



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 12:18 PM UTC

PDB ID : 9EVX / pdb_00009evx
EMDB ID : EMD-50019
Title : cryoEM structure of Photosystem II averaged across S2-S3 states at 1.71 Angstrom resolution
Authors : Hussein, R.; Graca, A.; Zouni, A.; Messinger, J.; Schroder, W.P.
Deposited on : 2024-04-02
Resolution : 1.71 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:

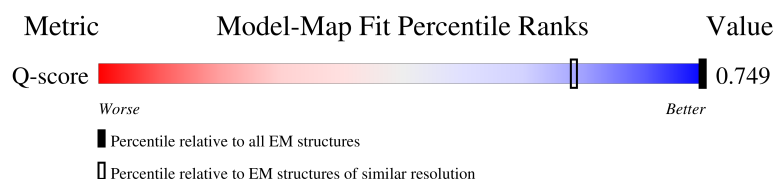
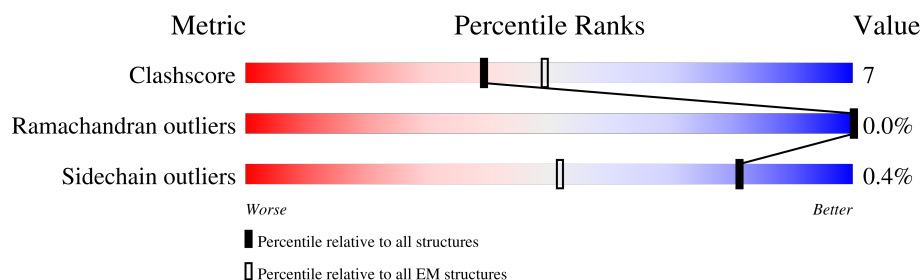
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 1.71 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	612 (1.21 - 2.21)

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

Mol	Chain	Length	Quality of chain
1	A	344	 82% 15% .
1	a	344	 82% 15% .
2	B	510	 88% 11% .
2	b	510	 88% 11% .

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Mol	Chain	Length	Quality of chain
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	

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Mol	Chain	Length	Quality of chain
15	u	134	
16	V	163	
16	v	163	
17	X	41	
17	x	41	
18	Y	46	
18	y	46	
19	Z	62	
19	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	404	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	A	419	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	C	501	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	507	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	406	X	-	-	-
22	CLA	a	419	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	c	501	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 104863 atoms, of which 52030 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 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	334	Total	C	H	N	O	S	3	0
			5164	1723	2530	433	463	15		
1	a	334	Total	C	H	N	O	S	3	0
			5164	1723	2530	433	463	15		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	505	Total	C	H	N	O	S	3	0
			7852	2620	3858	667	694	13		
2	b	505	Total	C	H	N	O	S	3	0
			7852	2620	3858	667	694	13		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	451	Total	C	H	N	O	S	2	0
			6899	2283	3408	585	610	13		
3	c	451	Total	C	H	N	O	S	2	0
			6899	2283	3408	585	610	13		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	0
			5338	1800	2621	444	461	12		
4	d	341	Total	C	H	N	O	S	0	0
			5338	1800	2621	444	461	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	82	Total	C	H	N	O	0	0
			1301	431	640	107	123		
5	e	82	Total	C	H	N	O	0	0
			1301	431	640	107	123		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	34	Total	C	H	N	O	S	0	0
			557	187	282	45	42	1		
6	f	34	Total	C	H	N	O	S	0	0
			557	187	282	45	42	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	H	65	Total 1045	C 338	H 534	N 83	O 87	S 3	2	0
7	h	65	Total 1045	C 338	H 534	N 83	O 87	S 3	2	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	41	CYS	PHE	variant	UNP Q8DJ43
h	41	CYS	PHE	variant	UNP Q8DJ43

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	I	38	Total 641	C 211	H 328	N 48	O 53	S 1	0	0
8	i	38	Total 641	C 211	H 328	N 48	O 53	S 1	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	J	36	Total	C	H	N	O	S	0	0
			525	174	268	40	42	1		
9	j	36	Total	C	H	N	O	S	0	0
			525	174	268	40	42	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	37	Total	C	H	N	O	0	0
			598	204	305	43	46		
10	k	37	Total	C	H	N	O	0	0
			598	204	305	43	46		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	L	37	Total 640	C 208	H 328	N 49	O 54	S 1	2	0
11	l	37	Total 640	C 208	H 328	N 49	O 54	S 1	2	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
12	M	33	Total	C	H	N	O	S	2	0
			545	177	281	38	48	1		
12	m	33	Total	C	H	N	O	S	2	0
			545	177	281	38	48	1		

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	O	243	Total	C	H	N	O	S	3	0
			3710	1171	1834	313	387	5		
13	o	243	Total	C	H	N	O	S	3	0
			3710	1171	1834	313	387	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
14	T	30	Total	C	H	N	O	S	0	0
			519	181	261	36	39	2		
14	t	30	Total	C	H	N	O	S	0	0
			519	181	261	36	39	2		

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	97	Total	C	H	N	O	0	0
			1547	491	773	129	154		
15	u	97	Total	C	H	N	O	0	0
			1547	491	773	129	154		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
16	V	137	Total	C	H	N	O	S	0	0
			2135	675	1071	177	208	4		
16	v	137	Total	C	H	N	O	S	0	0
			2135	675	1071	177	208	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	38	Total	C	H	N	O	0	0
			593	188	312	45	48		
17	x	38	Total	C	H	N	O	0	0
			593	188	312	45	48		

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	Y	27	Total	C	H	N	O	S	0	0
			423	131	224	35	30	3		
18	y	27	Total	C	H	N	O	S	0	0
			425	131	226	35	30	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
19	Z	62	Total	C	H	N	O	S	0	0
			995	328	516	72	77	2		
19	z	62	Total	C	H	N	O	S	0	0
			995	328	516	72	77	2		

- Molecule 20 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	AltConf
20	A	1	Total Fe 1 1	0

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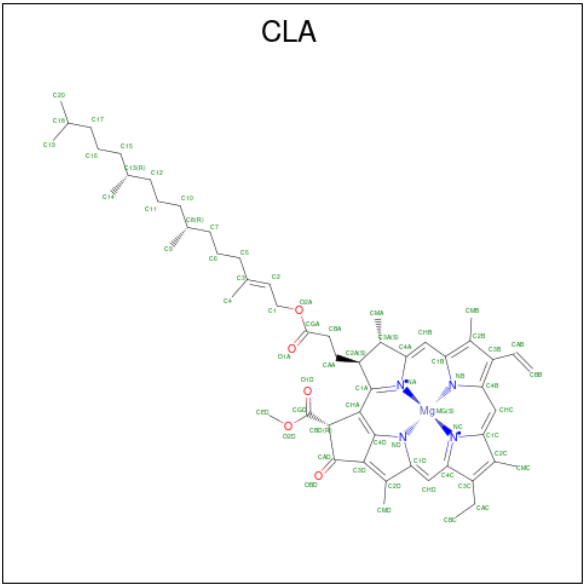
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Mol	Chain	Residues	Atoms		AltConf
20	a	1	Total	Fe	0
			1	1	

- Molecule 21 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
21	A	2	Total	Cl	0
			2	2	
21	a	2	Total	Cl	0
			2	2	

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms						AltConf
22	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	A	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	A	1	Total	C	H	Mg	N	O	0
			102	44	48	1	4	5	
22	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
22	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	C	1	Total	C	H	Mg	N	O	0
			117	49	58	1	4	5	
22	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	a	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
22	a	1	Total 102	C 44	H 48	Mg 1	N 4	O 5	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0

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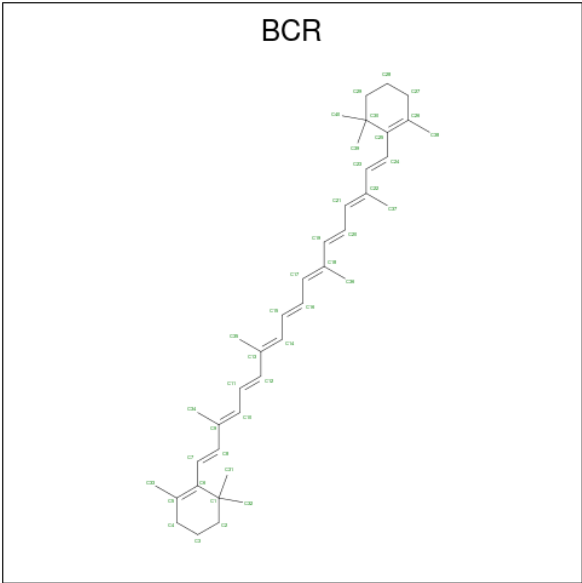
Mol	Chain	Residues	Atoms						AltConf
22	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	b	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	c	1	Total	C	H	Mg	N	O	0
			117	49	58	1	4	5	
22	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	d	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
22	d	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



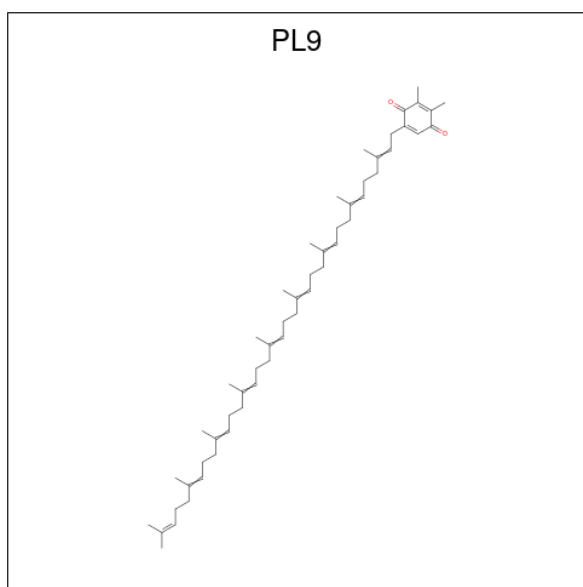
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23	A	1	Total	C	H	0
			96	40	56	
23	B	1	Total	C	H	0
			96	40	56	
23	B	1	Total	C	H	0
			96	40	56	
23	B	1	Total	C	H	0
			96	40	56	
23	C	1	Total	C	H	0
			96	40	56	
23	C	1	Total	C	H	0
			96	40	56	
23	D	1	Total	C	H	0
			96	40	56	
23	H	1	Total	C	H	0
			96	40	56	
23	K	1	Total	C	H	0
			96	40	56	
23	K	1	Total	C	H	0
			96	40	56	

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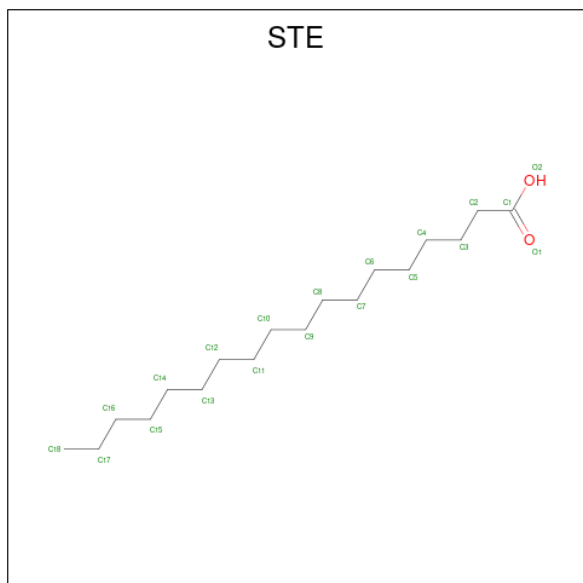
Mol	Chain	Residues	Atoms			AltConf
23	T	1	Total	C	H	0
			96	40	56	
23	a	1	Total	C	H	0
			96	40	56	
23	b	1	Total	C	H	0
			96	40	56	
23	b	1	Total	C	H	0
			96	40	56	
23	b	1	Total	C	H	0
			96	40	56	
23	c	1	Total	C	H	0
			96	40	56	
23	c	1	Total	C	H	0
			96	40	56	
23	d	1	Total	C	H	0
			96	40	56	
23	h	1	Total	C	H	0
			96	40	56	
23	k	1	Total	C	H	0
			96	40	56	
23	k	1	Total	C	H	0
			96	40	56	
23	t	1	Total	C	H	0
			96	40	56	

- Molecule 24 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	H	O	0
			135	53	80	2	
24	D	1	Total	C	H	O	0
			135	53	80	2	
24	a	1	Total	C	H	O	0
			135	53	80	2	
24	d	1	Total	C	H	O	0
			135	53	80	2	

- Molecule 25 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



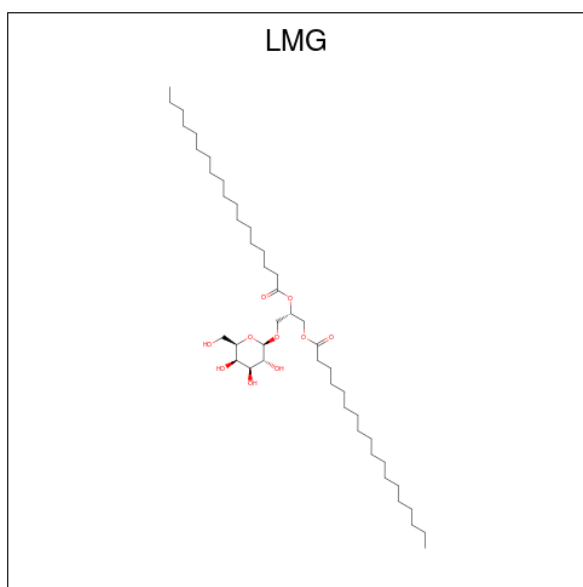
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C H 23 9 14	0
25	A	1	Total C H 23 8 15	0
25	A	1	Total C H 32 11 21	0
25	A	1	Total C H 32 11 21	0
25	A	1	Total C H O 28 10 16 2	0
25	B	1	Total C H O 43 15 26 2	0
25	B	1	Total C H O 28 10 16 2	0
25	B	1	Total C H 32 12 20	0
25	C	1	Total C H O 34 12 20 2	0
25	C	1	Total C H O 28 10 16 2	0
25	C	1	Total C H 23 8 15	0
25	D	1	Total C H O 55 18 35 2	0
25	D	1	Total C H 26 9 17	0
25	E	1	Total C H O 28 10 16 2	0
25	E	1	Total C H 35 12 23	0
25	E	1	Total C H O 55 18 35 2	0
25	I	1	Total C H 38 14 24	0
25	J	1	Total C H 32 12 20	0
25	K	1	Total C H 32 11 21	0
25	M	1	Total C H 26 10 16	0
25	T	1	Total C H 44 15 29	0
25	a	1	Total C H 23 9 14	0

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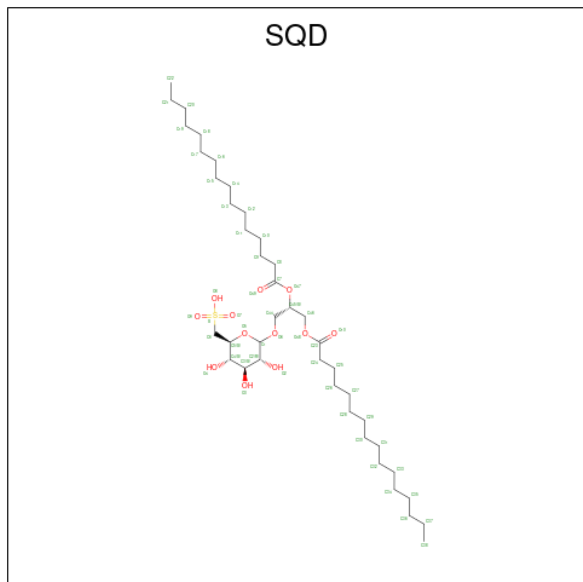
Mol	Chain	Residues	Atoms				AltConf
25	a	1	Total 23	C 8	H 15		0
25	a	1	Total 32	C 11	H 21		0
25	a	1	Total 32	C 11	H 21		0
25	a	1	Total 28	C 10	H 16	O 2	0
25	b	1	Total 32	C 12	H 20		0
25	b	1	Total 43	C 15	H 26	O 2	0
25	b	1	Total 28	C 10	H 16	O 2	0
25	c	1	Total 34	C 12	H 20	O 2	0
25	c	1	Total 28	C 10	H 16	O 2	0
25	c	1	Total 23	C 8	H 15		0
25	d	1	Total 55	C 18	H 35	O 2	0
25	d	1	Total 26	C 9	H 17		0
25	e	1	Total 28	C 10	H 16	O 2	0
25	e	1	Total 35	C 12	H 23		0
25	e	1	Total 55	C 18	H 35	O 2	0
25	i	1	Total 38	C 14	H 24		0
25	j	1	Total 32	C 12	H 20		0
25	k	1	Total 32	C 11	H 21		0
25	m	1	Total 26	C 10	H 16		0
25	t	1	Total 46	C 16	H 28	O 2	0

- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



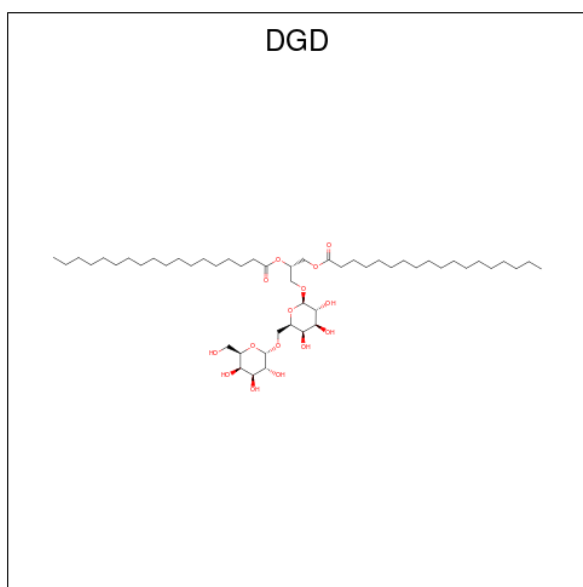
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	H	O	0
			114	38	66	10	
26	B	1	Total	C	H	O	0
			123	41	72	10	
26	C	1	Total	C	H	O	0
			114	38	66	10	
26	C	1	Total	C	H	O	0
			120	40	70	10	
26	D	1	Total	C	H	O	0
			83	29	49	5	
26	D	1	Total	C	H	O	0
			123	41	72	10	
26	H	1	Total	C	H	O	0
			98	34	59	5	
26	a	1	Total	C	H	O	0
			114	38	66	10	
26	b	1	Total	C	H	O	0
			123	41	72	10	
26	c	1	Total	C	H	O	0
			114	38	66	10	
26	c	1	Total	C	H	O	0
			120	40	70	10	
26	d	1	Total	C	H	O	0
			83	29	49	5	
26	d	1	Total	C	H	O	0
			123	41	72	10	
26	h	1	Total	C	H	O	0
			98	34	59	5	

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



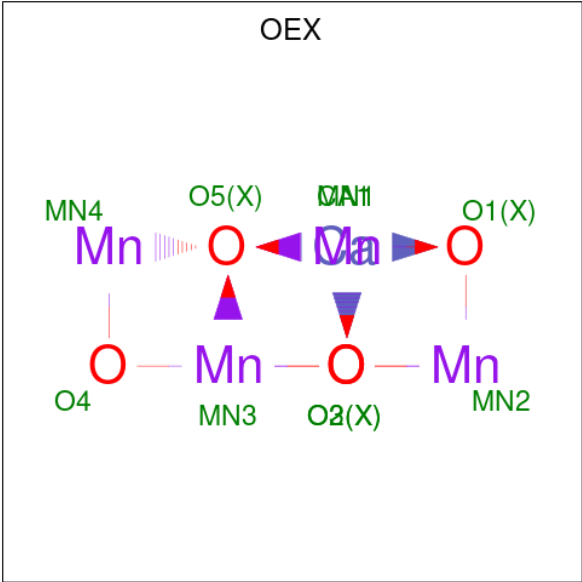
Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	H	O	S	0
			122	39	70	12	1	
27	A	1	Total	C	H	O	S	0
			131	41	77	12	1	
27	B	1	Total	C	H	O	S	0
			131	41	77	12	1	
27	X	1	Total	C	H	O	S	0
			81	25	45	10	1	
27	a	1	Total	C	H	O	S	0
			122	39	70	12	1	
27	a	1	Total	C	H	O	S	0
			131	41	77	12	1	
27	b	1	Total	C	H	O	S	0
			113	36	64	12	1	
27	x	1	Total	C	H	O	S	0
			81	25	45	10	1	

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



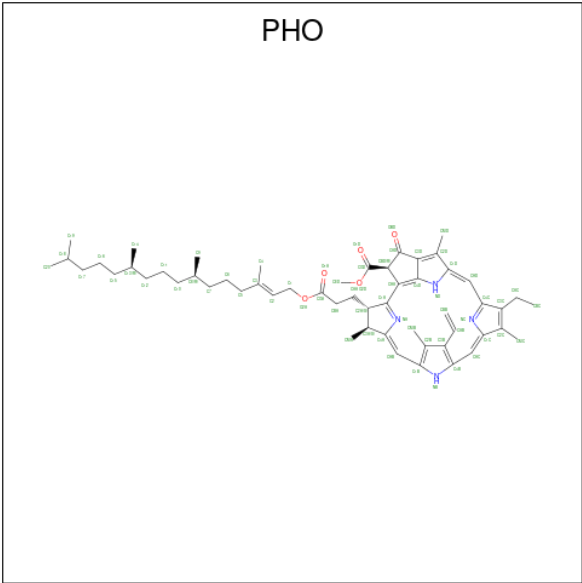
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	H	O	0
			162	51	96	15	
28	C	1	Total	C	H	O	0
			144	47	82	15	
28	C	1	Total	C	H	O	0
			129	42	72	15	
28	C	1	Total	C	H	O	0
			144	47	82	15	
28	H	1	Total	C	H	O	0
			144	47	82	15	
28	a	1	Total	C	H	O	0
			162	51	96	15	
28	c	1	Total	C	H	O	0
			144	47	82	15	
28	c	1	Total	C	H	O	0
			129	42	72	15	
28	c	1	Total	C	H	O	0
			144	47	82	15	
28	h	1	Total	C	H	O	0
			144	47	82	15	

- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
29	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 30 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



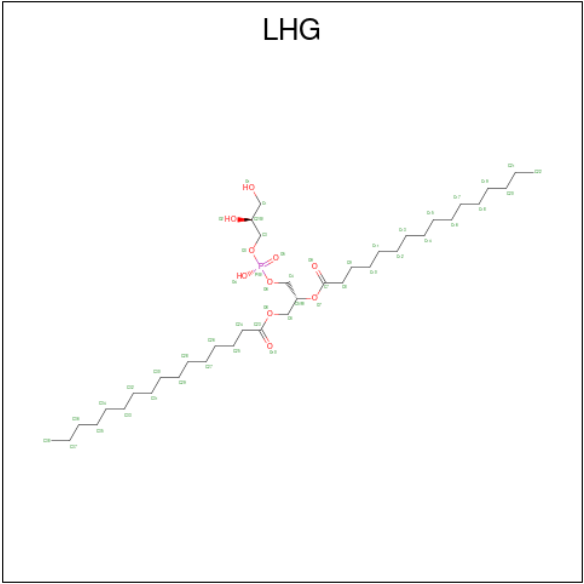
Mol	Chain	Residues	Atoms					AltConf
30	A	1	Total	C	H	N	O	0
			138	55	74	4	5	
30	D	1	Total	C	H	N	O	0
			138	55	74	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	a	1	Total	C	H	N	O	0
			138	55	74	4	5	
30	d	1	Total	C	H	N	O	0
			138	55	74	4	5	

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



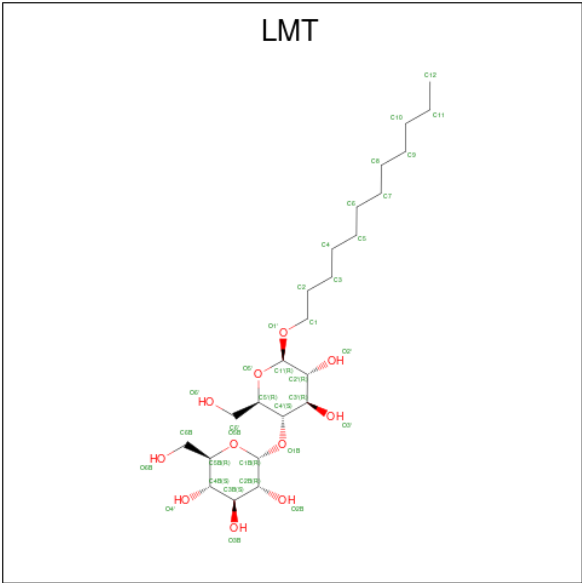
Mol	Chain	Residues	Atoms					AltConf
31	A	1	Total	C	H	O	P	0
			123	38	74	10	1	
31	D	1	Total	C	H	O	P	0
			123	38	74	10	1	
31	D	1	Total	C	H	O	P	0
			114	36	67	10	1	
31	D	1	Total	C	H	O	P	0
			123	38	74	10	1	
31	L	1	Total	C	H	O	P	0
			123	38	74	10	1	
31	a	1	Total	C	H	O	P	0
			123	38	74	10	1	
31	d	1	Total	C	H	O	P	0
			123	38	74	10	1	
31	d	1	Total	C	H	O	P	0
			114	36	67	10	1	
31	d	1	Total	C	H	O	P	0
			123	38	74	10	1	

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Mol	Chain	Residues	Atoms					AltConf
31	1	1	Total	C	H	O	P	0
			123	38	74	10	1	

- Molecule 32 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



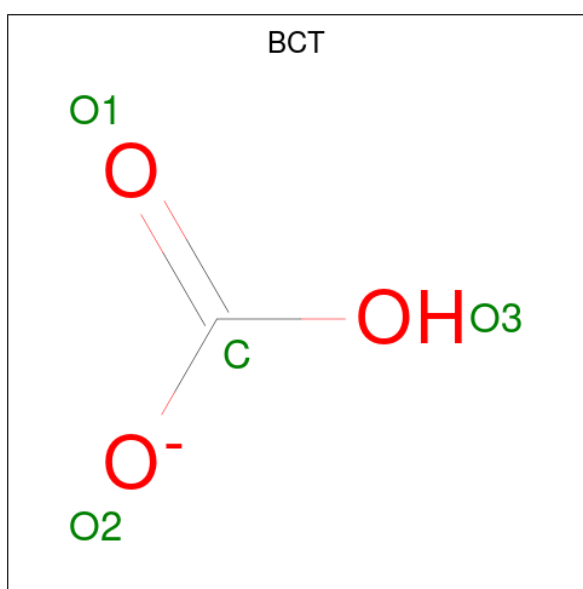
Mol	Chain	Residues	Atoms				AltConf
32	B	1	Total	C	H	O	0
			60	19	35	6	
32	C	1	Total	C	H	O	0
			59	18	35	6	
32	C	1	Total	C	H	O	0
			80	24	45	11	
32	E	1	Total	C	H	O	0
			57	18	33	6	
32	J	1	Total	C	H	O	0
			58	18	34	6	
32	M	1	Total	C	H	O	0
			79	24	44	11	
32	Z	1	Total	C	H	O	0
			79	24	44	11	
32	b	1	Total	C	H	O	0
			60	19	35	6	
32	c	1	Total	C	H	O	0
			59	18	35	6	
32	c	1	Total	C	H	O	0
			80	24	45	11	

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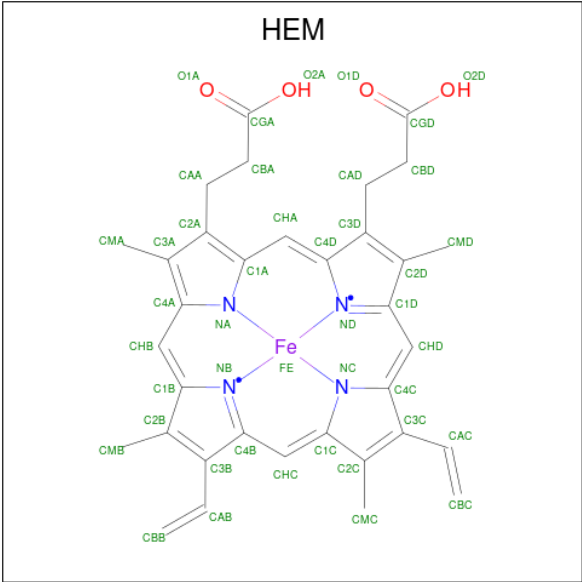
Mol	Chain	Residues	Atoms				AltConf
32	e	1	Total	C	H	O	0
			57	18	33	6	
32	j	1	Total	C	H	O	0
			58	18	34	6	
32	m	1	Total	C	H	O	0
			79	24	44	11	
32	z	1	Total	C	H	O	0
			79	24	44	11	

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



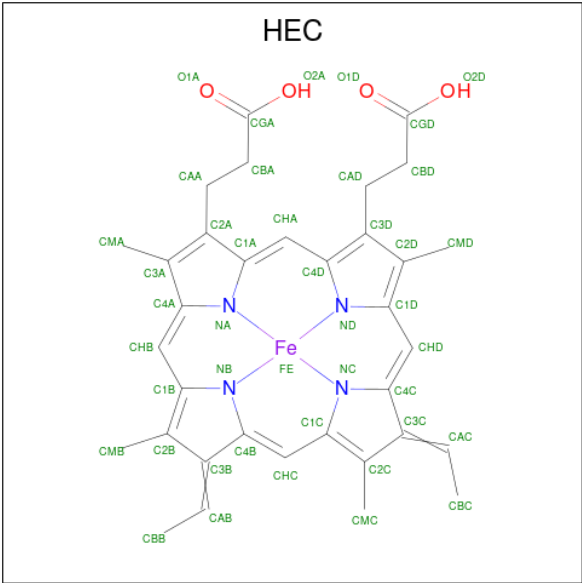
Mol	Chain	Residues	Atoms				AltConf
33	D	1	Total	C	H	O	0
			5	1	1	3	
33	d	1	Total	C	H	O	0
			5	1	1	3	

