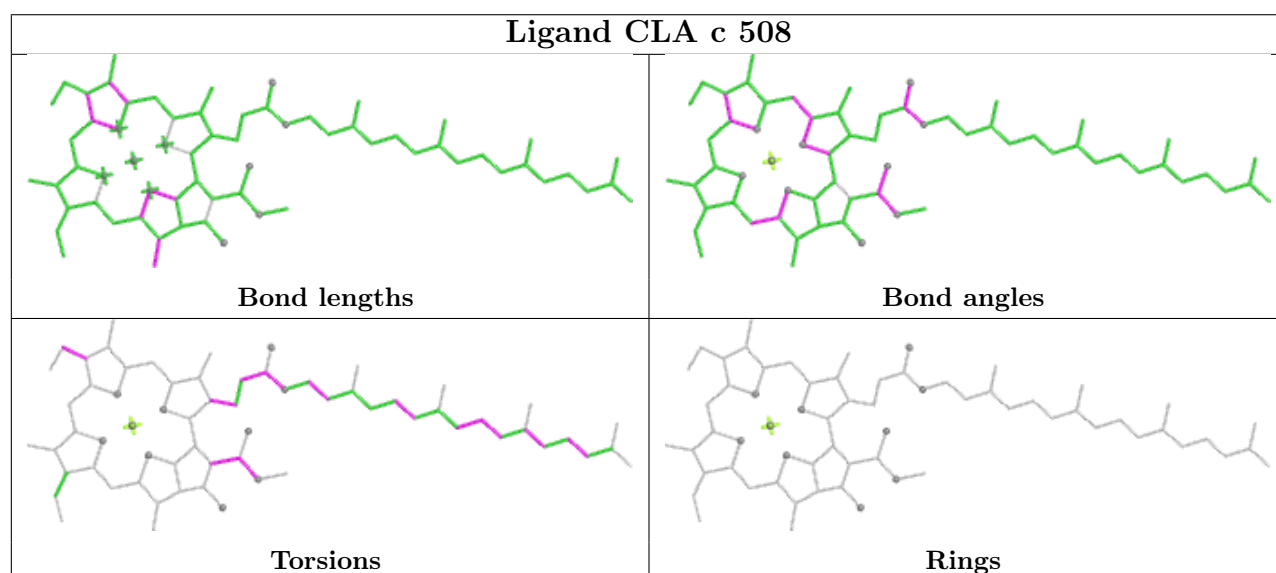
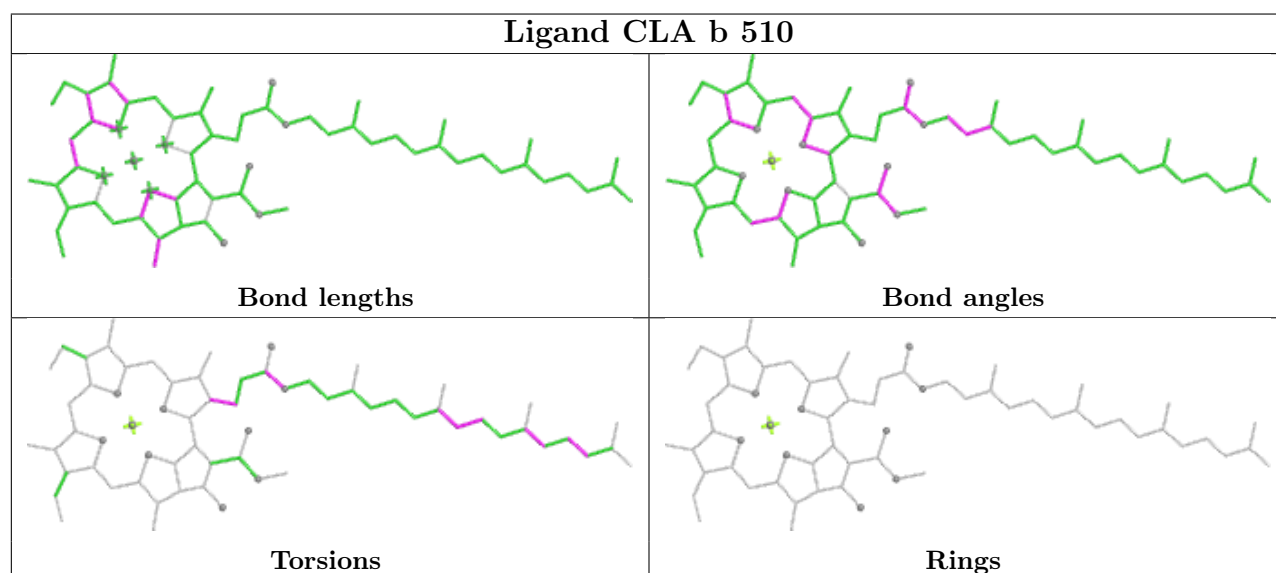
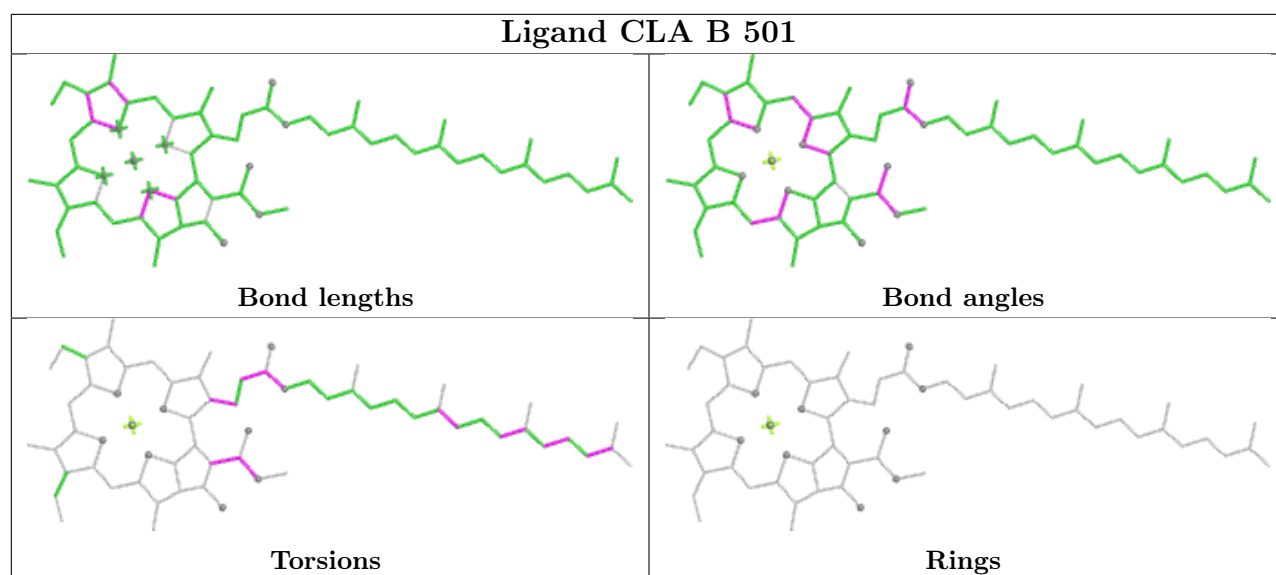


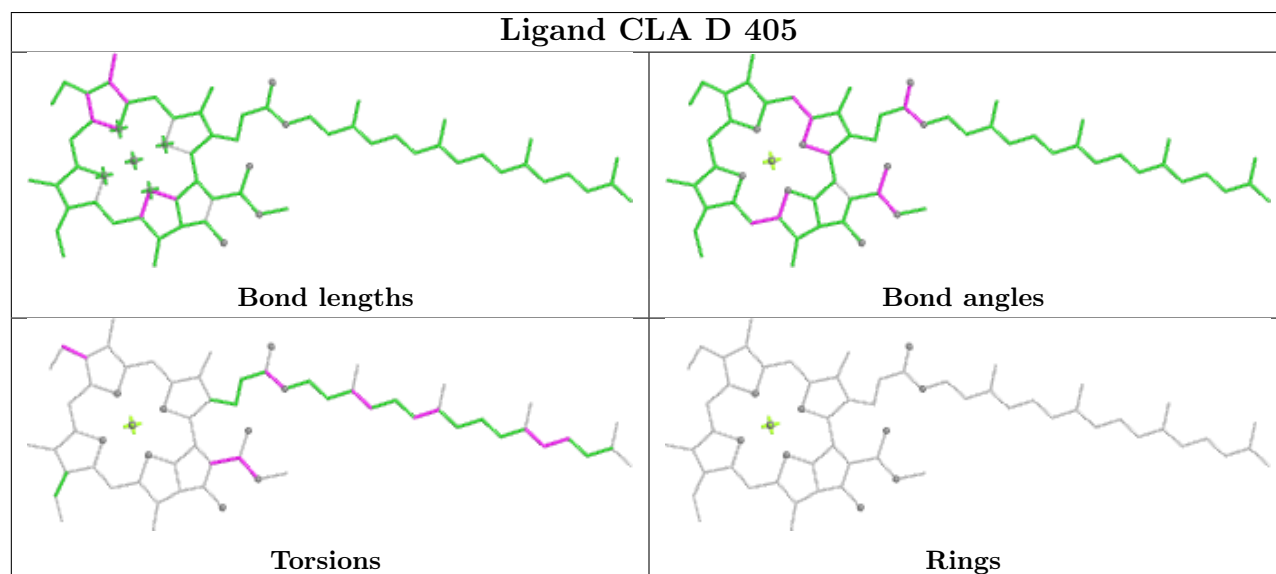
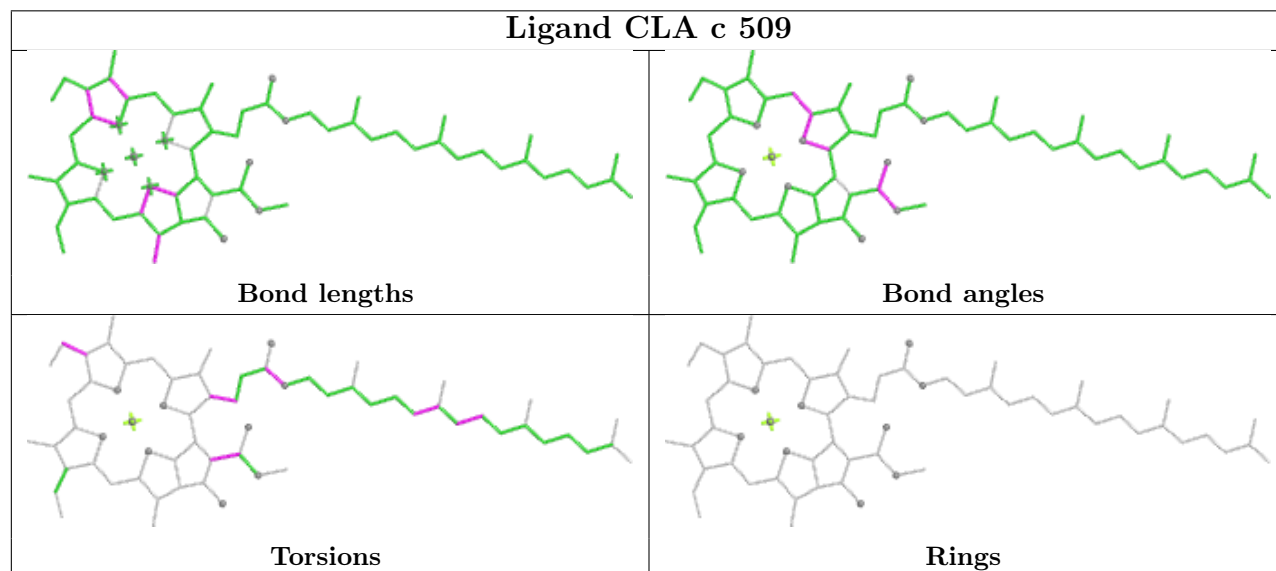
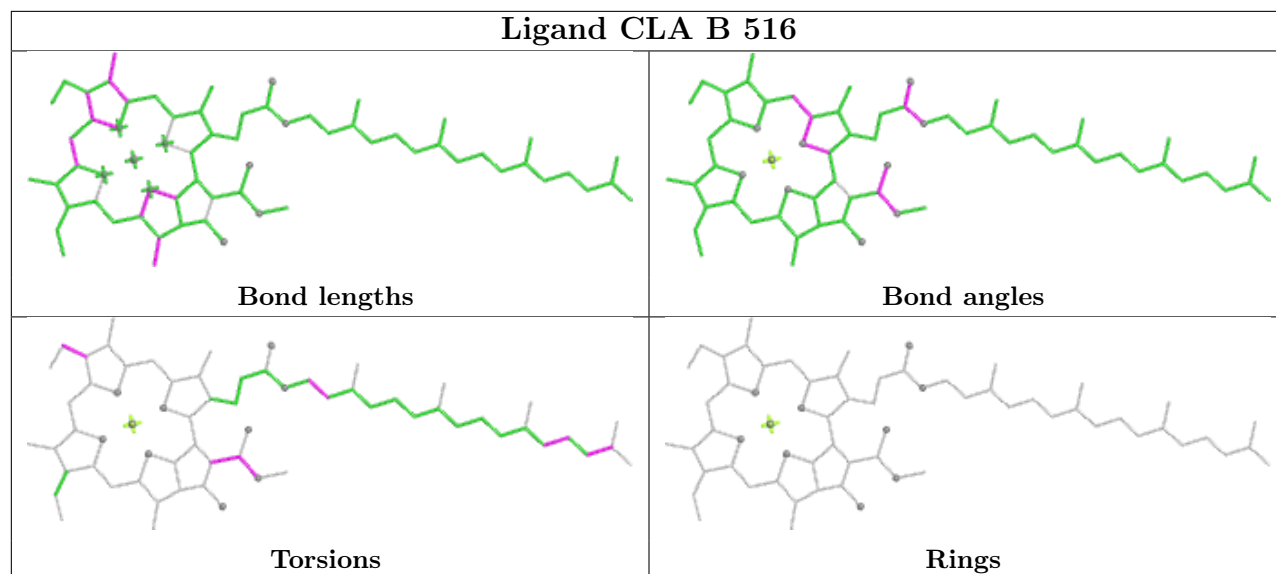


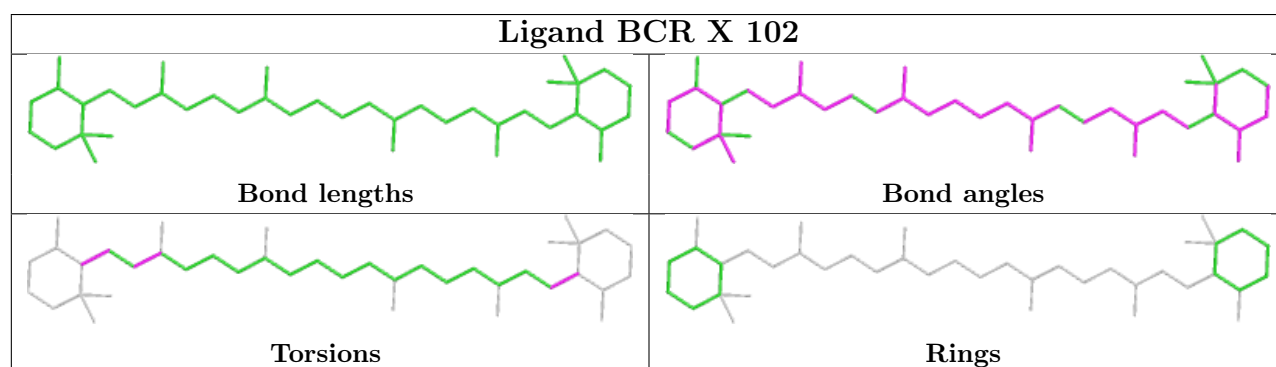
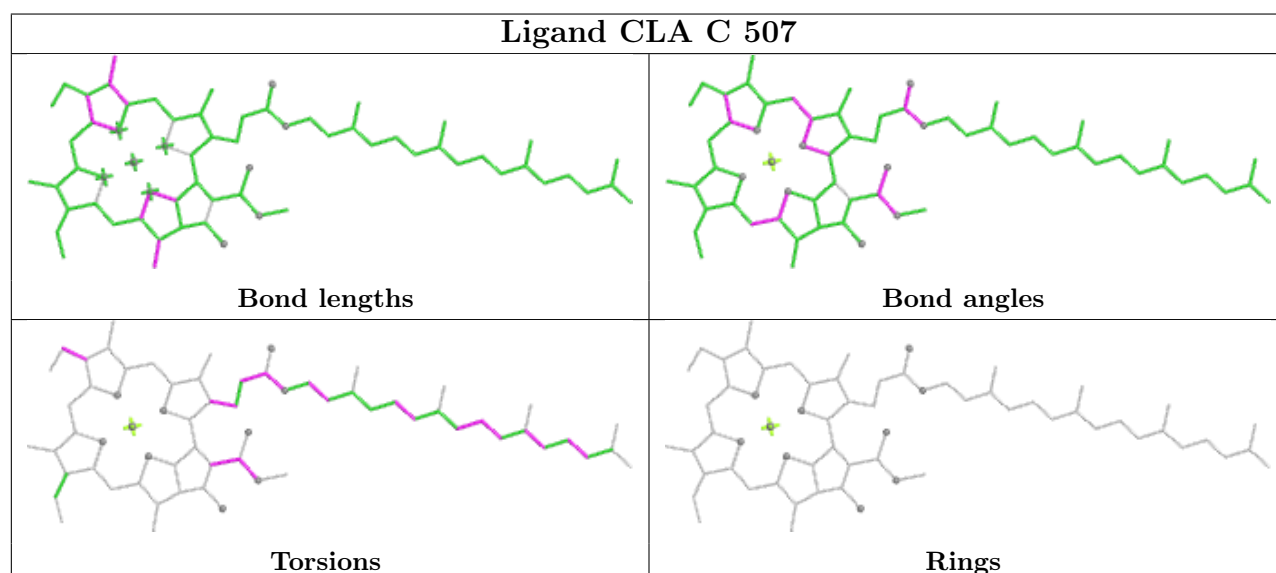
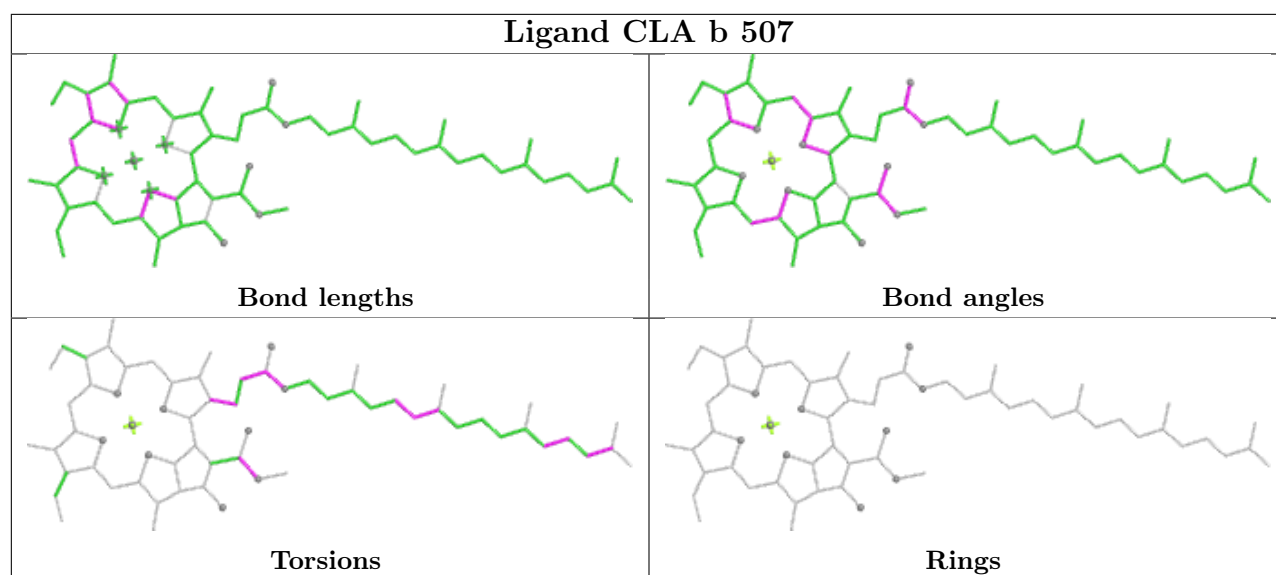


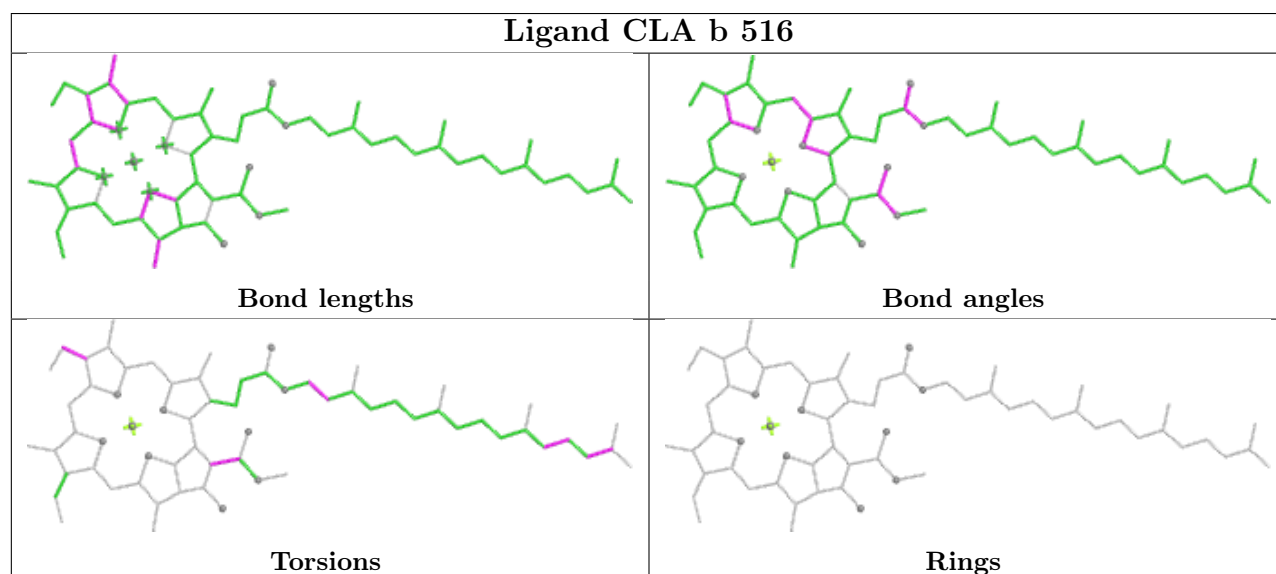
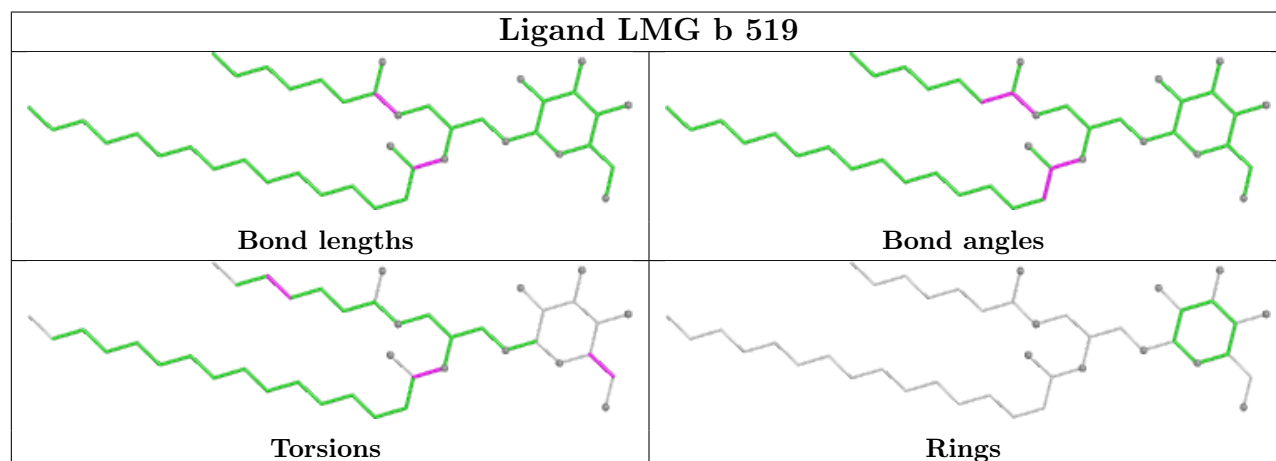
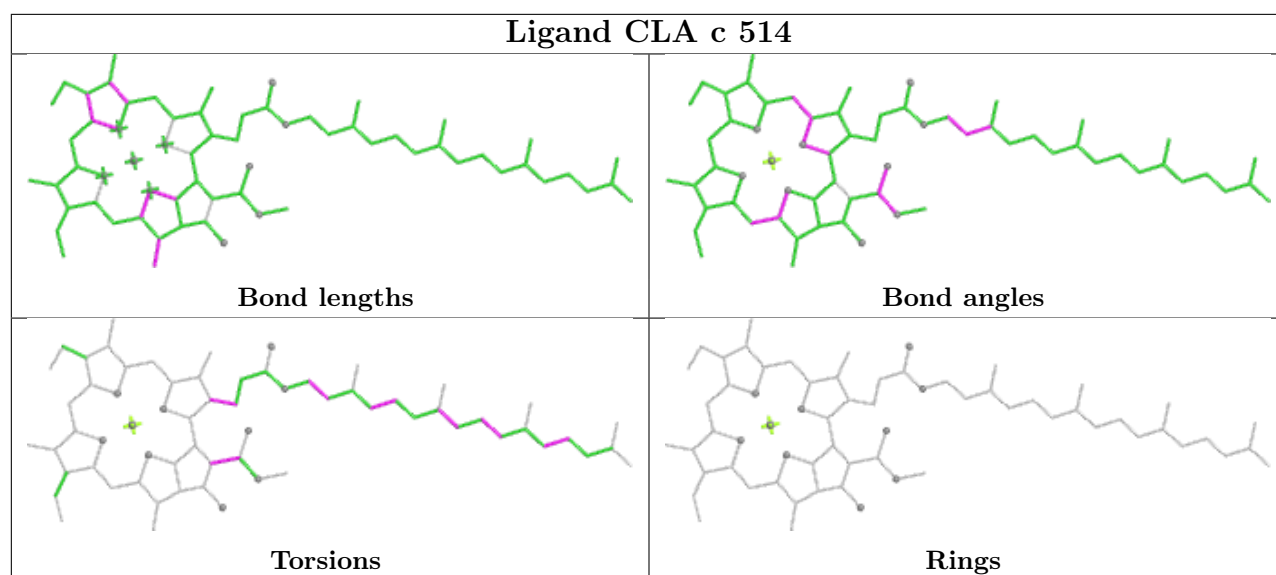