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms						AltConf
34	E	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
34	e	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 35 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms						AltConf
35	V	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
35	v	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		AltConf
36	A	172	Total 172	O 172	0
36	B	273	Total 273	O 273	0
36	C	200	Total 201	O 201	1
36	D	177	Total 177	O 177	0
36	E	38	Total 38	O 38	0
36	F	4	Total 4	O 4	0
36	H	28	Total 28	O 28	0
36	I	6	Total 6	O 6	0
36	J	14	Total 14	O 14	0
36	K	4	Total 4	O 4	0
36	L	16	Total 16	O 16	0
36	M	7	Total 7	O 7	0
36	O	99	Total 99	O 99	0
36	T	8	Total 8	O 8	0
36	U	61	Total 61	O 61	0
36	V	95	Total 95	O 95	0
36	X	9	Total 9	O 9	0
36	a	168	Total 168	O 168	0
36	b	273	Total 273	O 273	0
36	c	201	Total 202	O 202	1
36	d	177	Total 177	O 177	0

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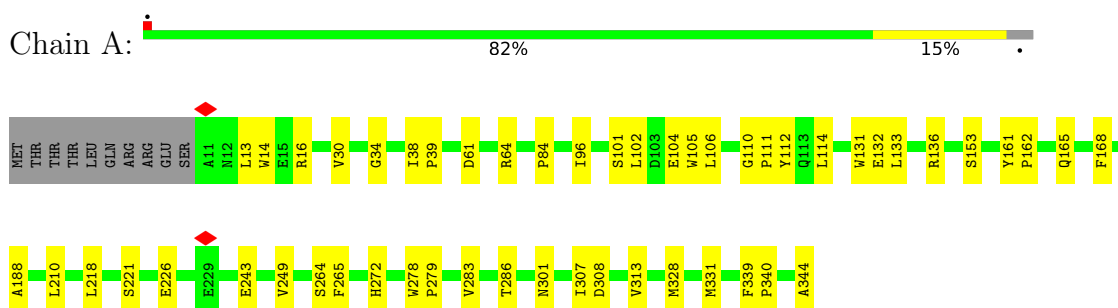
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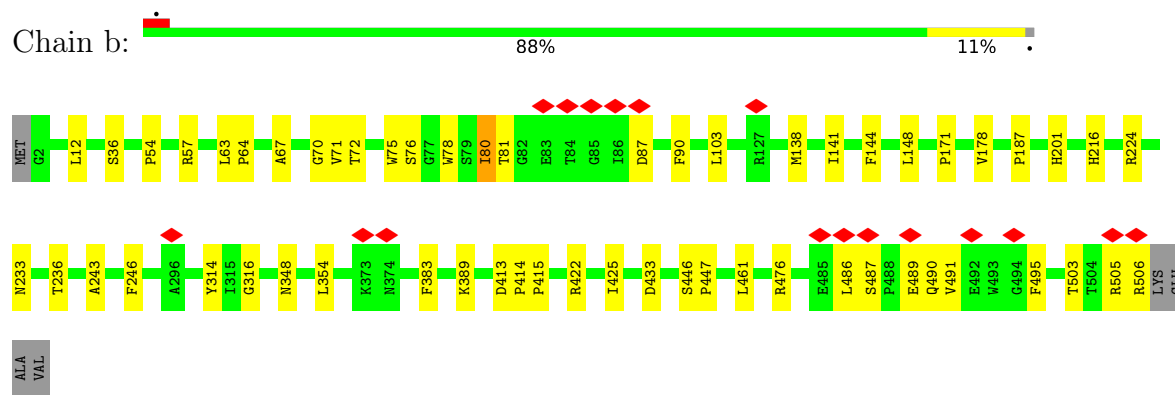
Mol	Chain	Residues	Atoms		AltConf
36	e	38	Total 38	O 38	0
36	f	4	Total 4	O 4	0
36	h	28	Total 28	O 28	0
36	i	6	Total 6	O 6	0
36	j	14	Total 14	O 14	0
36	k	4	Total 4	O 4	0
36	l	13	Total 13	O 13	0
36	m	3	Total 3	O 3	0
36	o	99	Total 99	O 99	0
36	t	7	Total 7	O 7	0
36	u	55	Total 55	O 55	0
36	v	95	Total 95	O 95	0
36	x	9	Total 9	O 9	0

3 Residue-property plots [i](#)

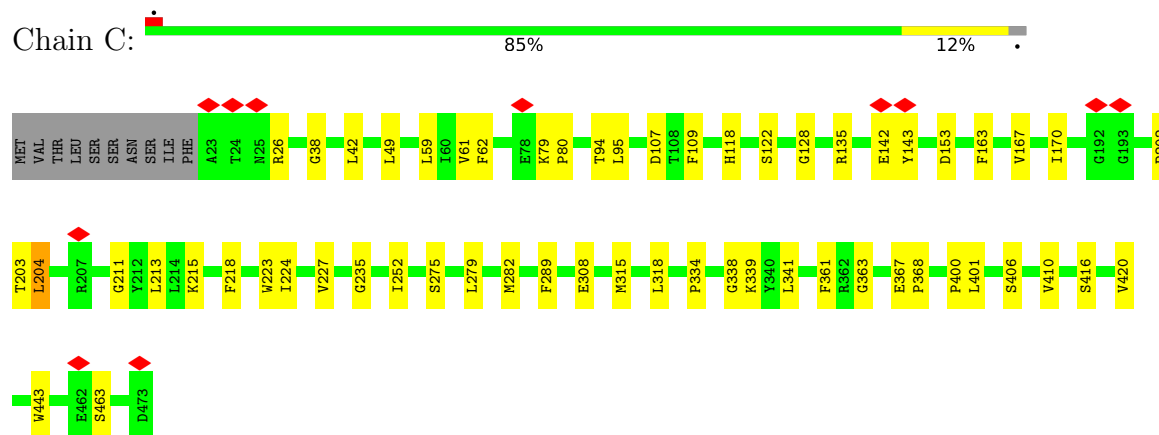
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem II protein D1 1

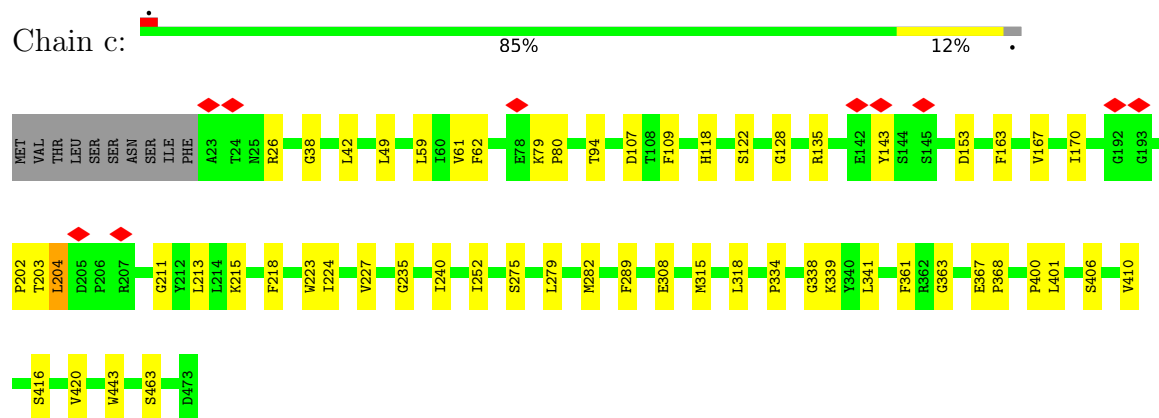




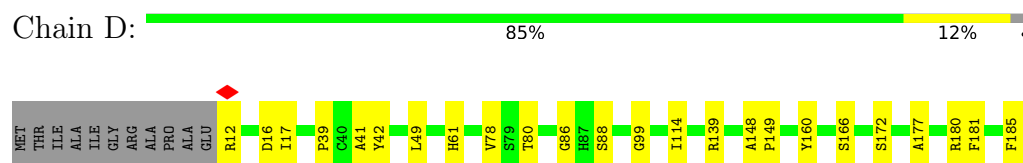
• Molecule 3: Photosystem II CP43 reaction center protein



• Molecule 3: Photosystem II CP43 reaction center protein



• Molecule 4: Photosystem II D2 protein





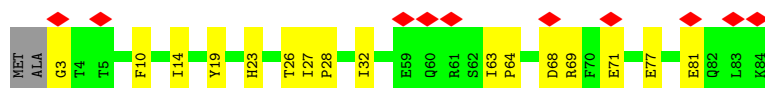
- Molecule 4: Photosystem II D2 protein

Chain d: 85% 12% .



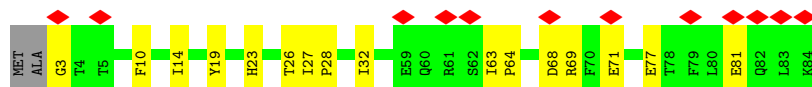
- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 12% 79% 19% .



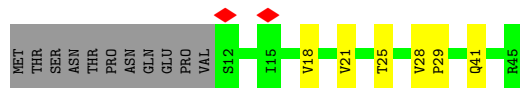
- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 14% 79% 19% .



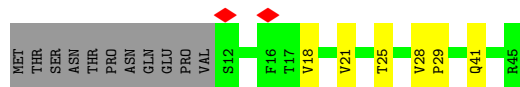
- Molecule 6: Cytochrome b559 subunit beta

Chain F: 62% 13% 24% .



- Molecule 6: Cytochrome b559 subunit beta

Chain f: 62% 13% 24% .

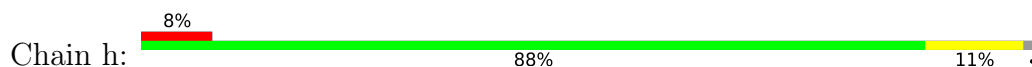


- Molecule 7: Photosystem II reaction center protein H

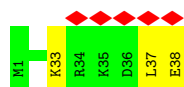
Chain H: 8% 88% 11% .



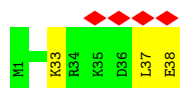
- Molecule 7: Photosystem II reaction center protein H



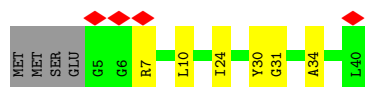
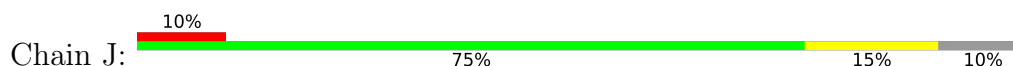
- Molecule 8: Photosystem II reaction center protein I



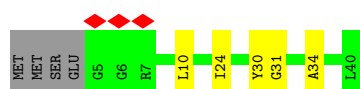
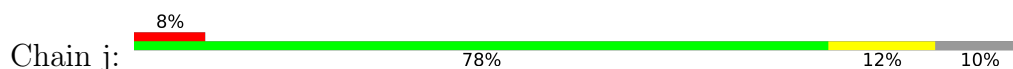
- Molecule 8: Photosystem II reaction center protein I



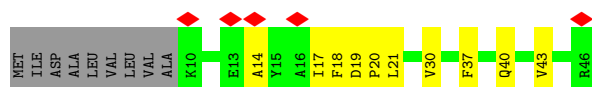
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



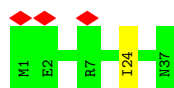
- Molecule 10: Photosystem II reaction center protein K



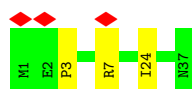
- Molecule 10: Photosystem II reaction center protein K



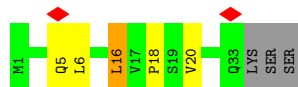
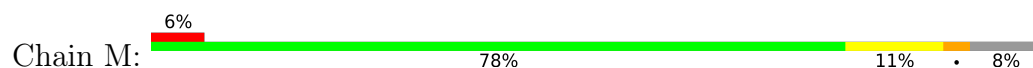
• Molecule 11: Photosystem II reaction center protein L



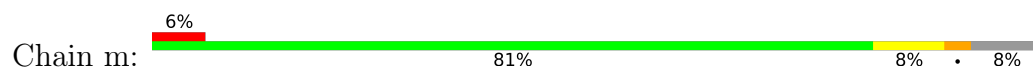
• Molecule 11: Photosystem II reaction center protein L



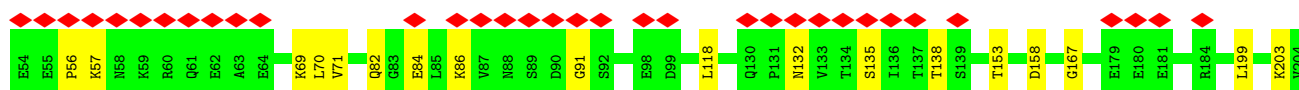
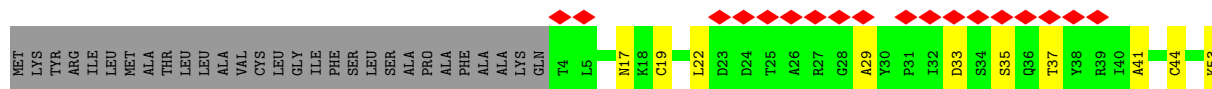
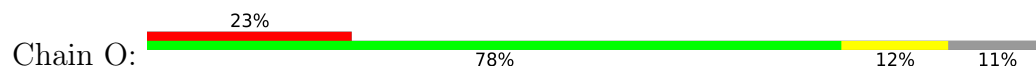
• Molecule 12: Photosystem II reaction center protein M



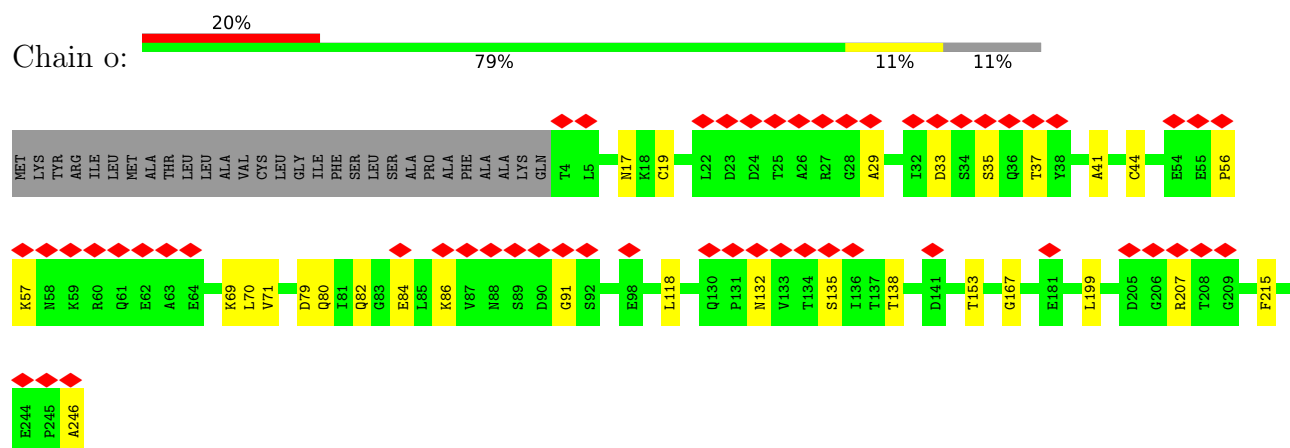
• Molecule 12: Photosystem II reaction center protein M



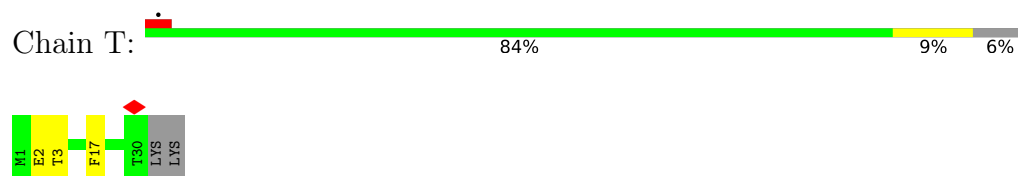
• Molecule 13: Photosystem II manganese-stabilizing polypeptide



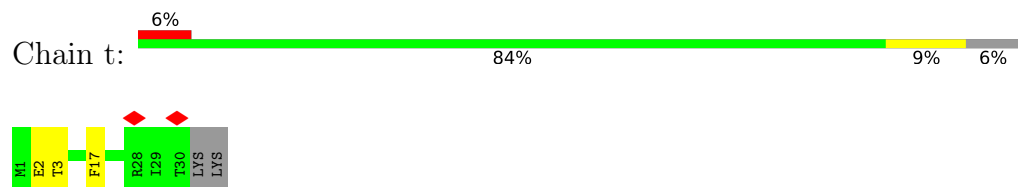
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



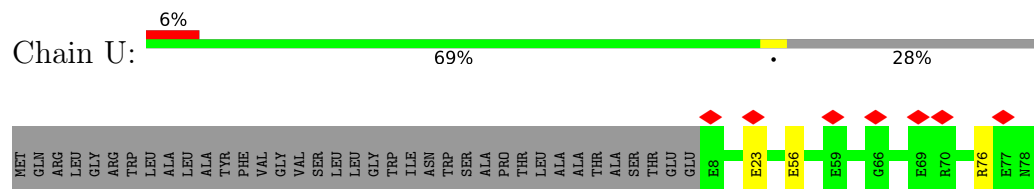
- Molecule 14: Photosystem II reaction center protein T



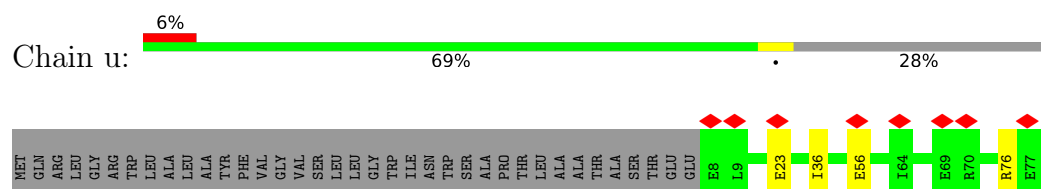
- Molecule 14: Photosystem II reaction center protein T



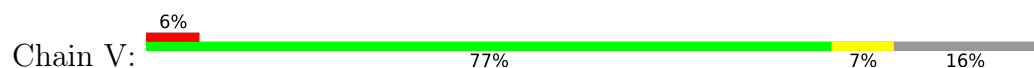
- Molecule 15: Photosystem II 12 kDa extrinsic protein

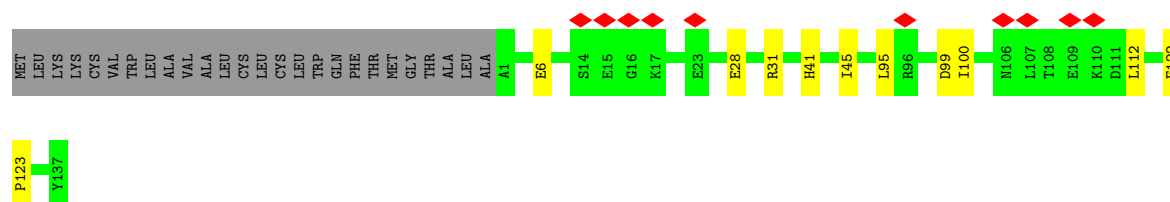


- Molecule 15: Photosystem II 12 kDa extrinsic protein

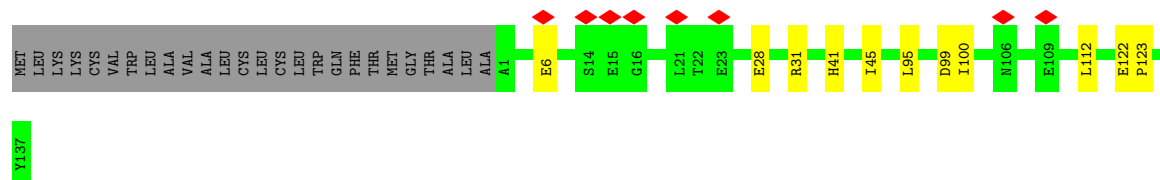
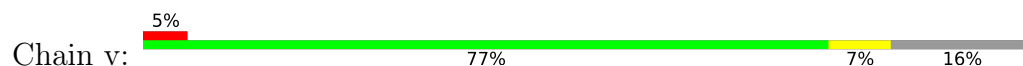


- Molecule 16: Cytochrome c-550

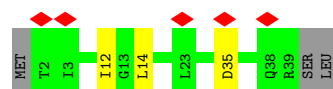
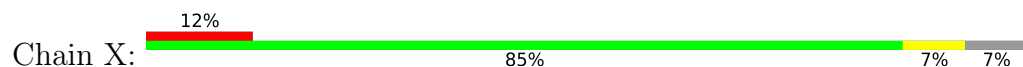




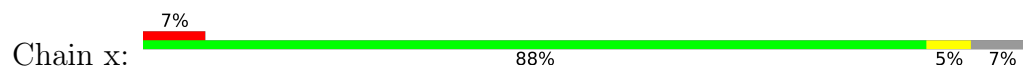
- Molecule 16: Cytochrome c-550



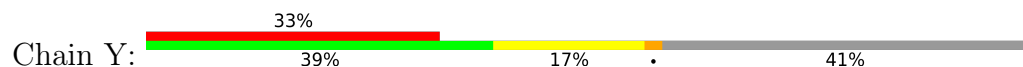
- Molecule 17: Photosystem II reaction center X protein



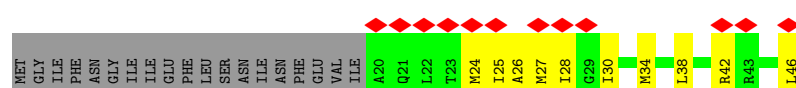
- Molecule 17: Photosystem II reaction center X protein



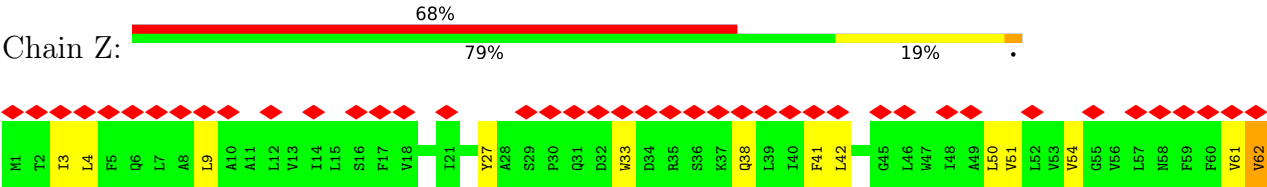
- Molecule 18: Photosystem II reaction center protein Ycf12



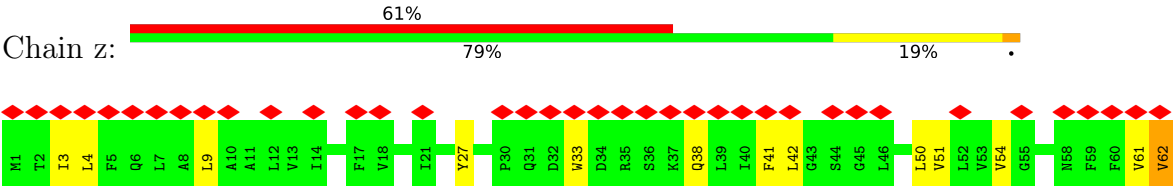
- Molecule 18: Photosystem II reaction center protein Ycf12



- Molecule 19: Photosystem II reaction center protein Z



● Molecule 19: Photosystem II reaction center protein Z



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	631270	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.426	Depositor
Minimum map value	-0.651	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	413.28, 413.28, 413.28	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.574, 0.574, 0.574	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.17	0/2723	0.39	0/3713
1	a	0.17	0/2723	0.39	0/3713
2	B	0.16	0/4140	0.35	0/5641
2	b	0.16	0/4140	0.35	0/5641
3	C	0.16	0/3612	0.34	0/4917
3	c	0.16	0/3612	0.34	0/4917
4	D	0.17	0/2812	0.37	0/3832
4	d	0.17	0/2812	0.37	0/3832
5	E	0.14	0/680	0.32	0/929
5	e	0.14	0/680	0.34	0/929
6	F	0.19	0/284	0.34	0/387
6	f	0.19	0/284	0.34	0/387
7	H	0.12	0/539	0.28	0/736
7	h	0.13	0/539	0.28	0/736
8	I	0.15	0/310	0.34	0/419
8	i	0.15	0/310	0.36	0/419
9	J	0.16	0/263	0.32	0/356
9	j	0.16	0/263	0.33	0/356
10	K	0.19	0/303	0.34	0/416
10	k	0.19	0/303	0.35	0/416
11	L	0.12	0/327	0.27	0/444
11	l	0.13	0/327	0.27	0/444
12	M	0.14	0/264	0.33	0/363
12	m	0.14	0/264	0.33	0/363
13	O	0.13	0/1910	0.34	0/2594
13	o	0.13	0/1910	0.33	0/2594
14	T	0.15	0/257	0.35	0/349
14	t	0.15	0/257	0.35	0/349
15	U	0.12	0/785	0.27	0/1064
15	u	0.12	0/785	0.27	0/1064
16	V	0.13	0/1085	0.25	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.14	0/1085	0.25	0/1473
17	X	0.11	0/284	0.22	0/384
17	x	0.11	0/284	0.22	0/384
18	Y	0.14	0/200	0.32	0/268
18	y	0.16	0/200	0.33	0/268
19	Z	0.14	0/490	0.36	0/669
19	z	0.15	0/490	0.36	0/669
All	All	0.16	0/42536	0.34	0/57908

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2634	2530	2525	47	0
1	a	2634	2530	2525	47	0
2	B	3994	3858	3851	50	0
2	b	3994	3858	3851	51	0
3	C	3491	3408	3395	45	0
3	c	3491	3408	3395	45	0
4	D	2717	2621	2621	34	0
4	d	2717	2621	2621	32	0
5	E	661	640	640	13	0
5	e	661	640	640	13	0
6	F	275	282	282	4	0
6	f	275	282	282	4	0
7	H	511	534	523	10	0
7	h	511	534	523	11	0
8	I	313	328	328	3	0
8	i	313	328	328	3	0
9	J	257	268	268	6	0
9	j	257	268	268	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	K	293	305	305	9	0
10	k	293	305	305	10	0
11	L	312	328	316	1	0
11	l	312	328	316	2	0
12	M	264	281	271	11	0
12	m	264	281	271	10	0
13	O	1876	1834	1832	28	0
13	o	1876	1834	1832	23	0
14	T	258	261	261	2	0
14	t	258	261	261	2	0
15	U	774	773	773	2	0
15	u	774	773	773	3	0
16	V	1064	1071	1073	10	0
16	v	1064	1071	1073	10	0
17	X	281	312	312	3	0
17	x	281	312	312	2	0
18	Y	199	224	226	9	0
18	y	199	226	226	8	0
19	Z	479	516	516	15	0
19	z	479	516	516	16	0
20	A	1	0	0	0	0
20	a	1	0	0	0	0
21	A	2	0	0	1	0
21	a	2	0	0	1	0
22	A	244	251	251	5	0
22	B	1035	1139	1139	23	0
22	C	839	922	922	24	0
22	D	130	144	144	3	0
22	a	244	251	251	5	0
22	b	1035	1139	1139	24	0
22	c	839	922	922	23	0
22	d	130	144	144	1	0
23	A	40	56	56	4	0
23	B	120	168	168	10	0
23	C	80	112	112	7	0
23	D	40	56	56	5	0
23	H	40	56	56	6	0
23	K	80	112	112	5	0
23	T	40	56	56	7	0
23	a	40	56	56	2	0
23	b	120	168	168	8	0
23	c	80	112	112	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	d	40	56	56	4	0
23	h	40	56	56	7	0
23	k	80	112	112	5	0
23	t	40	56	56	11	0
24	A	55	80	80	10	0
24	D	55	80	80	1	0
24	a	55	80	80	12	0
24	d	55	80	80	1	0
25	A	51	87	87	4	0
25	B	41	62	62	3	0
25	C	34	51	51	0	0
25	D	29	52	52	2	0
25	E	44	74	74	2	0
25	I	14	24	24	0	0
25	J	12	20	20	1	0
25	K	11	21	21	0	0
25	M	10	16	16	0	0
25	T	15	29	26	0	0
25	a	51	87	87	6	0
25	b	41	62	62	2	0
25	c	34	51	51	0	0
25	d	29	52	52	2	0
25	e	44	74	74	2	0
25	i	14	24	24	0	0
25	j	12	20	20	1	0
25	k	11	21	21	1	0
25	m	10	16	16	0	0
25	t	18	28	28	1	0
26	A	48	66	66	1	0
26	B	51	72	72	1	0
26	C	98	136	136	7	0
26	D	85	121	121	2	0
26	H	39	59	59	6	0
26	a	48	66	66	1	0
26	b	51	72	72	1	0
26	c	98	136	136	6	0
26	d	85	121	121	2	0
26	h	39	59	59	6	0
27	A	106	147	149	4	0
27	B	54	77	78	3	0
27	X	36	45	46	3	0
27	a	106	147	149	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	b	49	64	65	3	0
27	x	36	45	46	3	0
28	A	66	96	96	6	0
28	C	181	236	236	2	0
28	H	62	82	82	0	0
28	a	66	96	96	10	0
28	c	181	236	236	1	0
28	h	62	82	82	0	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	64	74	74	1	0
30	D	64	74	74	0	0
30	a	64	74	74	0	0
30	d	64	74	74	0	0
31	A	49	74	74	1	0
31	D	145	215	215	5	0
31	L	49	74	74	0	0
31	a	49	74	74	1	0
31	d	145	215	215	7	0
31	l	49	74	74	0	0
32	B	25	35	34	0	0
32	C	59	80	80	2	0
32	E	24	33	34	1	0
32	J	24	34	34	2	0
32	M	35	44	45	0	0
32	Z	35	44	45	3	0
32	b	25	35	34	0	0
32	c	59	80	80	2	0
32	e	24	33	34	1	0
32	j	24	34	34	2	0
32	m	35	44	45	0	0
32	z	35	44	45	3	0
33	D	4	1	1	0	0
33	d	4	1	1	0	0
34	E	43	30	30	6	0
34	e	43	30	30	6	0
35	V	43	30	30	1	0
35	v	43	30	30	1	0
36	A	172	0	0	7	0
36	B	273	0	0	9	0
36	C	201	0	0	5	0
36	D	177	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	E	38	0	0	2	0
36	F	4	0	0	0	0
36	H	28	0	0	0	0
36	I	6	0	0	0	0
36	J	14	0	0	2	0
36	K	4	0	0	0	0
36	L	16	0	0	0	0
36	M	7	0	0	0	0
36	O	99	0	0	4	0
36	T	8	0	0	0	0
36	U	61	0	0	0	0
36	V	95	0	0	0	0
36	X	9	0	0	1	0
36	a	168	0	0	7	0
36	b	273	0	0	9	0
36	c	202	0	0	5	0
36	d	177	0	0	2	0
36	e	38	0	0	2	0
36	f	4	0	0	0	0
36	h	28	0	0	0	0
36	i	6	0	0	0	0
36	j	14	0	0	2	0
36	k	4	0	0	0	0
36	l	13	0	0	0	0
36	m	3	0	0	0	0
36	o	99	0	0	4	0
36	t	7	0	0	0	0
36	u	55	0	0	0	0
36	v	95	0	0	0	0
36	x	9	0	0	1	0
All	All	52833	52030	51925	741	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 7.

All (741) 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:389:LYS:NZ	36:B:701:HOH:O	1.92	1.03
2:b:389:LYS:NZ	36:b:701:HOH:O	1.92	1.01
1:a:243:GLU:OE2	36:a:501:HOH:O	1.84	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:GLU:OE2	36:A:501:HOH:O	1.84	0.93
10:K:21:LEU:HD13	18:Y:24:MET:HE3	1.50	0.92
10:k:21:LEU:HD13	18:y:24:MET:HE3	1.51	0.92
19:Z:61:VAL:O	19:Z:62:VAL:HG13	1.72	0.89
3:C:142:GLU:OE1	3:C:142:GLU:N	2.05	0.88
19:z:61:VAL:O	19:z:62:VAL:HG13	1.72	0.88
23:d:406:BCR:H392	23:d:406:BCR:H23C	1.55	0.88
23:D:406:BCR:H392	23:D:406:BCR:H23C	1.55	0.88
2:b:490:GLN:OE1	36:b:702:HOH:O	1.96	0.83
3:C:107:ASP:OD2	26:C:524:LMG:O2	1.97	0.83
12:m:16[A]:LEU:HD13	12:m:16[A]:LEU:C	2.03	0.83
12:M:16[A]:LEU:HD13	12:M:16[A]:LEU:C	2.03	0.82
3:C:143:TYR:HH	32:C:523:LMT:H3O2	1.09	0.82
13:O:71:VAL:HG12	36:O:313:HOH:O	1.79	0.82
2:B:490:GLN:OE1	36:B:702:HOH:O	1.97	0.82
13:o:71:VAL:HG12	36:o:313:HOH:O	1.79	0.81
3:c:107:ASP:OD2	26:c:524:LMG:O2	1.99	0.78
3:c:410:VAL:HG13	36:c:639:HOH:O	1.85	0.76
3:C:410:VAL:HG13	36:C:639:HOH:O	1.85	0.76
1:a:226:GLU:OE2	36:a:502:HOH:O	2.04	0.75
23:k:103:BCR:H321	23:k:103:BCR:HC8	1.70	0.74
1:A:226:GLU:OE2	36:A:502:HOH:O	2.04	0.74
23:K:103:BCR:H321	23:K:103:BCR:HC8	1.70	0.73
2:b:187:PRO:HG3	22:b:602:CLA:HMD3	1.71	0.72
23:h:102:BCR:H331	23:h:102:BCR:C8	2.19	0.72
2:B:187:PRO:HG3	22:B:601:CLA:HMD3	1.72	0.71
23:H:102:BCR:H331	23:H:102:BCR:C8	2.19	0.71
25:e:102:STE:H101	9:j:10:LEU:HD21	1.73	0.71
3:c:143:TYR:HH	32:c:523:LMT:H3O2	1.22	0.70
25:E:102:STE:H101	9:J:10:LEU:HD21	1.72	0.70
4:d:352:LEU:HB2	36:d:514:HOH:O	1.91	0.70
19:Z:51:VAL:O	19:Z:54:VAL:O	2.09	0.70
16:v:45:ILE:C	16:v:45:ILE:HD12	2.17	0.70
19:z:51:VAL:O	19:z:54:VAL:O	2.09	0.69
4:D:352:LEU:HB2	36:D:513:HOH:O	1.91	0.69
21:A:403:CL:CL	36:A:587:HOH:O	2.47	0.69
21:a:403:CL:CL	36:a:585:HOH:O	2.47	0.69
10:k:14:ALA:HB2	19:z:62:VAL:HG23	1.75	0.69
16:V:45:ILE:C	16:V:45:ILE:HD12	2.17	0.69
22:a:406:CLA:H52	22:c:505:CLA:H191	1.75	0.69
19:z:38:GLN:O	19:z:42:LEU:HD23	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:64:ARG:NE	36:c:708[B]:HOH:O	2.26	0.68
7:H:41:CYS:SG	23:H:102:BCR:H363	2.34	0.68
18:Y:27:MET:HE3	18:Y:27:MET:HA	1.76	0.68
22:A:406:CLA:H52	22:C:505:CLA:H191	1.75	0.68
10:K:14:ALA:HB2	19:Z:62:VAL:HG23	1.75	0.68
1:A:64:ARG:NE	36:C:708[B]:HOH:O	2.26	0.68
18:y:25:ILE:O	18:y:28:ILE:O	2.11	0.68
19:Z:38:GLN:O	19:Z:42:LEU:HD23	1.93	0.67
22:C:513:CLA:H91	32:C:523:LMT:H101	1.77	0.67
4:D:99:GLY:HA3	25:D:412:STE:H21	1.77	0.67
7:h:41:CYS:SG	23:h:102:BCR:H363	2.33	0.67
7:h:32:ALA:HB1	26:h:101:LMG:H371	1.76	0.67
22:c:513:CLA:H91	32:c:523:LMT:H101	1.77	0.66
4:D:342:PRO:O	4:D:345:VAL:HG22	1.95	0.66
4:d:99:GLY:HA3	25:d:412:STE:H21	1.77	0.66
24:A:408:PL9:H311	24:A:408:PL9:H352	1.78	0.66
22:b:617:CLA:HMA1	22:b:617:CLA:H11	1.78	0.66
9:J:34:ALA:O	36:J:201:HOH:O	2.14	0.66
7:H:32:ALA:HB1	26:H:101:LMG:H371	1.76	0.66
4:d:342:PRO:O	4:d:345:VAL:HG22	1.95	0.65
22:c:505:CLA:H122	22:c:505:CLA:H93	1.78	0.65
22:B:616:CLA:HMA1	22:B:616:CLA:H11	1.78	0.65
19:Z:3:ILE:HD12	19:Z:4:LEU:N	2.11	0.65
2:B:76:SER:HG	2:B:78:TRP:CD1	2.15	0.64
34:e:105:HEM:HMB2	34:e:105:HEM:HBB2	1.79	0.64
24:A:408:PL9:H303	4:D:41:ALA:CB	2.28	0.64
2:b:495:PHE:CE2	2:b:505:ARG:HD3	2.32	0.64
19:z:3:ILE:HD12	19:z:4:LEU:N	2.11	0.64
2:B:495:PHE:CE2	2:B:505:ARG:HD3	2.33	0.64
22:C:505:CLA:H122	22:C:505:CLA:H93	1.78	0.64
24:a:408:PL9:H311	24:a:408:PL9:H352	1.78	0.64
9:j:34:ALA:O	36:j:201:HOH:O	2.14	0.64
34:E:105:HEM:O2A	36:E:201:HOH:O	2.15	0.64
34:e:105:HEM:O2A	36:e:201:HOH:O	2.15	0.64
23:B:618:BCR:H331	23:B:618:BCR:C8	2.27	0.63
23:b:619:BCR:H331	23:b:619:BCR:C8	2.27	0.63
3:c:26:ARG:NH2	18:y:46:LEU:O	2.29	0.63
22:C:512:CLA:H143	22:C:513:CLA:H142	1.80	0.63
24:a:408:PL9:H303	4:d:41:ALA:HB1	1.81	0.62
24:A:408:PL9:H303	4:D:41:ALA:HB1	1.81	0.62
34:E:105:HEM:HMB2	34:E:105:HEM:HBB2	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:272:LEU:C	4:d:272:LEU:HD23	2.24	0.62
22:c:512:CLA:H143	22:c:513:CLA:H142	1.80	0.62
12:M:16[A]:LEU:HD11	12:m:16[A]:LEU:HD11	1.81	0.62
3:C:26:ARG:NH2	18:Y:46:LEU:O	2.29	0.61
4:D:272:LEU:C	4:D:272:LEU:HD23	2.25	0.61
24:a:408:PL9:H303	4:d:41:ALA:CB	2.28	0.61
23:C:514:BCR:H332	19:Z:54:VAL:HG23	1.83	0.60
2:b:76:SER:HG	2:b:78:TRP:CD1	2.18	0.60
12:m:16[A]:LEU:C	12:m:16[A]:LEU:CD1	2.74	0.60
23:T:101:BCR:H321	23:T:101:BCR:HC8	1.84	0.60
7:H:41:CYS:SG	23:H:102:BCR:C16	2.90	0.60
12:M:16[A]:LEU:C	12:M:16[A]:LEU:CD1	2.74	0.60
26:c:520:LMG:H362	10:k:30:VAL:HG21	1.84	0.60
7:h:41:CYS:SG	23:h:102:BCR:C16	2.90	0.60
6:f:21:VAL:O	6:f:25:THR:HG23	2.02	0.60
7:h:41:CYS:SG	23:h:102:BCR:C17	2.90	0.60
26:C:520:LMG:H362	10:K:30:VAL:HG21	1.84	0.59
19:Z:61:VAL:HG23	19:Z:62:VAL:H	1.68	0.59
7:H:41:CYS:SG	23:H:102:BCR:C17	2.90	0.59
16:v:99:ASP:OD1	16:v:100:ILE:N	2.36	0.59
23:c:514:BCR:H332	19:z:54:VAL:HG23	1.83	0.59
6:F:21:VAL:O	6:F:25:THR:HG23	2.02	0.59
19:z:61:VAL:HG23	19:z:62:VAL:H	1.68	0.59
12:m:16[A]:LEU:HD13	12:m:16[A]:LEU:O	2.03	0.58
17:x:35:ASP:OD2	36:x:201:HOH:O	2.17	0.58
1:A:13:LEU:HD23	25:A:409:STE:H31	1.84	0.58
31:d:410:LHG:O5	31:d:410:LHG:O2	2.20	0.58
23:t:102:BCR:HC8	23:t:102:BCR:H321	1.84	0.58
3:C:334:PRO:HA	13:O:153:THR:OG1	2.04	0.58
13:o:69:LYS:NZ	13:o:70:LEU:O	2.30	0.58
2:B:224:ARG:HH11	26:H:101:LMG:C7	2.17	0.58
16:V:6:GLU:OE1	16:V:6:GLU:N	2.37	0.58
3:c:170:ILE:HG21	22:c:512:CLA:H101	1.86	0.58
16:v:6:GLU:N	16:v:6:GLU:OE1	2.37	0.58
4:D:209:LEU:HD23	4:D:209:LEU:C	2.29	0.57
13:o:56:PRO:O	13:o:57:LYS:HB3	2.04	0.57
3:C:170:ILE:HG21	22:C:512:CLA:H101	1.85	0.57
13:O:56:PRO:O	13:O:57:LYS:HB3	2.04	0.57
3:c:334:PRO:HA	13:o:153:THR:OG1	2.04	0.57
4:D:343:GLU:OE2	36:D:501:HOH:O	2.17	0.57
23:b:619:BCR:H19C	27:b:621:SQD:H223	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C:524:LMG:C11	26:C:524:LMG:HC92	2.34	0.57
12:M:16[A]:LEU:HD13	12:M:16[A]:LEU:O	2.03	0.57
10:K:18:PHE:CE2	19:Z:9:LEU:HD23	2.40	0.57
2:b:224:ARG:HH11	26:h:101:LMG:C7	2.17	0.57
34:e:105:HEM:HBB2	34:e:105:HEM:CMB	2.34	0.57
1:a:13:LEU:HD23	25:a:409:STE:H31	1.87	0.57
10:k:18:PHE:CE2	19:z:9:LEU:HD23	2.40	0.57
16:V:99:ASP:OD1	16:V:100:ILE:N	2.38	0.57
2:B:422:ARG:O	2:B:425:ILE:HG12	2.05	0.56
4:D:267:LEU:C	4:D:267:LEU:HD23	2.30	0.56
13:O:207:ARG:HD2	13:O:207:ARG:N	2.20	0.56
1:A:14:TRP:CG	25:A:421:STE:H42	2.41	0.56
2:B:144:PHE:CE2	2:B:148:LEU:HD11	2.40	0.56
2:b:144:PHE:CE2	2:b:148:LEU:HD11	2.40	0.56
4:d:343:GLU:OE2	36:d:501:HOH:O	2.17	0.56
3:c:153:ASP:OD2	36:c:601:HOH:O	2.18	0.56
4:d:209:LEU:HD23	4:d:209:LEU:C	2.30	0.56
18:y:27:MET:HE2	18:y:27:MET:HA	1.87	0.56
34:E:105:HEM:HBB2	34:E:105:HEM:CMB	2.34	0.56
23:T:101:BCR:C8	23:T:101:BCR:H311	2.36	0.56
17:X:35:ASP:OD2	36:X:201:HOH:O	2.17	0.56
2:b:422:ARG:O	2:b:425:ILE:HG12	2.05	0.56
23:t:102:BCR:HC8	23:t:102:BCR:H311	1.86	0.56
13:o:207:ARG:HD2	13:o:207:ARG:N	2.20	0.56
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.88	0.55
1:a:61:ASP:OD2	36:a:503:HOH:O	2.18	0.55
23:t:102:BCR:H311	23:t:102:BCR:C8	2.35	0.55
2:b:72:THR:HB	2:b:80:ILE:HD11	1.87	0.55
27:a:412:SQD:H312	28:a:413:DGD:CIA	2.35	0.55
8:i:37:LEU:O	8:i:38:GLU:HB2	2.06	0.55
19:z:3:ILE:HD12	19:z:3:ILE:C	2.32	0.55
23:T:101:BCR:HC8	23:T:101:BCR:H311	1.88	0.55
26:c:524:LMG:HC92	26:c:524:LMG:C11	2.34	0.55
19:z:41:PHE:CD2	19:z:42:LEU:HD22	2.42	0.55
8:I:37:LEU:O	8:I:38:GLU:HB2	2.07	0.55
1:a:14:TRP:CG	25:a:421:STE:H42	2.41	0.55
4:d:267:LEU:C	4:d:267:LEU:HD23	2.30	0.55
31:D:410:LHG:O5	31:D:410:LHG:O2	2.20	0.55
26:a:410:LMG:H132	3:c:218:PHE:HE2	1.72	0.55
4:d:148:ALA:HB3	4:d:149:PRO:HD3	1.88	0.54
24:A:408:PL9:H512	4:D:39:PRO:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:153:ASP:OD2	36:C:601:HOH:O	2.18	0.54
25:B:622:STE:H41	25:B:622:STE:H82	1.88	0.54
13:O:57:LYS:O	13:O:57:LYS:HG2	2.07	0.54
19:Z:41:PHE:CD2	19:Z:42:LEU:HD22	2.42	0.54
2:B:506:ARG:NH2	36:B:706:HOH:O	2.39	0.54
13:O:37:THR:OG1	13:O:246:ALA:OXT	2.26	0.54
2:b:216:HIS:HE1	22:b:610:CLA:C1A	2.21	0.54
22:b:608:CLA:H42	26:b:625:LMG:H301	1.88	0.54
26:A:410:LMG:H132	3:C:218:PHE:HE2	1.72	0.54
2:b:187:PRO:HG3	22:b:602:CLA:CMD	2.37	0.54
22:B:607:CLA:H42	26:B:624:LMG:H301	1.89	0.54
24:a:408:PL9:H512	4:d:39:PRO:HG3	1.88	0.54
25:b:623:STE:H41	25:b:623:STE:H82	1.90	0.54
2:B:72:THR:HB	2:B:80:ILE:HD11	1.87	0.54
2:b:233:ASN:O	2:b:236:THR:HG22	2.08	0.54
2:b:506:ARG:NH2	36:b:706:HOH:O	2.39	0.54
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.08	0.54
2:B:187:PRO:HG3	22:B:601:CLA:CMD	2.37	0.53
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.43	0.53
13:o:57:LYS:O	13:o:57:LYS:HG2	2.07	0.53
19:Z:3:ILE:HD12	19:Z:3:ILE:C	2.32	0.53
16:v:45:ILE:C	16:v:45:ILE:CD1	2.82	0.53
2:B:233:ASN:O	2:B:236:THR:HG22	2.09	0.53
1:a:38:ILE:HB	1:a:39:PRO:HD3	1.91	0.53
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.43	0.53
2:B:216:HIS:HE1	22:B:609:CLA:C1A	2.21	0.53
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.90	0.53
1:A:339:PHE:HB3	1:A:340:PRO:HD2	1.90	0.53
3:c:61:VAL:HG12	3:c:118:HIS:O	2.09	0.53
23:t:102:BCR:H382	23:t:102:BCR:H23C	1.91	0.53
2:B:413:ASP:OD1	2:B:415:PRO:HD2	2.08	0.53
2:b:476:ARG:NH1	36:b:708:HOH:O	2.42	0.53
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.08	0.52
2:b:413:ASP:OD1	2:b:415:PRO:HD2	2.08	0.52
2:b:489:GLU:HG2	2:b:495:PHE:CZ	2.44	0.52
23:B:618:BCR:H282	28:a:413:DGD:CGA	2.39	0.52
13:O:69:LYS:C	13:O:69:LYS:HD3	2.34	0.52
1:A:38:ILE:HB	1:A:39:PRO:HD3	1.91	0.52
3:C:61:VAL:HG12	3:C:118:HIS:O	2.09	0.52
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.92	0.52
16:V:45:ILE:C	16:V:45:ILE:CD1	2.82	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:419:CLA:HMA2	24:d:407:PL9:H411	1.92	0.52
2:b:36:SER:OG	23:b:619:BCR:H362	2.10	0.52
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.90	0.52
1:a:339:PHE:HB3	1:a:340:PRO:HD2	1.90	0.52
2:b:503:THR:O	2:b:503:THR:HG22	2.10	0.52
3:C:42:LEU:HD21	22:C:511:CLA:H2A	1.92	0.52
5:E:63:ILE:HG23	5:E:64:PRO:HD2	1.92	0.52
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.92	0.52
22:b:609:CLA:H172	22:b:610:CLA:H192	1.92	0.51
7:H:32:ALA:CB	26:H:101:LMG:H371	2.41	0.51
2:b:486[B]:LEU:C	2:b:486[B]:LEU:HD23	2.35	0.51
3:c:211:GLY:O	3:c:215:LYS:HG3	2.11	0.51
13:o:37:THR:OG1	13:o:246:ALA:OXT	2.27	0.51
2:B:489:GLU:HG2	2:B:495:PHE:CZ	2.45	0.51
23:T:101:BCR:H382	23:T:101:BCR:H23C	1.91	0.51
2:b:103:LEU:HD21	22:b:606:CLA:HMC3	1.93	0.51
3:c:42:LEU:HD21	22:c:511:CLA:H2A	1.91	0.51
16:v:41:HIS:HA	16:v:45:ILE:O	2.11	0.51
23:A:407:BCR:H352	27:A:412:SQD:H362	1.92	0.51
22:B:606:CLA:H121	28:a:413:DGD:HBE2	1.92	0.51
4:D:266:TRP:CD1	31:D:409:LHG:HC31	2.45	0.51
1:a:264:SER:HB2	36:a:504:HOH:O	2.10	0.51
23:b:619:BCR:C19	27:b:621:SQD:H223	2.41	0.51
22:A:419:CLA:HMA2	24:D:407:PL9:H411	1.92	0.51
5:e:63:ILE:HG23	5:e:64:PRO:HD2	1.92	0.51
13:o:69:LYS:HD3	13:o:69:LYS:C	2.36	0.51
1:A:61:ASP:OD2	36:A:503:HOH:O	2.18	0.51
2:B:486[B]:LEU:C	2:B:486[B]:LEU:HD23	2.35	0.51
5:e:10:PHE:HB3	25:e:102:STE:H132	1.92	0.51
3:C:211:GLY:O	3:C:215:LYS:HG3	2.11	0.50
1:A:264:SER:HB2	36:A:504:HOH:O	2.10	0.50
13:O:69:LYS:HD2	36:O:313:HOH:O	2.11	0.50
7:h:32:ALA:CB	26:h:101:LMG:H371	2.41	0.50
2:B:103:LEU:HD21	22:B:605:CLA:HMC3	1.93	0.50
2:B:201:HIS:HB2	22:B:602:CLA:CHB	2.41	0.50
27:B:620:SQD:H201	23:t:102:BCR:H351	1.93	0.50
3:C:109:PHE:CD2	26:C:524:LMG:HC1	2.47	0.50
3:C:308:GLU:HG3	3:C:361:PHE:CZ	2.47	0.50
22:C:508:CLA:H92	31:D:410:LHG:H152	1.93	0.50
22:b:602:CLA:CBB	22:b:602:CLA:HHC	2.42	0.50
2:B:36:SER:OG	23:B:618:BCR:H362	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:18:VAL:HG22	27:X:101:SQD:H241	1.93	0.50
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.47	0.50
4:d:266:TRP:CD1	31:d:409:LHG:HC31	2.45	0.50
2:B:503:THR:O	2:B:503:THR:HG22	2.10	0.50
22:B:608:CLA:H172	22:B:609:CLA:H192	1.92	0.50
2:b:201:HIS:HB2	22:b:603:CLA:CHB	2.41	0.50
13:o:69:LYS:HD2	36:o:313:HOH:O	2.11	0.50
18:y:26:ALA:O	18:y:30:ILE:HG22	2.11	0.50
5:E:10:PHE:HB3	25:E:102:STE:H132	1.92	0.50
12:M:5:GLN:OE1	12:M:5:GLN:N	2.42	0.50
6:f:18:VAL:HG22	27:x:101:SQD:H241	1.92	0.50
2:B:476:ARG:NH1	36:B:708:HOH:O	2.42	0.50
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.47	0.50
32:J:102:LMT:H3'	36:J:213:HOH:O	2.11	0.50
16:V:41:HIS:HA	16:V:45:ILE:O	2.11	0.50
1:a:30:VAL:O	1:a:34:GLY:HA3	2.12	0.50
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.47	0.50
23:B:617:BCR:H382	23:B:617:BCR:H23C	1.94	0.50
5:e:27:ILE:HG12	34:e:105:HEM:HMC3	1.94	0.50
3:c:109:PHE:CD2	26:c:524:LMG:HC1	2.47	0.49
3:C:463:SER:OG	8:I:33:LYS:NZ	2.45	0.49
5:E:68:ASP:OD2	5:E:71:GLU:HG2	2.12	0.49
3:c:213:LEU:HD11	23:c:515:BCR:C20	2.42	0.49
22:B:601:CLA:CBB	22:B:601:CLA:HHC	2.42	0.49
12:m:5:GLN:OE1	12:m:5:GLN:N	2.42	0.49
3:c:318:LEU:C	3:c:318:LEU:HD23	2.37	0.49
3:C:318:LEU:C	3:C:318:LEU:HD23	2.37	0.49
1:a:272:HIS:CD2	4:d:218:VAL:HG21	2.47	0.49
24:a:408:PL9:H352	24:a:408:PL9:C31	2.42	0.49
5:e:68:ASP:OD2	5:e:71:GLU:HG2	2.12	0.49
32:j:102:LMT:H3'	36:j:213:HOH:O	2.11	0.49
3:C:213:LEU:HD11	23:C:515:BCR:C20	2.42	0.49
5:E:23:HIS:HA	5:E:26:THR:OG1	2.13	0.49
19:Z:33:TRP:CZ2	32:Z:101:LMT:O3'	2.66	0.49
3:c:308:GLU:HG3	3:c:361:PHE:CZ	2.47	0.49
13:o:138:THR:O	13:o:138:THR:HG22	2.13	0.49
24:A:408:PL9:H352	24:A:408:PL9:C31	2.43	0.49
2:B:87:ASP:O	36:B:703:HOH:O	2.20	0.49
25:D:412:STE:H31	17:X:12:ILE:HG21	1.95	0.49
23:b:618:BCR:H382	23:b:618:BCR:H23C	1.94	0.49
24:A:408:PL9:H301	4:D:42:TYR:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:246:PHE:CD1	2:b:246:PHE:C	2.91	0.49
23:C:515:BCR:H331	23:C:515:BCR:C8	2.42	0.49
1:a:84:PRO:HA	1:a:112:TYR:CG	2.48	0.49
1:a:278:TRP:HB3	1:a:279:PRO:HD3	1.95	0.49
1:A:84:PRO:HA	1:A:112:TYR:CG	2.48	0.48
19:z:33:TRP:CZ2	32:z:101:LMT:O3'	2.66	0.48
13:O:138:THR:O	13:O:138:THR:HG22	2.13	0.48
1:a:105:TRP:NE1	1:a:110:GLY:HA3	2.28	0.48
3:c:443:TRP:CZ2	22:c:508:CLA:HMD1	2.48	0.48
24:A:408:PL9:C31	24:A:408:PL9:C35	2.91	0.48
3:C:443:TRP:CZ2	22:C:508:CLA:HMD1	2.48	0.48
28:C:518:DGD:HO4E	28:C:518:DGD:HO5E	1.57	0.48
3:c:49:LEU:HD11	22:c:509:CLA:C1C	2.43	0.48
1:A:278:TRP:HB3	1:A:279:PRO:HD3	1.95	0.48
23:a:407:BCR:H331	23:a:407:BCR:C8	2.43	0.48
12:m:16[A]:LEU:HD22	12:m:20:VAL:HG13	1.95	0.48
1:a:110:GLY:N	1:a:111:PRO:CD	2.76	0.48
3:c:463:SER:OG	8:i:33:LYS:NZ	2.47	0.48
23:c:515:BCR:C8	23:c:515:BCR:H331	2.42	0.48
1:A:105:TRP:NE1	1:A:110:GLY:HA3	2.28	0.48
23:K:103:BCR:C8	23:K:103:BCR:H311	2.43	0.48
11:L:24[B]:ILE:HD13	12:M:18:PRO:HB2	1.96	0.48
5:e:19:TYR:CE1	5:e:23:HIS:CE1	3.02	0.48
23:A:407:BCR:H331	23:A:407:BCR:C8	2.43	0.48
22:C:502:CLA:H61	22:C:512:CLA:H42	1.95	0.48
5:E:19:TYR:CE1	5:E:23:HIS:CE1	3.02	0.48
5:E:27:ILE:HG12	34:E:105:HEM:HMC3	1.94	0.48
1:a:133:LEU:HD23	4:d:256:ILE:HG12	1.96	0.48
24:a:408:PL9:C31	24:a:408:PL9:C35	2.91	0.48
3:c:223:TRP:CG	3:c:224:ILE:H	2.32	0.48
4:d:180:ARG:HD3	4:d:180:ARG:C	2.39	0.48
19:z:50:LEU:O	19:z:54:VAL:HG22	2.14	0.48
3:C:49:LEU:HD11	22:C:509:CLA:C1C	2.44	0.48
1:a:278:TRP:HB3	1:a:279:PRO:CD	2.44	0.48
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.49	0.48
19:Z:50:LEU:O	19:Z:54:VAL:HG22	2.14	0.48
23:k:103:BCR:C8	23:k:103:BCR:H311	2.43	0.48
1:A:30:VAL:O	1:A:34:GLY:HA3	2.13	0.47
3:C:279:LEU:HD12	3:C:282:MET:CE	2.44	0.47
25:d:412:STE:H31	17:x:12:ILE:HG21	1.95	0.47
5:e:23:HIS:HA	5:e:26:THR:OG1	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:TRP:HB3	1:A:279:PRO:CD	2.44	0.47
2:B:246:PHE:CD1	2:B:246:PHE:C	2.91	0.47
24:A:408:PL9:H501	27:X:101:SQD:H352	1.95	0.47
4:D:12:ARG:HB2	4:D:17:ILE:HD11	1.96	0.47
11:l:24[B]:ILE:HD13	12:m:18:PRO:HB2	1.96	0.47
4:D:180:ARG:HD3	4:D:180:ARG:C	2.39	0.47
3:c:279:LEU:HD12	3:c:282:MET:CE	2.43	0.47
15:u:76:ARG:HA	15:u:79:LEU:HG	1.97	0.47
1:A:110:GLY:N	1:A:111:PRO:CD	2.77	0.47
22:B:604:CLA:H92	22:B:604:CLA:H61	1.78	0.47
3:C:167:VAL:HG22	22:C:512:CLA:H152	1.96	0.47
5:E:81:GLU:OE1	5:E:81:GLU:HA	2.14	0.47
34:E:105:HEM:HBC2	34:E:105:HEM:CMC	2.45	0.47
12:M:16[A]:LEU:HD22	12:M:20:VAL:HG13	1.95	0.47
2:b:87:ASP:O	36:b:703:HOH:O	2.20	0.47
3:c:62:PHE:CD1	3:c:62:PHE:C	2.93	0.47
22:c:502:CLA:H61	22:c:512:CLA:H42	1.95	0.47
2:B:201:HIS:HB2	22:B:602:CLA:C1B	2.44	0.47
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.49	0.47
4:D:61:HIS:HE1	4:D:80:THR:O	1.98	0.47
22:b:614:CLA:HMB1	22:b:614:CLA:HBB1	1.96	0.47
22:c:508:CLA:H93	31:d:410:LHG:H161	1.96	0.47
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.96	0.47
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.96	0.47
1:a:249:VAL:HG12	2:b:491:VAL:HG21	1.97	0.47
24:a:408:PL9:H301	4:d:42:TYR:HA	1.96	0.47
2:b:201:HIS:HB2	22:b:603:CLA:C1B	2.44	0.47
19:z:33:TRP:HZ2	32:z:101:LMT:O3'	1.98	0.47
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.96	0.47
36:B:931:HOH:O	7:H:65:LEU:HD22	2.15	0.47
34:E:105:HEM:HBC2	34:E:105:HEM:HMC1	1.97	0.47
22:b:607:CLA:HMB3	22:b:607:CLA:HBB1	1.96	0.47
34:e:105:HEM:HBC2	34:e:105:HEM:CMC	2.45	0.47
1:A:153:SER:HB2	22:A:404:CLA:H43	1.97	0.47
24:a:408:PL9:H501	27:x:101:SQD:H352	1.96	0.47
27:a:412:SQD:H322	25:a:415:STE:C8	2.44	0.47
2:b:433:ASP:OD1	2:b:433:ASP:C	2.57	0.47
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.45	0.47
2:b:489:GLU:HB3	2:b:495:PHE:CD2	2.51	0.46
13:o:84:GLU:OE2	13:o:86:LYS:HD2	2.16	0.46
1:A:133:LEU:HD23	4:D:256:ILE:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:GLN:HG3	36:A:506:HOH:O	2.16	0.46
2:B:433:ASP:OD1	2:B:433:ASP:C	2.57	0.46
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.98	0.46
13:O:84:GLU:OE2	13:O:86:LYS:HD2	2.15	0.46
36:b:931:HOH:O	7:h:65:LEU:HD22	2.15	0.46
3:C:62:PHE:C	3:C:62:PHE:CD1	2.93	0.46
27:a:412:SQD:H312	28:a:413:DGD:HAG2	1.96	0.46
34:e:105:HEM:HBC2	34:e:105:HEM:HMC1	1.97	0.46
1:A:249:VAL:HG12	2:B:491:VAL:HG21	1.97	0.46
2:B:63:LEU:N	2:B:64:PRO:HD2	2.30	0.46
5:E:77:GLU:O	5:E:81:GLU:HG2	2.16	0.46
1:a:161:TYR:HB3	1:a:162:PRO:HD3	1.96	0.46
4:d:12:ARG:HB2	4:d:17:ILE:HD11	1.96	0.46
4:d:61:HIS:HE1	4:d:80:THR:O	1.98	0.46
15:U:76:ARG:HA	15:U:79:LEU:HG	1.97	0.46
1:a:344:ALA:HB3	36:a:507:HOH:O	2.15	0.46
2:b:63:LEU:N	2:b:64:PRO:HD2	2.30	0.46
2:b:80:ILE:HD12	2:b:81:THR:N	2.31	0.46
4:D:186:GLN:HB2	22:D:404:CLA:HBC1	1.98	0.46
3:c:109:PHE:HB2	26:c:524:LMG:HC3	1.98	0.46
1:A:102:LEU:HB2	28:A:413:DGD:O4D	2.16	0.46
22:B:613:CLA:HBB1	22:B:613:CLA:HMB1	1.96	0.46
3:C:223:TRP:CG	3:C:224:ILE:H	2.32	0.46
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.46	0.46
2:b:12:LEU:HB2	22:b:613:CLA:HMC2	1.98	0.46
3:C:163:PHE:CD1	3:C:252:ILE:HD11	2.51	0.46
13:O:69:LYS:NZ	13:O:70:LEU:O	2.27	0.46
3:c:94:THR:HG22	22:c:501:CLA:HED1	1.98	0.46