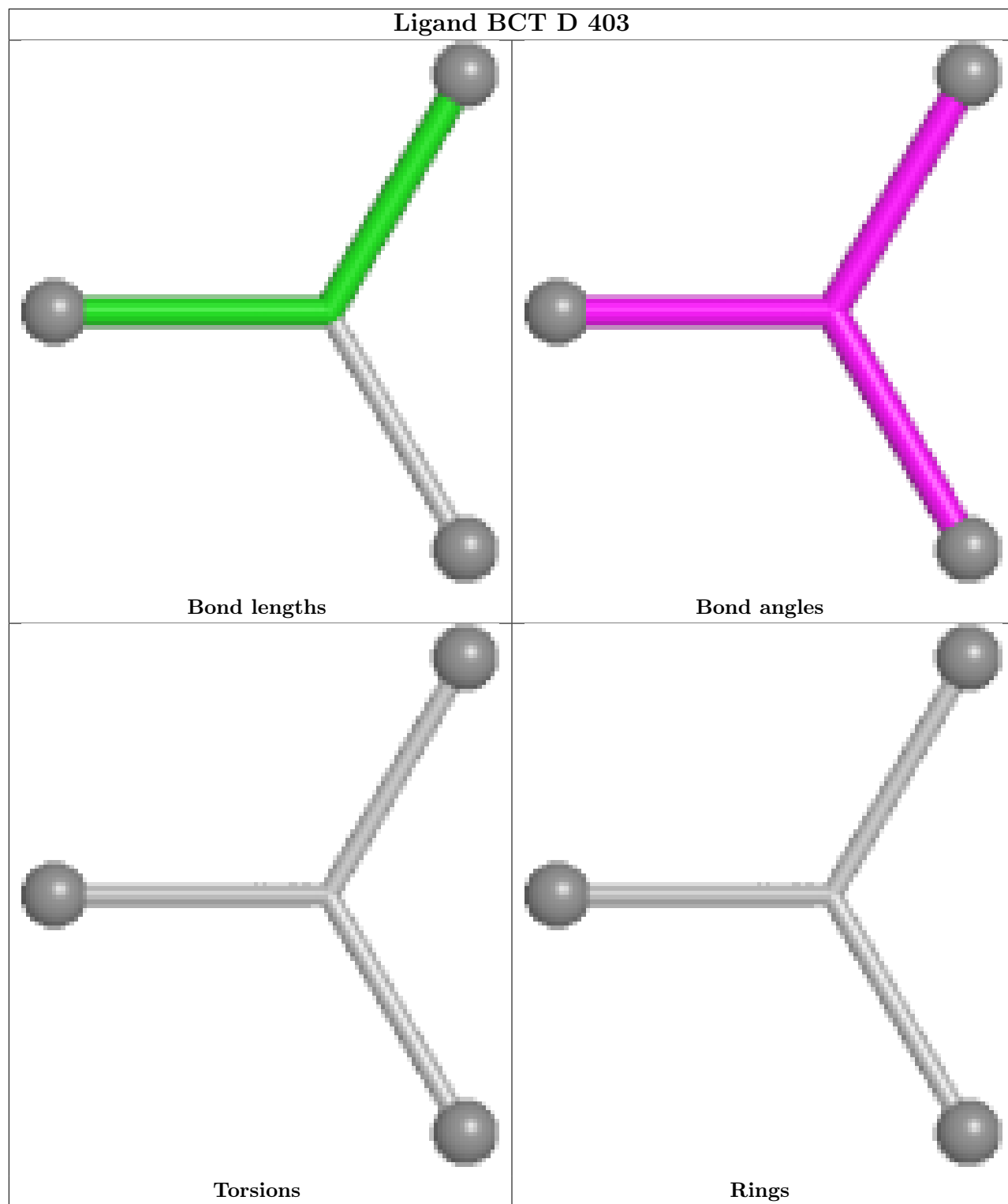


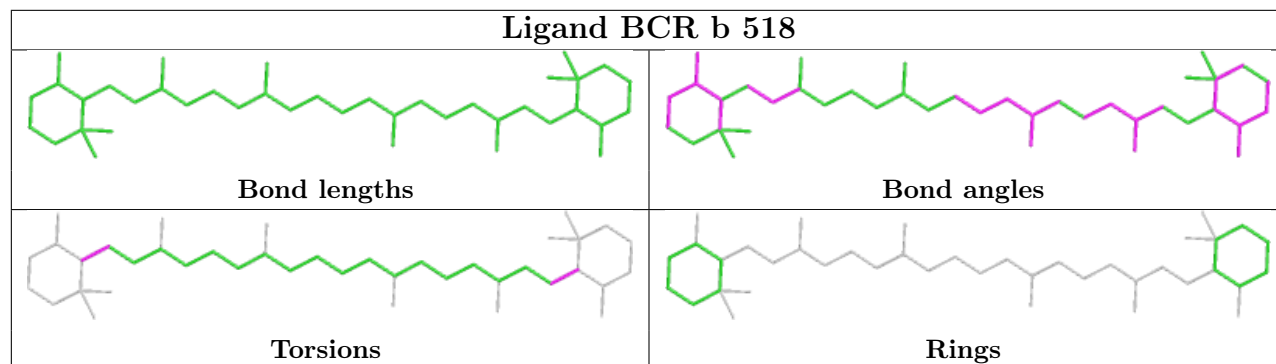
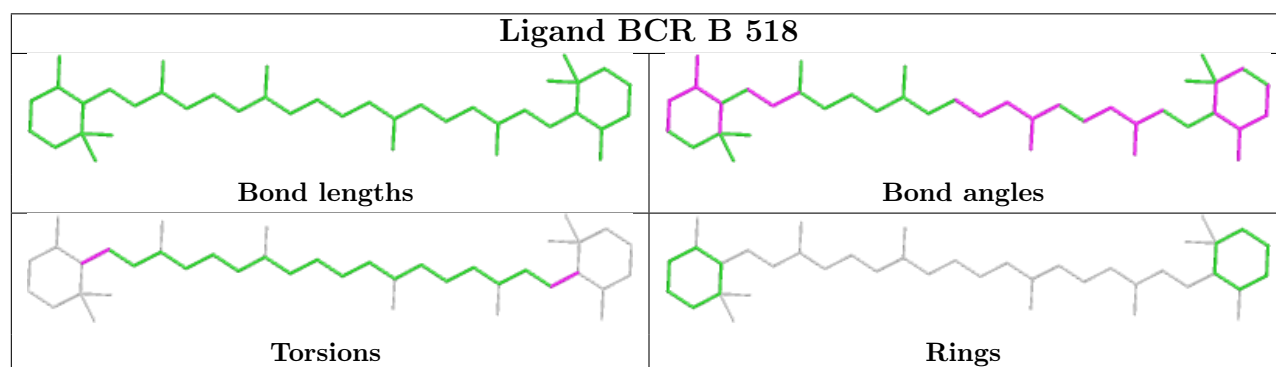
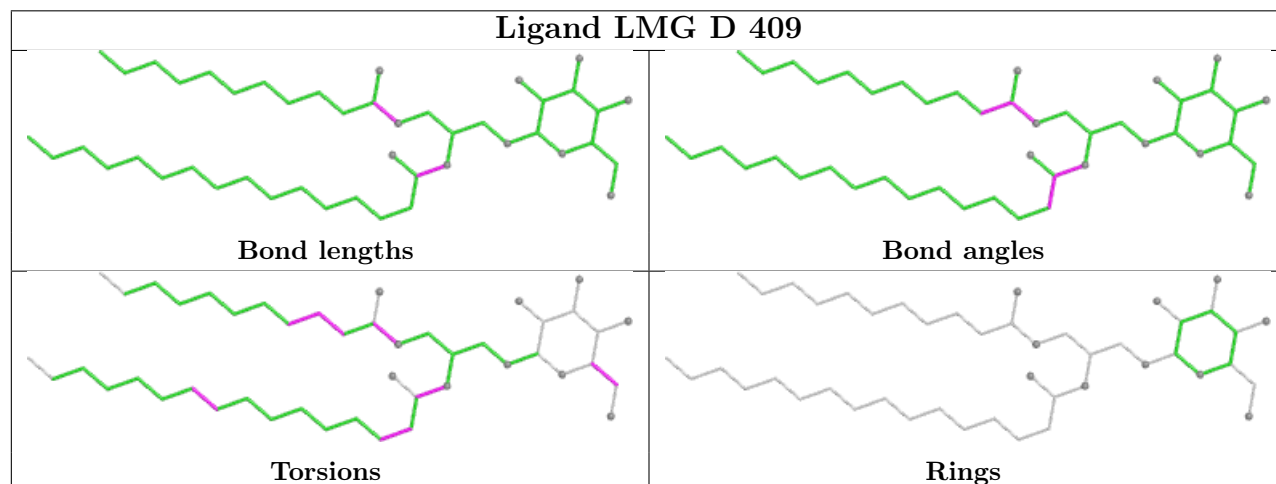
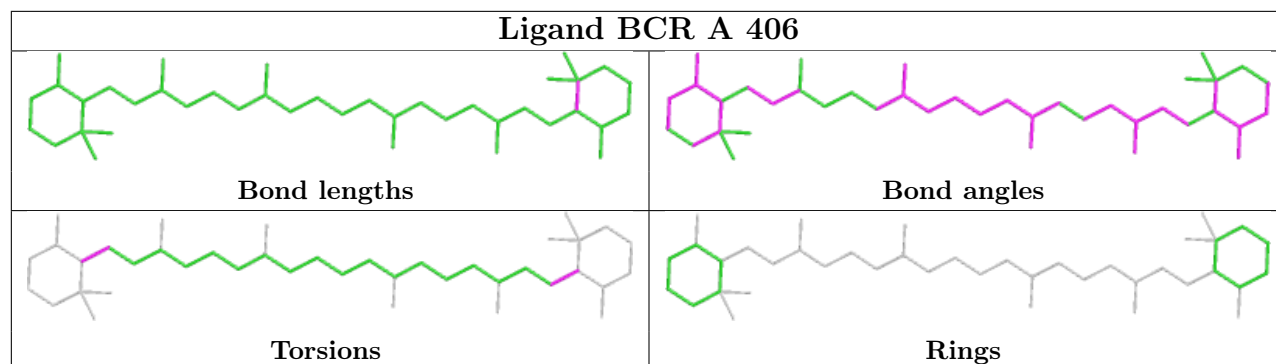


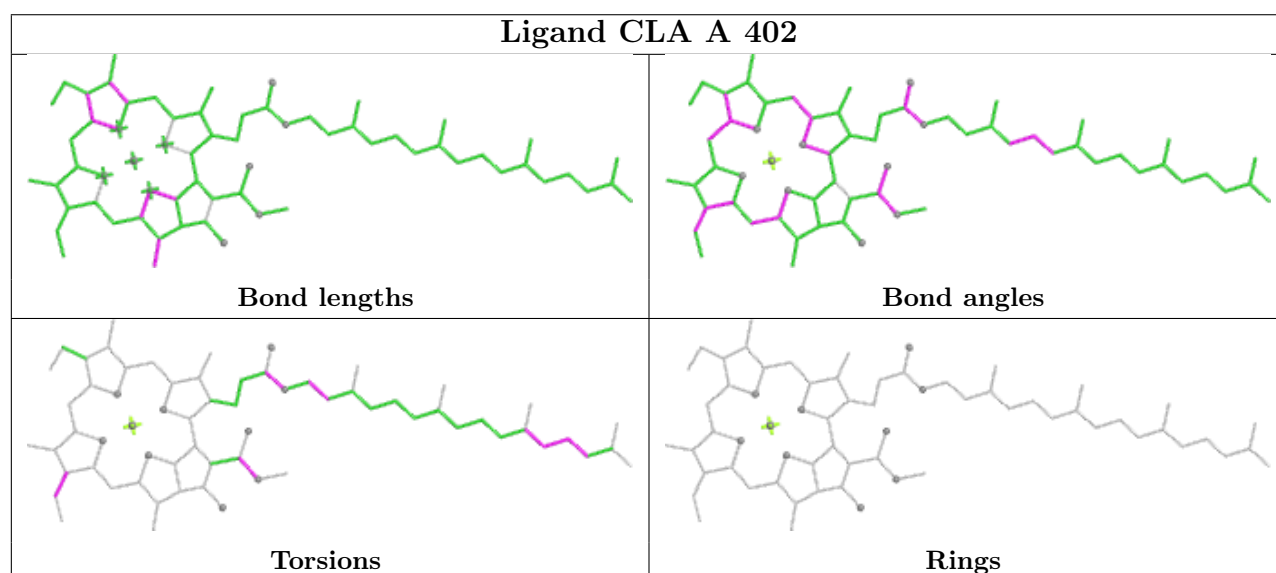
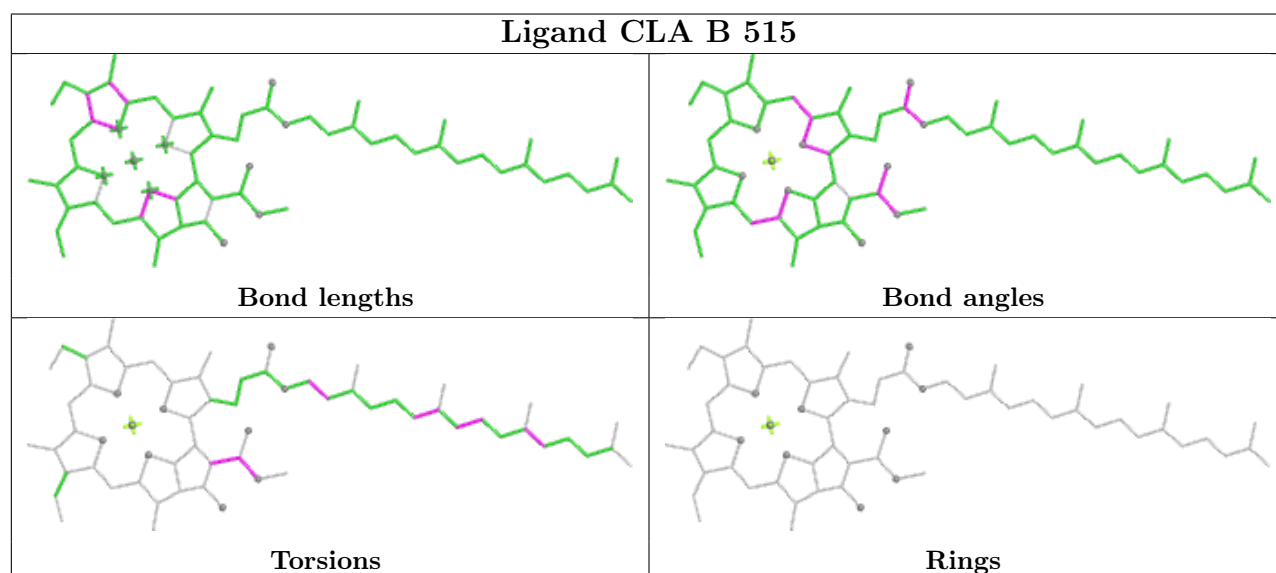
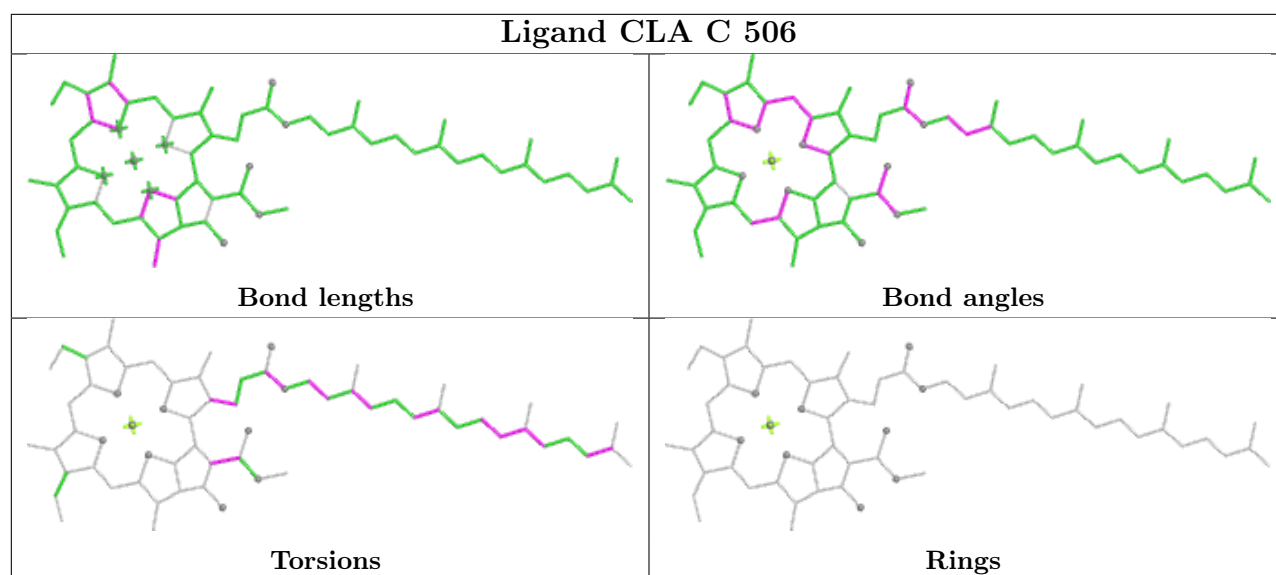