5:e:14:ILE:HD11	9:j:10:LEU:HD11	1.97	0.46
5:e:81:GLU:OE1	5:e:81:GLU:HA	2.15	0.46
2:B:80:ILE:HD12	2:B:81:THR:N	2.31	0.46
5:E:14:ILE:HD11	9:J:10:LEU:HD11	1.97	0.46
3:c:163:PHE:CD1	3:c:252:ILE:HD11	2.51	0.46
36:c:695:HOH:O	32:j:102:LMT:H2'	2.16	0.46
2:B:414:PRO:HB2	2:B:415:PRO:HD3	1.98	0.46
2:b:414:PRO:HB2	2:b:415:PRO:HD3	1.98	0.46
4:d:186:GLN:HB2	22:d:404:CLA:HBC1	1.97	0.46
23:k:101:BCR:H24C	23:k:101:BCR:H371	1.80	0.46
13:o:29:ALA:HB1	13:o:135:SER:OG	2.15	0.46
13:o:33:ASP:OD1	13:o:33:ASP:O	2.34	0.46
13:o:33:ASP:C	13:o:35:SER:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:LEU:HB2	22:B:612:CLA:HMC2	1.98	0.45
27:a:411:SQD:H341	10:k:37:PHE:CE1	2.51	0.45
16:V:6:GLU:H	16:V:6:GLU:CD	2.24	0.45
19:z:61:VAL:O	19:z:62:VAL:CG1	2.56	0.45
5:e:77:GLU:O	5:e:81:GLU:HG2	2.17	0.45
1:A:344:ALA:HB3	36:A:507:HOH:O	2.15	0.45
28:A:413:DGD:HBH1	22:b:607:CLA:H121	1.99	0.45
3:C:94:THR:HG22	22:C:501:CLA:HED1	1.98	0.45
3:C:109:PHE:HB2	26:C:524:LMG:HC3	1.97	0.45
36:C:694:HOH:O	32:J:102:LMT:H2'	2.16	0.45
12:M:16[B]:LEU:O	12:M:20:VAL:HG22	2.17	0.45
1:a:165:GLN:HG3	36:a:506:HOH:O	2.16	0.45
2:b:446:SER:HB2	2:b:447:PRO:HD2	1.99	0.45
13:o:91:GLY:HA3	13:o:132:ASN:HA	1.99	0.45
2:B:495:PHE:CZ	2:B:505:ARG:CZ	3.00	0.45
13:O:33:ASP:C	13:O:35:SER:H	2.25	0.45
1:a:46:ILE:HD13	28:a:413:DGD:HAT2	1.98	0.45
1:a:153:SER:HB2	22:a:404:CLA:H43	1.98	0.45
27:A:411:SQD:H341	10:K:37:PHE:CE1	2.51	0.45
13:O:53:LYS:NZ	13:O:232:GLU:OE1	2.40	0.45
1:a:102:LEU:HB2	28:a:413:DGD:O4D	2.16	0.45
3:c:338:GLY:HA3	3:c:341:LEU:O	2.17	0.45
3:c:363:GLY:O	3:c:367:GLU:HG2	2.17	0.45
16:v:6:GLU:CD	16:v:6:GLU:H	2.24	0.45
2:B:76:SER:HB3	28:a:413:DGD:HE4	1.98	0.45
3:C:363:GLY:O	3:C:367:GLU:HG2	2.17	0.45
13:O:33:ASP:OD1	13:O:33:ASP:O	2.34	0.45
3:c:79:LYS:HG3	3:c:80:PRO:HD2	1.99	0.45
3:c:367:GLU:N	3:c:368:PRO:CD	2.80	0.45
6:f:28:VAL:HB	6:f:29:PRO:HD3	1.98	0.45
12:m:16[B]:LEU:O	12:m:20:VAL:HG22	2.17	0.45
3:C:339:LYS:NZ	36:C:605:HOH:O	2.46	0.45
13:o:19[A]:CYS:HB3	13:o:44:CYS:SG	2.57	0.45
3:C:367:GLU:N	3:C:368:PRO:CD	2.80	0.45
1:a:131:TRP:CE3	1:a:132:GLU:HA	2.52	0.45
2:b:138:MET:HE3	22:b:616:CLA:CHD	2.47	0.45
3:c:167:VAL:HG22	22:c:512:CLA:H152	1.99	0.45
13:o:199:LEU:HD23	13:o:215:PHE:HB2	1.99	0.45
2:B:489:GLU:HB3	2:B:495:PHE:CD2	2.51	0.44
23:B:617:BCR:H24C	23:B:617:BCR:H371	1.84	0.44
18:Y:21:GLN:O	18:Y:25:ILE:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:495:PHE:CZ	2:b:505:ARG:CZ	3.00	0.44
4:d:160:TYR:HA	4:d:290:ALA:HB2	1.99	0.44
1:A:131:TRP:CE3	1:A:132:GLU:HA	2.52	0.44
19:Z:33:TRP:HZ2	32:Z:101:LMT:O3'	1.98	0.44
2:b:348:ASN:HB3	2:b:354:LEU:HD11	1.99	0.44
22:b:602:CLA:HHC	22:b:602:CLA:HBB1	1.99	0.44
22:B:606:CLA:C2D	25:B:621:STE:H41	2.48	0.44
36:B:717:HOH:O	26:D:402:LMG:HC91	2.18	0.44
3:C:79:LYS:HG3	3:C:80:PRO:HD2	1.99	0.44
3:C:338:GLY:HA3	3:C:341:LEU:O	2.17	0.44
3:c:406:SER:HA	3:c:420:VAL:HG23	1.99	0.44
4:d:49:LEU:HD13	23:d:406:BCR:C15	2.48	0.44
13:o:79:ASP:OD1	13:o:80:GLN:N	2.48	0.44
28:A:413:DGD:HBE2	22:b:607:CLA:H121	1.99	0.44
13:O:19[A]:CYS:HB3	13:O:44:CYS:SG	2.57	0.44
27:A:412:SQD:H322	25:A:415:STE:C8	2.48	0.44
1:a:16:ARG:HB3	25:a:416:STE:H152	2.00	0.44
23:h:102:BCR:H20C	23:h:102:BCR:H361	1.83	0.44
30:A:418:PHO:HBB1	30:A:418:PHO:HMB3	2.00	0.44
13:O:199:LEU:HD23	13:O:215:PHE:HB2	2.00	0.44
22:b:615:CLA:H162	23:b:618:BCR:H353	2.00	0.44
1:A:162:PRO:HB3	1:A:168:PHE:HA	2.00	0.44
13:O:29:ALA:HB1	13:O:135:SER:OG	2.18	0.44
13:O:91:GLY:HA3	13:O:132:ASN:HA	1.99	0.44
18:Y:27:MET:HE3	18:Y:27:MET:CA	2.47	0.44
22:b:609:CLA:C17	22:b:610:CLA:H192	2.48	0.44
13:O:19[A]:CYS:CB	13:O:44:CYS:SG	3.05	0.44
36:b:718:HOH:O	26:d:402:LMG:HC91	2.17	0.44
13:o:19[A]:CYS:CB	13:o:44:CYS:SG	3.06	0.44
3:C:202:PRO:O	3:C:204:LEU:HD22	2.18	0.44
13:O:207:ARG:N	13:O:207:ARG:CD	2.81	0.44
27:a:411:SQD:H271	31:d:410:LHG:H152	2.00	0.44
2:b:461:LEU:HD22	31:d:411:LHG:H312	1.99	0.44
22:b:607:CLA:C2D	25:b:622:STE:H41	2.48	0.44
9:j:30:TYR:CZ	25:j:101:STE:H51	2.53	0.44
16:v:45:ILE:HD12	16:v:45:ILE:O	2.18	0.44
2:B:476:ARG:HD3	36:B:708:HOH:O	2.18	0.43
22:B:601:CLA:HHC	22:B:601:CLA:HBB1	1.99	0.43
3:C:406:SER:HA	3:C:420:VAL:HG23	1.99	0.43
16:V:45:ILE:HD12	16:V:45:ILE:O	2.18	0.43
2:b:54:PRO:HD2	2:b:57:ARG:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:70:GLY:HA2	2:b:178:VAL:HG21	2.00	0.43
18:y:42:ARG:O	18:y:42:ARG:HG2	2.18	0.43
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.99	0.43
18:Y:42:ARG:O	18:Y:42:ARG:HG2	2.18	0.43
1:a:307:ILE:HD13	1:a:313:VAL:HA	2.00	0.43
3:c:202:PRO:O	3:c:204:LEU:HD22	2.17	0.43
13:o:41:ALA:O	13:o:82:GLN:HG2	2.18	0.43
18:y:34:MET:SD	18:y:38:LEU:HG	2.58	0.43
2:B:138:MET:HE3	22:B:615:CLA:CHD	2.47	0.43
27:B:620:SQD:H172	27:B:620:SQD:H371	2.00	0.43
7:H:6:TRP:CE2	7:H:10:ILE:HD11	2.53	0.43
10:K:17:ILE:HG23	10:K:18:PHE:CD2	2.54	0.43
14:T:2:GLU:HG2	14:T:3:THR:N	2.33	0.43
16:V:28:GLU:OE2	16:V:31:ARG:NH2	2.41	0.43
18:Y:34:MET:SD	18:Y:38:LEU:HG	2.58	0.43
14:t:2:GLU:HG2	14:t:3:THR:N	2.33	0.43
18:y:27:MET:HA	18:y:30:ILE:HG22	2.00	0.43
1:A:16:ARG:HB3	25:A:416:STE:H152	2.00	0.43
3:C:128:GLY:HA3	22:C:513:CLA:C3C	2.49	0.43
4:D:160:TYR:HA	4:D:290:ALA:HB2	1.99	0.43
23:T:101:BCR:HC7	23:T:101:BCR:H331	1.87	0.43
23:B:619:BCR:H24C	23:B:619:BCR:H371	1.87	0.43
4:D:49:LEU:HD13	23:D:406:BCR:C15	2.48	0.43
3:c:62:PHE:HB2	3:c:122:SER:HB2	2.01	0.43
3:c:128:GLY:HA3	22:c:513:CLA:C3C	2.49	0.43
8:i:37:LEU:O	8:i:38:GLU:CB	2.66	0.43
2:B:348:ASN:HB3	2:B:354:LEU:HD11	1.99	0.43
1:a:153:SER:CB	22:a:404:CLA:H43	2.49	0.43
3:c:135:ARG:NH1	19:z:27:TYR:O	2.47	0.43
22:c:508:CLA:C9	31:d:410:LHG:H161	2.48	0.43
4:d:86:GLY:O	4:d:166:SER:HB2	2.19	0.43
7:h:6:TRP:CE2	7:h:10:ILE:HD11	2.53	0.43
1:A:132:GLU:O	1:A:136:ARG:HG2	2.18	0.43
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.99	0.43
1:A:114:LEU:C	1:A:114:LEU:HD23	2.44	0.43
23:B:618:BCR:H282	28:a:413:DGD:CHA	2.49	0.43
3:C:62:PHE:HB2	3:C:122:SER:HB2	2.01	0.43
5:E:3:GLY:N	36:E:204:HOH:O	2.52	0.43
2:b:495:PHE:CZ	2:b:505:ARG:NH1	2.87	0.43
32:e:104:LMT:H121	9:j:24:ILE:HD11	2.01	0.43
13:o:57:LYS:O	13:o:57:LYS:CG	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:461:LEU:HD22	31:D:411:LHG:H312	2.00	0.43
4:D:86:GLY:O	4:D:166:SER:HB2	2.19	0.43
26:H:101:LMG:C7	26:H:101:LMG:O9	2.67	0.43
2:b:476:ARG:HD3	36:b:708:HOH:O	2.18	0.43
23:d:406:BCR:H15C	23:d:406:BCR:H351	1.91	0.43
22:B:608:CLA:C17	22:B:609:CLA:H192	2.48	0.43
3:C:62:PHE:HE2	23:K:103:BCR:H331	1.84	0.43
1:a:104:GLU:HB2	36:o:313:HOH:O	2.19	0.43
1:a:132:GLU:O	1:a:136:ARG:HG2	2.18	0.43
2:b:67:ALA:HA	2:b:71:VAL:O	2.19	0.43
22:c:509:CLA:HBB1	22:c:509:CLA:HMB3	2.00	0.43
1:A:153:SER:CB	22:A:404:CLA:H43	2.49	0.42
28:A:413:DGD:HE4	2:b:76:SER:HB3	2.01	0.42
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.00	0.42
22:C:509:CLA:HBB1	22:C:509:CLA:HMB3	2.00	0.42
23:C:514:BCR:H20C	23:C:514:BCR:H361	1.90	0.42
18:Y:31:ALA:O	18:Y:34:MET:HB3	2.19	0.42
22:a:405:CLA:HBB1	22:a:405:CLA:HMB1	2.01	0.42
27:a:412:SQD:H142	23:t:102:BCR:HC41	2.00	0.42
2:b:76:SER:OG	2:b:78:TRP:CD1	2.71	0.42
27:b:621:SQD:H112	27:b:621:SQD:H272	2.01	0.42
22:c:511:CLA:HBB1	22:c:511:CLA:HMB3	2.01	0.42
26:d:408:LMG:H211	26:d:408:LMG:H172	2.01	0.42
10:k:17:ILE:HG23	10:k:18:PHE:CD2	2.54	0.42
13:o:17:ASN:ND2	36:o:304:HOH:O	2.52	0.42
1:A:131:TRP:CE3	1:A:132:GLU:CA	3.03	0.42
2:B:495:PHE:CZ	2:B:505:ARG:NH1	2.87	0.42
3:C:109:PHE:CB	26:C:524:LMG:HC3	2.50	0.42
9:J:30:TYR:CZ	25:J:101:STE:H51	2.53	0.42
18:Y:27:MET:SD	18:Y:27:MET:N	2.92	0.42
1:a:114:LEU:C	1:a:114:LEU:HD23	2.44	0.42
3:c:109:PHE:CB	26:c:524:LMG:HC3	2.49	0.42
1:A:307:ILE:HD13	1:A:313:VAL:HA	2.00	0.42
23:A:407:BCR:H20C	23:A:407:BCR:H361	1.88	0.42
22:B:612:CLA:HBB1	22:B:612:CLA:HMB1	2.01	0.42
13:O:17:ASN:ND2	36:O:305:HOH:O	2.51	0.42
23:h:102:BCR:H331	23:h:102:BCR:HC8	2.00	0.42
1:a:162:PRO:HB3	1:a:168:PHE:HA	2.00	0.42
26:h:101:LMG:C7	26:h:101:LMG:O9	2.67	0.42
26:h:101:LMG:O9	26:h:101:LMG:HC72	2.19	0.42
16:v:95:LEU:HD11	16:v:112:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ASN:OD1	1:A:301:ASN:C	2.63	0.42
1:A:331:MET:SD	4:D:347:PRO:HB2	2.60	0.42
22:C:510:CLA:H191	10:K:30:VAL:HG22	2.02	0.42
26:H:101:LMG:C40	26:H:101:LMG:H362	2.49	0.42
13:O:57:LYS:O	13:O:57:LYS:CG	2.67	0.42
2:b:75:TRP:HA	36:b:716:HOH:O	2.20	0.42
4:d:78:VAL:HG11	4:d:114:ILE:HD12	2.02	0.42
1:A:101:SER:OG	13:O:69:LYS:HE3	2.20	0.42
1:A:102:LEU:HD12	28:A:413:DGD:O3G	2.20	0.42
2:B:486[B]:LEU:HD23	2:B:487:SER:O	2.19	0.42
23:B:617:BCR:H15C	23:B:617:BCR:H351	1.91	0.42
3:C:38:GLY:HA3	22:C:511:CLA:CMD	2.49	0.42
22:C:511:CLA:HBB1	22:C:511:CLA:HMB3	2.01	0.42
1:a:218:LEU:HD12	24:a:408:PL9:C4	2.50	0.42
2:b:486[B]:LEU:HD23	2:b:487:SER:O	2.19	0.42
3:c:59:LEU:HD21	23:k:101:BCR:H372	2.01	0.42
22:c:513:CLA:OBD	32:z:101:LMT:H6E	2.19	0.42
23:c:514:BCR:H24C	23:c:514:BCR:H371	1.85	0.42
4:d:12:ARG:NH2	4:d:16:ASP:HB3	2.35	0.42
23:t:102:BCR:C23	23:t:102:BCR:C38	2.98	0.42
26:C:524:LMG:HC92	26:C:524:LMG:H111	2.02	0.42
5:E:28:PRO:O	5:E:32:ILE:HG12	2.20	0.42
26:H:101:LMG:O9	26:H:101:LMG:HC72	2.19	0.42
23:H:102:BCR:C8	23:H:102:BCR:C33	2.92	0.42
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.55	0.42
24:a:408:PL9:C15	31:a:420:LHG:H311	2.49	0.42
22:c:510:CLA:H191	10:k:30:VAL:HG22	2.02	0.42
10:k:40:GLN:HA	10:k:43:VAL:HG22	2.02	0.42
2:B:67:ALA:HA	2:B:71:VAL:O	2.19	0.42
23:B:618:BCR:H331	23:B:618:BCR:HC8	2.00	0.42
3:C:135:ARG:NH1	19:Z:27:TYR:O	2.47	0.42
22:C:513:CLA:OBD	32:Z:101:LMT:H6E	2.19	0.42
23:D:406:BCR:H24C	23:D:406:BCR:H371	1.89	0.42
7:H:41:CYS:SG	23:H:102:BCR:C15	3.08	0.42
5:e:3:GLY:N	36:e:204:HOH:O	2.52	0.42
22:A:405:CLA:H112	22:D:404:CLA:H172	2.02	0.42
32:E:104:LMT:H121	9:J:24:ILE:HD11	2.01	0.42
19:Z:61:VAL:O	19:Z:62:VAL:CG1	2.57	0.42
1:a:106:LEU:CD1	28:a:413:DGD:HE1	2.50	0.42
5:e:28:PRO:O	5:e:32:ILE:HG12	2.20	0.42
26:h:101:LMG:C40	26:h:101:LMG:H362	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.55	0.42
26:D:408:LMG:H172	26:D:408:LMG:H211	2.01	0.42
13:O:22:LEU:HB2	13:O:203:LYS:HD2	2.02	0.42
1:a:131:TRP:CE3	1:a:132:GLU:CA	3.03	0.42
1:a:283:VAL:O	1:a:286:THR:HG22	2.20	0.42
1:a:301:ASN:OD1	1:a:301:ASN:C	2.63	0.42
23:b:618:BCR:H20C	23:b:618:BCR:H361	1.94	0.42
16:v:122:GLU:N	16:v:123:PRO:HD2	2.35	0.42
3:C:203:THR:O	3:C:235:GLY:HA3	2.20	0.41
23:C:515:BCR:H20C	23:C:515:BCR:H361	1.87	0.41
1:a:102:LEU:HD12	28:a:413:DGD:O3G	2.20	0.41
1:a:308:ASP:OD1	1:a:308:ASP:C	2.63	0.41
1:A:210:LEU:C	1:A:210:LEU:HD23	2.45	0.41
25:B:622:STE:O2	25:B:622:STE:C4	2.68	0.41
3:C:59:LEU:HD21	23:K:101:BCR:H372	2.01	0.41
4:D:78:VAL:HG11	4:D:114:ILE:HD12	2.02	0.41
23:T:101:BCR:H382	23:T:101:BCR:C23	2.50	0.41
16:V:122:GLU:N	16:V:123:PRO:HD2	2.35	0.41
3:c:38:GLY:HA3	22:c:511:CLA:CMD	2.49	0.41
1:A:106:LEU:CD1	28:A:413:DGD:HE1	2.50	0.41
23:a:407:BCR:H352	27:a:412:SQD:H362	2.02	0.41
23:b:619:BCR:H331	23:b:619:BCR:HC8	2.00	0.41
10:k:14:ALA:HB2	19:z:62:VAL:CG2	2.49	0.41
2:B:433:ASP:OD2	2:B:436:THR:OG1	2.39	0.41
3:C:227:VAL:O	3:C:227:VAL:HG13	2.20	0.41
8:I:37:LEU:O	8:I:38:GLU:CB	2.67	0.41
12:M:6:LEU:HD11	25:t:101:STE:H42	2.03	0.41
23:d:406:BCR:C8	23:d:406:BCR:H331	2.50	0.41
31:d:409:LHG:H282	14:t:17:PHE:CD1	2.55	0.41
16:v:28:GLU:OE2	16:v:31:ARG:NH2	2.41	0.41
2:B:76:SER:OG	2:B:78:TRP:CD1	2.73	0.41
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.56	0.41
4:D:272:LEU:C	4:D:272:LEU:CD2	2.94	0.41
1:a:331:MET:SD	4:d:347:PRO:HB2	2.60	0.41
2:b:171:PRO:HA	7:h:65:LEU:HD12	2.02	0.41
3:c:223:TRP:CE3	3:c:224:ILE:HG12	2.56	0.41
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.89	0.41
1:A:104:GLU:HB2	36:O:313:HOH:O	2.19	0.41
1:A:218:LEU:HD12	24:A:408:PL9:C4	2.50	0.41
23:A:407:BCR:H371	23:A:407:BCR:H24C	1.85	0.41
24:A:408:PL9:H501	27:X:101:SQD:C35	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:TRP:HA	36:B:716:HOH:O	2.20	0.41
3:C:275:SER:HB3	22:C:509:CLA:HED3	2.02	0.41
13:O:69:LYS:HD3	13:O:70:LEU:N	2.36	0.41
2:b:314:TYR:CE2	2:b:316:GLY:HA3	2.56	0.41
3:c:227:VAL:O	3:c:227:VAL:HG13	2.20	0.41
35:v:201:HEC:CMB	35:v:201:HEC:HBB3	2.51	0.41
1:A:131:TRP:CH2	22:C:505:CLA:HAA2	2.56	0.41
4:D:12:ARG:NH2	4:D:16:ASP:HB3	2.35	0.41
22:D:405:CLA:H61	17:X:14:LEU:HD12	2.03	0.41
16:V:95:LEU:HD11	16:V:112:LEU:HD11	2.02	0.41
25:a:415:STE:H162	25:a:415:STE:H132	1.82	0.41
3:c:62:PHE:HE2	23:k:103:BCR:H331	1.84	0.41
3:c:275:SER:HB3	22:c:509:CLA:HED3	2.02	0.41
23:t:102:BCR:H351	23:t:102:BCR:H15C	1.96	0.41
15:u:56:GLU:OE1	15:u:56:GLU:N	2.46	0.41
1:A:283:VAL:O	1:A:286:THR:HG22	2.20	0.41
27:B:620:SQD:H362	23:t:102:BCR:H362	2.03	0.41
1:a:210:LEU:C	1:a:210:LEU:HD23	2.45	0.41
23:c:515:BCR:H15C	23:c:515:BCR:H351	1.87	0.41
1:A:221[A]:SER:HA	4:D:139:ARG:HB2	2.03	0.41
1:A:308:ASP:C	1:A:308:ASP:OD1	2.63	0.41
22:B:614:CLA:H112	22:B:614:CLA:H152	1.93	0.41
3:C:95:LEU:HD21	22:C:501:CLA:OBD	2.21	0.41
23:C:515:BCR:H15C	23:C:515:BCR:H351	1.87	0.41
23:C:515:BCR:H24C	23:C:515:BCR:H371	1.84	0.41
31:D:409:LHG:H282	14:T:17:PHE:CD1	2.55	0.41
10:K:40:GLN:HA	10:K:43:VAL:HG22	2.02	0.41
13:O:41:ALA:O	13:O:82:GLN:HG2	2.21	0.41
13:O:158:ASP:OD1	13:O:158:ASP:C	2.64	0.41
1:a:210:LEU:HD23	1:a:214:MET:HG2	2.02	0.41
1:a:221[A]:SER:HA	4:d:139:ARG:HB2	2.03	0.41
2:b:141:ILE:HG21	22:b:616:CLA:HBB1	2.03	0.41
3:c:203:THR:O	3:c:235:GLY:HA3	2.20	0.41
23:c:515:BCR:H20C	23:c:515:BCR:H361	1.87	0.41
4:d:302:GLU:OE2	4:d:319:LEU:CD1	2.69	0.41
7:h:39:LEU:O	7:h:39:LEU:HD12	2.21	0.41
7:h:41:CYS:SG	23:h:102:BCR:C15	3.08	0.41
2:B:141:ILE:HG21	22:B:615:CLA:HBB1	2.03	0.41
22:B:601:CLA:H12	22:B:601:CLA:HBA2	1.92	0.41
4:D:302:GLU:OE2	4:D:319:LEU:CD1	2.69	0.41
7:H:39:LEU:O	7:H:39:LEU:HD12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:19:ASP:N	10:K:20:PRO:HD2	2.36	0.41
35:V:201:HEC:HBB3	35:V:201:HEC:CMB	2.51	0.41
2:b:90:PHE:CE2	22:b:607:CLA:H151	2.56	0.41
22:b:613:CLA:HBB1	22:b:613:CLA:HMB1	2.01	0.41
22:c:501:CLA:HHC	22:c:501:CLA:CBB	2.51	0.41
4:d:181:PHE:CZ	4:d:185:PHE:CE1	3.09	0.41
10:k:19:ASP:N	10:k:20:PRO:HD2	2.36	0.41
22:C:508:CLA:H203	28:C:518:DGD:HA92	2.02	0.40
22:C:513:CLA:H92	22:C:513:CLA:H62	1.87	0.40
23:T:101:BCR:C23	23:T:101:BCR:C38	2.98	0.40
23:c:514:BCR:H20C	23:c:514:BCR:H361	1.87	0.40
23:t:102:BCR:H11C	23:t:102:BCR:H341	1.97	0.40
3:C:400:PRO:C	3:C:401:LEU:HD12	2.46	0.40
22:C:501:CLA:CBB	22:C:501:CLA:HHC	2.51	0.40
23:D:406:BCR:C23	23:D:406:BCR:H403	2.52	0.40
15:U:56:GLU:OE1	15:U:56:GLU:N	2.46	0.40
3:c:400:PRO:C	3:c:401:LEU:HD12	2.46	0.40
22:c:508:CLA:H203	28:c:518:DGD:HA92	2.02	0.40
23:t:102:BCR:H382	23:t:102:BCR:C23	2.50	0.40
22:B:602:CLA:H43	7:H:45:ILE:HG22	2.03	0.40
23:D:406:BCR:C8	23:D:406:BCR:H331	2.50	0.40
1:a:14:TRP:CD1	25:a:421:STE:H42	2.56	0.40
24:a:408:PL9:H501	27:x:101:SQD:C35	2.51	0.40
3:c:339:LYS:NZ	36:c:605:HOH:O	2.46	0.40
4:d:38:PHE:N	4:d:39:PRO:HD2	2.37	0.40
27:A:411:SQD:H372	23:K:103:BCR:H392	2.04	0.40
4:D:181:PHE:CZ	4:D:185:PHE:CE1	3.09	0.40
24:a:408:PL9:H422	24:a:408:PL9:H401	1.97	0.40
22:b:603:CLA:H43	7:h:45:ILE:HG22	2.03	0.40
11:l:3:PRO:HB3	11:l:7:ARG:NH2	2.37	0.40
1:A:221[B]:SER:HA	4:D:139:ARG:HB2	2.04	0.40
1:A:265:PHE:CE1	31:A:420:LHG:H342	2.57	0.40
23:B:618:BCR:H15C	23:B:618:BCR:H351	1.87	0.40
4:D:236:ASN:O	4:D:239:GLN:HG2	2.22	0.40
1:a:131:TRP:CH2	22:c:505:CLA:HAA2	2.56	0.40
27:a:411:SQD:H292	25:k:102:STE:H183	2.04	0.40
15:u:36:ILE:O	15:u:36:ILE:HG22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	328 (98%)	7 (2%)	0	100	100
1	a	335/344 (97%)	328 (98%)	7 (2%)	0	100	100
2	B	506/510 (99%)	499 (99%)	7 (1%)	0	100	100
2	b	506/510 (99%)	499 (99%)	7 (1%)	0	100	100
3	C	451/461 (98%)	440 (98%)	10 (2%)	1 (0%)	43	31
3	c	451/461 (98%)	440 (98%)	10 (2%)	1 (0%)	43	31
4	D	339/352 (96%)	333 (98%)	6 (2%)	0	100	100
4	d	339/352 (96%)	333 (98%)	6 (2%)	0	100	100
5	E	80/84 (95%)	80 (100%)	0	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	65/66 (98%)	64 (98%)	1 (2%)	0	100	100
7	h	65/66 (98%)	64 (98%)	1 (2%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	34 (100%)	0	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	37/37 (100%)	37 (100%)	0	0	100	100
11	l	37/37 (100%)	37 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	33/36 (92%)	33 (100%)	0	0	100	100
13	O	244/272 (90%)	233 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	244/272 (90%)	235 (96%)	9 (4%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
15	u	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	V	135/163 (83%)	131 (97%)	4 (3%)	0	100	100
16	v	135/163 (83%)	131 (97%)	4 (3%)	0	100	100
17	X	36/41 (88%)	36 (100%)	0	0	100	100
17	x	36/41 (88%)	36 (100%)	0	0	100	100
18	Y	25/46 (54%)	25 (100%)	0	0	100	100
18	y	25/46 (54%)	24 (96%)	1 (4%)	0	100	100
19	Z	60/62 (97%)	60 (100%)	0	0	100	100
19	z	60/62 (97%)	60 (100%)	0	0	100	100
All	All	5212/5618 (93%)	5109 (98%)	101 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
3	c	416	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	272/280 (97%)	272 (100%)	0	100	100
1	a	272/280 (97%)	272 (100%)	0	100	100
2	B	406/407 (100%)	405 (100%)	1 (0%)	87	81
2	b	406/407 (100%)	405 (100%)	1 (0%)	87	81
3	C	354/362 (98%)	351 (99%)	3 (1%)	73	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	c	354/362 (98%)	351 (99%)	3 (1%)	73	61
4	D	276/283 (98%)	276 (100%)	0	100	100
4	d	276/283 (98%)	276 (100%)	0	100	100
5	E	71/73 (97%)	71 (100%)	0	100	100
5	e	71/73 (97%)	71 (100%)	0	100	100
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	28 (100%)	0	100	100
7	H	56/55 (102%)	56 (100%)	0	100	100
7	h	56/55 (102%)	56 (100%)	0	100	100
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	34 (100%)	0	100	100
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	6
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	37/35 (106%)	37 (100%)	0	100	100
11	l	37/35 (106%)	37 (100%)	0	100	100
12	M	30/32 (94%)	28 (93%)	2 (7%)	15	2
12	m	30/32 (94%)	28 (93%)	2 (7%)	15	2
13	O	207/228 (91%)	206 (100%)	1 (0%)	81	71
13	o	207/228 (91%)	206 (100%)	1 (0%)	81	71
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	84/112 (75%)	83 (99%)	1 (1%)	63	46
15	u	84/112 (75%)	83 (99%)	1 (1%)	63	46
16	V	117/138 (85%)	117 (100%)	0	100	100
16	v	117/138 (85%)	117 (100%)	0	100	100
17	X	31/34 (91%)	31 (100%)	0	100	100
17	x	31/34 (91%)	31 (100%)	0	100	100
18	Y	20/37 (54%)	19 (95%)	1 (5%)	22	4
18	y	20/37 (54%)	20 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	Z	52/52 (100%)	51 (98%)	1 (2%)	50	27
19	z	52/52 (100%)	51 (98%)	1 (2%)	50	27
All	All	4310/4588 (94%)	4290 (100%)	20 (0%)	81	71

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	80	ILE
3	C	204	LEU
3	C	289	PHE
3	C	315	MET
9	J	7	ARG
12	M	16[A]	LEU
12	M	16[B]	LEU
13	O	118	LEU
15	U	23	GLU
18	Y	27	MET
19	Z	62	VAL
2	b	80	ILE
3	c	204	LEU
3	c	289	PHE
3	c	315	MET
12	m	16[A]	LEU
12	m	16[B]	LEU
13	o	118	LEU
15	u	23	GLU
19	z	62	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
2	B	53	ASN
2	B	157	HIS
2	B	274	GLN
2	B	331	ASN
2	B	343	HIS
4	D	186	GLN
4	D	350	ASN
13	O	36	GLN

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Mol	Chain	Res	Type
13	O	155	ASN
15	U	78	ASN
16	V	86	GLN
17	X	38	GLN
19	Z	38	GLN
1	a	165	GLN
2	b	53	ASN
2	b	157	HIS
2	b	274	GLN
2	b	331	ASN
2	b	343	HIS
4	d	250	ASN
4	d	350	ASN
13	o	36	GLN
13	o	109	GLN
13	o	155	ASN
16	v	86	GLN
17	x	38	GLN
19	z	38	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	i	1	8	8,9,10	0.97	0	8,9,11	0.84	0
12	FME	m	1	12	8,9,10	0.95	0	8,9,11	0.74	0
8	FME	I	1	8	8,9,10	0.97	0	8,9,11	0.84	0
12	FME	M	1	12	8,9,10	0.96	0	8,9,11	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	FME	t	1	14	8,9,10	0.97	0	8,9,11	1.02	0
14	FME	T	1	14	8,9,10	0.97	0	8,9,11	1.02	0

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
8	FME	i	1	8	-	2/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
14	FME	t	1	14	-	0/7/9/11	-
14	FME	T	1	14	-	0/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O-C-CA-CB
8	i	1	FME	O-C-CA-CB
12	M	1	FME	CB-CA-N-CN
12	m	1	FME	CB-CA-N-CN
8	I	1	FME	CB-CG-SD-CE
8	i	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 212 ligands modelled in this entry, 6 are monoatomic - leaving 206 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
27	SQD	a	412	-	52,54,54	1.54	7 (13%)	62,65,65	1.29	6 (9%)
23	BCR	b	618	-	41,41,41	1.12	2 (4%)	56,56,56	1.20	6 (10%)
25	STE	B	621	-	16,16,19	0.59	0	16,16,19	1.09	0
25	STE	j	101	-	11,11,19	0.28	0	10,10,19	0.84	0
24	PL9	D	407	-	55,55,55	0.98	3 (5%)	68,69,69	1.44	11 (16%)
28	DGD	C	518	-	58,58,67	0.95	2 (3%)	72,72,81	1.30	5 (6%)
31	LHG	l	101	-	48,48,48	0.63	1 (2%)	51,54,54	1.22	5 (9%)
27	SQD	B	620	-	52,54,54	1.55	8 (15%)	62,65,65	1.34	6 (9%)
22	CLA	C	512	-	69,73,73	1.22	8 (11%)	82,113,113	1.26	6 (7%)
28	DGD	C	517	-	63,63,67	0.86	1 (1%)	77,77,81	1.33	7 (9%)
22	CLA	b	616	-	69,73,73	1.37	11 (15%)	82,113,113	1.23	4 (4%)
25	STE	b	601	-	11,11,19	0.29	0	10,10,19	0.79	0
26	LMG	H	101	-	38,38,55	0.53	0	40,40,63	1.33	2 (5%)
23	BCR	H	102	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	8 (14%)
25	STE	c	521	-	11,11,19	0.72	0	11,11,19	1.14	0
22	CLA	c	509	-	69,73,73	1.20	9 (13%)	82,113,113	1.33	6 (7%)
28	DGD	a	413	-	67,67,67	0.91	3 (4%)	81,81,81	1.35	12 (14%)
35	HEC	v	201	16	46,50,50	1.85	5 (10%)	58,82,82	1.95	4 (6%)
22	CLA	B	604	-	69,73,73	1.34	9 (13%)	82,113,113	1.37	7 (8%)
22	CLA	c	506	-	69,73,73	1.18	8 (11%)	82,113,113	1.23	5 (6%)
30	PHO	D	401	-	58,69,69	2.20	11 (18%)	55,99,99	1.33	6 (10%)
31	LHG	d	411	-	48,48,48	0.65	1 (2%)	51,54,54	1.23	6 (11%)
31	LHG	D	409	-	48,48,48	0.63	2 (4%)	51,54,54	1.18	5 (9%)
23	BCR	k	103	-	41,41,41	1.15	2 (4%)	56,56,56	1.15	4 (7%)
23	BCR	b	619	-	41,41,41	1.11	2 (4%)	56,56,56	1.12	4 (7%)
25	STE	d	412	-	19,19,19	0.56	0	19,19,19	1.01	0
25	STE	K	102	-	10,10,19	0.30	0	9,9,19	0.80	0
24	PL9	A	408	-	55,55,55	0.99	3 (5%)	68,69,69	1.50	11 (16%)
25	STE	C	522	-	7,7,19	0.30	0	6,6,19	0.72	0
22	CLA	A	405	36	64,68,73	1.21	8 (12%)	76,107,113	1.42	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	STE	A	416	-	10,10,19	0.30	0	9,9,19	0.78	0
22	CLA	a	419	36	69,73,73	1.15	8 (11%)	82,113,113	1.20	7 (8%)
22	CLA	c	512	-	69,73,73	1.21	8 (11%)	82,113,113	1.28	6 (7%)
25	STE	A	414	-	7,7,19	0.30	0	6,6,19	0.69	0
26	LMG	D	402	-	33,33,55	0.60	0	35,35,63	1.22	2 (5%)
32	LMT	j	102	-	24,24,36	1.04	3 (12%)	29,29,47	1.10	2 (6%)
25	STE	t	101	-	17,17,19	0.59	0	17,17,19	1.08	0
25	STE	E	101	-	11,11,19	0.70	0	11,11,19	1.14	0
22	CLA	C	505	-	69,73,73	1.32	9 (13%)	82,113,113	1.25	4 (4%)
32	LMT	C	523	-	24,24,36	1.11	4 (16%)	29,29,47	1.26	2 (6%)
27	SQD	A	411	-	50,52,54	1.55	7 (14%)	60,63,65	1.43	9 (15%)
23	BCR	B	619	-	41,41,41	1.08	2 (4%)	56,56,56	1.16	5 (8%)
30	PHO	d	401	-	58,69,69	2.21	11 (18%)	55,99,99	1.34	6 (10%)
32	LMT	b	624	-	25,25,36	0.99	2 (8%)	30,30,47	1.11	3 (10%)
24	PL9	d	407	-	55,55,55	0.98	3 (5%)	68,69,69	1.44	11 (16%)
28	DGD	H	103	-	63,63,67	0.94	2 (3%)	77,77,81	1.29	6 (7%)
25	STE	C	516	-	13,13,19	0.65	0	13,13,19	1.13	0
25	STE	a	409	-	8,8,19	0.31	0	7,7,19	0.74	0
23	BCR	K	101	-	41,41,41	1.10	3 (7%)	56,56,56	1.17	5 (8%)
22	CLA	B	605	-	69,73,73	1.31	8 (11%)	82,113,113	1.20	7 (8%)
22	CLA	b	603	-	69,73,73	1.21	9 (13%)	82,113,113	1.22	6 (7%)
22	CLA	b	611	36	69,73,73	1.20	9 (13%)	82,113,113	1.31	4 (4%)
22	CLA	B	609	-	69,73,73	1.34	10 (14%)	82,113,113	1.26	8 (9%)
22	CLA	a	406	-	58,62,73	1.43	7 (12%)	68,99,113	1.32	5 (7%)
22	CLA	b	617	-	64,68,73	1.38	7 (10%)	76,107,113	1.33	5 (6%)
23	BCR	D	406	-	41,41,41	1.12	2 (4%)	56,56,56	1.15	4 (7%)
29	OEX	a	417	1,3,36	0,15,15	-	-	-	-	-
25	STE	e	102	-	11,11,19	0.29	0	10,10,19	0.82	0
27	SQD	X	101	-	34,36,54	1.47	5 (14%)	42,45,65	1.50	7 (16%)
31	LHG	d	410	-	46,46,48	0.69	1 (2%)	49,52,54	1.20	4 (8%)
25	STE	E	103	-	19,19,19	0.56	0	19,19,19	1.06	0
25	STE	D	413	-	8,8,19	0.30	0	7,7,19	0.76	0
22	CLA	b	604	-	69,73,73	1.25	9 (13%)	82,113,113	1.12	5 (6%)
31	LHG	A	420	-	48,48,48	0.67	2 (4%)	51,54,54	1.30	7 (13%)
23	BCR	a	407	-	41,41,41	1.10	2 (4%)	56,56,56	1.12	3 (5%)
33	BCT	d	403	20	3,3,3	1.14	0	2,3,3	4.53	2 (100%)
22	CLA	D	405	-	69,73,73	1.37	10 (14%)	82,113,113	1.23	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMT	m	101	-	36,36,36	1.12	4 (11%)	47,47,47	0.98	2 (4%)
22	CLA	c	503	-	69,73,73	1.46	11 (15%)	82,113,113	1.15	5 (6%)
22	CLA	B	612	-	69,73,73	1.28	9 (13%)	82,113,113	1.33	5 (6%)
22	CLA	B	602	-	69,73,73	1.21	9 (13%)	82,113,113	1.22	6 (7%)
28	DGD	c	518	-	58,58,67	0.95	2 (3%)	72,72,81	1.30	5 (6%)
25	STE	b	623	-	11,11,19	0.69	0	11,11,19	1.21	1 (9%)
26	LMG	h	101	-	38,38,55	0.53	0	40,40,63	1.32	2 (5%)
23	BCR	C	515	-	41,41,41	1.11	2 (4%)	56,56,56	1.16	5 (8%)
24	PL9	a	408	-	55,55,55	0.98	3 (5%)	68,69,69	1.51	11 (16%)
27	SQD	b	621	-	47,49,54	1.63	8 (17%)	57,60,65	1.32	6 (10%)
25	STE	B	622	-	11,11,19	0.69	0	11,11,19	1.20	1 (9%)
26	LMG	d	408	-	51,51,55	0.78	1 (1%)	59,59,63	1.30	6 (10%)
25	STE	a	415	-	10,10,19	0.31	0	9,9,19	0.73	0
22	CLA	A	419	36	69,73,73	1.15	7 (10%)	82,113,113	1.20	7 (8%)
25	STE	k	102	-	10,10,19	0.30	0	9,9,19	0.79	0
22	CLA	B	616	-	64,68,73	1.38	7 (10%)	76,107,113	1.33	5 (6%)
22	CLA	c	510	-	69,73,73	1.18	8 (11%)	82,113,113	1.20	4 (4%)
23	BCR	c	515	-	41,41,41	1.11	2 (4%)	56,56,56	1.16	5 (8%)
22	CLA	b	613	-	69,73,73	1.29	9 (13%)	82,113,113	1.33	5 (6%)
22	CLA	B	607	36	69,73,73	1.18	7 (10%)	82,113,113	1.22	4 (4%)
22	CLA	D	404	-	69,73,73	1.35	9 (13%)	82,113,113	1.28	6 (7%)
26	LMG	c	524	-	50,50,55	0.74	1 (2%)	58,58,63	1.34	7 (12%)
34	HEM	E	105	6,5	50,50,50	1.48	7 (14%)	67,82,82	1.11	6 (8%)
22	CLA	c	513	-	69,73,73	1.15	8 (11%)	82,113,113	1.18	6 (7%)
22	CLA	b	610	-	69,73,73	1.33	10 (14%)	82,113,113	1.25	8 (9%)
22	CLA	c	504	36	63,67,73	1.22	8 (12%)	74,105,113	1.28	4 (5%)
22	CLA	C	501	-	69,73,73	1.16	8 (11%)	82,113,113	1.21	6 (7%)
22	CLA	b	615	-	69,73,73	1.18	8 (11%)	82,113,113	1.20	5 (6%)
23	BCR	h	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.21	7 (12%)
22	CLA	d	405	-	69,73,73	1.37	10 (14%)	82,113,113	1.24	5 (6%)
26	LMG	d	402	-	33,33,55	0.60	0	35,35,63	1.22	2 (5%)
28	DGD	h	103	-	63,63,67	0.94	2 (3%)	77,77,81	1.29	6 (7%)
25	STE	C	521	-	11,11,19	0.72	0	11,11,19	1.14	0
25	STE	c	516	-	13,13,19	0.65	0	13,13,19	1.13	0
22	CLA	B	613	-	69,73,73	1.32	10 (14%)	82,113,113	1.32	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	b	605	-	69,73,73	1.35	9 (13%)	82,113,113	1.37	7 (8%)
30	PHO	A	418	-	58,69,69	2.20	10 (17%)	55,99,99	1.32	5 (9%)
25	STE	T	102	-	14,14,19	0.29	0	13,13,19	0.82	0
22	CLA	C	503	-	69,73,73	1.46	11 (15%)	82,113,113	1.15	5 (6%)
25	STE	a	414	-	7,7,19	0.29	0	6,6,19	0.69	0
25	STE	d	413	-	8,8,19	0.31	0	7,7,19	0.76	0
23	BCR	A	407	-	41,41,41	1.10	2 (4%)	56,56,56	1.12	3 (5%)
32	LMT	J	102	-	24,24,36	1.03	3 (12%)	29,29,47	1.10	2 (6%)
34	HEM	e	105	6,5	50,50,50	1.48	6 (12%)	67,82,82	1.11	6 (8%)
26	LMG	D	408	-	51,51,55	0.78	1 (1%)	59,59,63	1.29	6 (10%)
28	DGD	A	413	-	67,67,67	0.92	2 (2%)	81,81,81	1.35	11 (13%)
23	BCR	B	618	-	41,41,41	1.12	2 (4%)	56,56,56	1.13	5 (8%)
22	CLA	B	615	-	69,73,73	1.38	11 (15%)	82,113,113	1.24	4 (4%)
25	STE	B	625	-	11,11,19	0.29	0	10,10,19	0.79	0
22	CLA	B	606	-	69,73,73	1.19	9 (13%)	82,113,113	1.26	4 (4%)
31	LHG	D	411	-	48,48,48	0.65	1 (2%)	51,54,54	1.23	6 (11%)
32	LMT	M	102	-	36,36,36	1.12	5 (13%)	47,47,47	0.98	2 (4%)
25	STE	a	421	-	11,11,19	0.70	0	11,11,19	1.16	0
22	CLA	b	608	36	69,73,73	1.17	7 (10%)	82,113,113	1.22	4 (4%)
26	LMG	B	624	-	51,51,55	0.72	1 (1%)	59,59,63	1.34	6 (10%)
25	STE	e	101	-	11,11,19	0.72	0	11,11,19	1.14	0
25	STE	m	102	-	9,9,19	0.28	0	8,8,19	0.84	0
26	LMG	a	410	-	48,48,55	0.79	1 (2%)	56,56,63	1.26	5 (8%)
32	LMT	e	104	-	24,24,36	1.01	2 (8%)	29,29,47	1.09	2 (6%)
22	CLA	B	611	-	69,73,73	1.34	9 (13%)	82,113,113	1.31	8 (9%)
22	CLA	A	404	-	69,73,73	1.33	7 (10%)	82,113,113	1.18	3 (3%)
22	CLA	C	509	-	69,73,73	1.20	9 (13%)	82,113,113	1.33	6 (7%)
25	STE	A	421	-	11,11,19	0.70	0	11,11,19	1.16	0
27	SQD	A	412	-	52,54,54	1.54	7 (13%)	62,65,65	1.29	6 (9%)
22	CLA	a	404	-	69,73,73	1.33	7 (10%)	82,113,113	1.18	3 (3%)
22	CLA	C	511	3	69,73,73	1.19	7 (10%)	82,113,113	1.27	5 (6%)
23	BCR	K	103	-	41,41,41	1.15	2 (4%)	56,56,56	1.16	3 (5%)
22	CLA	b	607	-	69,73,73	1.19	9 (13%)	82,113,113	1.26	4 (4%)
22	CLA	c	501	-	69,73,73	1.15	8 (11%)	82,113,113	1.21	6 (7%)
23	BCR	T	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.18	5 (8%)
32	LMT	z	101	-	36,36,36	1.17	6 (16%)	47,47,47	0.98	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	t	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.19	5 (8%)
25	STE	J	101	-	11,11,19	0.28	0	10,10,19	0.84	0
32	LMT	B	623	-	25,25,36	1.00	2 (8%)	30,30,47	1.11	3 (10%)
31	LHG	d	409	-	48,48,48	0.64	2 (4%)	51,54,54	1.18	5 (9%)
26	LMG	c	520	-	48,48,55	0.81	1 (2%)	56,56,63	1.31	6 (10%)
32	LMT	C	525	-	36,36,36	1.13	5 (13%)	47,47,47	0.92	2 (4%)
22	CLA	B	608	-	69,73,73	1.30	10 (14%)	82,113,113	1.22	5 (6%)
22	CLA	b	602	36	69,73,73	1.16	6 (8%)	82,113,113	1.19	6 (7%)
23	BCR	k	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.17	5 (8%)
31	LHG	a	420	-	48,48,48	0.67	2 (4%)	51,54,54	1.29	7 (13%)
30	PHO	a	418	-	58,69,69	2.19	10 (17%)	55,99,99	1.32	6 (10%)
27	SQD	x	101	-	34,36,54	1.47	5 (14%)	42,45,65	1.50	7 (16%)
31	LHG	D	410	-	46,46,48	0.68	1 (2%)	49,52,54	1.19	4 (8%)
25	STE	i	101	-	13,13,19	0.26	0	12,12,19	0.87	0
22	CLA	b	614	-	69,73,73	1.32	10 (14%)	82,113,113	1.32	7 (8%)
22	CLA	c	507	36	69,73,73	1.19	8 (11%)	82,113,113	1.27	6 (7%)
25	STE	A	415	-	10,10,19	0.31	0	9,9,19	0.74	0
23	BCR	C	514	-	41,41,41	1.13	2 (4%)	56,56,56	1.19	5 (8%)
22	CLA	B	614	-	69,73,73	1.19	8 (11%)	82,113,113	1.20	6 (7%)
22	CLA	C	502	-	69,73,73	1.26	10 (14%)	82,113,113	1.25	3 (3%)
22	CLA	C	508	-	69,73,73	1.30	10 (14%)	82,113,113	1.26	6 (7%)
26	LMG	C	524	-	50,50,55	0.74	1 (2%)	58,58,63	1.33	7 (12%)
22	CLA	c	505	-	69,73,73	1.32	9 (13%)	82,113,113	1.25	4 (4%)
32	LMT	Z	101	-	36,36,36	1.17	6 (16%)	47,47,47	0.98	1 (2%)
22	CLA	C	506	-	69,73,73	1.17	8 (11%)	82,113,113	1.23	5 (6%)
22	CLA	B	603	-	69,73,73	1.25	9 (13%)	82,113,113	1.12	5 (6%)
23	BCR	c	514	-	41,41,41	1.13	2 (4%)	56,56,56	1.19	5 (8%)
23	BCR	d	406	-	41,41,41	1.13	2 (4%)	56,56,56	1.14	4 (7%)
25	STE	c	522	-	7,7,19	0.30	0	6,6,19	0.72	0
35	HEC	V	201	16	46,50,50	1.85	5 (10%)	58,82,82	1.95	4 (6%)
22	CLA	C	504	36	63,67,73	1.22	8 (12%)	74,105,113	1.28	4 (5%)
26	LMG	A	410	-	48,48,55	0.79	1 (2%)	56,56,63	1.26	5 (8%)
25	STE	D	412	-	19,19,19	0.57	0	19,19,19	1.01	0
32	LMT	c	525	-	36,36,36	1.13	5 (13%)	47,47,47	0.92	2 (4%)
22	CLA	C	510	-	69,73,73	1.18	8 (11%)	82,113,113	1.20	4 (4%)
23	BCR	B	617	-	41,41,41	1.12	2 (4%)	56,56,56	1.19	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	BCT	D	403	20	3,3,3	1.14	0	2,3,3	4.52	2 (100%)
22	CLA	B	610	36	69,73,73	1.20	8 (11%)	82,113,113	1.31	4 (4%)
32	LMT	E	104	-	24,24,36	1.01	2 (8%)	29,29,47	1.08	2 (6%)
25	STE	E	102	-	11,11,19	0.29	0	10,10,19	0.83	0
25	STE	b	622	-	16,16,19	0.60	0	16,16,19	1.09	0
22	CLA	a	405	36	64,68,73	1.20	6 (9%)	76,107,113	1.35	6 (7%)
22	CLA	c	511	3	69,73,73	1.19	8 (11%)	82,113,113	1.26	5 (6%)
31	LHG	L	101	-	48,48,48	0.63	1 (2%)	51,54,54	1.21	5 (9%)
26	LMG	C	520	-	48,48,55	0.81	1 (2%)	56,56,63	1.30	6 (10%)
29	OEX	A	417	1,3,36	0,15,15	-	-	-	-	-
22	CLA	C	513	-	69,73,73	1.15	8 (11%)	82,113,113	1.18	6 (7%)
28	DGD	c	519	-	63,63,67	0.88	1 (1%)	77,77,81	1.26	5 (6%)
22	CLA	b	609	-	69,73,73	1.30	10 (14%)	82,113,113	1.22	5 (6%)
25	STE	a	416	-	10,10,19	0.30	0	9,9,19	0.77	0
25	STE	I	101	-	13,13,19	0.26	0	12,12,19	0.86	0
22	CLA	c	502	-	69,73,73	1.26	10 (14%)	82,113,113	1.25	3 (3%)
23	BCR	b	620	-	41,41,41	1.09	2 (4%)	56,56,56	1.16	6 (10%)
25	STE	e	103	-	19,19,19	0.57	0	19,19,19	1.06	0
22	CLA	d	404	-	69,73,73	1.35	9 (13%)	82,113,113	1.28	6 (7%)
22	CLA	b	606	-	69,73,73	1.31	8 (11%)	82,113,113	1.20	7 (8%)
22	CLA	C	507	36	69,73,73	1.19	8 (11%)	82,113,113	1.27	6 (7%)
22	CLA	c	508	-	69,73,73	1.30	10 (14%)	82,113,113	1.25	6 (7%)
22	CLA	b	612	-	69,73,73	1.34	9 (13%)	82,113,113	1.31	8 (9%)
25	STE	A	409	-	8,8,19	0.31	0	7,7,19	0.74	0
27	SQD	a	411	-	50,52,54	1.55	7 (14%)	60,63,65	1.43	9 (15%)
28	DGD	c	517	-	63,63,67	0.85	1 (1%)	77,77,81	1.33	7 (9%)
32	LMT	c	523	-	24,24,36	1.12	4 (16%)	29,29,47	1.29	2 (6%)
25	STE	M	101	-	9,9,19	0.28	0	8,8,19	0.84	0
28	DGD	C	519	-	63,63,67	0.88	1 (1%)	77,77,81	1.26	5 (6%)
22	CLA	B	601	36	69,73,73	1.16	8 (11%)	82,113,113	1.19	6 (7%)
26	LMG	b	625	-	51,51,55	0.72	1 (1%)	59,59,63	1.34	6 (10%)
22	CLA	A	406	-	58,62,73	1.44	7 (12%)	68,99,113	1.32	5 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	a	412	-	-	19/49/69/69	0/1/1/1
23	BCR	b	618	-	-	2/29/63/63	0/2/2/2
25	STE	B	621	-	-	5/14/14/17	-
25	STE	j	101	-	-	2/9/9/17	-
24	PL9	D	407	-	-	7/53/73/73	0/1/1/1
28	DGD	C	518	-	-	15/46/86/95	0/2/2/2
31	LHG	l	101	-	-	15/53/53/53	-
27	SQD	B	620	-	-	29/49/69/69	0/1/1/1
22	CLA	C	512	-	1/1/20/20	12/39/115/115	-
28	DGD	C	517	-	-	18/51/91/95	0/2/2/2
22	CLA	b	616	-	1/1/20/20	7/39/115/115	-
25	STE	b	601	-	-	3/9/9/17	-
26	LMG	H	101	-	-	18/40/40/70	-
23	BCR	H	102	-	-	8/29/63/63	0/2/2/2
25	STE	c	521	-	-	7/9/9/17	-
22	CLA	c	509	-	1/1/20/20	5/39/115/115	-
28	DGD	a	413	-	-	26/55/95/95	0/2/2/2
35	HEC	v	201	16	-	6/14/54/54	-
22	CLA	B	604	-	1/1/20/20	7/39/115/115	-
22	CLA	c	506	-	1/1/20/20	13/39/115/115	-
30	PHO	D	401	-	-	0/37/103/103	0/5/6/6
31	LHG	d	411	-	-	9/53/53/53	-
31	LHG	D	409	-	-	12/53/53/53	-
23	BCR	k	103	-	-	2/29/63/63	0/2/2/2
23	BCR	b	619	-	-	3/29/63/63	0/2/2/2
25	STE	d	412	-	-	6/17/17/17	-
25	STE	K	102	-	-	5/8/8/17	-
24	PL9	A	408	-	-	20/53/73/73	0/1/1/1
25	STE	C	522	-	-	1/5/5/17	-
22	CLA	A	405	36	1/1/19/20	6/33/109/115	-
25	STE	A	416	-	-	5/8/8/17	-
22	CLA	a	419	36	1/1/20/20	2/39/115/115	-
22	CLA	c	512	-	1/1/20/20	11/39/115/115	-
25	STE	A	414	-	-	1/5/5/17	-
26	LMG	D	402	-	-	8/35/35/70	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMT	j	102	-	-	10/15/35/61	0/1/1/2
25	STE	t	101	-	-	10/15/15/17	-
25	STE	E	101	-	-	4/9/9/17	-
22	CLA	C	505	-	1/1/20/20	5/39/115/115	-
32	LMT	C	523	-	-	2/15/35/61	0/1/1/2
27	SQD	A	411	-	-	18/47/67/69	0/1/1/1
23	BCR	B	619	-	-	1/29/63/63	0/2/2/2
30	PHO	d	401	-	-	0/37/103/103	0/5/6/6
32	LMT	b	624	-	-	6/17/37/61	0/1/1/2
24	PL9	d	407	-	-	7/53/73/73	0/1/1/1
28	DGD	H	103	-	-	14/51/91/95	0/2/2/2
25	STE	C	516	-	-	7/11/11/17	-
25	STE	a	409	-	-	5/6/6/17	-
23	BCR	K	101	-	-	0/29/63/63	0/2/2/2
22	CLA	B	605	-	-	7/39/115/115	-
22	CLA	b	603	-	1/1/20/20	2/39/115/115	-
22	CLA	b	611	36	1/1/20/20	0/39/115/115	-
22	CLA	a	406	-	1/1/17/20	5/26/102/115	-
22	CLA	b	617	-	1/1/19/20	8/33/109/115	-
22	CLA	B	609	-	-	5/39/115/115	-
23	BCR	D	406	-	-	3/29/63/63	0/2/2/2
25	STE	e	102	-	-	6/9/9/17	-
27	SQD	X	101	-	-	12/28/48/69	0/1/1/1
31	LHG	d	410	-	-	11/51/51/53	-
25	STE	E	103	-	-	8/17/17/17	-
25	STE	D	413	-	-	1/6/6/17	-
22	CLA	b	604	-	1/1/20/20	8/39/115/115	-
31	LHG	A	420	-	-	23/53/53/53	-
23	BCR	a	407	-	-	0/29/63/63	0/2/2/2
22	CLA	D	405	-	-	5/39/115/115	-
32	LMT	m	101	-	-	3/21/61/61	0/2/2/2
22	CLA	c	503	-	-	5/39/115/115	-
22	CLA	B	612	-	1/1/20/20	5/39/115/115	-
22	CLA	B	602	-	1/1/20/20	2/39/115/115	-
28	DGD	c	518	-	-	15/46/86/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	STE	b	623	-	-	5/9/9/17	-
26	LMG	h	101	-	-	17/40/40/70	-
23	BCR	C	515	-	-	0/29/63/63	0/2/2/2
24	PL9	a	408	-	-	20/53/73/73	0/1/1/1
27	SQD	b	621	-	-	21/44/64/69	0/1/1/1
25	STE	B	622	-	-	5/9/9/17	-
26	LMG	d	408	-	-	16/46/66/70	0/1/1/1
25	STE	a	415	-	-	5/8/8/17	-
22	CLA	A	419	36	1/1/20/20	2/39/115/115	-
25	STE	k	102	-	-	5/8/8/17	-
22	CLA	B	616	-	1/1/19/20	8/33/109/115	-
22	CLA	c	510	-	1/1/20/20	6/39/115/115	-
23	BCR	c	515	-	-	0/29/63/63	0/2/2/2
22	CLA	b	613	-	1/1/20/20	5/39/115/115	-
22	CLA	B	607	36	1/1/20/20	2/39/115/115	-
22	CLA	D	404	-	-	6/39/115/115	-
26	LMG	c	524	-	-	20/45/65/70	0/1/1/1
34	HEM	E	105	6,5	-	0/14/54/54	-
22	CLA	c	513	-	1/1/20/20	8/39/115/115	-
22	CLA	c	504	36	1/1/18/20	5/32/108/115	-
22	CLA	b	610	-	-	5/39/115/115	-
22	CLA	C	501	-	1/1/20/20	1/39/115/115	-
22	CLA	b	615	-	1/1/20/20	12/39/115/115	-
23	BCR	h	102	-	-	8/29/63/63	0/2/2/2
22	CLA	d	405	-	-	5/39/115/115	-
26	LMG	d	402	-	-	8/35/35/70	-
28	DGD	h	103	-	-	14/51/91/95	0/2/2/2
25	STE	C	521	-	-	7/9/9/17	-
25	STE	c	516	-	-	8/11/11/17	-
22	CLA	B	613	-	1/1/20/20	5/39/115/115	-
22	CLA	b	605	-	1/1/20/20	7/39/115/115	-
30	PHO	A	418	-	-	2/37/103/103	0/5/6/6
25	STE	T	102	-	-	5/12/12/17	-
22	CLA	C	503	-	-	5/39/115/115	-
25	STE	a	414	-	-	1/5/5/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	STE	d	413	-	-	1/6/6/17	-
23	BCR	A	407	-	-	0/29/63/63	0/2/2/2
32	LMT	J	102	-	-	10/15/35/61	0/1/1/2
34	HEM	e	105	6,5	-	0/14/54/54	-
26	LMG	D	408	-	-	16/46/66/70	0/1/1/1
28	DGD	A	413	-	-	28/55/95/95	0/2/2/2
23	BCR	B	618	-	-	1/29/63/63	0/2/2/2
22	CLA	B	615	-	1/1/20/20	7/39/115/115	-
25	STE	B	625	-	-	4/9/9/17	-
22	CLA	B	606	-	1/1/20/20	8/39/115/115	-
31	LHG	D	411	-	-	9/53/53/53	-
32	LMT	M	102	-	-	3/21/61/61	0/2/2/2
25	STE	a	421	-	-	5/9/9/17	-
22	CLA	b	608	36	1/1/20/20	2/39/115/115	-
26	LMG	B	624	-	-	17/46/66/70	0/1/1/1
25	STE	e	101	-	-	4/9/9/17	-
25	STE	m	102	-	-	3/7/7/17	-
26	LMG	a	410	-	-	25/43/63/70	0/1/1/1
32	LMT	e	104	-	-	9/15/35/61	0/1/1/2
22	CLA	B	611	-	1/1/20/20	3/39/115/115	-
22	CLA	A	404	-	1/1/20/20	2/39/115/115	-
22	CLA	C	509	-	1/1/20/20	5/39/115/115	-
25	STE	A	421	-	-	5/9/9/17	-
27	SQD	A	412	-	-	19/49/69/69	0/1/1/1
22	CLA	a	404	-	1/1/20/20	2/39/115/115	-
22	CLA	C	511	3	1/1/20/20	0/39/115/115	-
23	BCR	K	103	-	-	2/29/63/63	0/2/2/2
22	CLA	b	607	-	1/1/20/20	8/39/115/115	-
22	CLA	c	501	-	1/1/20/20	1/39/115/115	-
23	BCR	T	101	-	-	3/29/63/63	0/2/2/2
32	LMT	z	101	-	-	12/21/61/61	0/2/2/2
23	BCR	t	102	-	-	3/29/63/63	0/2/2/2
25	STE	J	101	-	-	2/9/9/17	-
32	LMT	B	623	-	-	6/17/37/61	0/1/1/2
31	LHG	d	409	-	-	12/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LMG	c	520	-	-	19/43/63/70	0/1/1/1
32	LMT	C	525	-	-	8/21/61/61	0/2/2/2
22	CLA	B	608	-	1/1/20/20	5/39/115/115	-
22	CLA	b	602	36	1/1/20/20	22/39/115/115	-
23	BCR	k	101	-	-	0/29/63/63	0/2/2/2
31	LHG	a	420	-	-	24/53/53/53	-
30	PHO	a	418	-	-	2/37/103/103	0/5/6/6
27	SQD	x	101	-	-	12/28/48/69	0/1/1/1
31	LHG	D	410	-	-	10/51/51/53	-
25	STE	i	101	-	-	6/11/11/17	-
22	CLA	b	614	-	1/1/20/20	5/39/115/115	-
22	CLA	c	507	36	1/1/20/20	8/39/115/115	-
25	STE	A	415	-	-	3/8/8/17	-
23	BCR	C	514	-	-	0/29/63/63	0/2/2/2
22	CLA	B	614	-	1/1/20/20	11/39/115/115	-
22	CLA	C	502	-	-	4/39/115/115	-
22	CLA	C	508	-	-	1/39/115/115	-
26	LMG	C	524	-	-	20/45/65/70	0/1/1/1
22	CLA	c	505	-	1/1/20/20	5/39/115/115	-
32	LMT	Z	101	-	-	12/21/61/61	0/2/2/2
22	CLA	C	506	-	1/1/20/20	13/39/115/115	-
22	CLA	B	603	-	1/1/20/20	8/39/115/115	-
23	BCR	c	514	-	-	0/29/63/63	0/2/2/2
23	BCR	d	406	-	-	3/29/63/63	0/2/2/2
25	STE	c	522	-	-	1/5/5/17	-
35	HEC	V	201	16	-	6/14/54/54	-
22	CLA	C	504	36	1/1/18/20	5/32/108/115	-
26	LMG	A	410	-	-	25/43/63/70	0/1/1/1
25	STE	D	412	-	-	6/17/17/17	-
32	LMT	c	525	-	-	8/21/61/61	0/2/2/2
22	CLA	C	510	-	1/1/20/20	6/39/115/115	-
23	BCR	B	617	-	-	2/29/63/63	0/2/2/2
22	CLA	B	610	36	1/1/20/20	0/39/115/115	-
32	LMT	E	104	-	-	9/15/35/61	0/1/1/2
25	STE	E	102	-	-	5/9/9/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	STE	b	622	-	-	5/14/14/17	-
22	CLA	a	405	36	1/1/19/20	2/33/109/115	-
22	CLA	c	511	3	1/1/20/20	0/39/115/115	-
31	LHG	L	101	-	-	15/53/53/53	-
26	LMG	C	520	-	-	19/43/63/70	0/1/1/1
22	CLA	C	513	-	1/1/20/20	9/39/115/115	-
28	DGD	c	519	-	-	15/51/91/95	0/2/2/2
22	CLA	b	609	-	1/1/20/20	5/39/115/115	-
25	STE	a	416	-	-	5/8/8/17	-
25	STE	I	101	-	-	6/11/11/17	-
22	CLA	c	502	-	-	4/39/115/115	-
23	BCR	b	620	-	-	1/29/63/63	0/2/2/2
25	STE	e	103	-	-	8/17/17/17	-
22	CLA	d	404	-	-	6/39/115/115	-
22	CLA	b	606	-	-	6/39/115/115	-
22	CLA	C	507	36	1/1/20/20	8/39/115/115	-
22	CLA	c	508	-	-	1/39/115/115	-
22	CLA	b	612	-	1/1/20/20	3/39/115/115	-
25	STE	A	409	-	-	5/6/6/17	-
27	SQD	a	411	-	-	18/47/67/69	0/1/1/1
28	DGD	c	517	-	-	18/51/91/95	0/2/2/2
32	LMT	c	523	-	-	2/15/35/61	0/1/1/2
25	STE	M	101	-	-	3/7/7/17	-
28	DGD	C	519	-	-	15/51/91/95	0/2/2/2
22	CLA	B	601	36	1/1/20/20	22/39/115/115	-
26	LMG	b	625	-	-	16/46/66/70	0/1/1/1
22	CLA	A	406	-	1/1/17/20	5/26/102/115	-