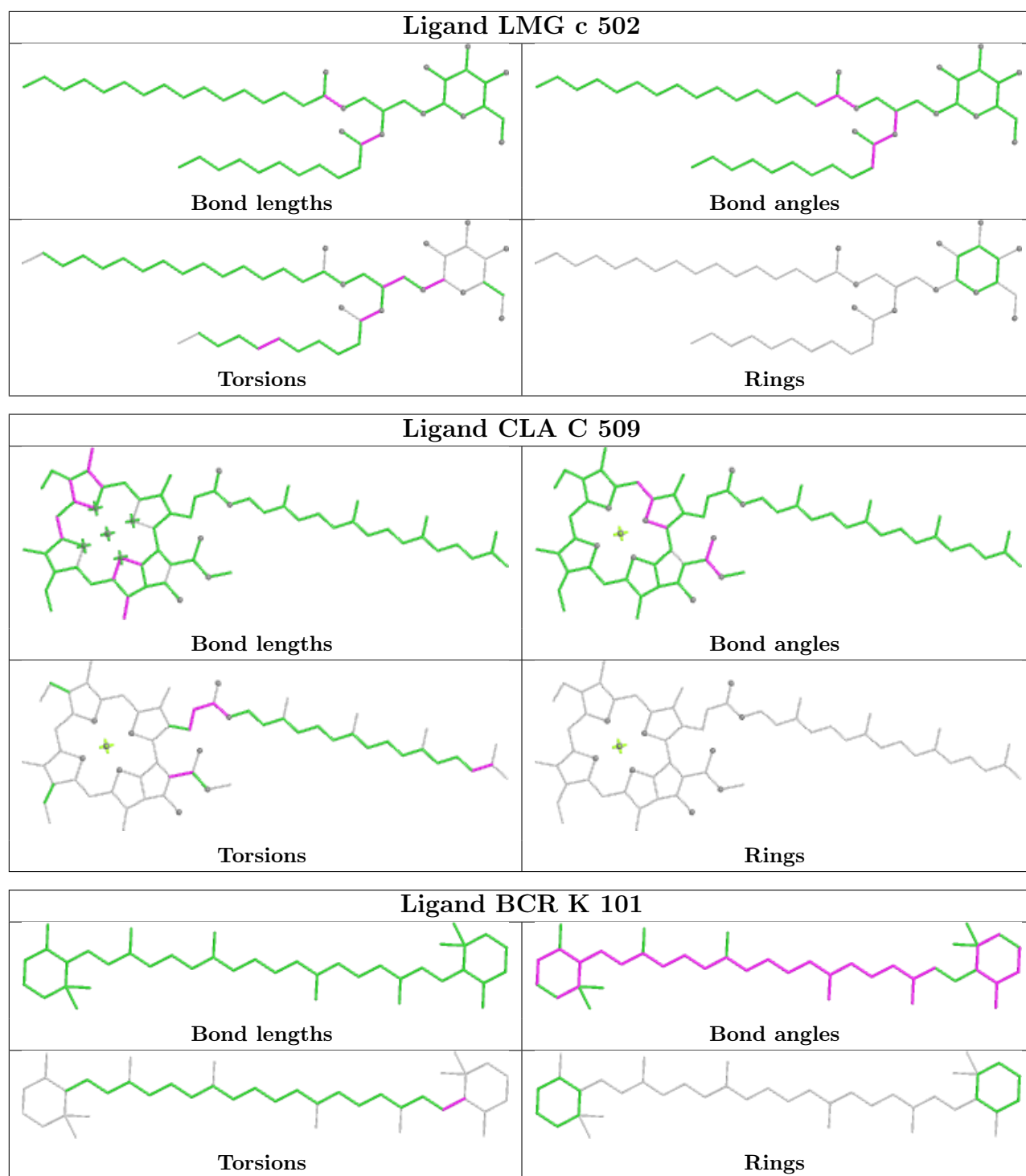


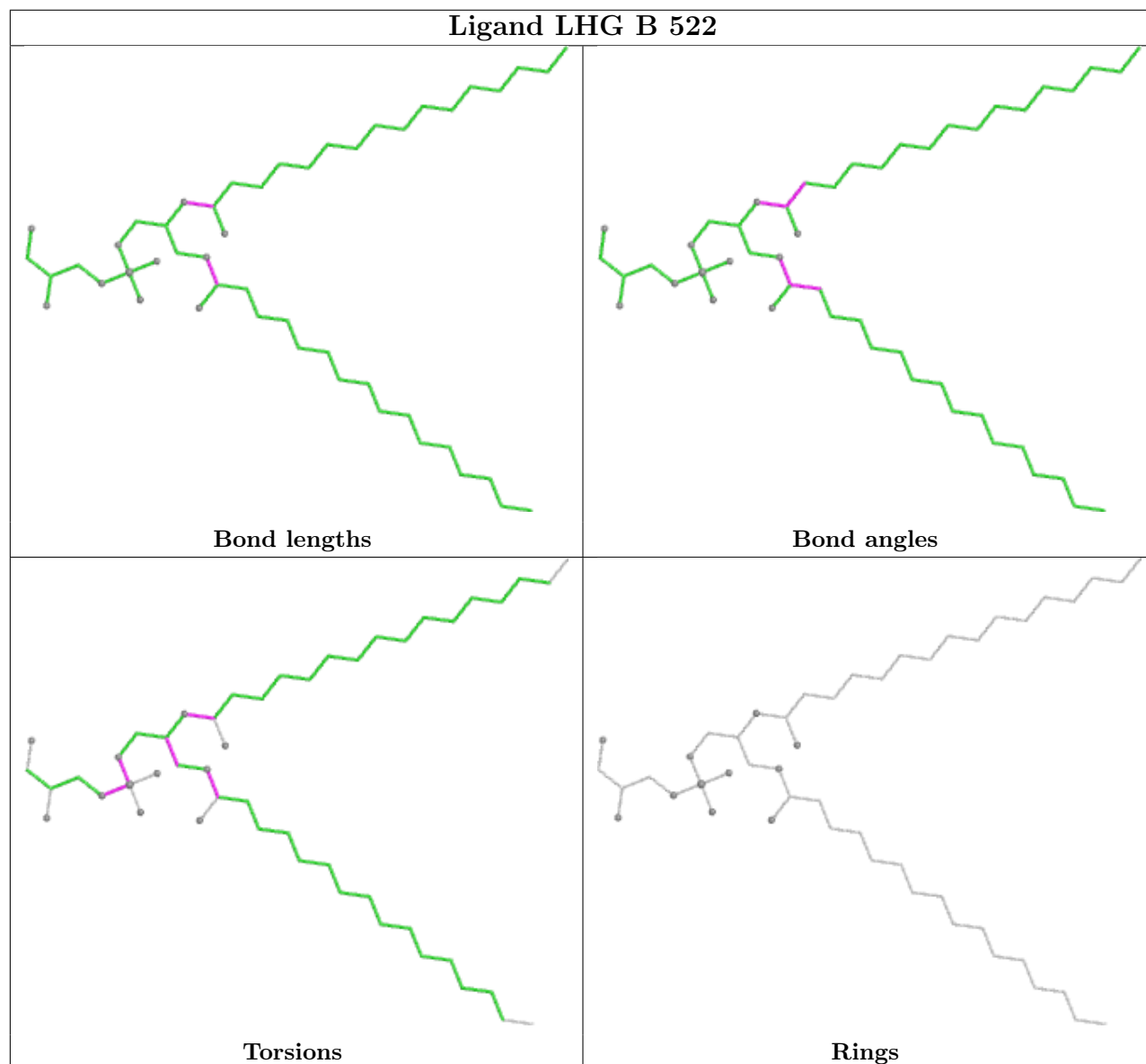
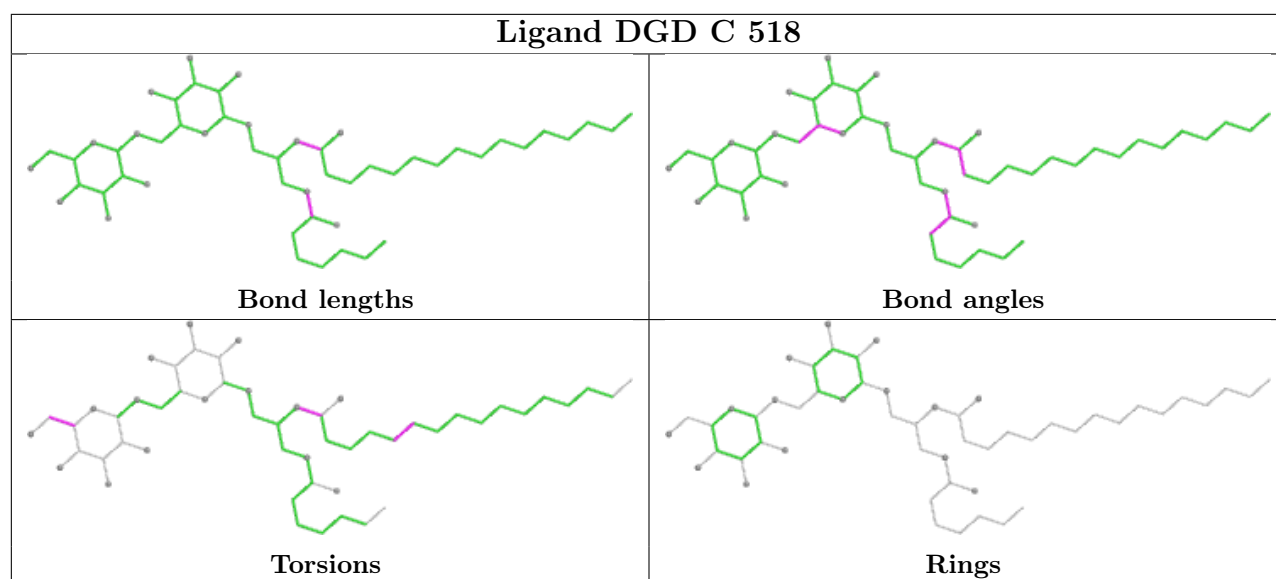


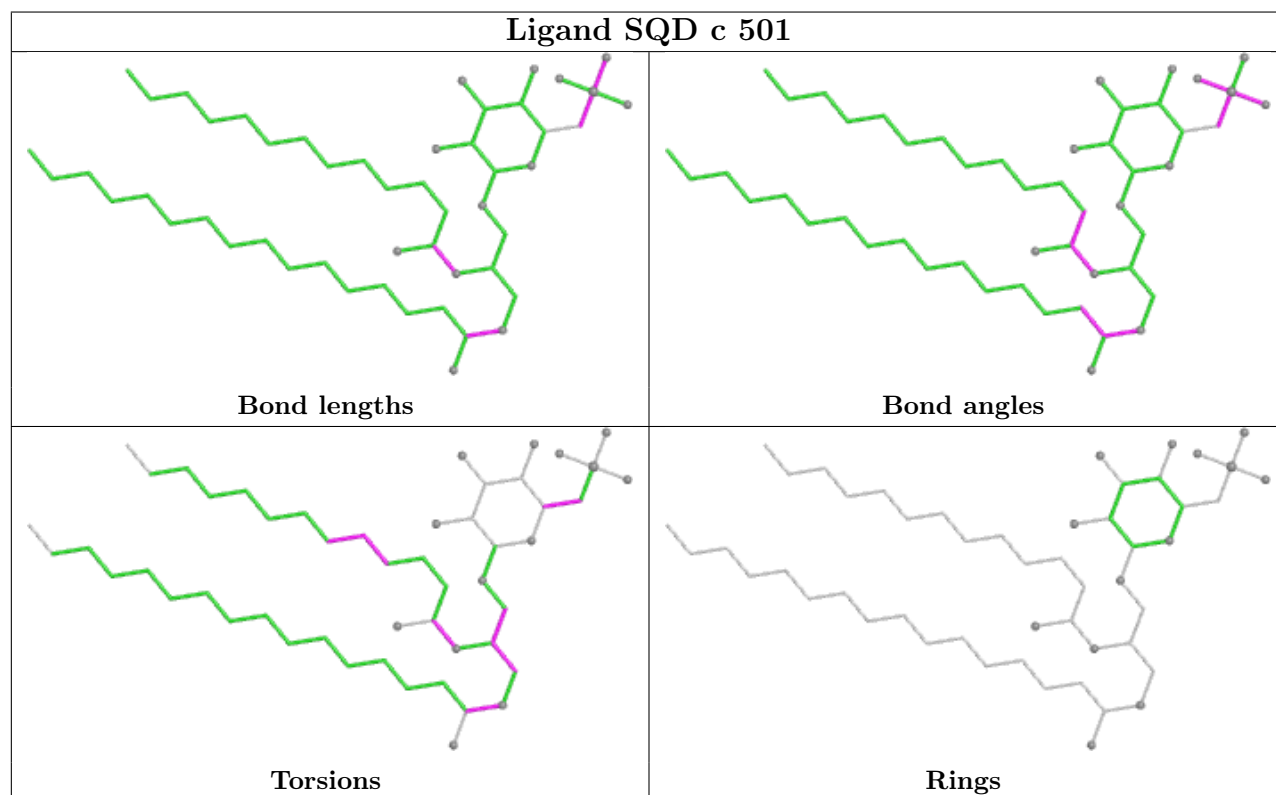
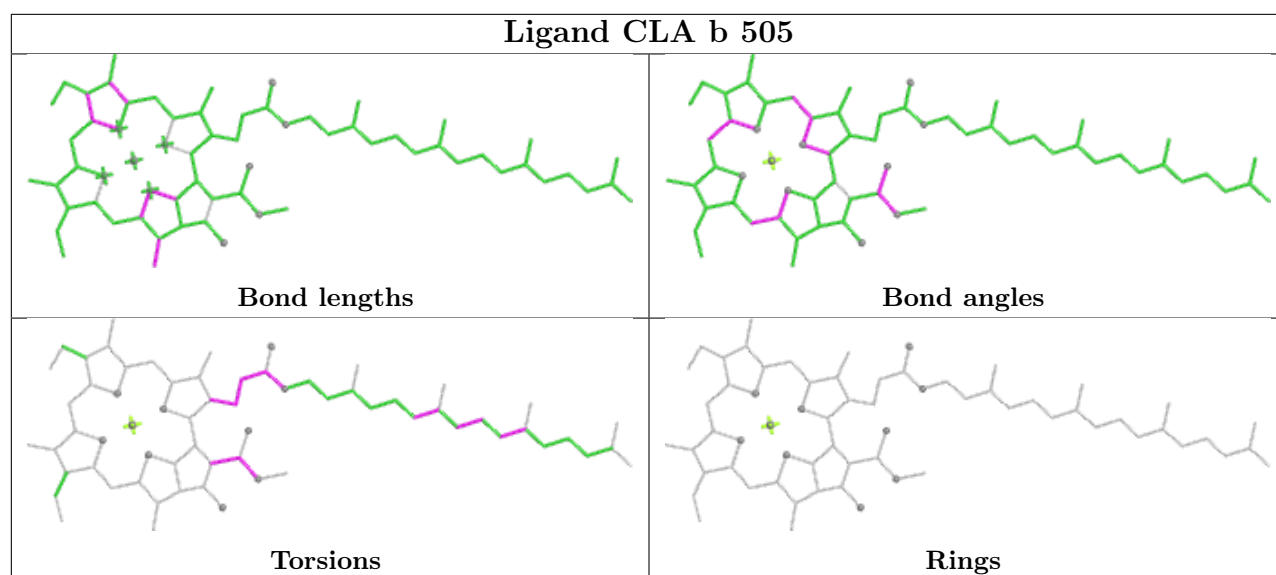




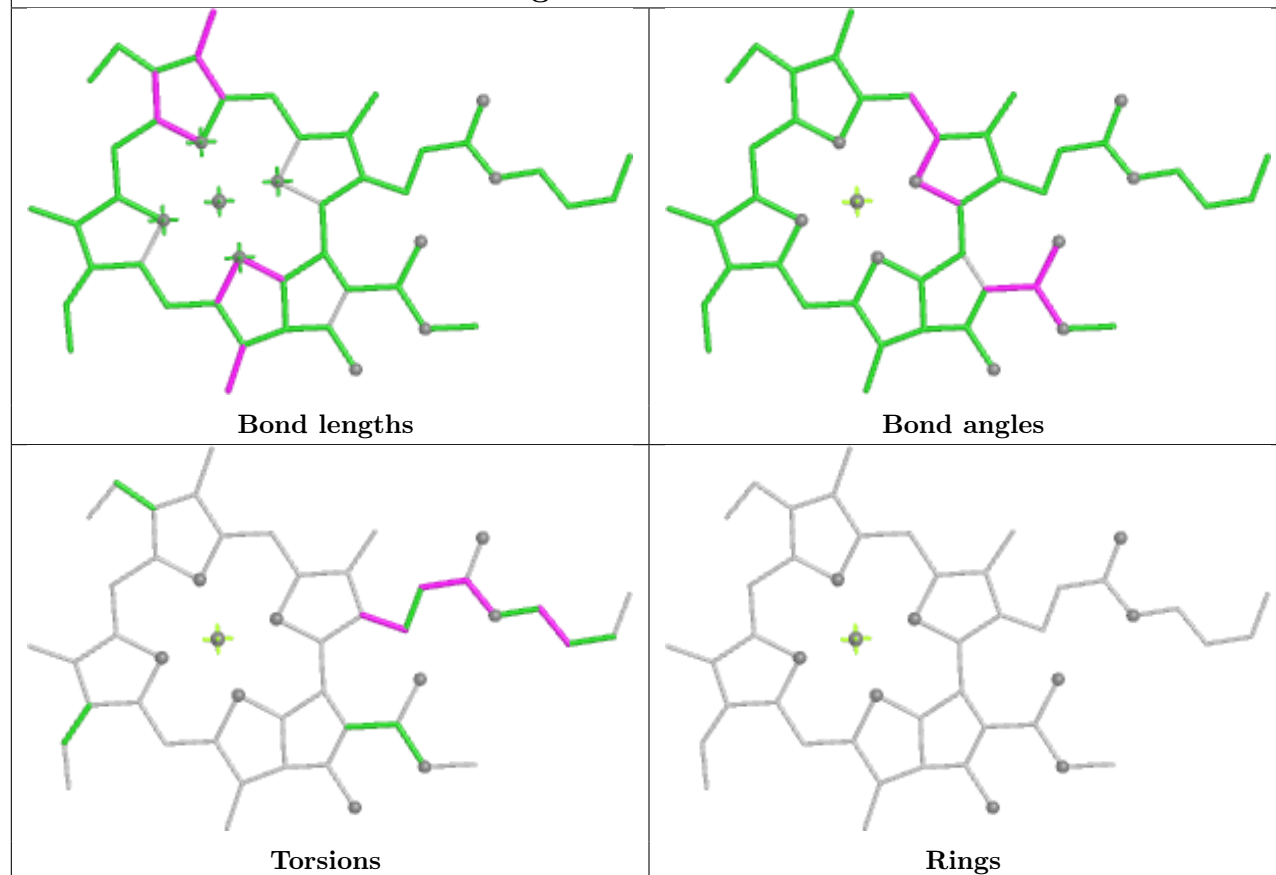




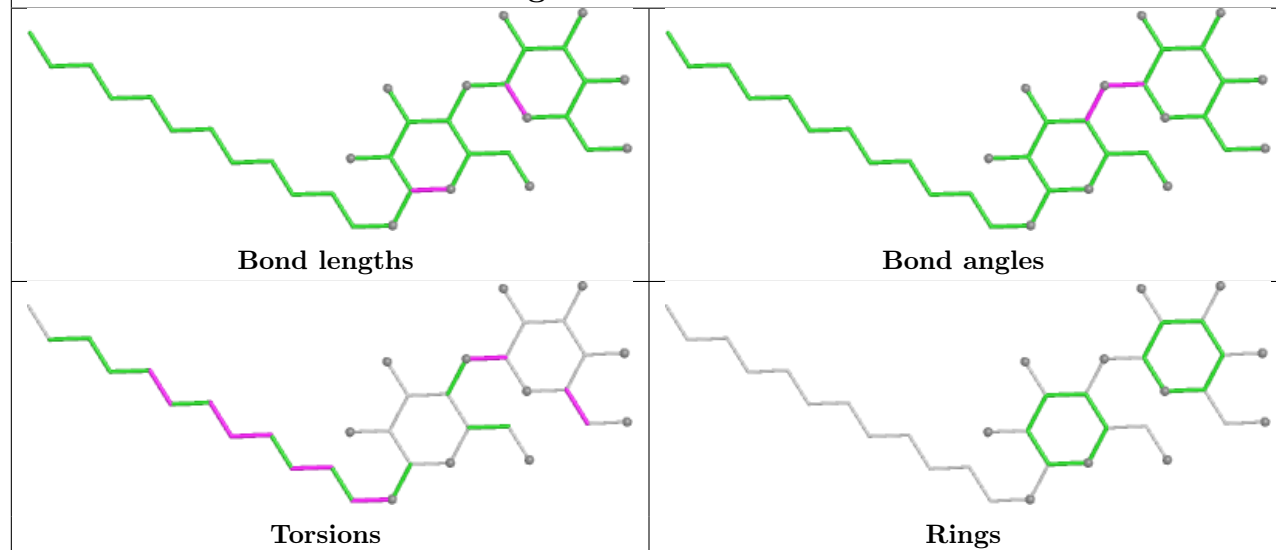


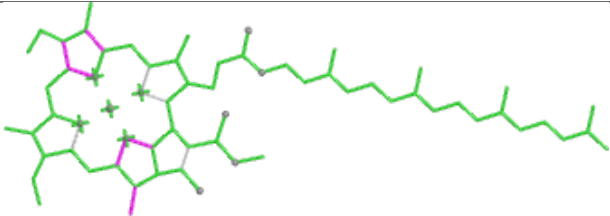
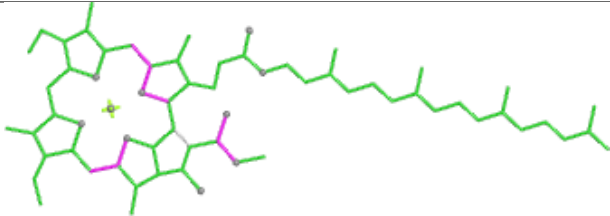
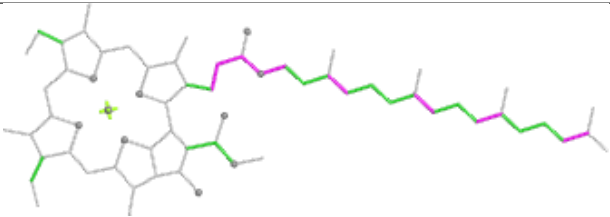
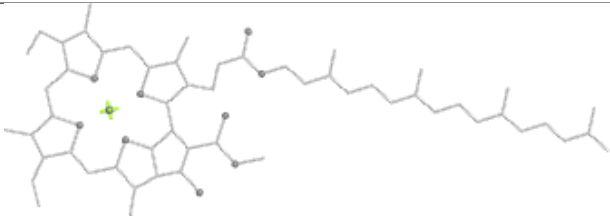
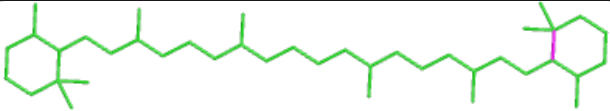
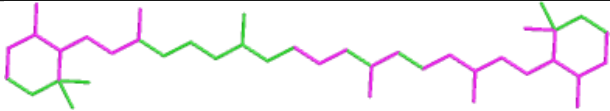
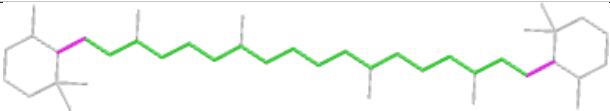
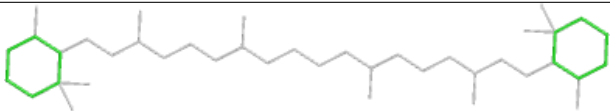


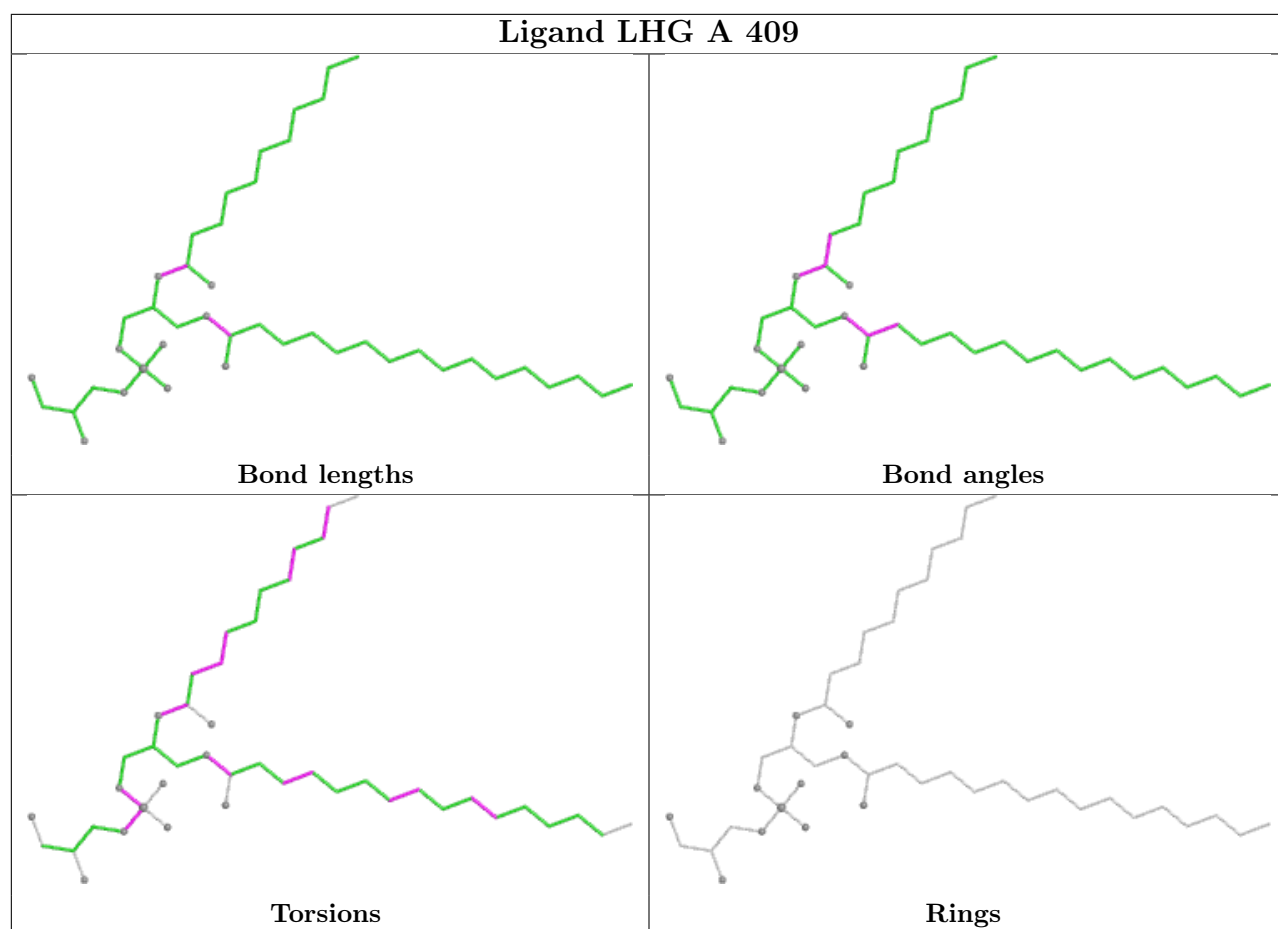
Ligand CLA A 403

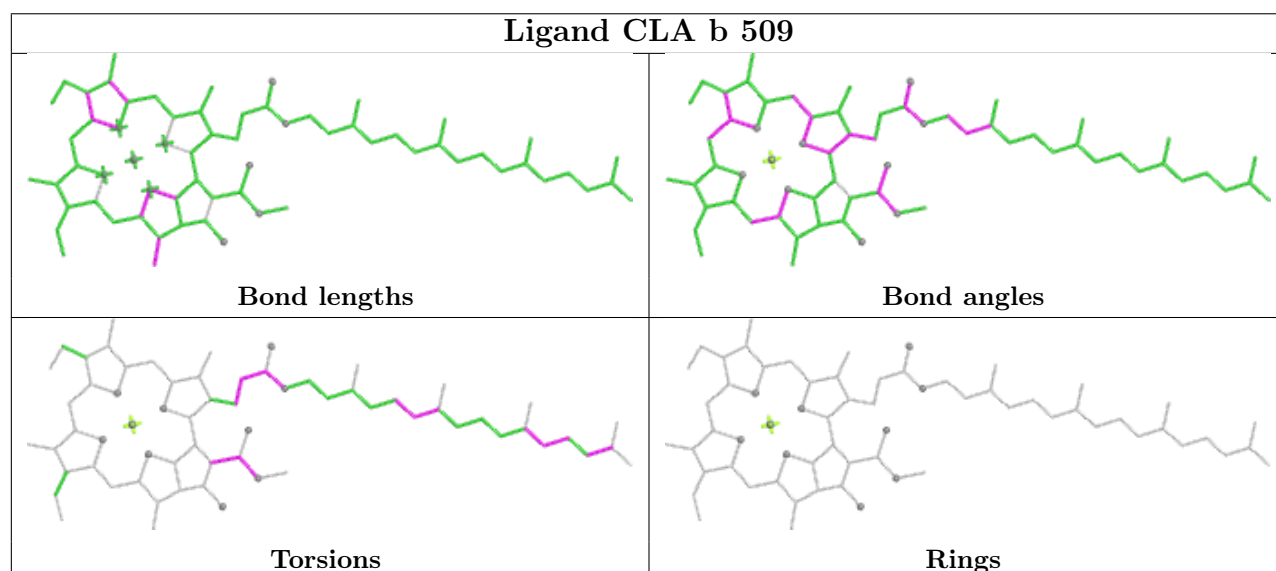
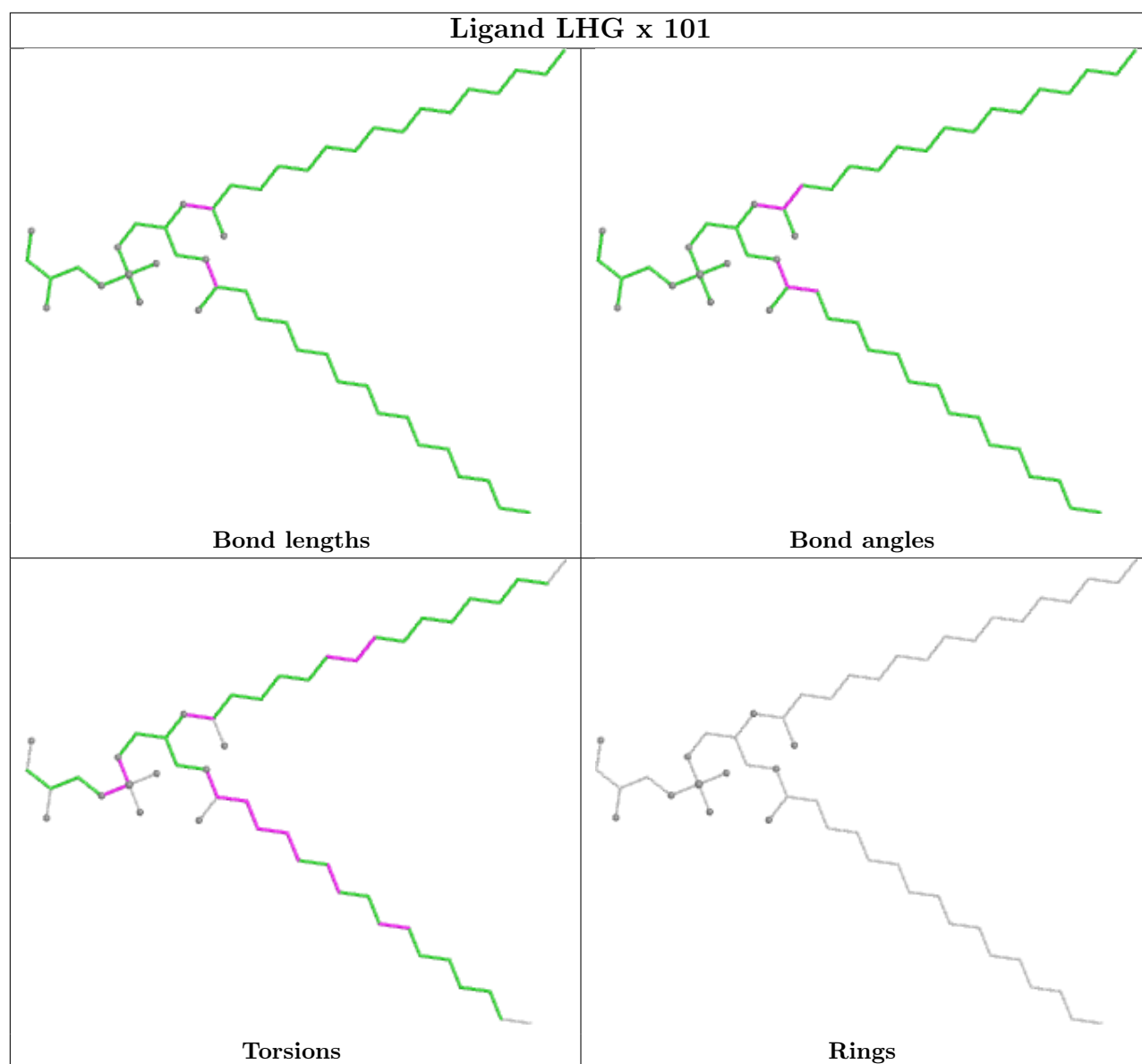


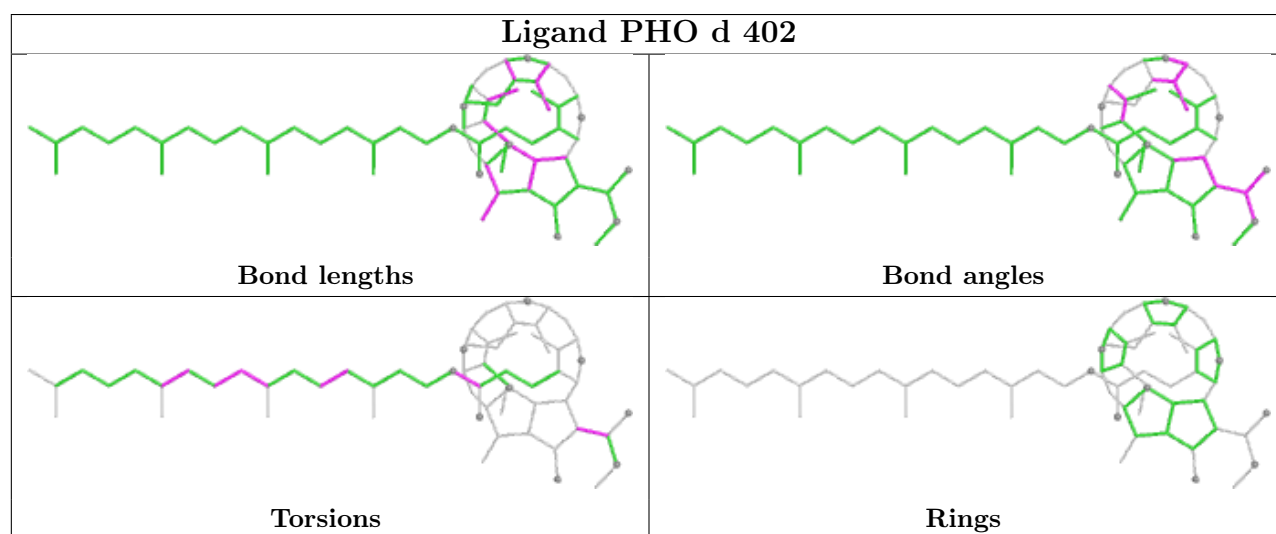
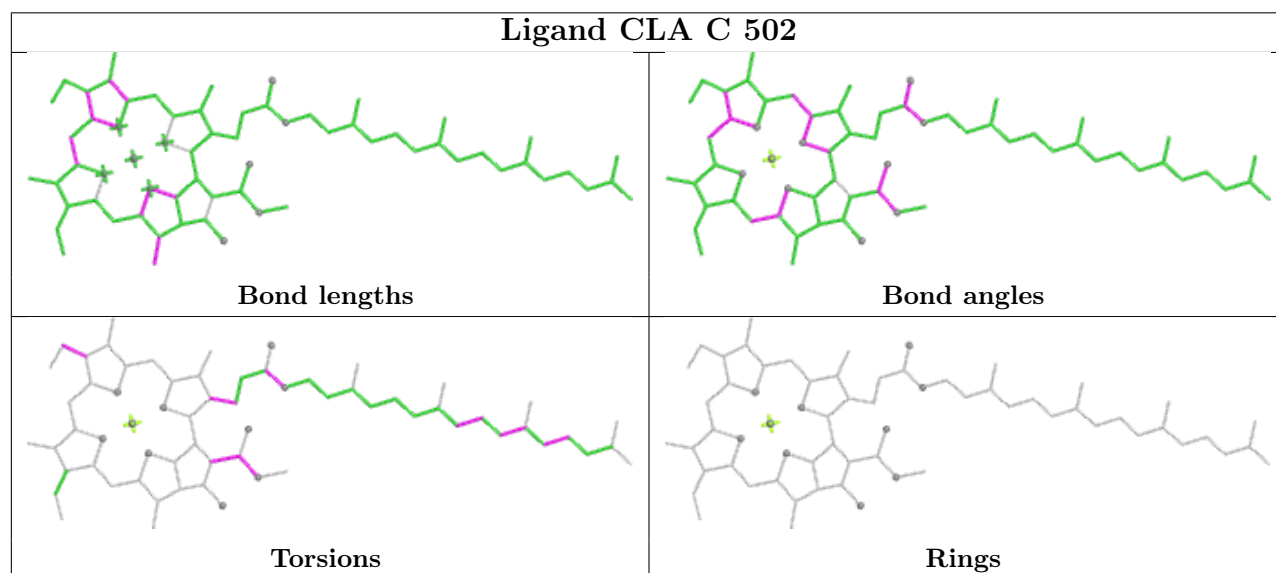
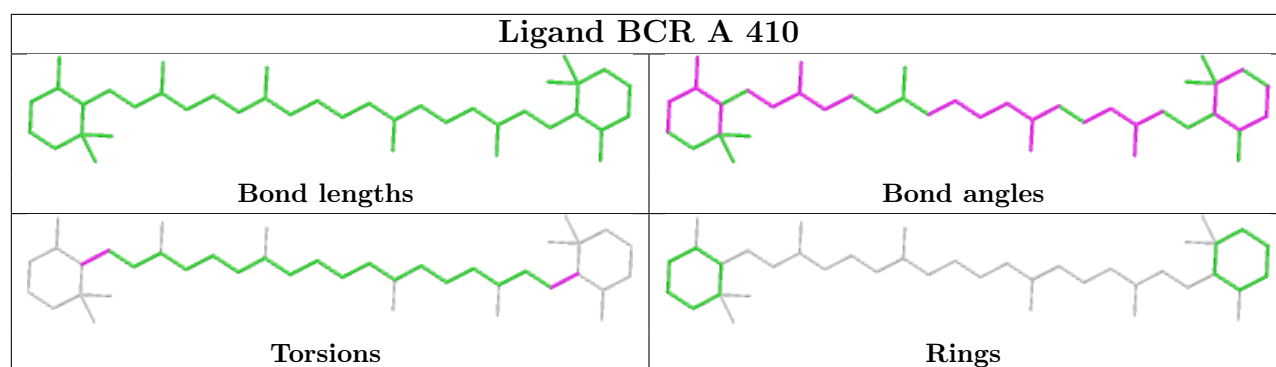
Ligand LMU C 522

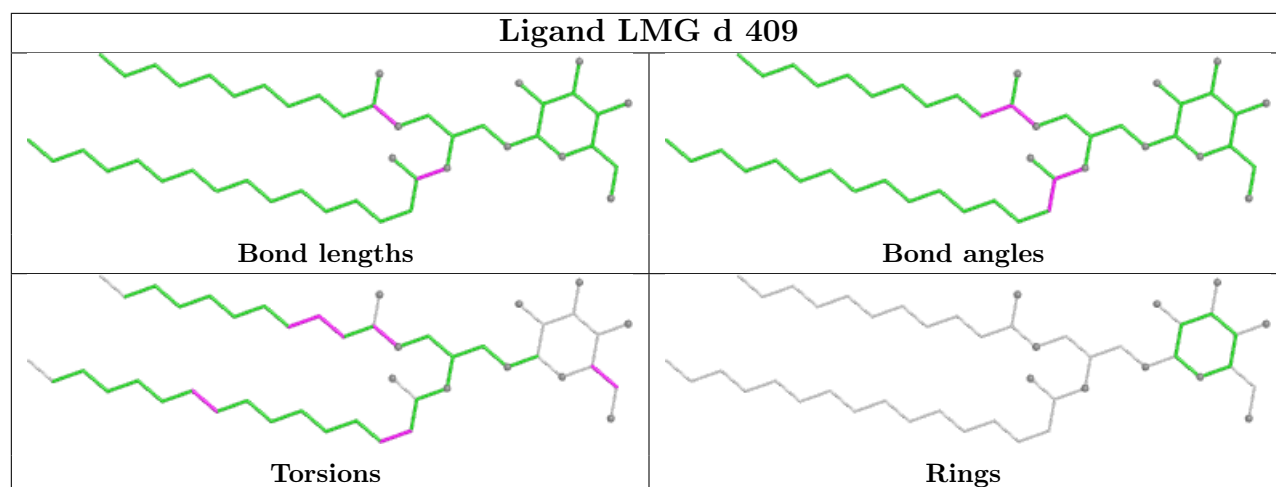
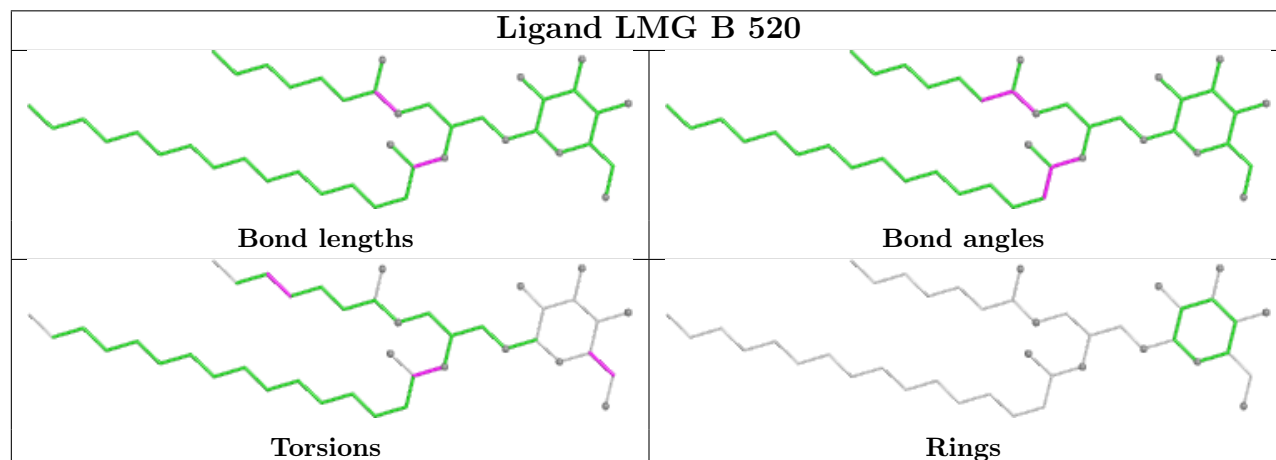
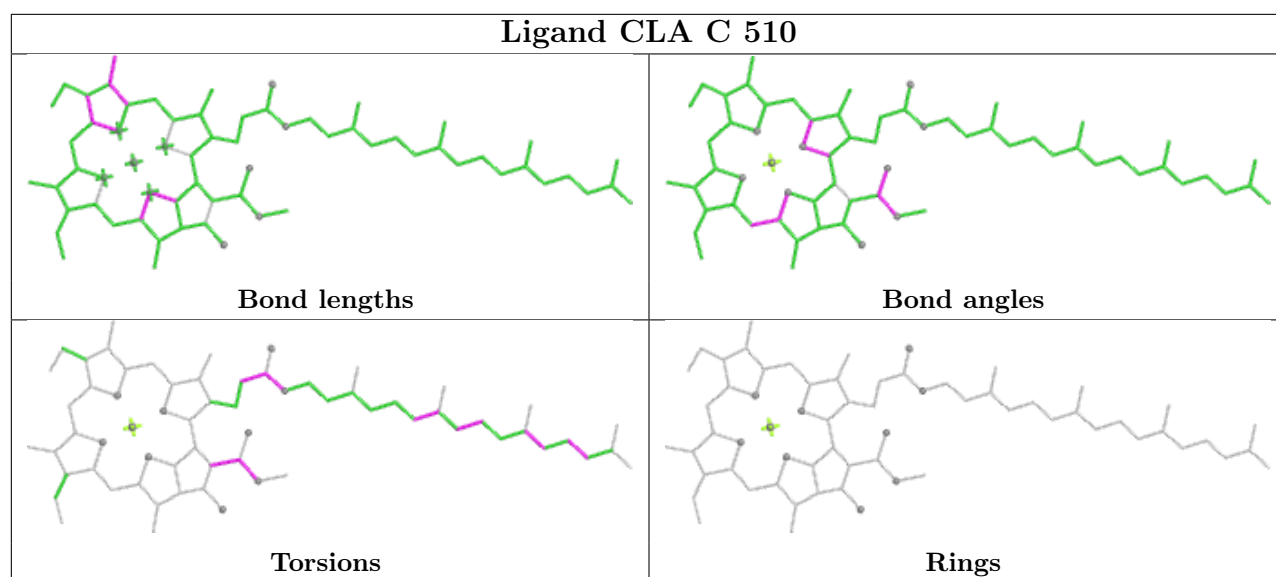


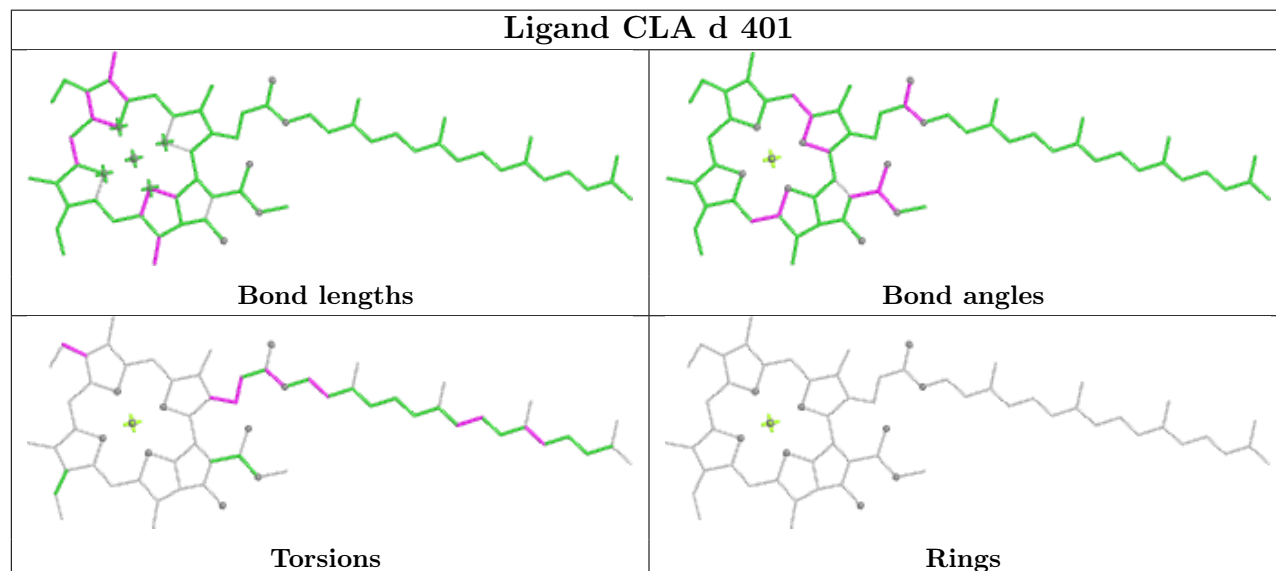
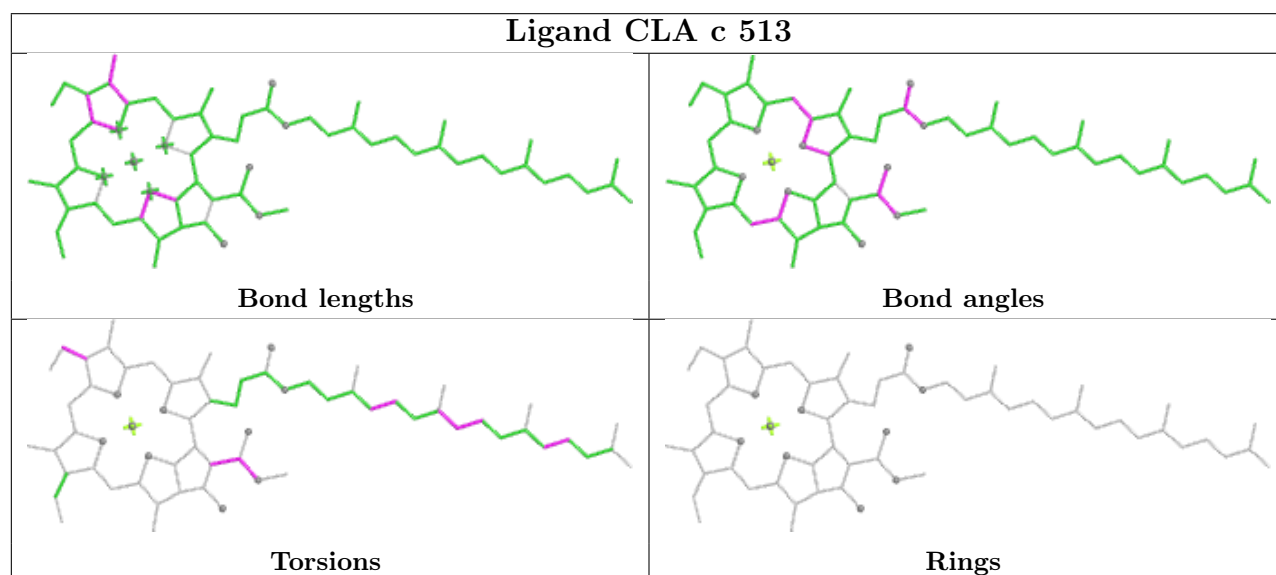
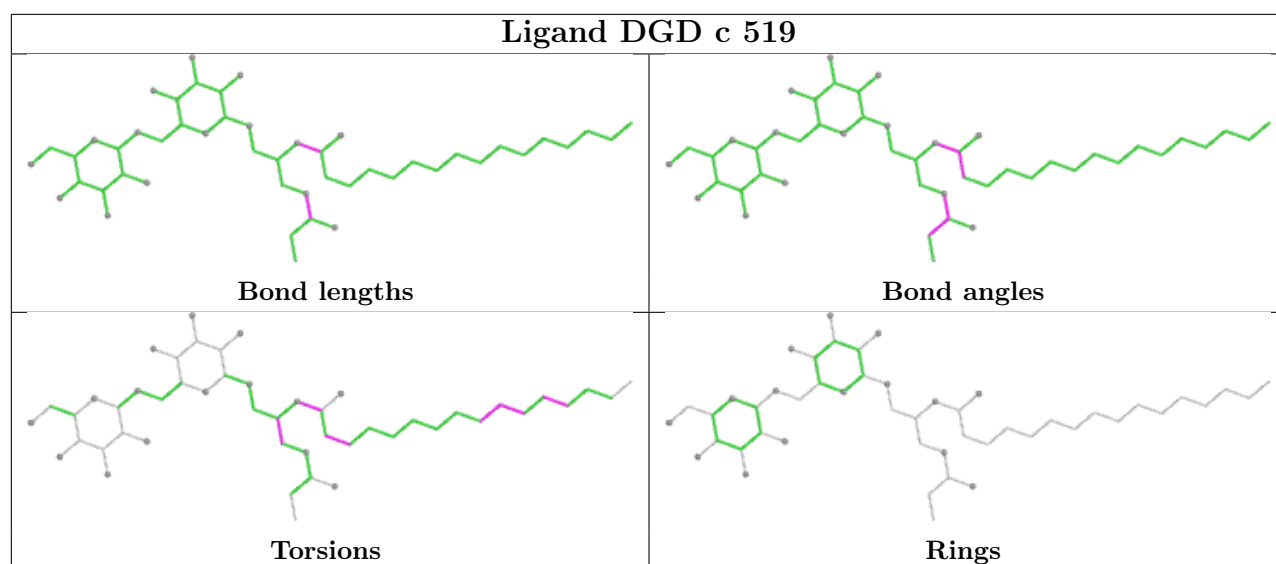
Ligand CLA C 511	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 516	
 Bond lengths	 Bond angles
 Torsions	 Rings