All (871) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	418	PHO	C1B-C2B	9.76	1.50	1.39
30	A	418	PHO	C1B-C2B	9.73	1.50	1.39
30	d	401	PHO	C1B-C2B	9.49	1.49	1.39
30	D	401	PHO	C1B-C2B	9.47	1.49	1.39
30	d	401	PHO	C3B-C4B	9.40	1.51	1.41
30	D	401	PHO	C3B-C4B	9.33	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	418	PHO	C3B-C4B	8.66	1.50	1.41
30	a	418	PHO	C3B-C4B	8.59	1.50	1.41
35	V	201	HEC	CAC-C3C	6.29	1.55	1.35
35	v	201	HEC	CAC-C3C	6.29	1.55	1.35
35	V	201	HEC	CAB-C3B	6.23	1.55	1.35
35	v	201	HEC	CAB-C3B	6.23	1.55	1.35
35	V	201	HEC	C3D-C2D	5.70	1.53	1.38
35	v	201	HEC	C3D-C2D	5.67	1.53	1.38
22	A	406	CLA	MG-NC	5.54	2.19	2.06
22	a	406	CLA	MG-NC	5.48	2.19	2.06
22	C	503	CLA	MG-NA	5.45	2.19	2.06
22	c	503	CLA	MG-NA	5.45	2.19	2.06
22	D	405	CLA	MG-NC	5.38	2.19	2.06
22	d	405	CLA	MG-NC	5.38	2.19	2.06
22	C	505	CLA	MG-NA	5.28	2.18	2.06
22	c	505	CLA	MG-NA	5.28	2.18	2.06
22	B	616	CLA	MG-NA	4.98	2.18	2.06
22	b	617	CLA	MG-NA	4.98	2.18	2.06
22	A	404	CLA	MG-NC	4.83	2.17	2.06
22	a	404	CLA	MG-NC	4.83	2.17	2.06
22	b	605	CLA	MG-NA	4.83	2.17	2.06
22	B	604	CLA	MG-NA	4.80	2.17	2.06
22	b	610	CLA	MG-NC	4.74	2.17	2.06
22	B	609	CLA	MG-NC	4.74	2.17	2.06
22	D	404	CLA	MG-NA	4.73	2.17	2.06
22	d	404	CLA	MG-NA	4.73	2.17	2.06
27	A	411	SQD	O48-C23	4.67	1.46	1.33
27	a	411	SQD	O48-C23	4.66	1.46	1.33
27	x	101	SQD	O48-C23	4.66	1.46	1.33
27	A	412	SQD	O48-C23	4.66	1.46	1.33
27	X	101	SQD	O48-C23	4.65	1.46	1.33
27	a	412	SQD	O48-C23	4.63	1.46	1.33
27	b	621	SQD	O48-C23	4.62	1.46	1.33
22	B	605	CLA	MG-NA	4.62	2.17	2.06
22	b	606	CLA	MG-NA	4.62	2.17	2.06
27	B	620	SQD	O48-C23	4.61	1.46	1.33
22	B	608	CLA	MG-NC	4.48	2.16	2.06
22	b	609	CLA	MG-NC	4.48	2.16	2.06
22	B	611	CLA	MG-NC	4.42	2.16	2.06
22	b	612	CLA	MG-NC	4.42	2.16	2.06
22	b	613	CLA	MG-NC	4.38	2.16	2.06
22	B	612	CLA	MG-NC	4.37	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	d	401	PHO	C1D-C2D	4.35	1.44	1.39
22	B	615	CLA	MG-NC	4.35	2.16	2.06
22	b	616	CLA	MG-NC	4.35	2.16	2.06
30	D	401	PHO	C1D-C2D	4.33	1.44	1.39
30	A	418	PHO	C1D-C2D	4.19	1.44	1.39
30	a	418	PHO	C1D-C2D	4.19	1.44	1.39
34	E	105	HEM	FE-ND	4.03	2.07	1.94
22	C	503	CLA	MG-NC	4.03	2.15	2.06
22	c	503	CLA	MG-NC	4.03	2.15	2.06
34	e	105	HEM	FE-ND	4.00	2.07	1.94
23	K	103	BCR	C1-C6	-3.87	1.48	1.53
22	B	613	CLA	MG-NA	3.87	2.15	2.06
23	k	103	BCR	C1-C6	-3.87	1.48	1.53
27	a	411	SQD	O47-C45	-3.86	1.37	1.46
23	H	102	BCR	C1-C6	-3.85	1.48	1.53
23	h	102	BCR	C1-C6	-3.85	1.48	1.53
23	B	617	BCR	C1-C6	-3.85	1.48	1.53
23	b	618	BCR	C1-C6	-3.85	1.48	1.53
27	A	411	SQD	O47-C45	-3.84	1.37	1.46
22	b	614	CLA	MG-NA	3.84	2.15	2.06
22	B	610	CLA	C1D-ND	3.81	1.42	1.37
27	a	412	SQD	O47-C45	-3.80	1.37	1.46
22	a	404	CLA	C1D-ND	3.77	1.42	1.37
22	C	508	CLA	MG-NC	3.76	2.15	2.06
22	A	404	CLA	C1D-ND	3.75	1.42	1.37
27	A	412	SQD	O47-C45	-3.75	1.37	1.46
22	B	604	CLA	C1D-ND	3.75	1.42	1.37
22	b	605	CLA	C1D-ND	3.75	1.42	1.37
22	b	611	CLA	C1D-ND	3.74	1.42	1.37
34	E	105	HEM	FE-NA	3.72	2.07	1.95
34	e	105	HEM	FE-NA	3.72	2.07	1.95
30	A	418	PHO	C4D-CHA	3.70	1.45	1.39
22	c	508	CLA	MG-NC	3.68	2.15	2.06
22	B	615	CLA	MG-NA	3.67	2.15	2.06
22	b	616	CLA	MG-NA	3.67	2.15	2.06
27	b	621	SQD	O47-C45	-3.66	1.38	1.46
30	a	418	PHO	C4D-CHA	3.65	1.45	1.39
23	d	406	BCR	C1-C6	-3.64	1.49	1.53
23	D	406	BCR	C1-C6	-3.64	1.49	1.53
23	c	514	BCR	C1-C6	-3.64	1.49	1.53
22	c	509	CLA	C1D-ND	3.63	1.42	1.37
22	d	404	CLA	C1D-ND	3.62	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	612	CLA	C1D-ND	3.61	1.42	1.37
22	b	613	CLA	C1D-ND	3.61	1.42	1.37
22	B	613	CLA	C1D-ND	3.61	1.42	1.37
22	b	614	CLA	C1D-ND	3.61	1.42	1.37
23	K	101	BCR	C1-C6	-3.60	1.49	1.53
22	C	509	CLA	C1D-ND	3.58	1.42	1.37
23	C	515	BCR	C1-C6	-3.57	1.49	1.53
23	c	515	BCR	C1-C6	-3.57	1.49	1.53
23	b	619	BCR	C30-C25	-3.56	1.49	1.53
23	C	514	BCR	C1-C6	-3.55	1.49	1.53
22	D	404	CLA	C1D-ND	3.55	1.42	1.37
22	C	510	CLA	C1D-ND	3.54	1.42	1.37
22	c	510	CLA	C1D-ND	3.54	1.42	1.37
22	C	506	CLA	C1D-ND	3.54	1.42	1.37
22	c	506	CLA	C1D-ND	3.54	1.42	1.37
22	B	602	CLA	C1D-ND	3.53	1.42	1.37
22	b	603	CLA	C1D-ND	3.53	1.42	1.37
22	A	405	CLA	C1D-ND	3.52	1.42	1.37
23	B	618	BCR	C30-C25	-3.52	1.49	1.53
22	B	616	CLA	C1D-ND	3.51	1.42	1.37
22	b	617	CLA	C1D-ND	3.51	1.42	1.37
22	B	609	CLA	C1D-ND	3.51	1.42	1.37
22	b	610	CLA	C1D-ND	3.51	1.42	1.37
23	k	101	BCR	C1-C6	-3.51	1.49	1.53
27	B	620	SQD	O47-C45	-3.51	1.38	1.46
22	c	502	CLA	C1D-ND	3.49	1.42	1.37
22	b	602	CLA	C1D-ND	3.46	1.42	1.37
22	C	502	CLA	C1D-ND	3.46	1.42	1.37
22	B	601	CLA	C1D-ND	3.46	1.42	1.37
22	B	605	CLA	C1D-ND	3.45	1.42	1.37
22	b	606	CLA	C1D-ND	3.45	1.42	1.37
22	C	505	CLA	C1D-ND	3.45	1.42	1.37
22	c	505	CLA	C1D-ND	3.45	1.42	1.37
23	A	407	BCR	C1-C6	-3.45	1.49	1.53
22	B	611	CLA	C1D-ND	3.45	1.42	1.37
22	b	612	CLA	C1D-ND	3.45	1.42	1.37
22	a	406	CLA	C1D-ND	3.45	1.42	1.37
22	A	406	CLA	C1D-ND	3.44	1.42	1.37
23	a	407	BCR	C1-C6	-3.44	1.49	1.53
22	b	614	CLA	MG-NC	3.43	2.14	2.06
22	B	615	CLA	C1D-ND	3.43	1.42	1.37
22	C	507	CLA	C1D-ND	3.42	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	507	CLA	C1D-ND	3.42	1.42	1.37
22	B	606	CLA	C1D-ND	3.42	1.42	1.37
22	B	608	CLA	C1D-ND	3.41	1.42	1.37
22	b	609	CLA	C1D-ND	3.41	1.42	1.37
22	C	504	CLA	C1D-ND	3.40	1.42	1.37
22	c	504	CLA	C1D-ND	3.40	1.42	1.37
22	b	607	CLA	C1D-ND	3.38	1.42	1.37
22	B	613	CLA	MG-NC	3.38	2.14	2.06
22	a	405	CLA	C1D-ND	3.38	1.42	1.37
27	b	621	SQD	O5-C1	3.37	1.50	1.41
22	B	603	CLA	C1D-ND	3.37	1.42	1.37
22	b	604	CLA	C1D-ND	3.37	1.42	1.37
22	B	607	CLA	C1D-ND	3.37	1.42	1.37
22	b	608	CLA	C1D-ND	3.37	1.42	1.37
34	e	105	HEM	FE-NB	3.36	2.05	1.94
23	b	619	BCR	C1-C6	-3.36	1.49	1.53
22	D	405	CLA	C1D-ND	3.36	1.42	1.37
22	b	616	CLA	C1D-ND	3.36	1.42	1.37
22	C	508	CLA	C1D-ND	3.36	1.42	1.37
22	c	508	CLA	C1D-ND	3.36	1.42	1.37
23	D	406	BCR	C30-C25	-3.35	1.49	1.53
23	d	406	BCR	C30-C25	-3.35	1.49	1.53
22	C	513	CLA	C1D-ND	3.35	1.42	1.37
22	c	513	CLA	C1D-ND	3.35	1.42	1.37
22	d	405	CLA	C1D-ND	3.35	1.42	1.37
23	B	618	BCR	C1-C6	-3.34	1.49	1.53
34	E	105	HEM	FE-NB	3.34	2.05	1.94
22	B	603	CLA	MG-NC	3.34	2.14	2.06
22	b	604	CLA	MG-NC	3.34	2.14	2.06
22	D	404	CLA	C4B-NB	3.34	1.42	1.37
22	d	404	CLA	C4B-NB	3.34	1.42	1.37
22	c	511	CLA	C1D-ND	3.34	1.42	1.37
22	C	512	CLA	C1D-ND	3.33	1.42	1.37
23	H	102	BCR	C30-C25	-3.33	1.49	1.53
22	B	615	CLA	C4B-NB	3.32	1.42	1.37
22	B	611	CLA	MG-NA	3.32	2.14	2.06
22	b	612	CLA	MG-NA	3.32	2.14	2.06
22	C	502	CLA	C4B-NB	3.32	1.42	1.37
22	c	502	CLA	C4B-NB	3.32	1.42	1.37
30	D	401	PHO	C4D-CHA	3.31	1.44	1.39
30	d	401	PHO	C4D-CHA	3.31	1.44	1.39
23	k	103	BCR	C30-C25	-3.31	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	602	CLA	MG-NC	3.30	2.14	2.06
22	b	603	CLA	MG-NC	3.30	2.14	2.06
23	T	101	BCR	C1-C6	-3.30	1.49	1.53
22	c	512	CLA	C1D-ND	3.30	1.42	1.37
23	K	103	BCR	C30-C25	-3.29	1.49	1.53
23	c	514	BCR	C30-C25	-3.29	1.49	1.53
22	B	614	CLA	C1D-ND	3.29	1.42	1.37
22	C	503	CLA	C1D-ND	3.29	1.42	1.37
22	c	503	CLA	C1D-ND	3.29	1.42	1.37
24	D	407	PL9	C3-C4	-3.29	1.44	1.49
24	d	407	PL9	C3-C4	-3.29	1.44	1.49
22	C	511	CLA	C1D-ND	3.29	1.42	1.37
27	b	621	SQD	O47-C7	3.29	1.43	1.34
23	b	620	BCR	C1-C6	-3.29	1.49	1.53
27	B	620	SQD	O5-C1	3.28	1.50	1.41
23	T	101	BCR	C30-C25	-3.28	1.49	1.53
23	t	102	BCR	C30-C25	-3.28	1.49	1.53
27	B	620	SQD	O47-C7	3.27	1.43	1.34
22	C	512	CLA	MG-NC	3.27	2.14	2.06
23	t	102	BCR	C1-C6	-3.27	1.49	1.53
22	B	614	CLA	MG-NC	3.27	2.14	2.06
22	B	616	CLA	MG-NC	3.26	2.14	2.06
22	b	617	CLA	MG-NC	3.26	2.14	2.06
22	C	501	CLA	C1D-ND	3.26	1.42	1.37
22	c	501	CLA	C1D-ND	3.26	1.42	1.37
23	h	102	BCR	C30-C25	-3.26	1.49	1.53
22	b	616	CLA	C4B-NB	3.25	1.42	1.37
22	b	615	CLA	MG-NC	3.25	2.14	2.06
23	B	619	BCR	C1-C6	-3.25	1.49	1.53
22	b	615	CLA	C1D-ND	3.24	1.42	1.37
22	D	404	CLA	MG-NC	3.24	2.14	2.06
22	d	404	CLA	MG-NC	3.24	2.14	2.06
22	C	503	CLA	MG-ND	3.23	2.12	2.05
22	c	503	CLA	MG-ND	3.23	2.12	2.05
23	C	514	BCR	C30-C25	-3.23	1.49	1.53
22	c	512	CLA	MG-NC	3.23	2.13	2.06
22	B	603	CLA	MG-NA	3.23	2.13	2.06
22	b	604	CLA	MG-NA	3.23	2.13	2.06
23	C	515	BCR	C30-C25	-3.19	1.49	1.53
23	c	515	BCR	C30-C25	-3.19	1.49	1.53
22	B	605	CLA	MG-NC	3.18	2.13	2.06
23	A	407	BCR	C30-C25	-3.17	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	407	BCR	C30-C25	-3.17	1.49	1.53
22	d	405	CLA	MG-ND	3.17	2.12	2.05
22	B	602	CLA	C4B-NB	3.16	1.42	1.37
27	A	412	SQD	O5-C1	3.15	1.50	1.41
27	a	412	SQD	O5-C1	3.15	1.50	1.41
22	C	508	CLA	MG-NA	3.15	2.13	2.06
22	c	508	CLA	MG-NA	3.15	2.13	2.06
22	b	606	CLA	MG-NC	3.14	2.13	2.06
23	b	620	BCR	C30-C25	-3.14	1.49	1.53
27	A	412	SQD	O47-C7	3.14	1.43	1.34
22	C	511	CLA	C4B-NB	3.14	1.42	1.37
27	a	412	SQD	O47-C7	3.13	1.43	1.34
22	b	603	CLA	C4B-NB	3.13	1.42	1.37
22	D	405	CLA	MG-ND	3.13	2.12	2.05
27	a	411	SQD	O47-C7	3.12	1.43	1.34
22	C	512	CLA	C4B-NB	3.12	1.42	1.37
22	B	605	CLA	C4B-NB	3.11	1.41	1.37
22	b	606	CLA	C4B-NB	3.11	1.41	1.37
22	C	507	CLA	C4B-NB	3.11	1.41	1.37
22	c	507	CLA	C4B-NB	3.11	1.41	1.37
22	C	509	CLA	C4B-NB	3.10	1.41	1.37
22	b	610	CLA	MG-NA	3.10	2.13	2.06
22	c	512	CLA	C4B-NB	3.09	1.41	1.37
27	A	411	SQD	O47-C7	3.09	1.43	1.34
22	B	604	CLA	MG-NC	3.08	2.13	2.06
22	B	609	CLA	MG-NA	3.08	2.13	2.06
23	K	101	BCR	C30-C25	-3.08	1.49	1.53
23	k	101	BCR	C30-C25	-3.08	1.49	1.53
27	b	621	SQD	C24-C23	3.07	1.59	1.50
22	c	511	CLA	C4B-NB	3.07	1.41	1.37
23	B	619	BCR	C30-C25	-3.07	1.49	1.53
22	B	607	CLA	C4B-NB	3.06	1.41	1.37
22	b	605	CLA	MG-NC	3.06	2.13	2.06
22	c	509	CLA	C4B-NB	3.06	1.41	1.37
22	B	608	CLA	C4B-NB	3.05	1.41	1.37
22	b	609	CLA	C4B-NB	3.05	1.41	1.37
22	A	406	CLA	C4B-NB	3.05	1.41	1.37
27	a	411	SQD	C24-C23	3.04	1.59	1.50
27	x	101	SQD	O5-C1	3.04	1.49	1.41
34	E	105	HEM	FE-NC	3.03	2.05	1.95
34	e	105	HEM	FE-NC	3.03	2.05	1.95
27	a	412	SQD	C24-C23	3.03	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	404	CLA	C1B-C2B	3.02	1.50	1.43
27	A	411	SQD	C24-C23	3.02	1.59	1.50
22	b	607	CLA	C4B-NB	3.02	1.41	1.37
22	B	613	CLA	C1B-C2B	3.02	1.50	1.43
22	b	614	CLA	C1B-C2B	3.02	1.50	1.43
22	a	406	CLA	C4B-NB	3.01	1.41	1.37
22	B	603	CLA	C4B-NB	3.01	1.41	1.37
27	X	101	SQD	O5-C1	3.01	1.49	1.41
22	C	505	CLA	C4B-NB	3.00	1.41	1.37
22	b	608	CLA	C4B-NB	3.00	1.41	1.37
22	c	505	CLA	C4B-NB	3.00	1.41	1.37
22	A	419	CLA	C1D-ND	3.00	1.41	1.37
22	a	419	CLA	C1D-ND	3.00	1.41	1.37
22	B	613	CLA	C4B-NB	3.00	1.41	1.37
22	C	503	CLA	C4B-NB	2.99	1.41	1.37
22	c	503	CLA	C4B-NB	2.99	1.41	1.37
27	A	412	SQD	C24-C23	2.99	1.59	1.50
22	B	607	CLA	C1B-C2B	2.99	1.50	1.43
22	b	608	CLA	C1B-C2B	2.99	1.50	1.43
22	a	404	CLA	C1B-C2B	2.98	1.50	1.43
22	C	508	CLA	C4B-NB	2.97	1.41	1.37
22	c	508	CLA	C4B-NB	2.97	1.41	1.37
22	B	612	CLA	C1B-C2B	2.97	1.50	1.43
22	b	613	CLA	C1B-C2B	2.97	1.50	1.43
27	x	101	SQD	C24-C23	2.97	1.59	1.50
22	b	617	CLA	C1B-C2B	2.96	1.50	1.43
27	B	620	SQD	C24-C23	2.96	1.59	1.50
22	B	604	CLA	C4B-NB	2.96	1.41	1.37
22	B	606	CLA	C4B-NB	2.96	1.41	1.37
22	B	610	CLA	C4B-NB	2.95	1.41	1.37
22	b	611	CLA	C4B-NB	2.95	1.41	1.37
22	B	601	CLA	C4B-NB	2.95	1.41	1.37
23	b	618	BCR	C30-C25	-2.95	1.50	1.53
22	B	616	CLA	C1B-C2B	2.94	1.50	1.43
22	c	511	CLA	C1B-C2B	2.94	1.50	1.43
22	B	609	CLA	C4B-NB	2.94	1.41	1.37
22	b	610	CLA	C4B-NB	2.94	1.41	1.37
22	C	501	CLA	C4B-NB	2.94	1.41	1.37
22	D	405	CLA	C4B-NB	2.94	1.41	1.37
22	d	405	CLA	C4B-NB	2.94	1.41	1.37
22	B	612	CLA	C4B-NB	2.94	1.41	1.37
22	b	613	CLA	C4B-NB	2.94	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	604	CLA	C1B-C2B	2.94	1.50	1.43
22	b	605	CLA	C1B-C2B	2.94	1.50	1.43
27	X	101	SQD	C24-C23	2.94	1.59	1.50
22	b	614	CLA	C4B-NB	2.94	1.41	1.37
22	C	511	CLA	C1B-C2B	2.93	1.50	1.43
22	b	612	CLA	C4B-NB	2.93	1.41	1.37
23	B	617	BCR	C30-C25	-2.93	1.50	1.53
27	A	411	SQD	O5-C1	2.93	1.49	1.41
22	b	605	CLA	C4B-NB	2.92	1.41	1.37
22	B	614	CLA	C1B-C2B	2.92	1.50	1.43
22	b	615	CLA	C1B-C2B	2.92	1.50	1.43
22	C	504	CLA	C4B-NB	2.92	1.41	1.37
22	c	504	CLA	C4B-NB	2.92	1.41	1.37
22	b	602	CLA	C4B-NB	2.92	1.41	1.37
22	b	604	CLA	C4B-NB	2.92	1.41	1.37
22	C	506	CLA	C4B-NB	2.92	1.41	1.37
22	c	506	CLA	C4B-NB	2.92	1.41	1.37
22	B	614	CLA	C4B-NB	2.90	1.41	1.37
22	b	615	CLA	C4B-NB	2.90	1.41	1.37
27	a	411	SQD	O5-C1	2.90	1.49	1.41
22	C	506	CLA	C1B-C2B	2.90	1.49	1.43
22	c	506	CLA	C1B-C2B	2.90	1.49	1.43
22	C	510	CLA	MG-NA	2.90	2.13	2.06
22	A	405	CLA	C4B-NB	2.90	1.41	1.37
22	C	504	CLA	C1B-C2B	2.89	1.49	1.43
22	c	504	CLA	C1B-C2B	2.89	1.49	1.43
22	B	606	CLA	C1B-C2B	2.88	1.49	1.43
22	C	507	CLA	C1B-C2B	2.88	1.49	1.43
22	b	607	CLA	C1B-C2B	2.88	1.49	1.43
22	c	507	CLA	C1B-C2B	2.88	1.49	1.43
22	D	404	CLA	C1B-C2B	2.88	1.49	1.43
22	B	615	CLA	C1B-C2B	2.88	1.49	1.43
22	c	501	CLA	C4B-NB	2.87	1.41	1.37
22	c	510	CLA	MG-NA	2.87	2.13	2.06
22	b	616	CLA	C1B-C2B	2.87	1.49	1.43
22	B	611	CLA	C4B-NB	2.86	1.41	1.37
22	d	404	CLA	C1B-C2B	2.86	1.49	1.43
22	a	404	CLA	C4B-NB	2.86	1.41	1.37
34	E	105	HEM	CAB-C3B	2.85	1.55	1.47
34	e	105	HEM	CAB-C3B	2.85	1.55	1.47
34	E	105	HEM	CAC-C3C	2.85	1.55	1.47
22	c	502	CLA	MG-NC	2.85	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	405	CLA	C1B-C2B	2.84	1.49	1.43
22	b	602	CLA	C1B-C2B	2.84	1.49	1.43
22	a	405	CLA	C4B-NB	2.84	1.41	1.37
22	C	509	CLA	C1B-C2B	2.83	1.49	1.43
22	c	509	CLA	C1B-C2B	2.83	1.49	1.43
22	C	503	CLA	C1B-C2B	2.83	1.49	1.43
22	c	503	CLA	C1B-C2B	2.83	1.49	1.43
22	C	502	CLA	MG-NC	2.83	2.13	2.06
22	a	405	CLA	C1B-C2B	2.82	1.49	1.43
22	B	603	CLA	C1B-C2B	2.81	1.49	1.43
22	b	604	CLA	C1B-C2B	2.81	1.49	1.43
34	e	105	HEM	CAC-C3C	2.81	1.54	1.47
22	A	419	CLA	C4B-NB	2.81	1.41	1.37
22	a	419	CLA	C4B-NB	2.81	1.41	1.37
22	B	608	CLA	C1B-C2B	2.81	1.49	1.43
22	b	609	CLA	C1B-C2B	2.81	1.49	1.43
22	C	508	CLA	C1B-C2B	2.81	1.49	1.43
22	c	508	CLA	C1B-C2B	2.81	1.49	1.43
22	C	511	CLA	MG-NA	2.80	2.12	2.06
22	c	511	CLA	MG-NA	2.80	2.12	2.06
22	B	601	CLA	C1B-C2B	2.80	1.49	1.43
22	B	609	CLA	C1B-C2B	2.80	1.49	1.43
22	C	510	CLA	C4B-NB	2.80	1.41	1.37
22	c	510	CLA	C4B-NB	2.80	1.41	1.37
28	A	413	DGD	O1G-C1G	-2.80	1.38	1.45
22	b	606	CLA	C1B-C2B	2.80	1.49	1.43
22	A	404	CLA	C4B-NB	2.80	1.41	1.37
22	B	605	CLA	C1B-C2B	2.79	1.49	1.43
22	B	610	CLA	C1B-C2B	2.79	1.49	1.43
22	b	611	CLA	C1B-C2B	2.79	1.49	1.43
22	C	510	CLA	C1B-C2B	2.78	1.49	1.43
22	c	510	CLA	C1B-C2B	2.78	1.49	1.43
22	A	406	CLA	C1B-C2B	2.78	1.49	1.43
22	a	406	CLA	C1B-C2B	2.78	1.49	1.43
22	A	419	CLA	C1B-C2B	2.78	1.49	1.43
22	a	419	CLA	C1B-C2B	2.78	1.49	1.43
32	Z	101	LMT	O3'-C3'	-2.78	1.36	1.43
22	C	513	CLA	C1B-C2B	2.77	1.49	1.43
30	A	418	PHO	C3D-C4D	2.77	1.45	1.41
22	C	509	CLA	MG-NA	2.77	2.12	2.06
22	c	509	CLA	MG-NA	2.77	2.12	2.06
22	b	610	CLA	C1B-C2B	2.77	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	525	LMT	O3'-C3'	-2.76	1.36	1.43
32	z	101	LMT	O3'-C3'	-2.76	1.36	1.43
22	c	513	CLA	C1B-C2B	2.76	1.49	1.43
30	a	418	PHO	C3D-C4D	2.76	1.45	1.41
22	B	611	CLA	C1B-C2B	2.76	1.49	1.43
22	b	612	CLA	C1B-C2B	2.76	1.49	1.43
22	B	616	CLA	C4B-NB	2.76	1.41	1.37
22	b	617	CLA	C4B-NB	2.76	1.41	1.37
22	C	502	CLA	C1B-C2B	2.75	1.49	1.43
22	c	502	CLA	C1B-C2B	2.75	1.49	1.43
22	C	513	CLA	C4B-NB	2.74	1.41	1.37
22	c	513	CLA	C4B-NB	2.74	1.41	1.37
32	c	525	LMT	O3'-C3'	-2.74	1.36	1.43
22	C	505	CLA	C1B-C2B	2.73	1.49	1.43
22	c	505	CLA	C1B-C2B	2.73	1.49	1.43
22	D	405	CLA	C1B-C2B	2.73	1.49	1.43
22	d	405	CLA	C1B-C2B	2.73	1.49	1.43
22	C	501	CLA	C1B-C2B	2.71	1.49	1.43
22	c	501	CLA	C1B-C2B	2.71	1.49	1.43
24	A	408	PL9	C7-C3	-2.71	1.47	1.51
24	a	408	PL9	C7-C3	-2.71	1.47	1.51
22	B	602	CLA	C1B-C2B	2.71	1.49	1.43
22	b	603	CLA	C1B-C2B	2.71	1.49	1.43
22	C	512	CLA	C1B-C2B	2.70	1.49	1.43
28	A	413	DGD	O2G-C2G	-2.70	1.40	1.46
22	C	508	CLA	MG-NB	2.69	2.11	2.05
22	c	512	CLA	C1B-C2B	2.68	1.49	1.43
30	A	418	PHO	CMC-C2C	-2.67	1.46	1.50
28	a	413	DGD	O2G-C2G	-2.67	1.40	1.46
30	a	418	PHO	CMC-C2C	-2.67	1.46	1.50
22	c	508	CLA	MG-NB	2.67	2.11	2.05
22	C	502	CLA	MG-NA	2.65	2.12	2.06
22	c	502	CLA	MG-NA	2.65	2.12	2.06
28	c	518	DGD	O1G-C1G	-2.65	1.39	1.45
30	d	401	PHO	CMC-C2C	-2.65	1.46	1.50
30	D	401	PHO	CMC-C2C	-2.65	1.46	1.50
28	a	413	DGD	O1G-C1G	-2.64	1.39	1.45
28	C	518	DGD	O1G-C1G	-2.62	1.39	1.45
22	B	613	CLA	MG-NB	2.61	2.11	2.05
22	B	607	CLA	MG-NA	2.61	2.12	2.06
22	b	608	CLA	MG-NA	2.61	2.12	2.06
32	j	102	LMT	O3'-C3'	-2.61	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	m	101	LMT	O3'-C3'	-2.60	1.36	1.43
22	b	614	CLA	MG-NB	2.59	2.10	2.05
32	J	102	LMT	O3'-C3'	-2.59	1.36	1.43
30	a	418	PHO	CMD-C2D	-2.58	1.46	1.51
32	E	104	LMT	O3'-C3'	-2.58	1.36	1.43
32	e	104	LMT	O3'-C3'	-2.58	1.36	1.43
26	C	520	LMG	O7-C8	-2.57	1.40	1.46
32	M	102	LMT	O3'-C3'	-2.57	1.36	1.43
30	D	401	PHO	C3D-C4D	2.56	1.44	1.41
30	d	401	PHO	C3D-C4D	2.56	1.44	1.41
30	A	418	PHO	CAC-C3C	-2.55	1.47	1.51
30	a	418	PHO	CAC-C3C	-2.55	1.47	1.51