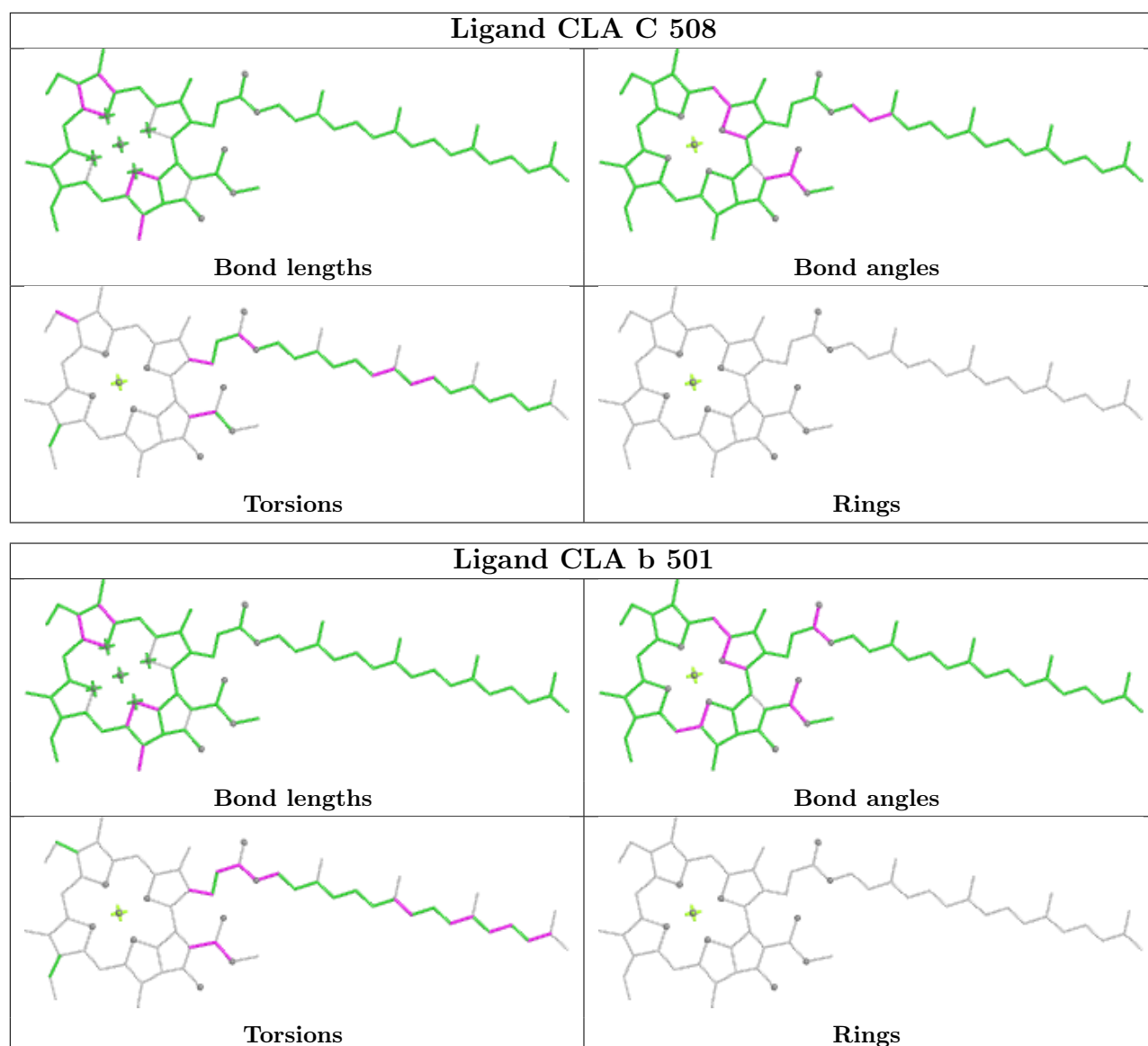


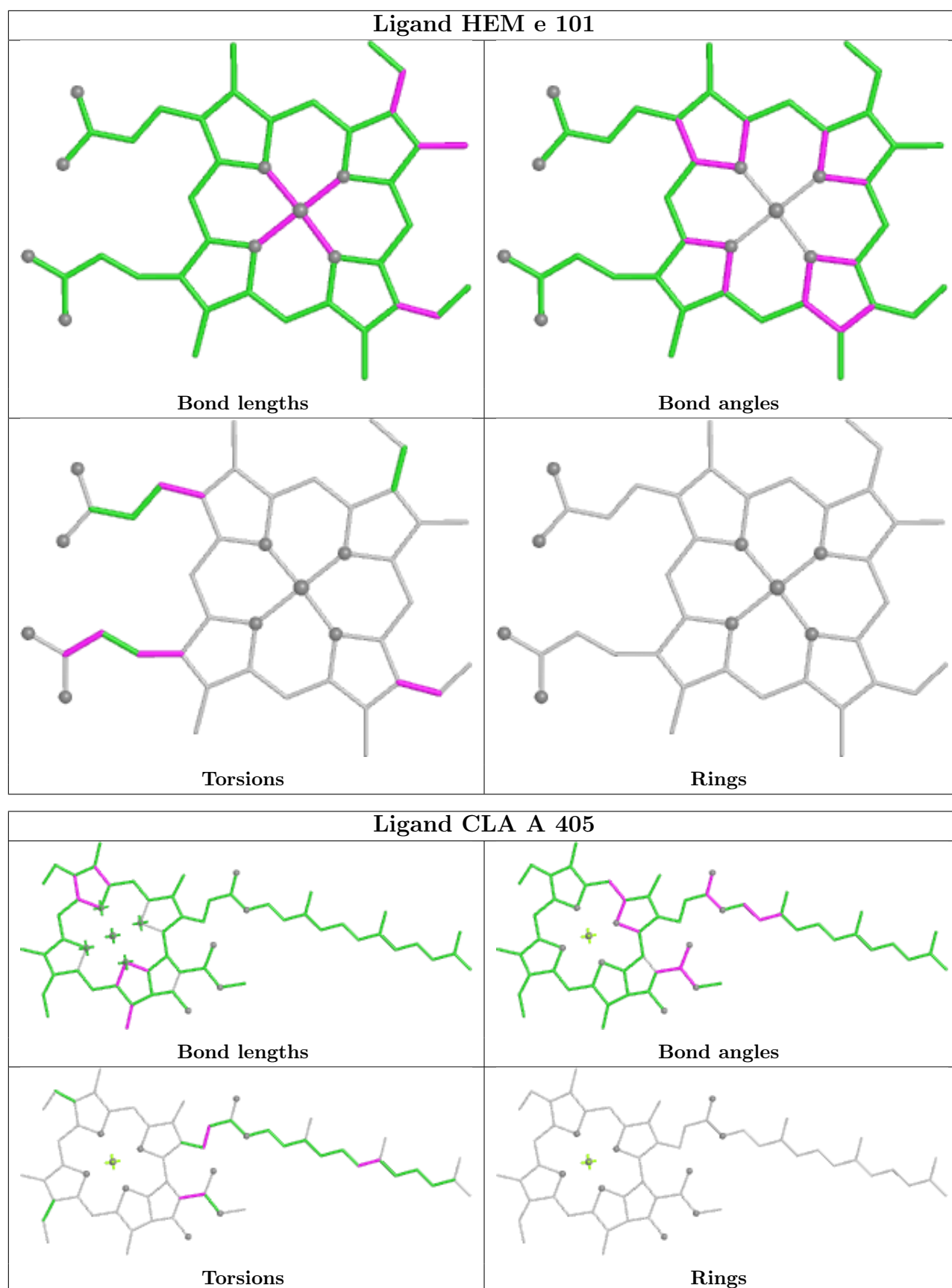


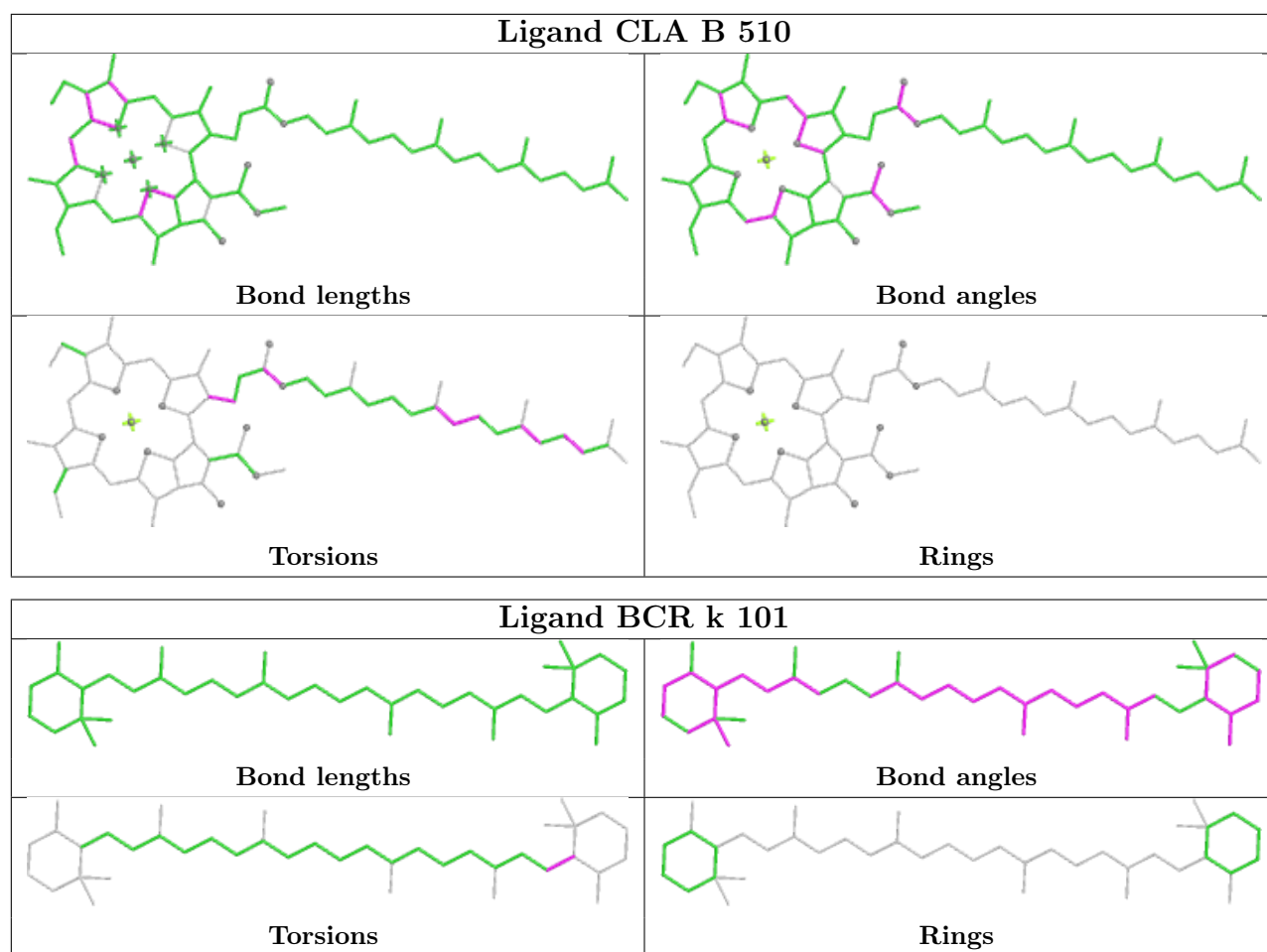


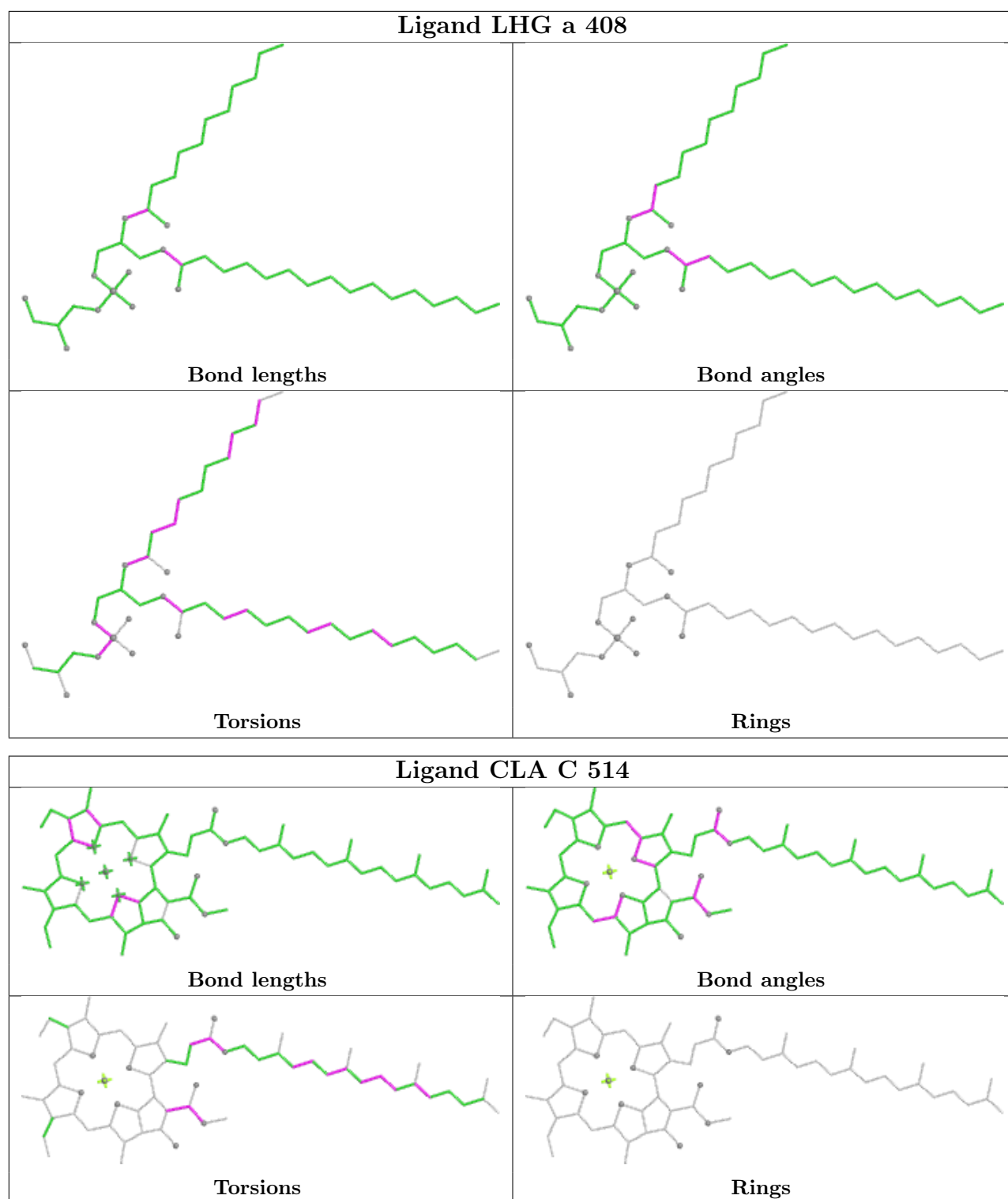


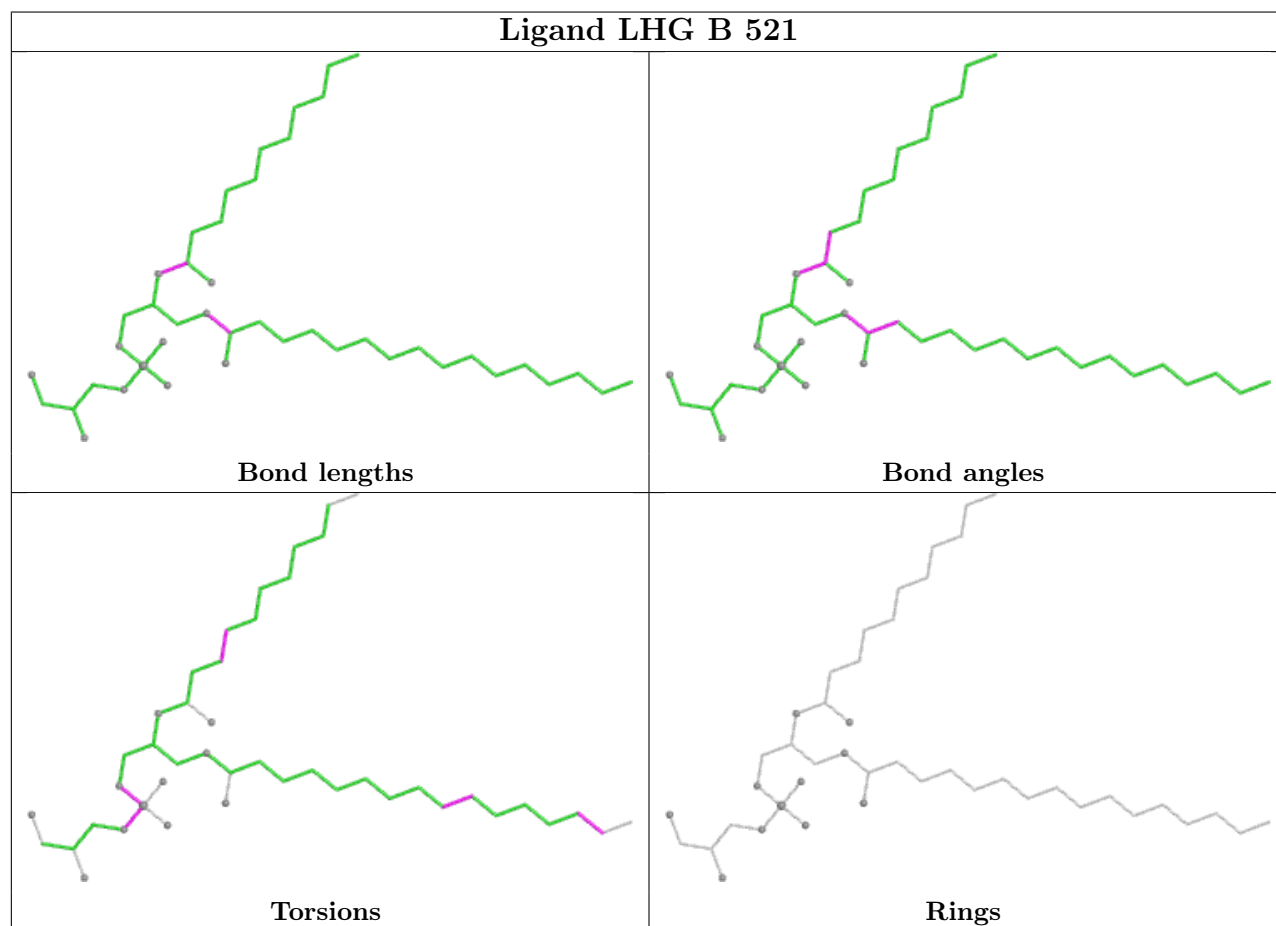
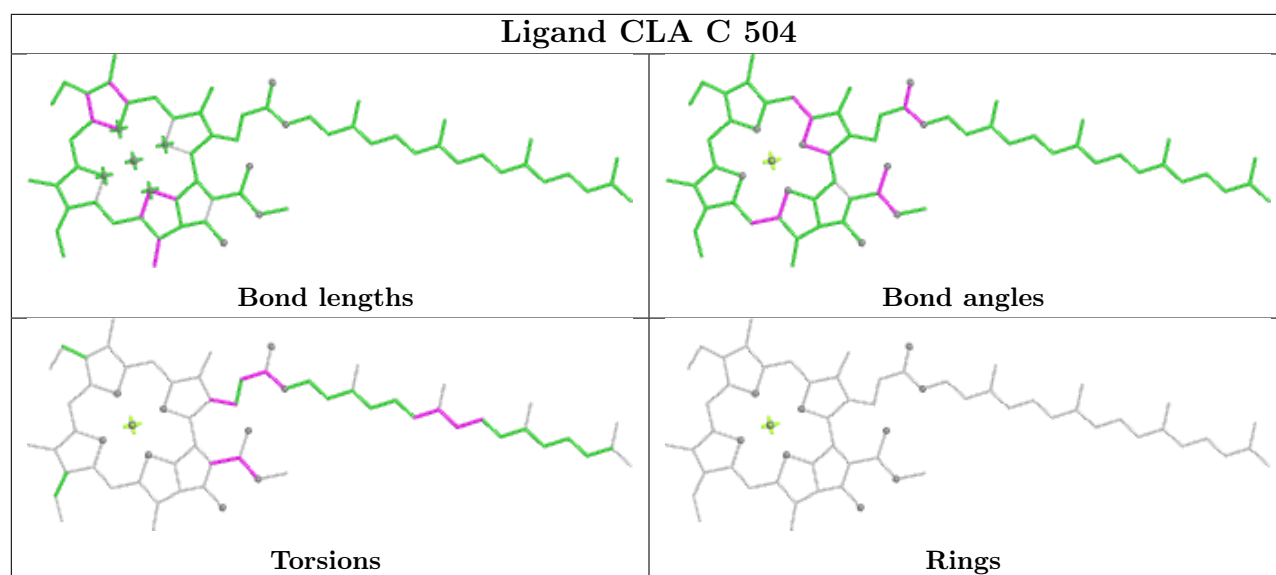


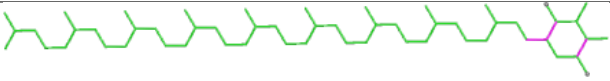
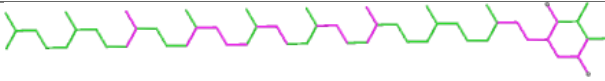
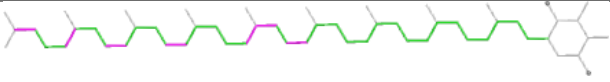
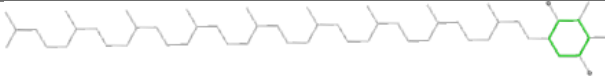
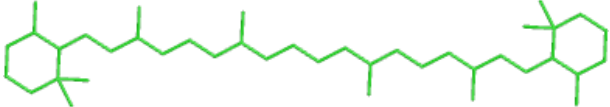
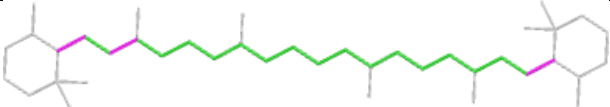
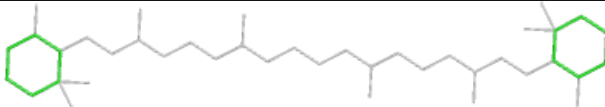
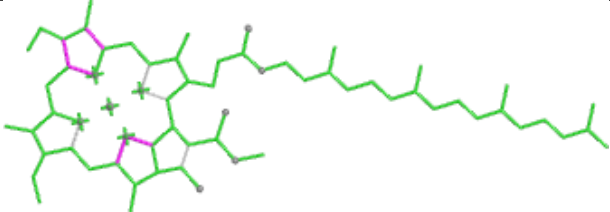
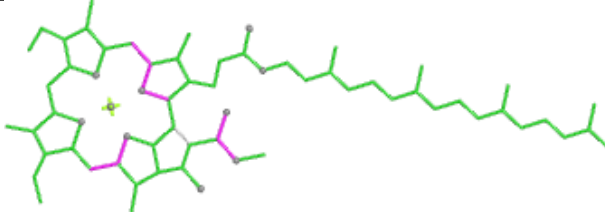
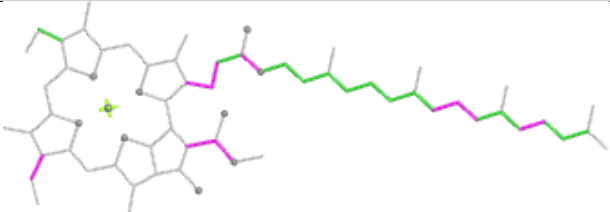
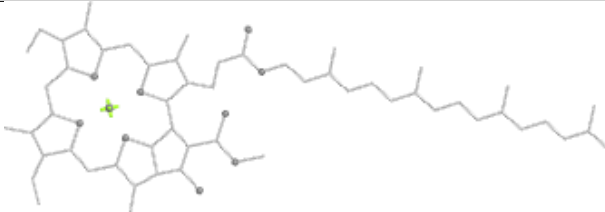