30	A	418	PHO	CMD-C2D	-2.54	1.46	1.51
22	b	612	CLA	MG-ND	2.54	2.10	2.05
26	c	520	LMG	O7-C8	-2.51	1.40	1.46
30	a	418	PHO	CMB-C2B	-2.51	1.46	1.51
22	C	513	CLA	MG-NA	2.51	2.12	2.06
24	D	407	PL9	C6-C1	-2.50	1.44	1.48
24	d	407	PL9	C6-C1	-2.50	1.44	1.48
24	A	408	PL9	C6-C1	-2.50	1.44	1.48
24	a	408	PL9	C6-C1	-2.50	1.44	1.48
31	A	420	LHG	O7-C5	-2.50	1.40	1.46
22	B	611	CLA	MG-ND	2.50	2.10	2.05
31	a	420	LHG	O7-C5	-2.50	1.40	1.46
32	B	623	LMT	O3'-C3'	-2.50	1.36	1.43
22	B	607	CLA	C3B-C4B	2.50	1.50	1.42
22	b	608	CLA	C3B-C4B	2.50	1.50	1.42
22	C	503	CLA	MG-NB	2.49	2.10	2.05
22	c	503	CLA	MG-NB	2.49	2.10	2.05
22	C	505	CLA	MG-NC	2.49	2.12	2.06
22	c	505	CLA	MG-NC	2.49	2.12	2.06
22	A	404	CLA	MG-NA	2.49	2.12	2.06
22	a	404	CLA	MG-NA	2.49	2.12	2.06
31	D	411	LHG	O7-C5	-2.49	1.40	1.46
31	d	411	LHG	O7-C5	-2.49	1.40	1.46
30	A	418	PHO	CMB-C2B	-2.48	1.46	1.51
30	D	401	PHO	CMB-C2B	-2.48	1.46	1.51
31	d	410	LHG	P-O6	2.48	1.69	1.59
22	B	612	CLA	MG-NA	2.47	2.12	2.06
22	c	513	CLA	MG-NA	2.47	2.12	2.06
32	b	624	LMT	O3'-C3'	-2.47	1.36	1.43
22	b	613	CLA	MG-NA	2.47	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	523	LMT	O3'-C3'	-2.46	1.36	1.43
30	d	401	PHO	CMB-C2B	-2.46	1.46	1.51
22	a	419	CLA	MG-NA	2.45	2.12	2.06
30	D	401	PHO	CMD-C2D	-2.45	1.46	1.51
31	D	410	LHG	P-O6	2.45	1.69	1.59
22	B	610	CLA	C3B-C4B	2.45	1.49	1.42
22	b	611	CLA	C3B-C4B	2.45	1.49	1.42
22	c	511	CLA	C3B-C4B	2.44	1.49	1.42
22	a	404	CLA	C3B-C4B	2.44	1.49	1.42
30	d	401	PHO	CMD-C2D	-2.44	1.46	1.51
22	A	419	CLA	MG-NA	2.43	2.12	2.06
22	A	404	CLA	C3B-C4B	2.43	1.49	1.42
22	b	616	CLA	C3B-C4B	2.42	1.49	1.42
22	B	615	CLA	C3B-C4B	2.42	1.49	1.42
32	c	523	LMT	O3'-C3'	-2.42	1.37	1.43
22	C	511	CLA	C3B-C4B	2.42	1.49	1.42
32	M	102	LMT	O2B-C2B	-2.41	1.37	1.43
32	m	101	LMT	O2B-C2B	-2.41	1.37	1.43
22	A	419	CLA	C3B-C4B	2.41	1.49	1.42
22	a	419	CLA	C3B-C4B	2.41	1.49	1.42
22	B	607	CLA	CHC-C1C	2.40	1.43	1.38
22	C	501	CLA	C3B-C4B	2.40	1.49	1.42
22	c	501	CLA	C3B-C4B	2.40	1.49	1.42
22	C	501	CLA	MG-NA	2.37	2.11	2.06
22	c	501	CLA	MG-NA	2.37	2.11	2.06
22	B	606	CLA	MG-NA	2.37	2.11	2.06
22	b	607	CLA	MG-NA	2.37	2.11	2.06
22	C	507	CLA	C3B-C4B	2.36	1.49	1.42
22	c	507	CLA	C3B-C4B	2.36	1.49	1.42
22	B	609	CLA	C3B-C4B	2.36	1.49	1.42
22	b	610	CLA	C3B-C4B	2.36	1.49	1.42
22	B	609	CLA	MG-NB	2.36	2.10	2.05
22	b	605	CLA	C3B-C4B	2.36	1.49	1.42
22	b	610	CLA	MG-NB	2.36	2.10	2.05
22	b	606	CLA	C3B-C4B	2.35	1.49	1.42
22	C	511	CLA	CHC-C1C	2.35	1.43	1.38
22	a	405	CLA	CHC-C1C	2.35	1.43	1.38
22	B	608	CLA	C3B-C4B	2.35	1.49	1.42
22	b	609	CLA	C3B-C4B	2.35	1.49	1.42
22	b	604	CLA	C3B-C4B	2.35	1.49	1.42
22	B	610	CLA	CHC-C1C	2.34	1.43	1.38
22	b	611	CLA	CHC-C1C	2.34	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	406	CLA	C3B-C4B	2.34	1.49	1.42
22	a	406	CLA	C3B-C4B	2.34	1.49	1.42
22	B	603	CLA	C3B-C4B	2.34	1.49	1.42
22	B	605	CLA	C3B-C4B	2.34	1.49	1.42
22	C	504	CLA	C3B-C4B	2.34	1.49	1.42
22	D	404	CLA	C3B-C4B	2.34	1.49	1.42
22	c	504	CLA	C3B-C4B	2.34	1.49	1.42
22	d	404	CLA	C3B-C4B	2.34	1.49	1.42
22	B	615	CLA	CHC-C1C	2.34	1.43	1.38
22	B	604	CLA	C3B-C4B	2.33	1.49	1.42
22	B	608	CLA	MG-NA	2.33	2.11	2.06
22	b	609	CLA	MG-NA	2.33	2.11	2.06
22	b	608	CLA	CHC-C1C	2.33	1.43	1.38
22	B	612	CLA	C3B-C4B	2.33	1.49	1.42
22	b	613	CLA	C3B-C4B	2.33	1.49	1.42
22	c	511	CLA	CHC-C1C	2.32	1.43	1.38
22	b	603	CLA	C3B-C4B	2.32	1.49	1.42
22	C	508	CLA	C3B-C4B	2.32	1.49	1.42
22	c	508	CLA	C3B-C4B	2.32	1.49	1.42
22	a	405	CLA	C3B-C4B	2.32	1.49	1.42
22	b	611	CLA	MG-NC	2.32	2.11	2.06
22	c	507	CLA	CHC-C1C	2.32	1.43	1.38
22	c	513	CLA	C3B-C4B	2.32	1.49	1.42
22	b	616	CLA	CHC-C1C	2.31	1.43	1.38
22	C	502	CLA	C3B-C4B	2.31	1.49	1.42
22	C	510	CLA	C3B-C4B	2.31	1.49	1.42
22	c	502	CLA	C3B-C4B	2.31	1.49	1.42
22	c	510	CLA	C3B-C4B	2.31	1.49	1.42
31	L	101	LHG	O7-C5	-2.31	1.41	1.46
31	l	101	LHG	O7-C5	-2.31	1.41	1.46
22	C	510	CLA	CHC-C1C	2.30	1.43	1.38
22	C	501	CLA	CHC-C1C	2.30	1.43	1.38
22	c	501	CLA	CHC-C1C	2.30	1.43	1.38
24	D	407	PL9	C53-C6	-2.30	1.46	1.50
24	d	407	PL9	C53-C6	-2.30	1.46	1.50
22	B	608	CLA	CHC-C1C	2.30	1.43	1.38
22	b	609	CLA	CHC-C1C	2.30	1.43	1.38
22	B	602	CLA	C3B-C4B	2.30	1.49	1.42
22	B	610	CLA	MG-NC	2.30	2.11	2.06
22	B	613	CLA	C3B-C4B	2.29	1.49	1.42
22	b	614	CLA	C3B-C4B	2.29	1.49	1.42
22	D	405	CLA	C3B-C4B	2.29	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	405	CLA	C3B-C4B	2.29	1.49	1.42
22	c	506	CLA	MG-NC	2.29	2.11	2.06
22	C	512	CLA	C3B-C4B	2.28	1.49	1.42
22	C	513	CLA	C3B-C4B	2.28	1.49	1.42
22	C	503	CLA	C3B-C4B	2.28	1.49	1.42
22	c	503	CLA	C3B-C4B	2.28	1.49	1.42
28	C	517	DGD	O1G-C1G	-2.28	1.40	1.45
28	c	517	DGD	O1G-C1G	-2.28	1.40	1.45
22	c	510	CLA	CHC-C1C	2.28	1.43	1.38
22	A	405	CLA	CHC-C1C	2.28	1.43	1.38
22	B	605	CLA	CHC-C1C	2.28	1.43	1.38
22	b	606	CLA	CHC-C1C	2.28	1.43	1.38
22	B	611	CLA	C3B-C4B	2.28	1.49	1.42
22	C	505	CLA	C3B-C4B	2.28	1.49	1.42
22	c	505	CLA	C3B-C4B	2.28	1.49	1.42
22	b	612	CLA	C3B-C4B	2.28	1.49	1.42
22	A	406	CLA	CHC-C1C	2.27	1.43	1.38
22	a	406	CLA	CHC-C1C	2.27	1.43	1.38
22	B	606	CLA	MG-ND	-2.27	2.01	2.05
22	b	607	CLA	MG-ND	-2.27	2.01	2.05
22	C	503	CLA	CHC-C1C	2.27	1.43	1.38
22	c	502	CLA	CHC-C1C	2.27	1.43	1.38
22	c	503	CLA	CHC-C1C	2.27	1.43	1.38
30	D	401	PHO	C4D-ND	-2.27	1.35	1.38
22	B	606	CLA	C3B-C4B	2.26	1.49	1.42
32	C	525	LMT	O2'-C2'	-2.26	1.37	1.43
22	c	512	CLA	C3B-C4B	2.26	1.49	1.42
22	c	513	CLA	CHC-C1C	2.26	1.43	1.38
22	C	506	CLA	MG-NC	2.25	2.11	2.06
22	b	607	CLA	C3B-C4B	2.25	1.49	1.42
22	B	614	CLA	C3B-C4B	2.25	1.49	1.42
22	b	615	CLA	C3B-C4B	2.25	1.49	1.42
32	z	101	LMT	O2'-C2'	-2.25	1.37	1.43
32	Z	101	LMT	O2'-C2'	-2.25	1.37	1.43
22	C	502	CLA	CHC-C1C	2.25	1.43	1.38
22	C	507	CLA	CHC-C1C	2.25	1.43	1.38
24	A	408	PL9	C3-C4	-2.25	1.46	1.49
22	b	613	CLA	CHC-C1C	2.24	1.43	1.38
22	C	509	CLA	MG-NC	2.24	2.11	2.06
22	B	609	CLA	CHC-C1C	2.24	1.43	1.38
22	b	610	CLA	CHC-C1C	2.24	1.43	1.38
22	C	505	CLA	CHC-C1C	2.24	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	505	CLA	CHC-C1C	2.24	1.43	1.38
22	A	405	CLA	C3B-C4B	2.24	1.49	1.42
32	c	525	LMT	O2'-C2'	-2.24	1.37	1.43
30	d	401	PHO	C4D-ND	-2.24	1.35	1.38
22	C	506	CLA	MG-NA	2.24	2.11	2.06
22	c	506	CLA	MG-NA	2.24	2.11	2.06
22	C	506	CLA	C3B-C4B	2.23	1.49	1.42
22	c	506	CLA	C3B-C4B	2.23	1.49	1.42
22	a	405	CLA	CMD-C2D	-2.23	1.46	1.50
22	c	509	CLA	C3B-C4B	2.23	1.49	1.42
22	C	513	CLA	CHC-C1C	2.22	1.42	1.38
22	B	612	CLA	CHC-C1C	2.22	1.42	1.38
22	B	616	CLA	C3B-C4B	2.22	1.49	1.42
22	b	617	CLA	C3B-C4B	2.22	1.49	1.42
22	B	604	CLA	CHC-C1C	2.22	1.42	1.38
32	C	523	LMT	O1'-C1'	-2.22	1.36	1.40
22	C	512	CLA	CHC-C1C	2.21	1.42	1.38
27	b	621	SQD	O9-S	2.21	1.51	1.45
22	B	602	CLA	CHC-C1C	2.21	1.42	1.38
22	b	603	CLA	CHC-C1C	2.21	1.42	1.38
32	c	525	LMT	O3B-C3B	-2.21	1.37	1.43
32	z	101	LMT	O2B-C2B	-2.21	1.37	1.43
22	b	605	CLA	CHC-C1C	2.21	1.42	1.38
24	a	408	PL9	C3-C4	-2.21	1.46	1.49
27	B	620	SQD	O9-S	2.20	1.51	1.45
22	A	405	CLA	CMD-C2D	-2.20	1.46	1.50
22	c	509	CLA	MG-NC	2.20	2.11	2.06
28	C	518	DGD	O2G-C2G	-2.20	1.41	1.46
32	B	623	LMT	O2'-C2'	-2.20	1.37	1.43
32	b	624	LMT	O2'-C2'	-2.20	1.37	1.43
22	b	602	CLA	C3B-C4B	2.20	1.49	1.42
32	C	523	LMT	O2'-C2'	-2.20	1.37	1.43
32	C	525	LMT	O3B-C3B	-2.20	1.37	1.43
32	Z	101	LMT	O2B-C2B	-2.20	1.37	1.43
22	C	509	CLA	C3B-C4B	2.20	1.49	1.42
22	b	614	CLA	CHC-C1C	2.19	1.42	1.38
27	A	412	SQD	O9-S	2.19	1.51	1.45
22	D	404	CLA	CHC-C1C	2.19	1.42	1.38
22	d	404	CLA	CHC-C1C	2.19	1.42	1.38
32	c	523	LMT	O1'-C1'	-2.19	1.36	1.40
28	H	103	DGD	O2G-C2G	-2.19	1.41	1.46
27	b	621	SQD	O7-S	2.19	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	505	CLA	CMB-C2B	-2.19	1.46	1.50
22	c	505	CLA	CMB-C2B	-2.19	1.46	1.50
22	c	512	CLA	CHC-C1C	2.19	1.42	1.38
22	B	601	CLA	CHC-C1C	2.19	1.42	1.38
22	b	602	CLA	CHC-C1C	2.19	1.42	1.38
35	v	201	HEC	C3B-C2B	-2.18	1.33	1.41
22	b	605	CLA	CMB-C2B	-2.18	1.46	1.50
22	B	611	CLA	CHC-C1C	2.18	1.42	1.38
22	b	612	CLA	CHC-C1C	2.18	1.42	1.38
22	B	615	CLA	MG-NB	2.18	2.10	2.05
22	b	616	CLA	MG-NB	2.18	2.10	2.05
22	C	503	CLA	CMD-C2D	-2.18	1.46	1.50
22	c	503	CLA	CMD-C2D	-2.18	1.46	1.50
28	c	518	DGD	O2G-C2G	-2.17	1.41	1.46
22	C	506	CLA	CHC-C1C	2.17	1.42	1.38
22	c	506	CLA	CHC-C1C	2.17	1.42	1.38
22	B	615	CLA	MG-ND	2.17	2.10	2.05
22	b	616	CLA	MG-ND	2.17	2.10	2.05
22	C	508	CLA	CMB-C2B	-2.17	1.46	1.50
22	c	508	CLA	CMB-C2B	-2.17	1.46	1.50
35	V	201	HEC	C3B-C2B	-2.16	1.33	1.41
27	a	412	SQD	O9-S	2.16	1.51	1.45
22	B	613	CLA	CMD-C2D	-2.16	1.46	1.50
22	b	614	CLA	CMD-C2D	-2.16	1.46	1.50
28	h	103	DGD	O2G-C2G	-2.16	1.41	1.46
22	C	507	CLA	MG-NC	2.16	2.11	2.06
22	c	507	CLA	MG-NC	2.16	2.11	2.06
32	c	523	LMT	O2'-C2'	-2.16	1.37	1.43
22	C	512	CLA	CMB-C2B	-2.16	1.46	1.50
22	B	613	CLA	CHC-C1C	2.16	1.42	1.38
22	A	419	CLA	CHC-C1C	2.16	1.42	1.38
22	a	419	CLA	CHC-C1C	2.16	1.42	1.38
22	B	601	CLA	C3B-C4B	2.15	1.49	1.42
30	D	401	PHO	CAC-C3C	-2.15	1.47	1.51
30	d	401	PHO	CAC-C3C	-2.15	1.47	1.51
22	B	604	CLA	CMB-C2B	-2.15	1.46	1.50
22	C	509	CLA	CHC-C1C	2.15	1.42	1.38
22	c	509	CLA	CHC-C1C	2.15	1.42	1.38
22	B	612	CLA	CMD-C2D	-2.15	1.46	1.50
22	b	613	CLA	CMD-C2D	-2.15	1.46	1.50
22	B	612	CLA	CMB-C2B	-2.15	1.46	1.50
22	b	613	CLA	CMB-C2B	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	502	CLA	CMB-C2B	-2.14	1.46	1.50
22	C	512	CLA	CMD-C2D	-2.14	1.46	1.50
22	B	603	CLA	CMD-C2D	-2.14	1.46	1.50
22	b	604	CLA	CMD-C2D	-2.14	1.46	1.50
22	B	602	CLA	MG-NA	2.14	2.11	2.06
22	b	603	CLA	MG-NA	2.14	2.11	2.06
22	B	603	CLA	CHC-C1C	2.14	1.42	1.38
22	b	604	CLA	CHC-C1C	2.14	1.42	1.38
22	B	606	CLA	CHC-C1C	2.14	1.42	1.38
22	b	607	CLA	CHC-C1C	2.14	1.42	1.38
22	B	608	CLA	CMD-C2D	-2.13	1.46	1.50
22	b	609	CLA	CMD-C2D	-2.13	1.46	1.50
22	A	406	CLA	CMB-C2B	-2.13	1.46	1.50
32	z	101	LMT	O3B-C3B	-2.13	1.37	1.43
22	A	419	CLA	CMD-C2D	-2.13	1.46	1.50
22	a	419	CLA	CMD-C2D	-2.13	1.46	1.50
22	C	508	CLA	CMD-C2D	-2.13	1.46	1.50
22	c	508	CLA	CMD-C2D	-2.13	1.46	1.50
22	C	501	CLA	CMD-C2D	-2.13	1.46	1.50
22	c	501	CLA	CMD-C2D	-2.13	1.46	1.50
22	D	405	CLA	CHC-C1C	2.12	1.42	1.38
22	d	405	CLA	CHC-C1C	2.12	1.42	1.38
35	v	201	HEC	C3C-C2C	-2.12	1.34	1.41
22	C	502	CLA	MG-ND	-2.12	2.01	2.05
22	C	504	CLA	CHC-C1C	2.12	1.42	1.38
22	c	504	CLA	CHC-C1C	2.12	1.42	1.38
26	B	624	LMG	O7-C8	-2.12	1.41	1.46
26	b	625	LMG	O7-C8	-2.12	1.41	1.46
22	c	512	CLA	CMB-C2B	-2.12	1.46	1.50
27	B	620	SQD	O7-S	2.12	1.51	1.45
27	A	412	SQD	O7-S	2.12	1.51	1.45
31	D	409	LHG	O7-C5	-2.11	1.41	1.46
31	d	409	LHG	O7-C5	-2.11	1.41	1.46
27	a	412	SQD	O7-S	2.11	1.51	1.45
22	C	501	CLA	CMB-C2B	-2.11	1.46	1.50
22	c	501	CLA	CMB-C2B	-2.11	1.46	1.50
32	j	102	LMT	O2'-C2'	-2.11	1.37	1.43
22	B	606	CLA	CMB-C2B	-2.11	1.46	1.50
22	C	510	CLA	CMB-C2B	-2.11	1.46	1.50
22	b	607	CLA	CMB-C2B	-2.11	1.46	1.50
22	c	510	CLA	CMB-C2B	-2.11	1.46	1.50
22	B	614	CLA	CHC-C1C	2.11	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	610	CLA	MG-NA	2.11	2.11	2.06
22	c	502	CLA	MG-ND	-2.11	2.01	2.05
32	c	525	LMT	O2B-C2B	-2.11	1.37	1.43
32	c	523	LMT	O5'-C5'	-2.11	1.39	1.44
31	A	420	LHG	P-O6	2.11	1.67	1.59
22	C	513	CLA	CMD-C2D	-2.11	1.46	1.50
22	c	513	CLA	CMD-C2D	-2.11	1.46	1.50
32	Z	101	LMT	O3B-C3B	-2.10	1.37	1.43
35	V	201	HEC	C3C-C2C	-2.10	1.34	1.41
22	C	504	CLA	CMD-C2D	-2.10	1.46	1.50
22	c	504	CLA	CMD-C2D	-2.10	1.46	1.50
32	z	101	LMT	O4'-C4B	-2.10	1.37	1.43
22	B	602	CLA	CMD-C2D	-2.10	1.46	1.50
22	b	603	CLA	CMD-C2D	-2.10	1.46	1.50
22	B	616	CLA	CMD-C2D	-2.10	1.46	1.50
22	c	502	CLA	CMB-C2B	-2.10	1.46	1.50
26	D	408	LMG	O7-C8	-2.10	1.41	1.46
26	d	408	LMG	O7-C8	-2.10	1.41	1.46
22	D	405	CLA	MG-NA	2.10	2.11	2.06
22	d	405	CLA	MG-NA	2.10	2.11	2.06
32	E	104	LMT	O2'-C2'	-2.10	1.37	1.43
32	e	104	LMT	O2'-C2'	-2.10	1.37	1.43
22	B	604	CLA	CMD-C2D	-2.10	1.46	1.50
22	b	611	CLA	MG-NA	2.10	2.11	2.06
32	Z	101	LMT	O4'-C4B	-2.09	1.37	1.43
22	B	615	CLA	CMD-C2D	-2.09	1.46	1.50
22	b	616	CLA	CMD-C2D	-2.09	1.46	1.50
22	b	615	CLA	CMD-C2D	-2.09	1.46	1.50
22	C	502	CLA	CMD-C2D	-2.09	1.46	1.50
22	c	502	CLA	CMD-C2D	-2.09	1.46	1.50
22	d	404	CLA	CMB-C2B	-2.09	1.46	1.50
32	C	525	LMT	O2B-C2B	-2.09	1.37	1.43
22	C	504	CLA	CMB-C2B	-2.09	1.46	1.50
22	c	504	CLA	CMB-C2B	-2.09	1.46	1.50
22	c	512	CLA	CMD-C2D	-2.09	1.46	1.50
22	C	506	CLA	CMB-C2B	-2.09	1.46	1.50
22	c	506	CLA	CMB-C2B	-2.09	1.46	1.50
22	b	615	CLA	CHC-C1C	2.09	1.42	1.38
22	A	405	CLA	CMB-C2B	-2.09	1.46	1.50
22	b	617	CLA	CMD-C2D	-2.09	1.46	1.50
22	a	406	CLA	CMB-C2B	-2.09	1.46	1.50
22	c	511	CLA	CMD-C2D	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	410	LMG	O7-C8	-2.08	1.41	1.46
22	C	507	CLA	CMC-C2C	-2.08	1.46	1.50
22	c	507	CLA	CMC-C2C	-2.08	1.46	1.50
32	J	102	LMT	O2'-C2'	-2.08	1.37	1.43
22	B	609	CLA	CMB-C2B	-2.08	1.46	1.50
22	D	405	CLA	CMB-C2B	-2.07	1.46	1.50
22	d	405	CLA	CMB-C2B	-2.07	1.46	1.50
22	B	608	CLA	CMB-C2B	-2.07	1.46	1.50
22	b	609	CLA	CMB-C2B	-2.07	1.46	1.50
27	X	101	SQD	O9-S	2.07	1.51	1.45
30	d	401	PHO	C3B-C2B	-2.07	1.37	1.40
23	K	101	BCR	C33-C5	-2.07	1.47	1.50
27	x	101	SQD	O7-S	2.07	1.51	1.45
31	a	420	LHG	P-O6	2.07	1.67	1.59
27	x	101	SQD	O9-S	2.07	1.51	1.45
22	B	614	CLA	CMD-C2D	-2.07	1.46	1.50
22	C	508	CLA	CHC-C1C	2.07	1.42	1.38
22	c	508	CLA	CHC-C1C	2.07	1.42	1.38
22	c	504	CLA	MG-NA	2.07	2.11	2.06
22	b	610	CLA	CMB-C2B	-2.07	1.46	1.50
22	B	609	CLA	CMD-C2D	-2.07	1.46	1.50
32	J	102	LMT	O1'-C1'	-2.07	1.36	1.40
32	j	102	LMT	O1'-C1'	-2.07	1.36	1.40
30	A	418	PHO	C4D-ND	-2.07	1.35	1.38
22	D	405	CLA	CMD-C2D	-2.07	1.46	1.50
22	b	605	CLA	CMD-C2D	-2.07	1.46	1.50
22	d	405	CLA	CMD-C2D	-2.07	1.46	1.50
32	M	102	LMT	O2'-C2'	-2.06	1.37	1.43
22	B	611	CLA	CMB-C2B	-2.06	1.46	1.50
22	b	612	CLA	CMB-C2B	-2.06	1.46	1.50
27	X	101	SQD	O7-S	2.06	1.50	1.45
22	C	505	CLA	CMD-C2D	-2.06	1.46	1.50
22	c	505	CLA	CMD-C2D	-2.06	1.46	1.50
22	B	605	CLA	CMB-C2B	-2.06	1.46	1.50
22	b	606	CLA	CMB-C2B	-2.06	1.46	1.50
27	B	620	SQD	C8-C7	2.06	1.56	1.50
32	M	102	LMT	O3B-C3B	-2.06	1.37	1.43
32	m	101	LMT	O3B-C3B	-2.06	1.37	1.43
22	b	610	CLA	CMD-C2D	-2.06	1.46	1.50
28	H	103	DGD	C6D-C5D	2.06	1.57	1.51
28	h	103	DGD	C6D-C5D	2.06	1.57	1.51
22	D	404	CLA	CMB-C2B	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	616	CLA	CMB-C2B	-2.05	1.46	1.50
22	C	504	CLA	MG-NA	2.05	2.11	2.06
27	A	411	SQD	O9-S	2.05	1.50	1.45
27	a	411	SQD	O9-S	2.05	1.50	1.45
22	B	614	CLA	CMB-C2B	-2.05	1.46	1.50
31	d	409	LHG	P-O6	2.05	1.67	1.59
22	b	614	CLA	CMB-C2B	-2.05	1.46	1.50
22	A	405	CLA	MG-NC	2.05	2.11	2.06
26	C	524	LMG	C7-C8	2.05	1.57	1.50
26	a	410	LMG	O7-C8	-2.05	1.41	1.46
22	c	511	CLA	CMB-C2B	-2.04	1.46	1.50
22	B	610	CLA	CMB-C2B	-2.04	1.46	1.50
22	B	615	CLA	CMB-C2B	-2.04	1.46	1.50
22	b	611	CLA	CMB-C2B	-2.04	1.46	1.50
22	c	510	CLA	CMD-C2D	-2.04	1.46	1.50
22	a	404	CLA	CHC-C1C	2.04	1.42	1.38
32	m	101	LMT	O2'-C2'	-2.04	1.37	1.43
28	c	519	DGD	O2G-C2G	-2.04	1.41	1.46
32	C	525	LMT	O4'-C4B	-2.04	1.37	1.43
22	C	509	CLA	CMB-C2B	-2.04	1.46	1.50
22	c	509	CLA	CMB-C2B	-2.04	1.46	1.50
27	A	411	SQD	O7-S	2.04	1.50	1.45
22	B	603	CLA	CMB-C2B	-2.04	1.46	1.50
22	b	604	CLA	CMB-C2B	-2.04	1.46	1.50
32	z	101	LMT	O1'-C1'	-2.03	1.36	1.40
32	c	525	LMT	O4'-C4B	-2.03	1.37	1.43
26	c	524	LMG	C7-C8	2.03	1.57	1.50
28	C	519	DGD	O2G-C2G	-2.03	1.41	1.46
22	C	507	CLA	CMB-C2B	-2.03	1.46	1.50
22	c	507	CLA	CMB-C2B	-2.03	1.46	1.50
22	B	601	CLA	MG-NB	-2.03	2.01	2.05
22	b	602	CLA	MG-NB	-2.03	2.01	2.05
22	B	601	CLA	CMB-C2B	-2.03	1.46	1.50
22	C	513	CLA	CMB-C2B	-2.03	1.46	1.50
22	c	513	CLA	CMB-C2B	-2.03	1.46	1.50
22	B	613	CLA	CMB-C2B	-2.03	1.46	1.50
32	C	523	LMT	O5'-C5'	-2.03	1.39	1.44
22	B	601	CLA	CMD-C2D	-2.03	1.46	1.50
22	b	615	CLA	CMB-C2B	-2.03	1.46	1.50
22	A	404	CLA	CHC-C1C	2.02	1.42	1.38
31	D	409	LHG	P-O6	2.02	1.67	1.59
27	a	411	SQD	O7-S	2.02	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	503	CLA	CMB-C2B	-2.02	1.46	1.50
22	c	503	CLA	CMB-C2B	-2.02	1.46	1.50
22	B	608	CLA	CMC-C2C	-2.02	1.46	1.50
22	b	609	CLA	CMC-C2C	-2.02	1.46	1.50
27	b	621	SQD	C8-C7	2.02	1.56	1.50
22	C	509	CLA	CMD-C2D	-2.02	1.46	1.50
22	c	509	CLA	CMD-C2D	-2.02	1.46	1.50
30	D	401	PHO	C3B-C2B	-2.02	1.37	1.40
22	b	607	CLA	CMD-C2D	-2.02	1.46	1.50
22	B	602	CLA	CMB-C2B	-2.02	1.46	1.50
22	b	603	CLA	CMB-C2B	-2.02	1.46	1.50
22	C	510	CLA	CMD-C2D	-2.02	1.46	1.50
22	B	606	CLA	CMD-C2D	-2.02	1.46	1.50
22	C	511	CLA	CMB-C2B	-2.02	1.46	1.50
22	a	419	CLA	CMB-C2B	-2.01	1.46	1.50
32	Z	101	LMT	O1'-C1'	-2.01	1.36	1.40
30	a	418	PHO	C4D-ND	-2.01	1.35	1.38
32	M	102	LMT	O4'-C4B	-2.01	1.38	1.43
22	D	404	CLA	CMD-C2D	-2.01	1.46	1.50
22	d	404	CLA	CMD-C2D	-2.01	1.46	1.50
22	B	607	CLA	CMD-C2D	-2.00	1.46	1.50
22	b	608	CLA	CMD-C2D	-2.00	1.46	1.50
28	a	413	DGD	O3G-C3G	-2.00	1.40	1.43
34	E	105	HEM	CMD-C2D	2.00	1.54	1.50
22	b	611	CLA	CMD-C2D	-2.00	1.46	1.50