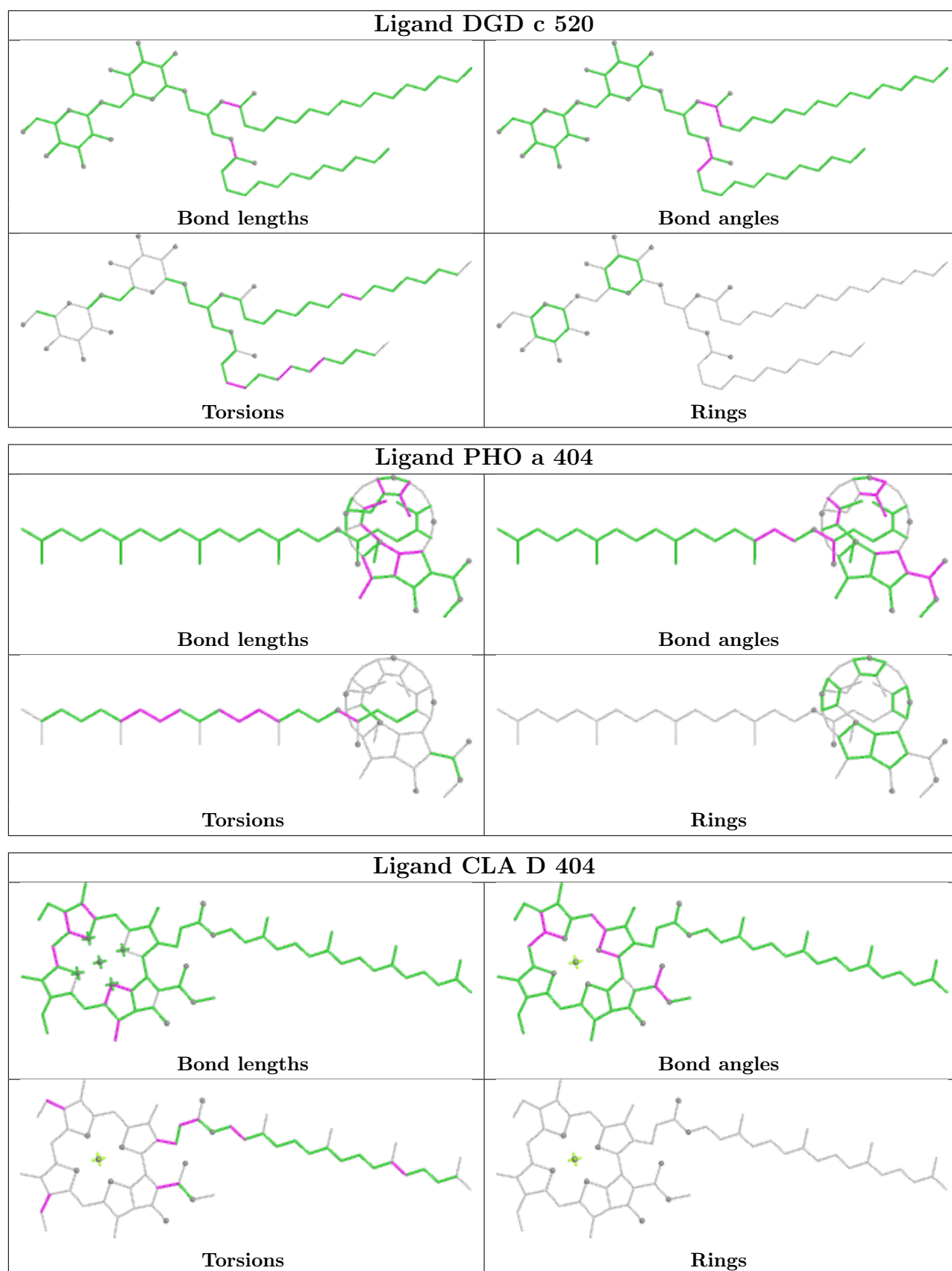


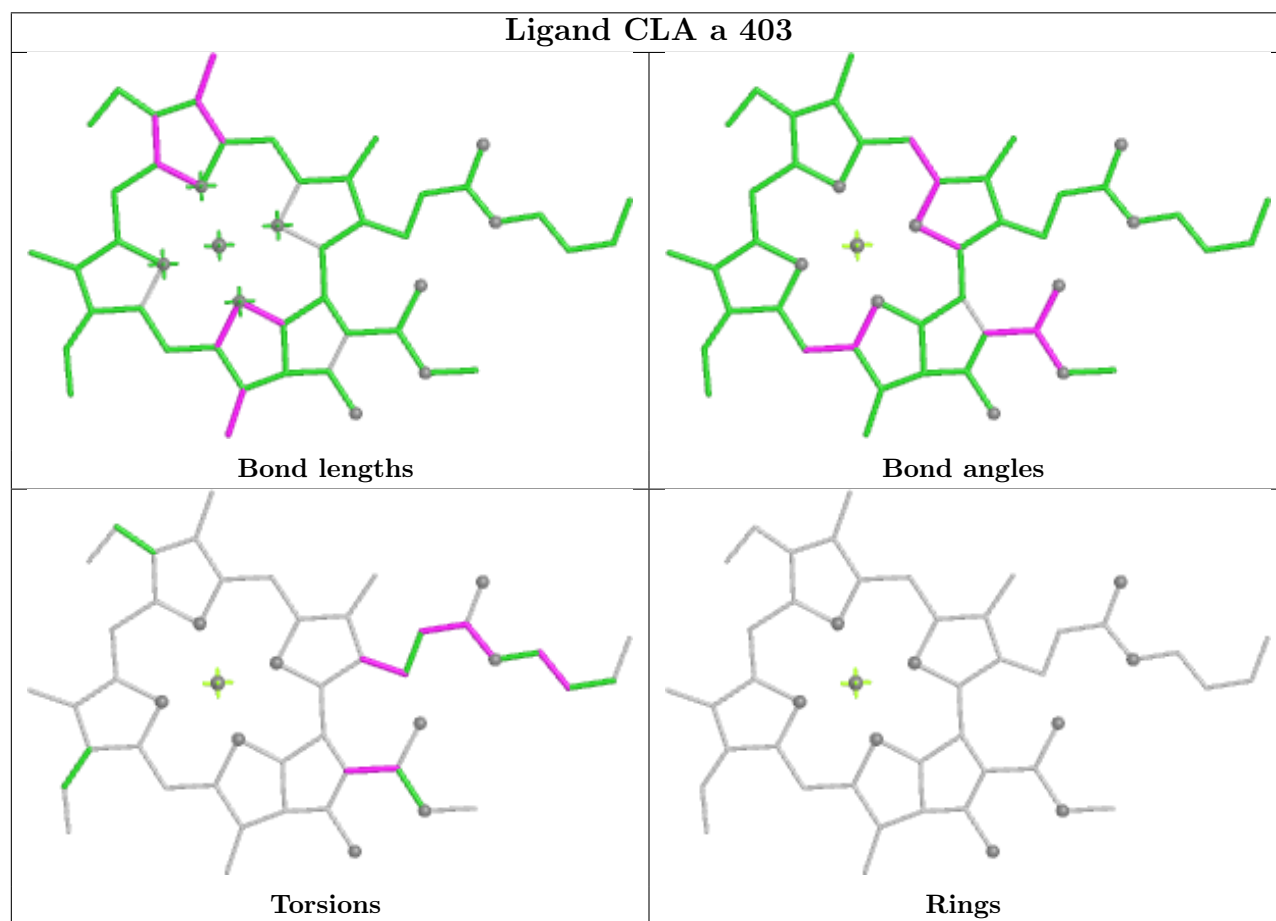
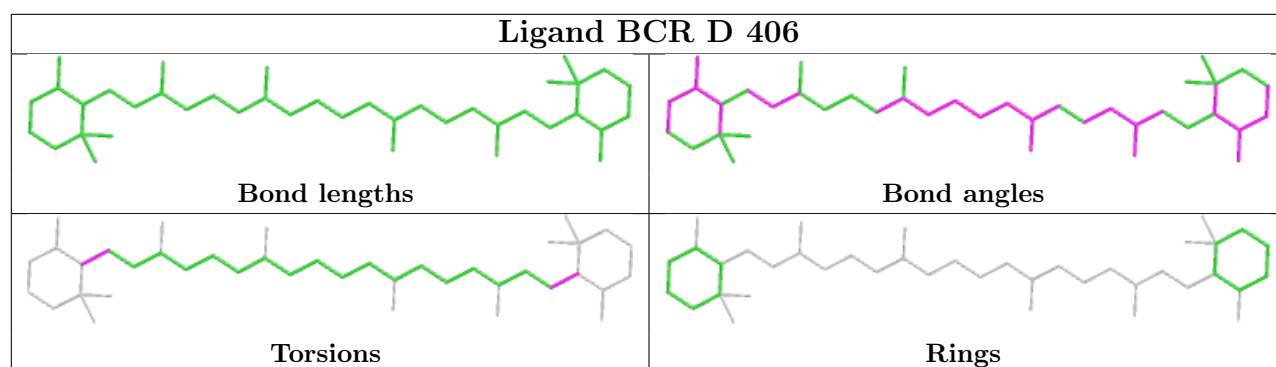


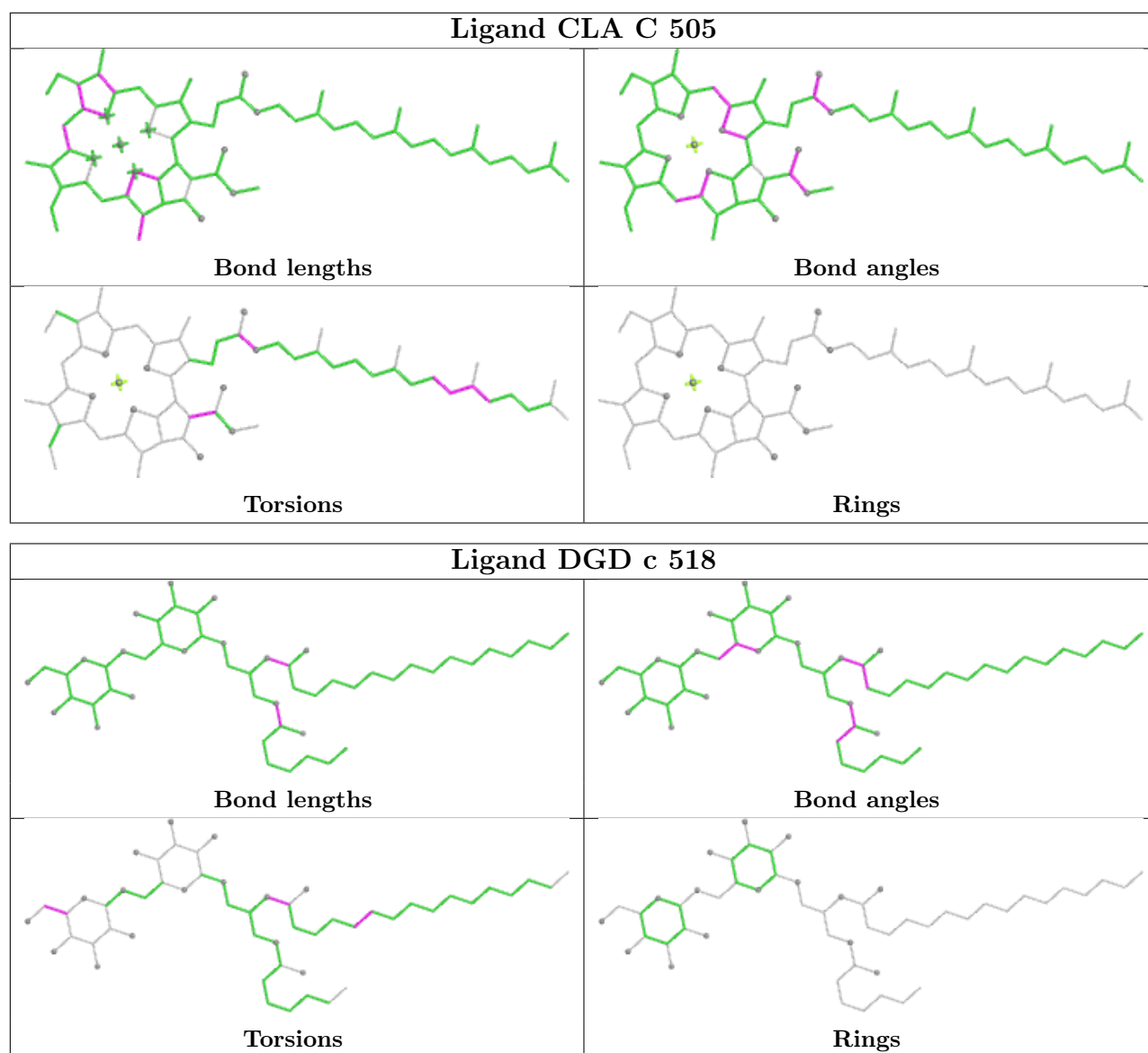


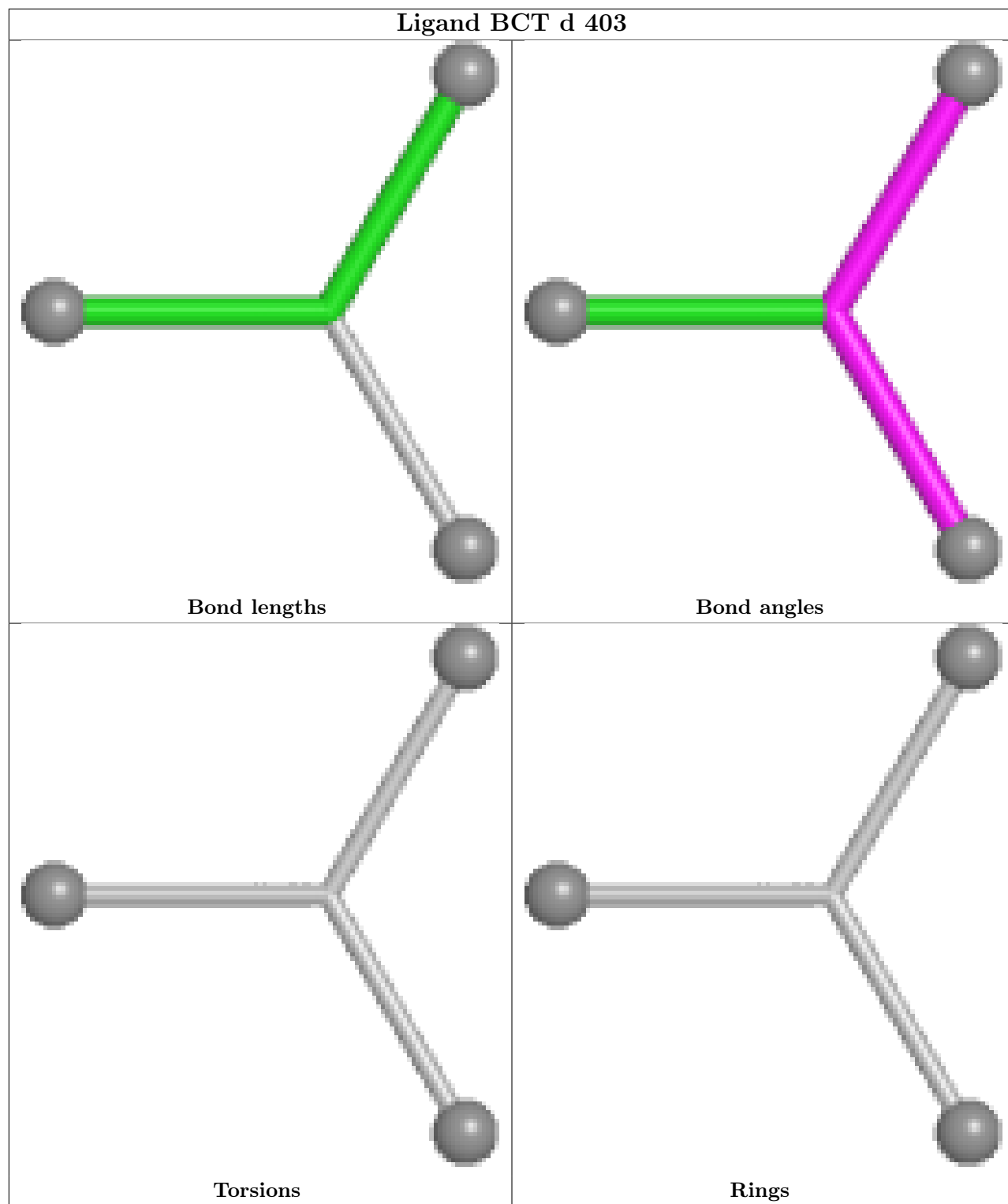


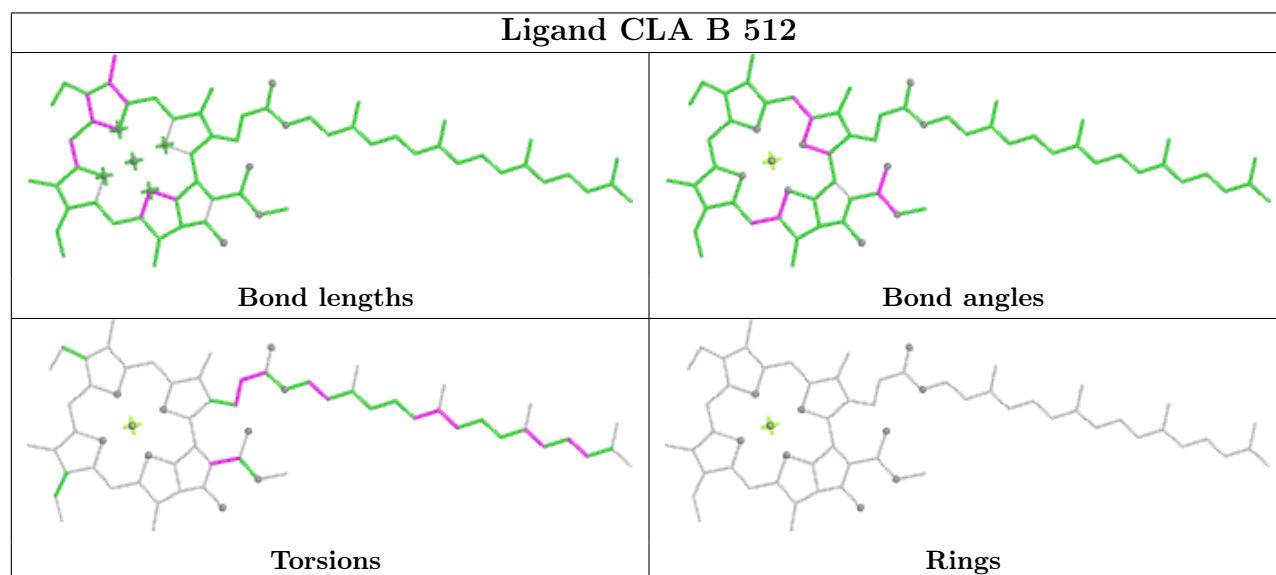
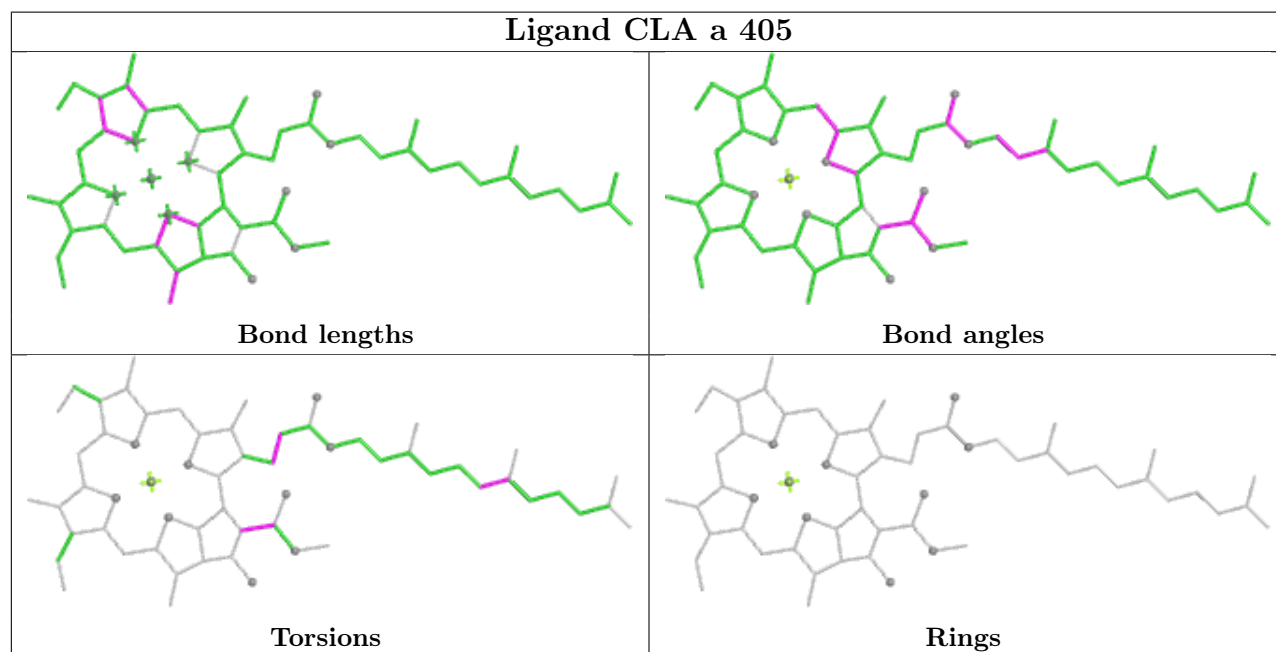
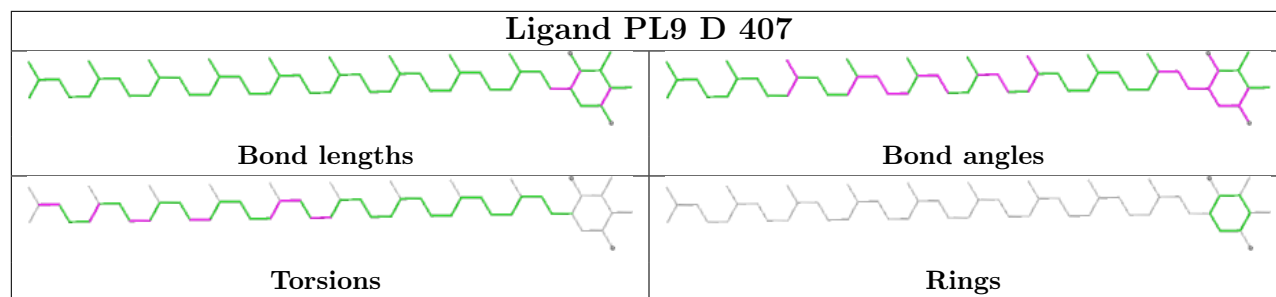
Ligand PL9 d 407	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR z 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

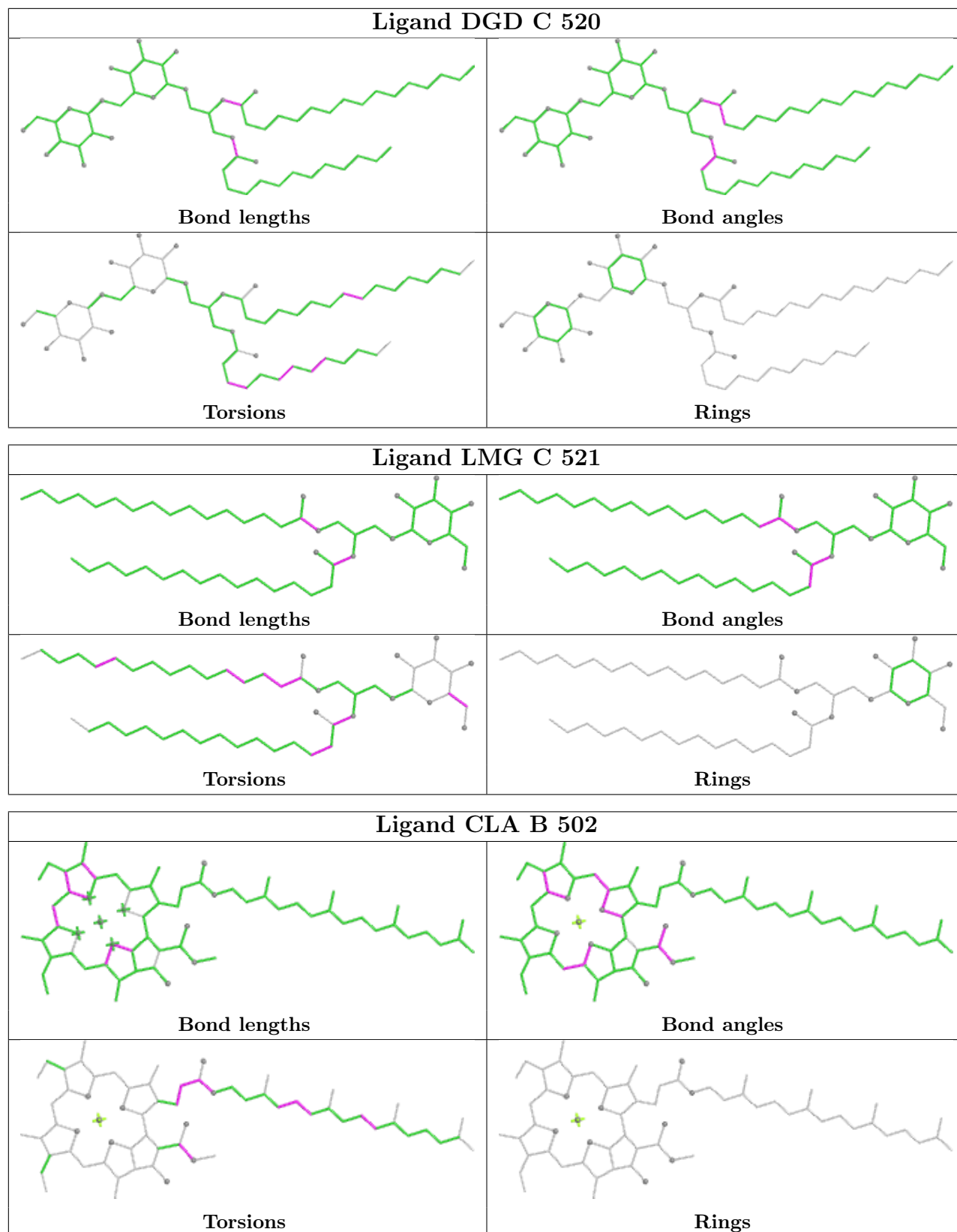


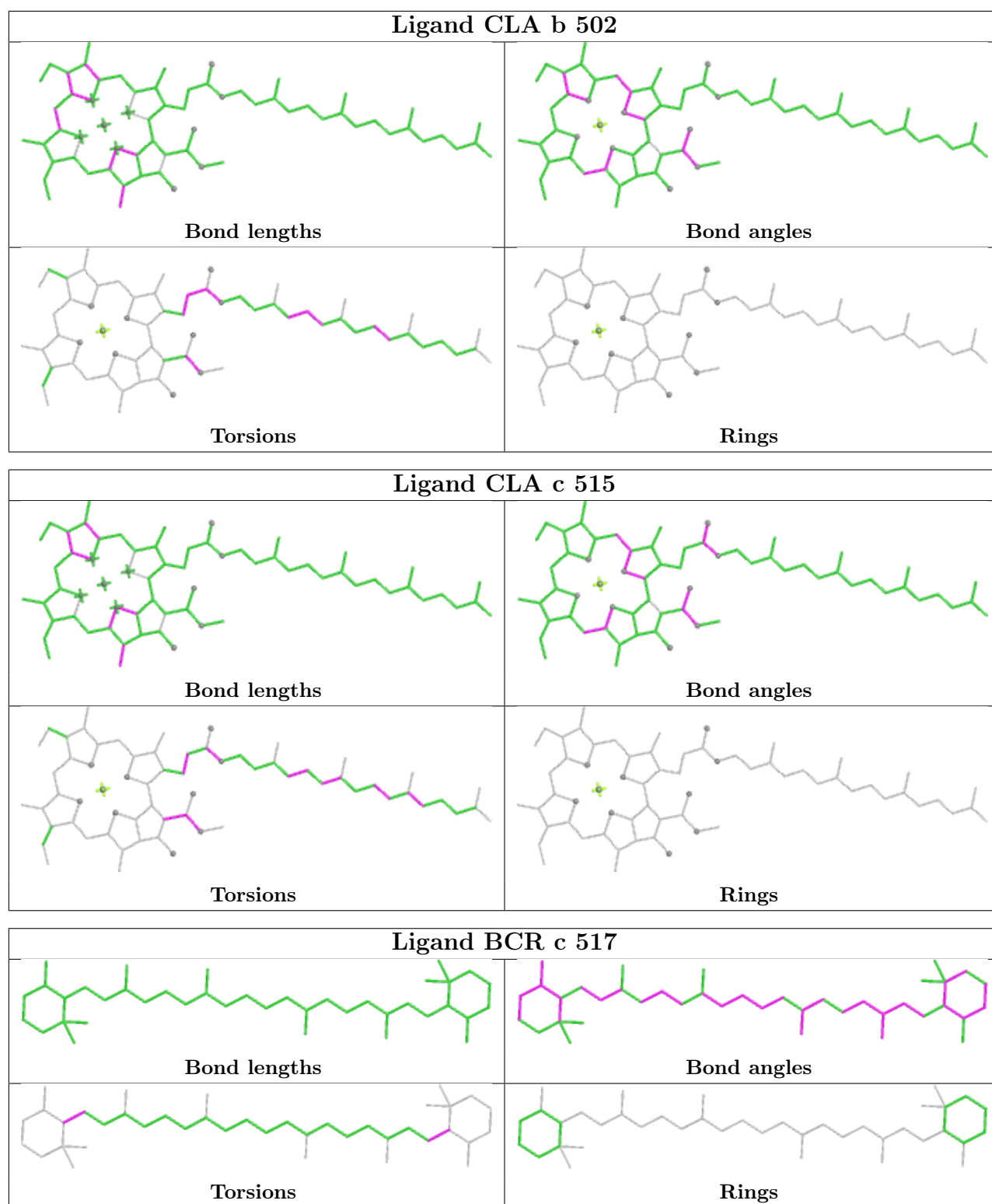












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

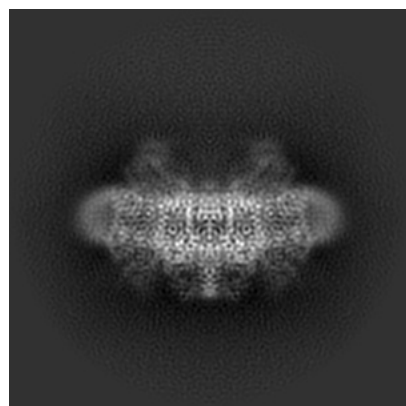
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60748. These allow visual inspection of the internal detail of the map and identification of artifacts.

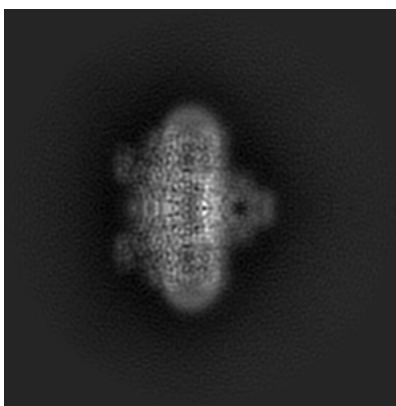
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

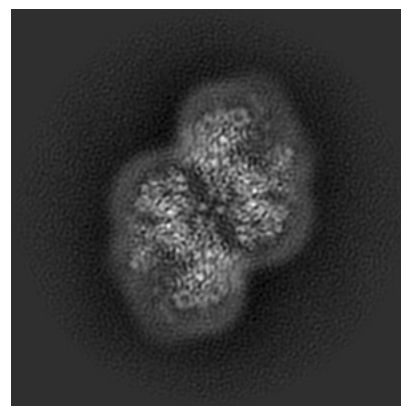
6.1.1 Primary map



X

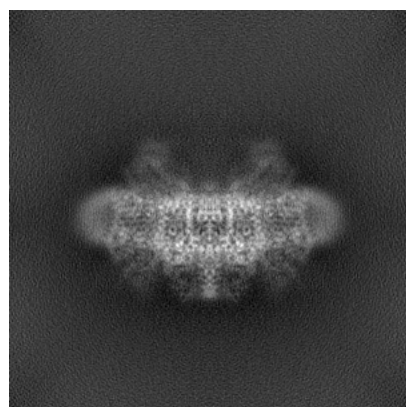


Y

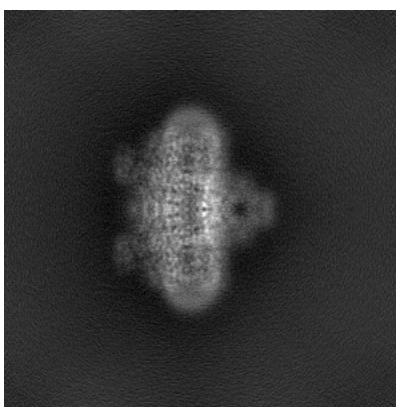


Z

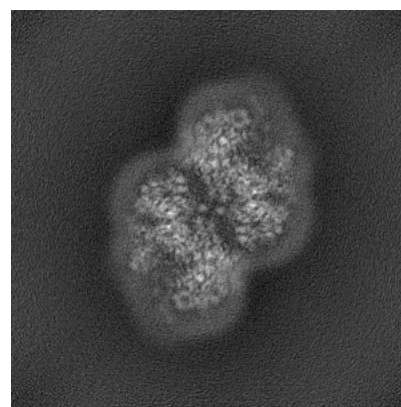
6.1.2 Raw map



X



Y

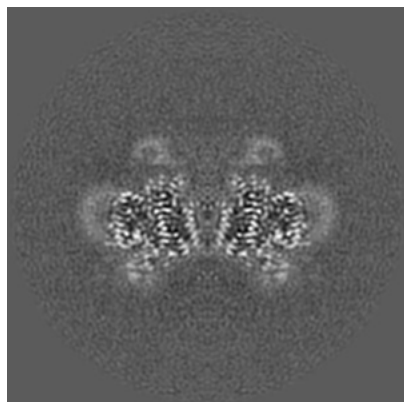


Z

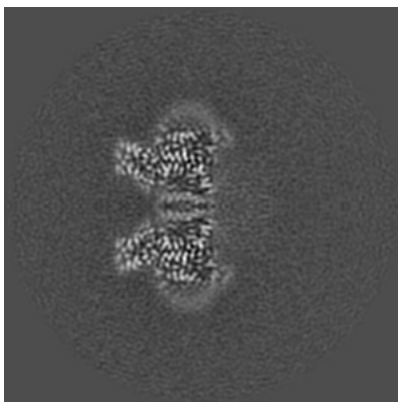
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

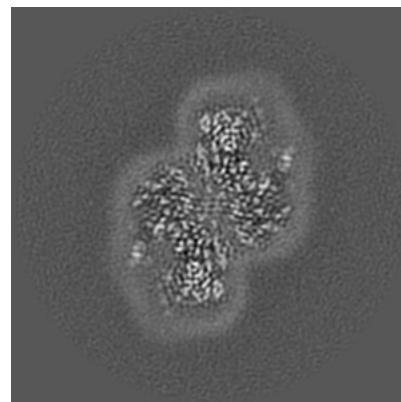
6.2.1 Primary map



X Index: 150

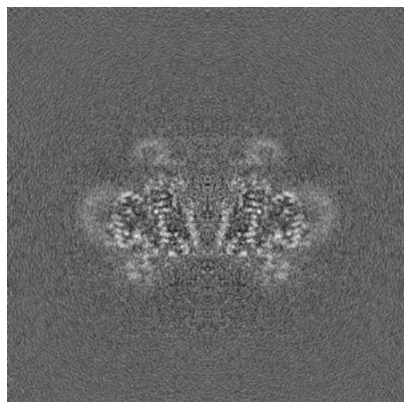


Y Index: 150

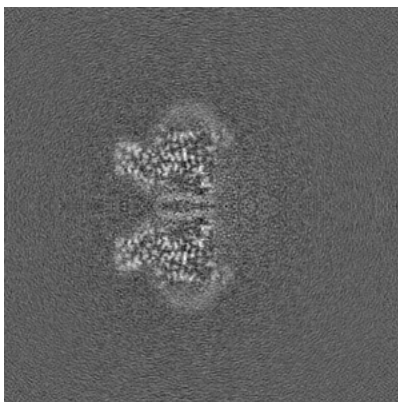


Z Index: 150

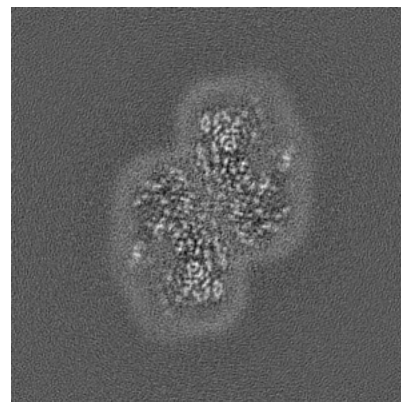
6.2.2 Raw map



X Index: 150



Y Index: 150

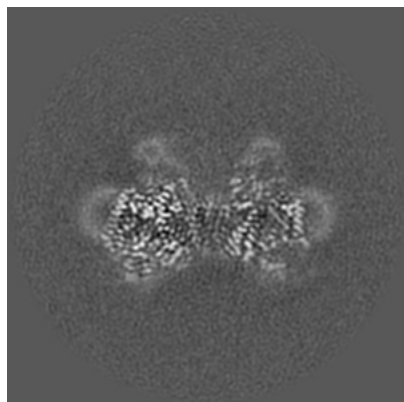


Z Index: 150

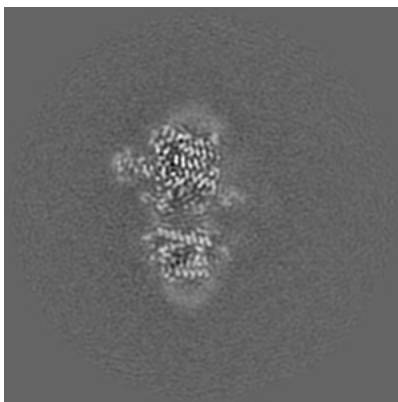
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

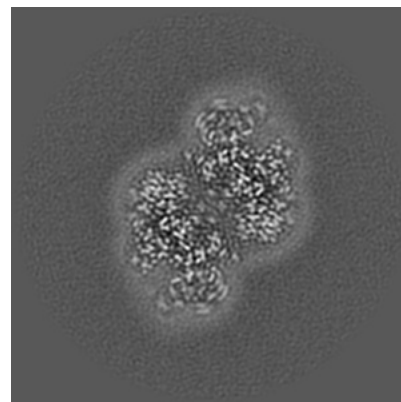
6.3.1 Primary map



X Index: 147

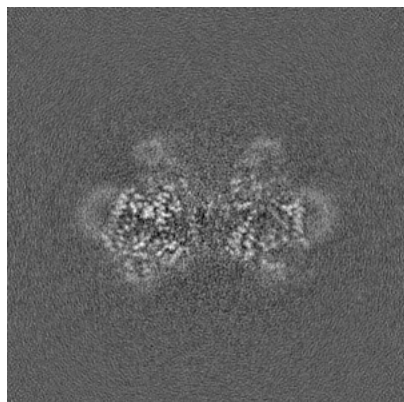


Y Index: 166

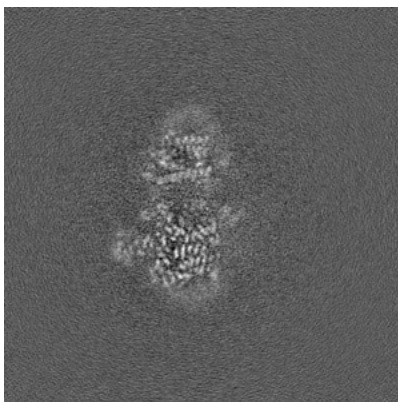


Z Index: 128

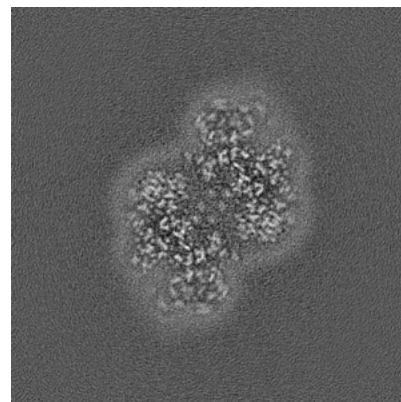
6.3.2 Raw map



X Index: 147



Y Index: 134

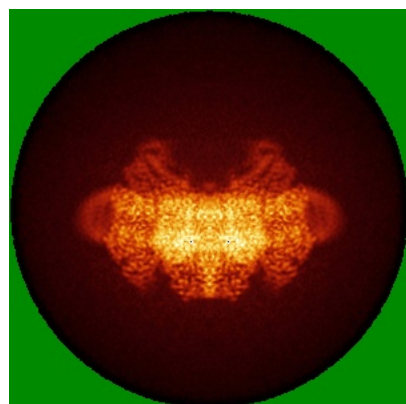


Z Index: 128

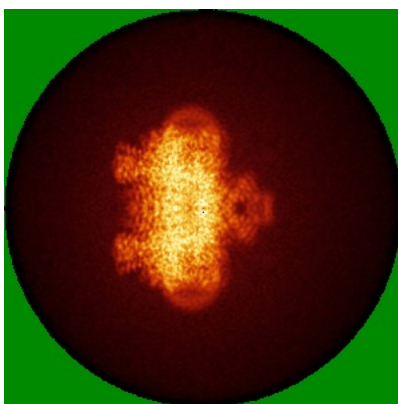
The images above show the largest variance slices of the map in three orthogonal directions.

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

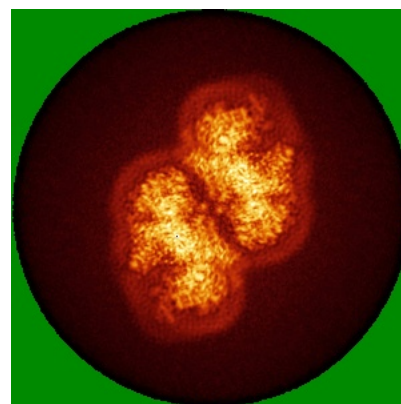
6.4.1 Primary map



X

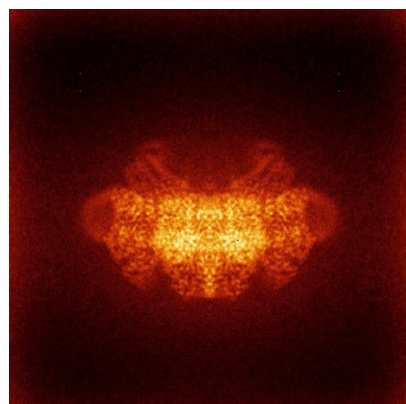


Y

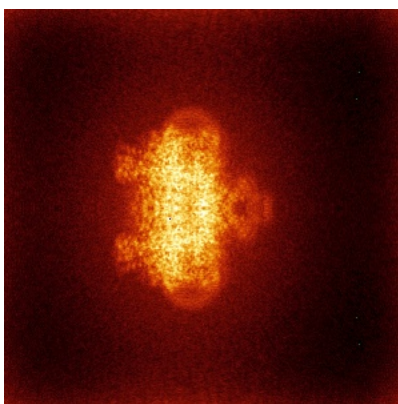


Z

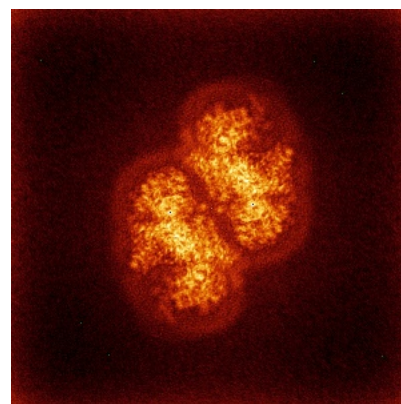
6.4.2 Raw map



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.

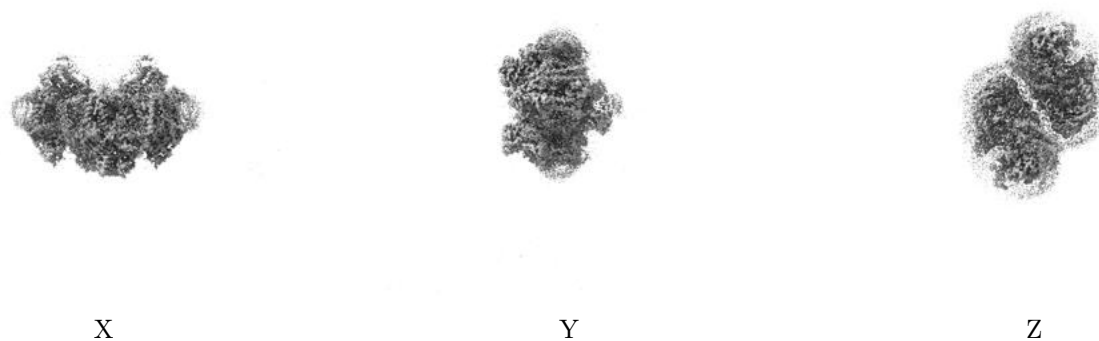
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.165. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

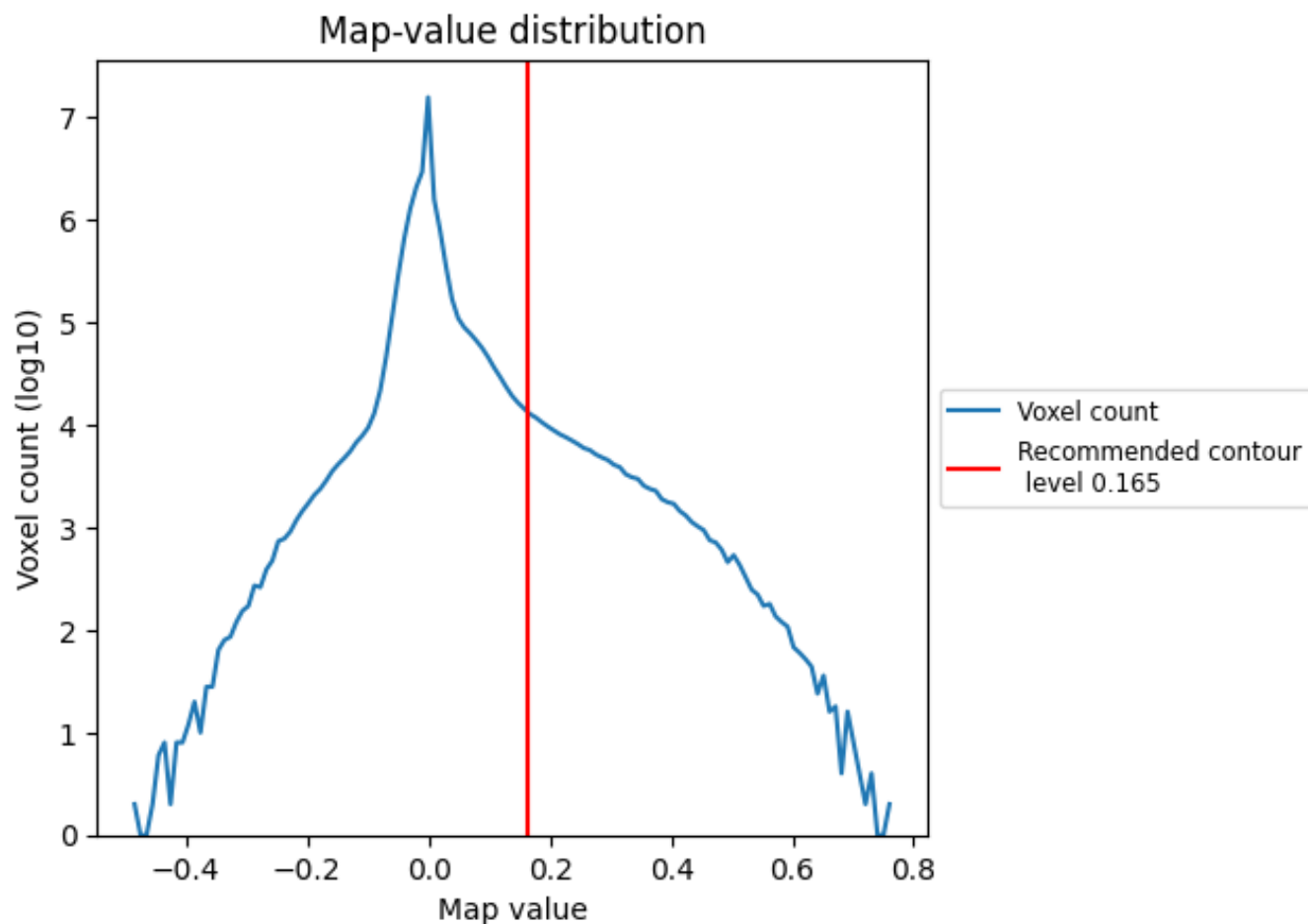
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

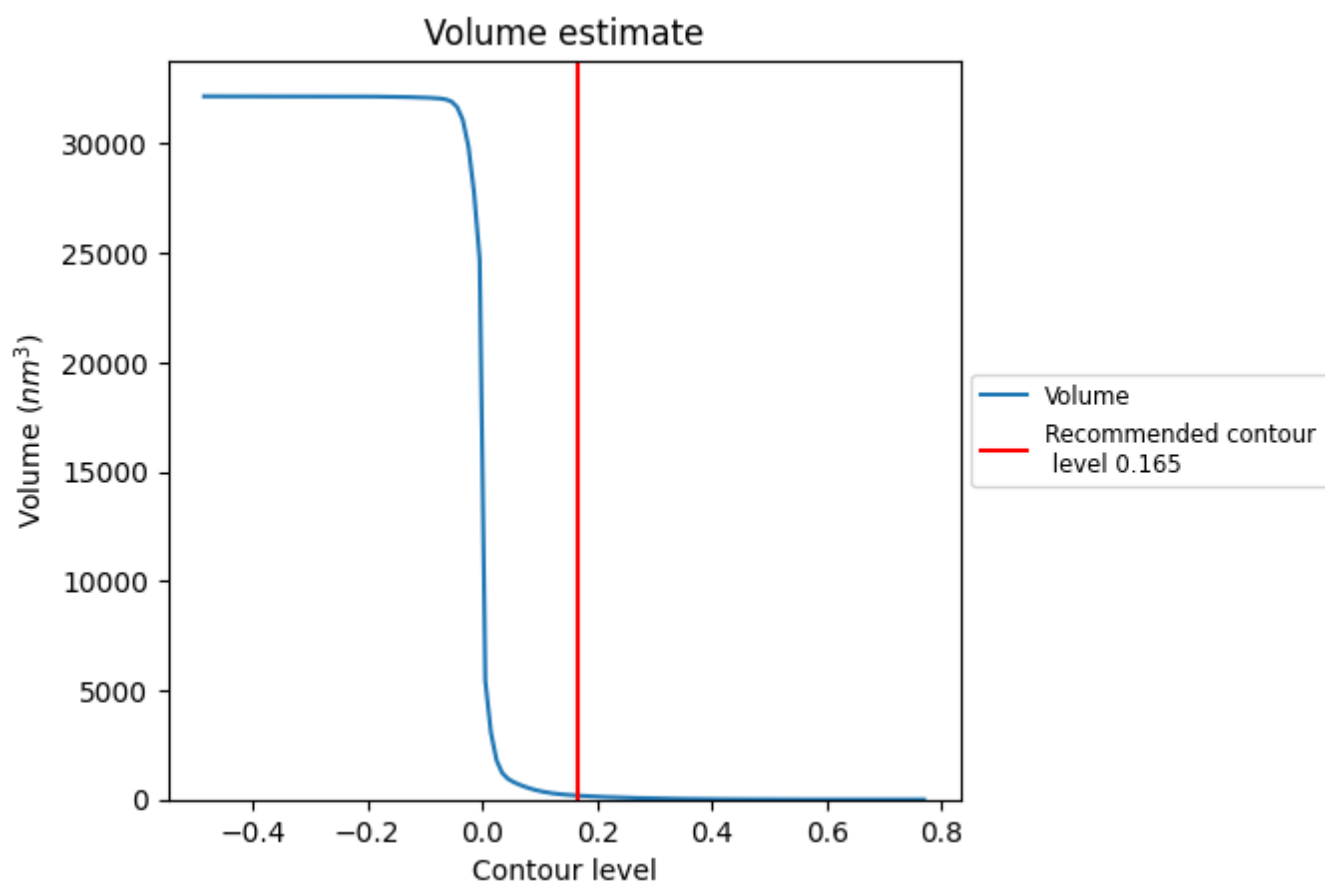
This section contains the results of statistical analysis of the map.

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.

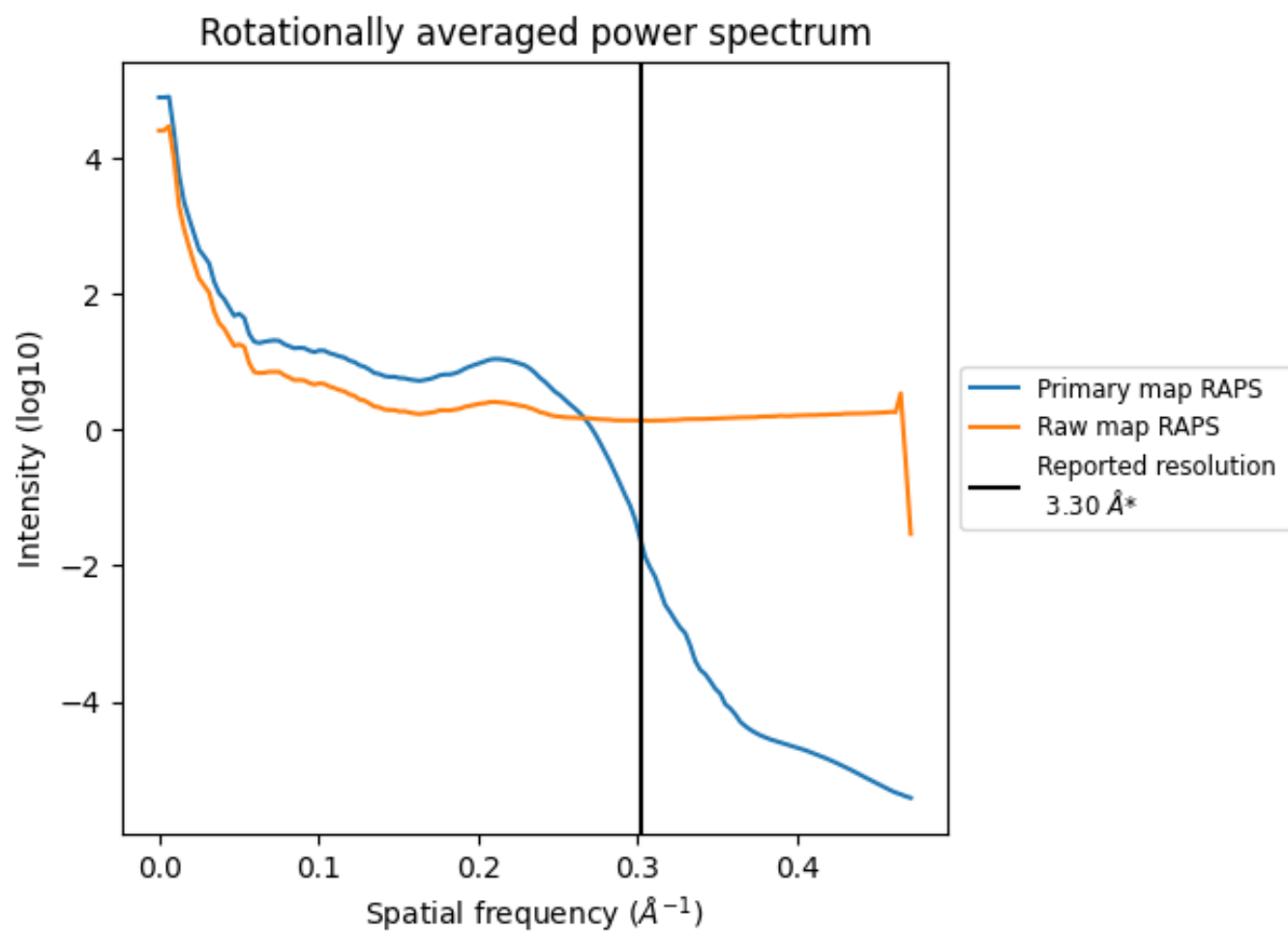
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 184 nm³; this corresponds to an approximate mass of 166 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

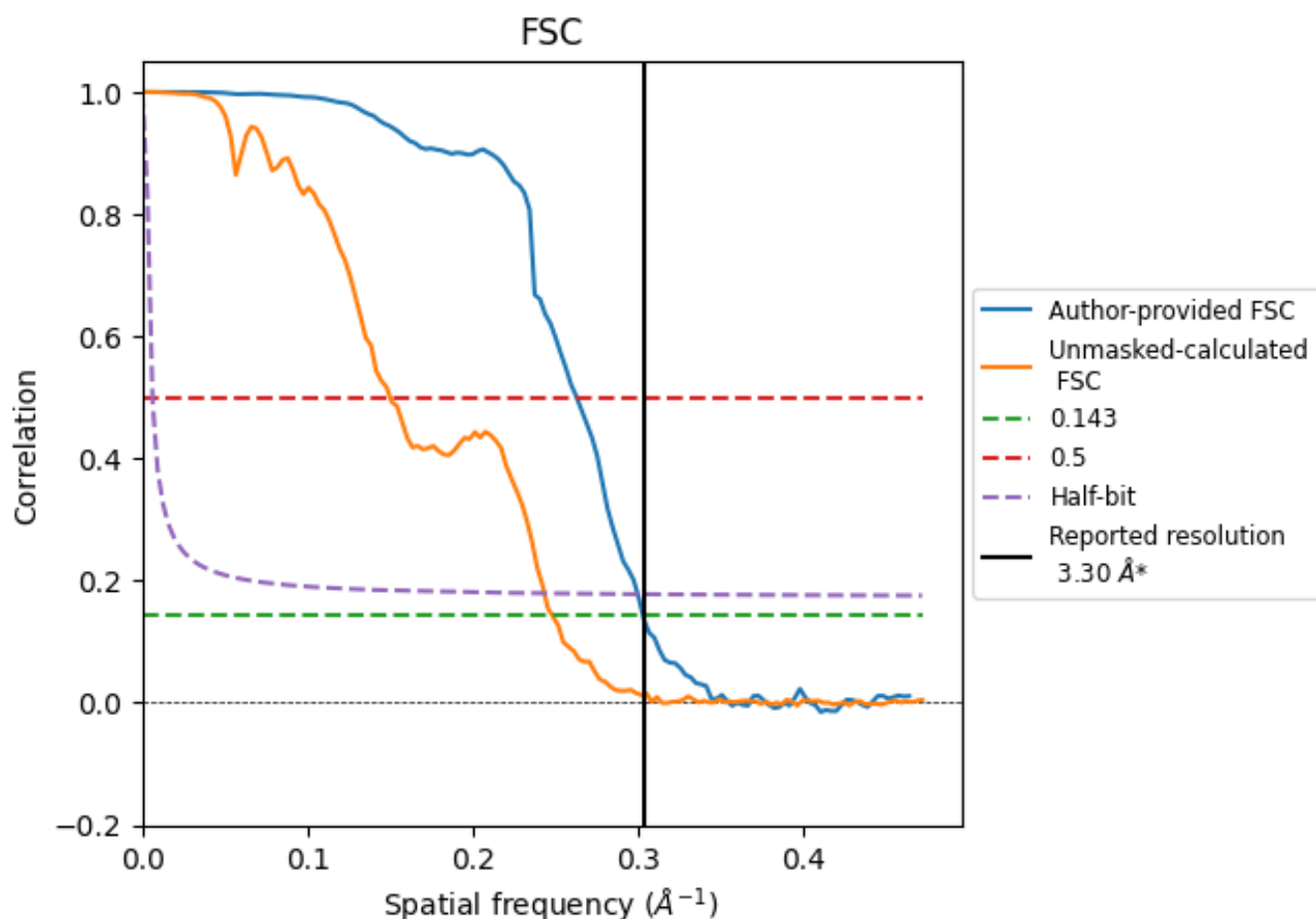


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

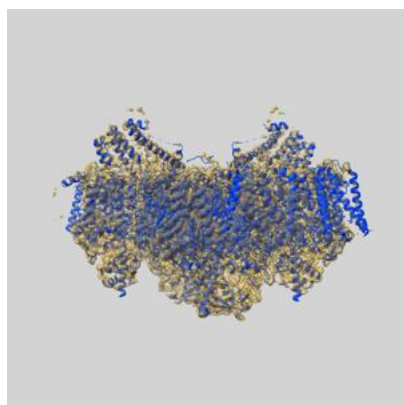
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.81	3.34
Unmasked-calculated*	4.03	6.67	4.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.03 differs from the reported value 3.3 by more than 10 %

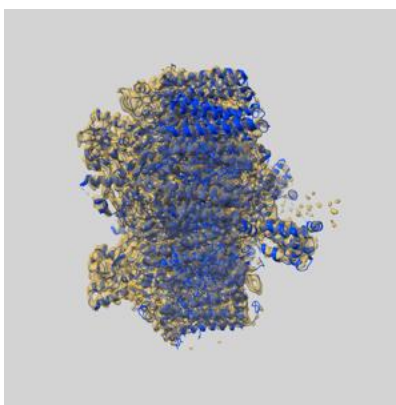
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60748 and PDB model 9IOX. Per-residue inclusion information can be found in section 3 on page 21.

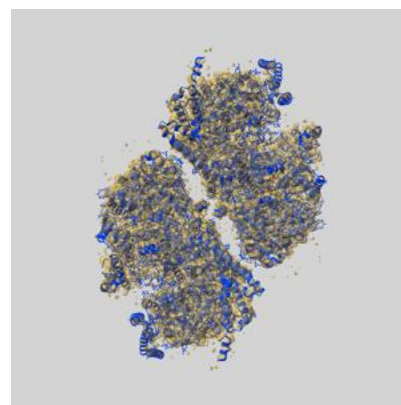
9.1 Map-model overlay [i](#)



X



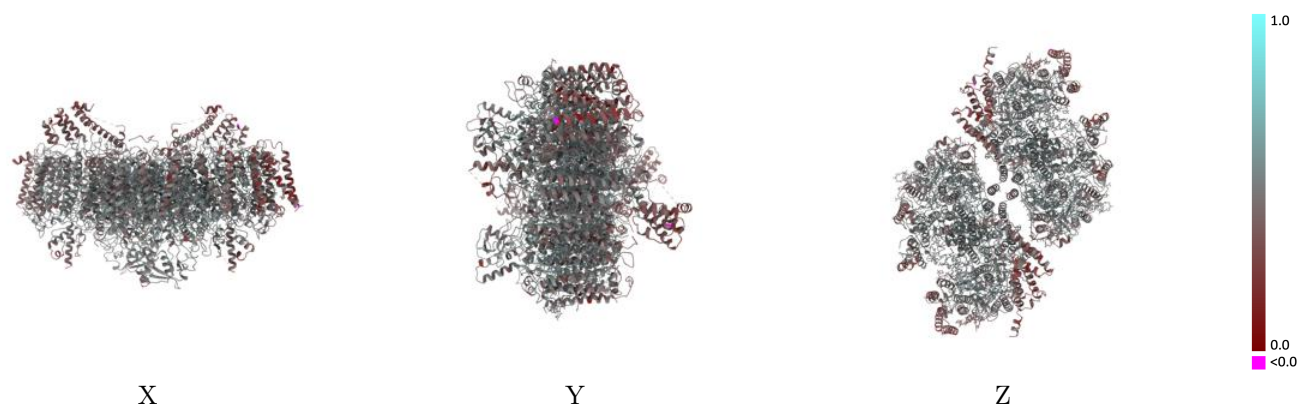
Y



Z

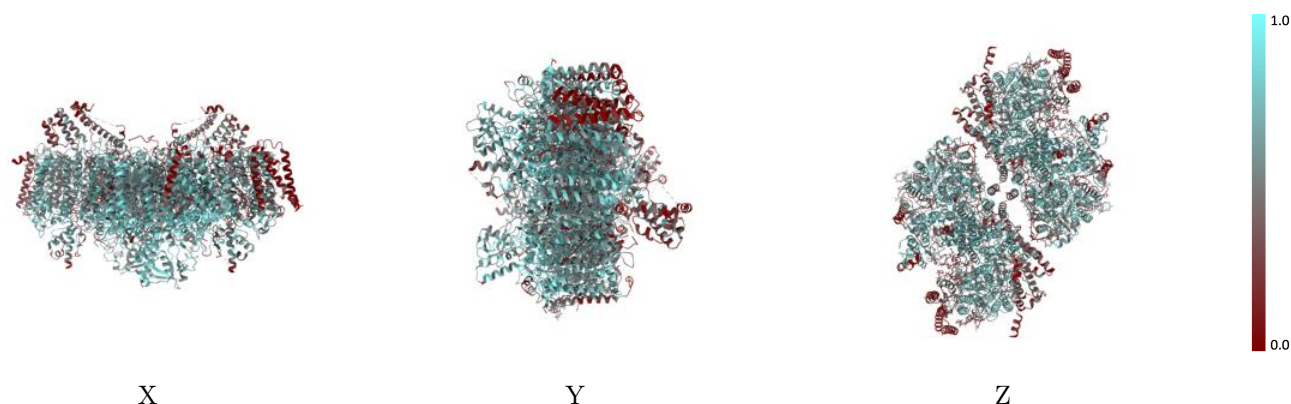
The images above show the 3D surface view of the map at the recommended contour level 0.165 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



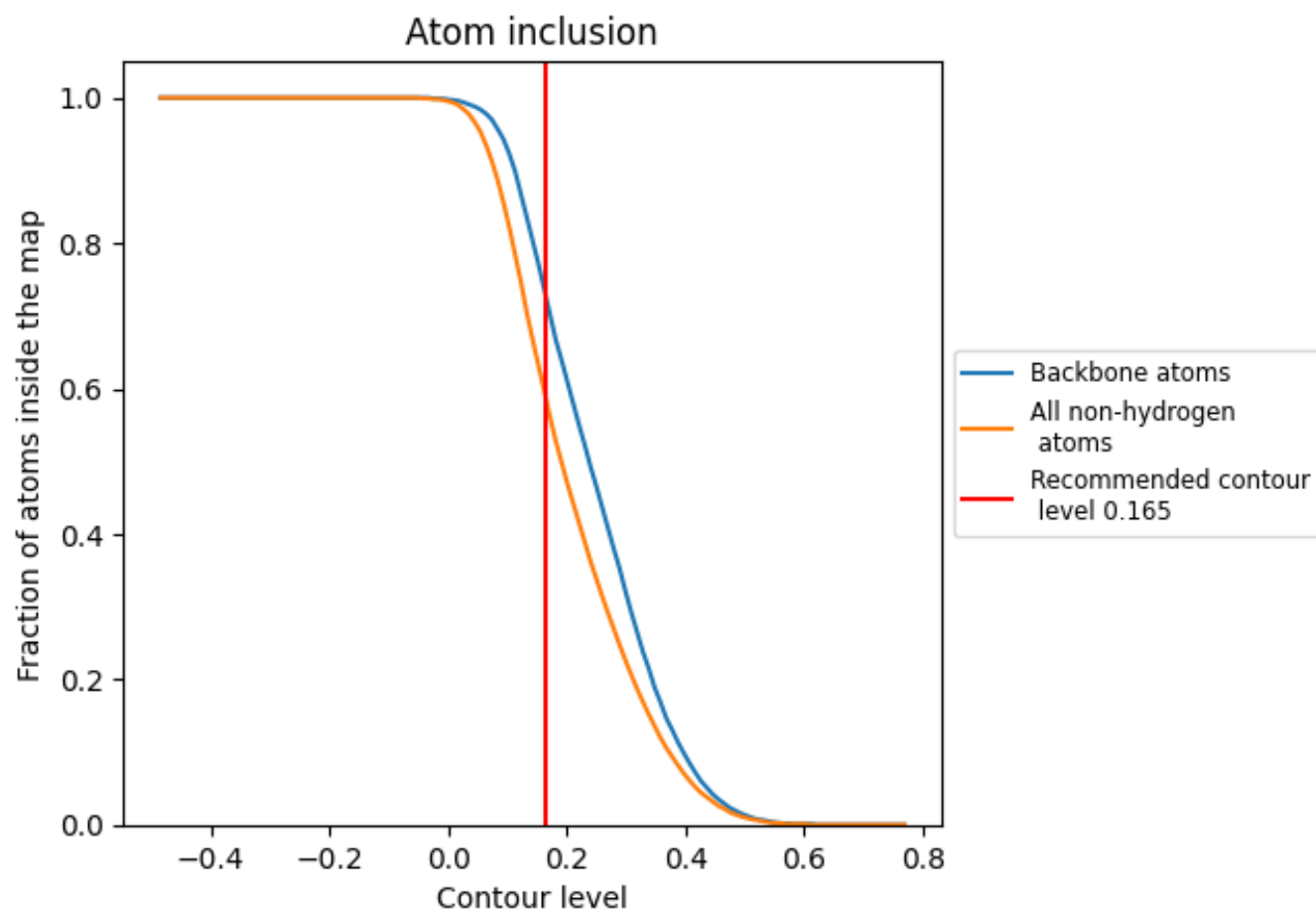
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.165).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 59% 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 (0.165) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5870	 0.4630
A	 0.6460	 0.4890
B	 0.6580	 0.4850
C	 0.5900	 0.4630
D	 0.7080	 0.5100
E	 0.5470	 0.4150
F	 0.6250	 0.4380
G	 0.3550	 0.3560
H	 0.5530	 0.4260
I	 0.5510	 0.4500
K	 0.4230	 0.4270
L	 0.4920	 0.4720
M	 0.4330	 0.4330
T	 0.4560	 0.4420
V	 0.0930	 0.3270
X	 0.2470	 0.4050
Z	 0.0970	 0.2960
a	 0.6650	 0.4930
b	 0.6650	 0.4890
c	 0.5930	 0.4640
d	 0.7090	 0.5090
e	 0.5450	 0.4210
f	 0.6380	 0.4230
g	 0.3580	 0.3580
h	 0.5480	 0.4380
i	 0.5590	 0.4530
k	 0.4170	 0.4300
l	 0.4890	 0.4720
m	 0.4330	 0.4270
t	 0.4510	 0.4390
v	 0.0890	 0.3280
x	 0.2570	 0.4110
z	 0.0910	 0.2970