All (855) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	v	201	HEC	CBB-CAB-C3B	-8.79	109.87	127.43
35	V	201	HEC	CBB-CAB-C3B	-8.77	109.91	127.43
35	V	201	HEC	CBC-CAC-C3C	-8.11	111.22	127.43
35	v	201	HEC	CBC-CAC-C3C	-8.11	111.22	127.43
22	B	604	CLA	C4A-NA-C1A	8.11	110.38	106.68
22	b	605	CLA	C4A-NA-C1A	8.11	110.38	106.68
22	B	612	CLA	C4A-NA-C1A	7.68	110.18	106.68
22	b	613	CLA	C4A-NA-C1A	7.68	110.18	106.68
22	b	614	CLA	C4A-NA-C1A	7.38	110.05	106.68
22	B	613	CLA	C4A-NA-C1A	7.37	110.04	106.68
22	C	509	CLA	C4A-NA-C1A	7.32	110.02	106.68
22	c	509	CLA	C4A-NA-C1A	7.32	110.02	106.68
22	A	405	CLA	C4A-NA-C1A	7.15	109.94	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	616	CLA	C4A-NA-C1A	7.13	109.93	106.68
22	b	617	CLA	C4A-NA-C1A	7.13	109.93	106.68
22	a	405	CLA	C4A-NA-C1A	7.06	109.90	106.68
22	C	511	CLA	C4A-NA-C1A	6.99	109.87	106.68
22	B	610	CLA	C4A-NA-C1A	6.97	109.86	106.68
22	D	404	CLA	C4A-NA-C1A	6.97	109.86	106.68
22	b	611	CLA	C4A-NA-C1A	6.97	109.86	106.68
22	d	404	CLA	C4A-NA-C1A	6.97	109.86	106.68
22	c	511	CLA	C4A-NA-C1A	6.87	109.81	106.68
22	C	507	CLA	C4A-NA-C1A	6.75	109.76	106.68
22	c	507	CLA	C4A-NA-C1A	6.75	109.76	106.68
22	C	505	CLA	C4A-NA-C1A	6.68	109.73	106.68
22	c	505	CLA	C4A-NA-C1A	6.68	109.73	106.68
22	B	611	CLA	C4A-NA-C1A	6.55	109.67	106.68
22	b	612	CLA	C4A-NA-C1A	6.55	109.67	106.68
22	C	502	CLA	C4A-NA-C1A	6.54	109.66	106.68
22	C	508	CLA	C4A-NA-C1A	6.47	109.63	106.68
22	c	502	CLA	C4A-NA-C1A	6.47	109.63	106.68
22	C	504	CLA	C4A-NA-C1A	6.46	109.62	106.68
22	c	504	CLA	C4A-NA-C1A	6.42	109.61	106.68
22	d	405	CLA	C4A-NA-C1A	6.40	109.60	106.68
22	B	615	CLA	C4A-NA-C1A	6.38	109.59	106.68
22	B	606	CLA	C4A-NA-C1A	6.37	109.58	106.68
22	b	607	CLA	C4A-NA-C1A	6.37	109.58	106.68
22	D	405	CLA	C4A-NA-C1A	6.32	109.56	106.68
22	b	616	CLA	C4A-NA-C1A	6.32	109.56	106.68
22	C	506	CLA	C4A-NA-C1A	6.32	109.56	106.68
22	c	506	CLA	C4A-NA-C1A	6.32	109.56	106.68
22	c	508	CLA	C4A-NA-C1A	6.30	109.55	106.68
22	B	609	CLA	C4A-NA-C1A	6.25	109.53	106.68
22	b	610	CLA	C4A-NA-C1A	6.23	109.52	106.68
22	c	512	CLA	C4A-NA-C1A	6.17	109.50	106.68
22	B	614	CLA	C4A-NA-C1A	6.15	109.48	106.68
22	b	615	CLA	C4A-NA-C1A	6.12	109.47	106.68
22	a	406	CLA	C4A-NA-C1A	6.07	109.45	106.68
22	A	406	CLA	C4A-NA-C1A	6.05	109.44	106.68
22	B	607	CLA	C4A-NA-C1A	6.01	109.42	106.68
22	b	608	CLA	C4A-NA-C1A	6.01	109.42	106.68
22	C	512	CLA	C4A-NA-C1A	5.99	109.41	106.68
22	c	510	CLA	C4A-NA-C1A	5.96	109.40	106.68
22	C	510	CLA	C4A-NA-C1A	5.93	109.38	106.68
22	C	501	CLA	C4A-NA-C1A	5.80	109.33	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	501	CLA	C4A-NA-C1A	5.80	109.33	106.68
22	a	404	CLA	C4A-NA-C1A	5.79	109.32	106.68
22	A	404	CLA	C4A-NA-C1A	5.79	109.32	106.68
22	B	602	CLA	C4A-NA-C1A	5.71	109.29	106.68
22	C	513	CLA	C4A-NA-C1A	5.71	109.29	106.68
22	b	603	CLA	C4A-NA-C1A	5.71	109.29	106.68
22	c	513	CLA	C4A-NA-C1A	5.71	109.29	106.68
22	C	503	CLA	C4A-NA-C1A	5.71	109.28	106.68
22	c	503	CLA	C4A-NA-C1A	5.71	109.28	106.68
22	B	608	CLA	C4A-NA-C1A	5.68	109.27	106.68
22	b	609	CLA	C4A-NA-C1A	5.68	109.27	106.68
33	d	403	BCT	O2-C-O1	5.58	133.95	119.68
22	A	419	CLA	C4A-NA-C1A	5.57	109.22	106.68
22	a	419	CLA	C4A-NA-C1A	5.57	109.22	106.68
33	D	403	BCT	O2-C-O1	5.56	133.91	119.68
24	a	408	PL9	C7-C3-C4	5.54	121.47	116.91
24	A	408	PL9	C7-C3-C4	5.50	121.44	116.91
22	B	605	CLA	C4A-NA-C1A	5.23	109.06	106.68
22	b	606	CLA	C4A-NA-C1A	5.23	109.06	106.68
30	a	418	PHO	C4D-CHA-CBD	-5.22	105.95	108.45
30	A	418	PHO	C4D-CHA-CBD	-5.19	105.97	108.45
24	D	407	PL9	C7-C3-C4	4.93	120.97	116.91
24	d	407	PL9	C7-C3-C4	4.91	120.95	116.91
30	D	401	PHO	C4D-CHA-CBD	-4.83	106.14	108.45
30	d	401	PHO	C4D-CHA-CBD	-4.82	106.14	108.45
22	B	601	CLA	C4A-NA-C1A	4.75	108.85	106.68
22	b	602	CLA	C4A-NA-C1A	4.70	108.82	106.68
31	a	420	LHG	O4-P-O5	4.40	132.91	112.44
31	A	420	LHG	O4-P-O5	4.39	132.88	112.44
31	l	101	LHG	O4-P-O5	4.36	132.70	112.44
31	L	101	LHG	O4-P-O5	4.33	132.61	112.44
31	d	410	LHG	O4-P-O5	4.33	132.60	112.44
31	D	410	LHG	O4-P-O5	4.32	132.56	112.44
31	D	411	LHG	O4-P-O5	4.27	132.30	112.44
31	d	411	LHG	O4-P-O5	4.26	132.28	112.44
31	d	409	LHG	O4-P-O5	4.20	132.00	112.44
31	D	409	LHG	O4-P-O5	4.20	131.98	112.44
22	B	603	CLA	C4A-NA-C1A	4.13	108.56	106.68
22	b	604	CLA	C4A-NA-C1A	4.13	108.56	106.68
24	A	408	PL9	C7-C3-C2	-4.10	118.56	123.39
24	a	408	PL9	C7-C3-C2	-4.10	118.56	123.39
27	b	621	SQD	O9-S-O7	-4.08	100.54	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	620	SQD	O9-S-O7	-4.05	100.67	113.82
28	a	413	DGD	O3G-C3G-C2G	-4.03	101.01	110.82
28	A	413	DGD	O3G-C3G-C2G	-4.03	101.02	110.82
27	A	411	SQD	O9-S-O7	-4.02	100.75	113.82
27	a	411	SQD	O9-S-O7	-4.01	100.78	113.82
27	B	620	SQD	O47-C7-C8	3.94	120.00	111.48
27	x	101	SQD	O9-S-O7	-3.92	101.07	113.82
27	X	101	SQD	O9-S-O7	-3.91	101.10	113.82
28	C	518	DGD	O3G-C3G-C2G	-3.86	101.43	110.82
24	D	407	PL9	C7-C3-C2	-3.86	118.84	123.39
27	A	412	SQD	O9-S-O7	-3.85	101.30	113.82
28	c	518	DGD	O3G-C3G-C2G	-3.85	101.46	110.82
27	a	412	SQD	O9-S-O7	-3.84	101.34	113.82
24	d	407	PL9	C7-C3-C2	-3.84	118.86	123.39
27	a	412	SQD	O47-C7-C8	3.79	119.68	111.48
32	c	523	LMT	C1'-O5'-C5'	-3.78	106.34	113.72
27	A	412	SQD	O47-C7-C8	3.77	119.64	111.48
27	b	621	SQD	O47-C7-C8	3.76	119.62	111.48
28	C	517	DGD	O3G-C3G-C2G	-3.75	101.69	110.82
28	c	517	DGD	O3G-C3G-C2G	-3.73	101.74	110.82
32	C	523	LMT	C1'-O5'-C5'	-3.67	106.55	113.72
35	v	201	HEC	C4D-ND-C1D	3.65	111.77	105.82
35	V	201	HEC	C4D-ND-C1D	3.61	111.71	105.82
30	a	418	PHO	C2B-C1B-NB	-3.57	106.85	109.43
30	A	418	PHO	C2B-C1B-NB	-3.54	106.87	109.43
27	A	411	SQD	O47-C7-C8	3.54	119.13	111.48
27	a	411	SQD	O47-C7-C8	3.53	119.12	111.48
22	C	511	CLA	C3B-C4B-NB	-3.42	107.48	110.53
27	X	101	SQD	C3-C4-C5	3.42	116.42	110.23
22	c	511	CLA	C3B-C4B-NB	-3.40	107.49	110.53
27	B	620	SQD	O7-S-C6	3.40	111.83	106.76
27	x	101	SQD	C3-C4-C5	3.39	116.38	110.23
27	A	411	SQD	O6-C1-C2	3.37	113.39	108.27
28	H	103	DGD	O3G-C3G-C2G	-3.36	102.65	110.82
27	a	411	SQD	O6-C1-C2	3.35	113.37	108.27
28	h	103	DGD	O3G-C3G-C2G	-3.35	102.66	110.82
22	C	502	CLA	C3B-C4B-NB	-3.33	107.56	110.53
22	c	502	CLA	C3B-C4B-NB	-3.33	107.56	110.53
28	C	519	DGD	O3G-C3G-C2G	-3.32	102.73	110.82
28	c	519	DGD	O3G-C3G-C2G	-3.32	102.75	110.82
30	d	401	PHO	O1D-CGD-CBD	3.31	129.75	124.72
22	c	512	CLA	O2D-CGD-O1D	-3.30	117.43	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	621	SQD	O7-S-C6	3.29	111.67	106.76
27	a	411	SQD	C1-O5-C5	-3.29	107.30	113.72
22	C	505	CLA	C3B-C4B-NB	-3.29	107.60	110.53
22	c	505	CLA	C3B-C4B-NB	-3.29	107.60	110.53
22	b	612	CLA	C3B-C4B-NB	-3.28	107.60	110.53
27	A	411	SQD	C1-O5-C5	-3.27	107.33	113.72
28	c	518	DGD	O6D-C1D-O3G	-3.27	102.31	110.04
28	C	518	DGD	O6D-C1D-O3G	-3.27	102.32	110.04
22	C	512	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
30	D	401	PHO	O1D-CGD-CBD	3.26	129.66	124.72
22	B	610	CLA	C3B-C4B-NB	-3.24	107.64	110.53
22	b	611	CLA	C3B-C4B-NB	-3.24	107.64	110.53
22	D	404	CLA	C3B-C4B-NB	-3.23	107.64	110.53
22	d	404	CLA	C3B-C4B-NB	-3.23	107.64	110.53
22	B	611	CLA	C3B-C4B-NB	-3.23	107.65	110.53
22	A	406	CLA	C3B-C4B-NB	-3.23	107.65	110.53
22	B	602	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
22	B	607	CLA	C3B-C4B-NB	-3.21	107.66	110.53
22	a	405	CLA	C3B-C4B-NB	-3.21	107.66	110.53
22	b	603	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
22	B	615	CLA	C3B-C4B-NB	-3.20	107.67	110.53
22	B	612	CLA	C3B-C4B-NB	-3.19	107.68	110.53
22	b	613	CLA	C3B-C4B-NB	-3.19	107.68	110.53
22	a	406	CLA	C3B-C4B-NB	-3.19	107.69	110.53
22	A	405	CLA	C3B-C4B-NB	-3.18	107.69	110.53
22	b	608	CLA	C3B-C4B-NB	-3.18	107.69	110.53
22	b	616	CLA	C3B-C4B-NB	-3.18	107.69	110.53
22	c	504	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
22	B	615	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
22	b	616	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
22	c	509	CLA	C3B-C4B-NB	-3.16	107.71	110.53
28	c	519	DGD	O6D-C1D-O3G	-3.16	102.58	110.04
28	C	519	DGD	O6D-C1D-O3G	-3.15	102.60	110.04
22	B	608	CLA	C3B-C4B-NB	-3.15	107.72	110.53
22	b	609	CLA	C3B-C4B-NB	-3.15	107.72	110.53
22	C	504	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
22	C	509	CLA	C3B-C4B-NB	-3.14	107.73	110.53
33	d	403	BCT	O3-C-O1	-3.14	111.65	119.68
22	b	612	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
33	D	403	BCT	O3-C-O1	-3.13	111.66	119.68
22	B	611	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
22	b	603	CLA	C3B-C4B-NB	-3.13	107.74	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	419	CLA	CHB-C4A-NA	3.12	128.90	124.40
22	a	419	CLA	CHB-C4A-NA	3.12	128.90	124.40
22	B	613	CLA	C3B-C4B-NB	-3.12	107.75	110.53
22	c	501	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
22	b	614	CLA	C3B-C4B-NB	-3.10	107.76	110.53
22	B	602	CLA	C3B-C4B-NB	-3.10	107.77	110.53
22	C	501	CLA	O2D-CGD-O1D	-3.08	117.84	123.85
27	A	411	SQD	O9-S-C6	3.08	111.35	106.76
22	C	501	CLA	C3B-C4B-NB	-3.07	107.79	110.53
22	b	606	CLA	C3B-C4B-NB	-3.06	107.79	110.53
32	e	104	LMT	C3'-C4'-C5'	-3.06	104.68	110.23
22	B	605	CLA	C3B-C4B-NB	-3.06	107.80	110.53
27	a	411	SQD	O9-S-C6	3.06	111.32	106.76
22	c	501	CLA	C3B-C4B-NB	-3.05	107.80	110.53
22	d	404	CLA	O2D-CGD-O1D	-3.05	117.90	123.85
22	D	404	CLA	O2D-CGD-O1D	-3.05	117.90	123.85
22	C	507	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
22	c	507	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
32	E	104	LMT	C3'-C4'-C5'	-3.04	104.71	110.23
22	B	609	CLA	C3B-C4B-NB	-3.04	107.82	110.53
22	b	610	CLA	C3B-C4B-NB	-3.04	107.82	110.53
27	A	412	SQD	O7-S-C6	3.03	111.27	106.76
22	C	509	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
22	c	509	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
22	B	603	CLA	C3B-C4B-NB	-3.00	107.85	110.53
22	b	604	CLA	C3B-C4B-NB	-3.00	107.85	110.53
27	b	621	SQD	O9-S-C6	2.99	111.22	106.76
22	c	512	CLA	CHB-C4A-NA	2.99	128.71	124.40
23	B	619	BCR	C2-C1-C6	2.99	114.78	110.44
23	b	620	BCR	C2-C1-C6	2.98	114.77	110.44
23	K	101	BCR	C27-C26-C25	2.98	126.73	122.70
23	k	101	BCR	C27-C26-C25	2.98	126.73	122.70
22	B	603	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
27	a	412	SQD	O7-S-C6	2.98	111.20	106.76
22	C	508	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
22	c	508	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
32	J	102	LMT	C3'-C4'-C5'	-2.97	104.84	110.23
22	C	512	CLA	CHB-C4A-NA	2.97	128.68	124.40
22	a	405	CLA	O2D-CGD-CBD	2.96	116.41	111.23
32	j	102	LMT	C3'-C4'-C5'	-2.96	104.86	110.23
22	a	405	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
31	A	420	LHG	O8-C23-C24	2.96	120.86	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	405	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
22	b	604	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
27	a	412	SQD	O9-S-C6	2.96	111.17	106.76
22	B	614	CLA	C3B-C4B-NB	-2.96	107.89	110.53
22	b	615	CLA	C3B-C4B-NB	-2.96	107.89	110.53
22	A	405	CLA	O2D-CGD-CBD	2.95	116.39	111.23
22	C	510	CLA	C3B-C4B-NB	-2.95	107.90	110.53
22	c	510	CLA	C3B-C4B-NB	-2.95	107.90	110.53
22	A	419	CLA	C3B-C4B-NB	-2.95	107.90	110.53
22	a	419	CLA	C3B-C4B-NB	-2.95	107.90	110.53
22	C	508	CLA	CHB-C4A-NA	2.94	128.65	124.40
22	b	617	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
22	B	614	CLA	CHB-C4A-NA	2.94	128.64	124.40
22	A	404	CLA	C3B-C4B-NB	-2.94	107.91	110.53
22	b	615	CLA	CHB-C4A-NA	2.94	128.64	124.40
24	A	408	PL9	C27-C28-C29	-2.93	120.91	127.62
27	x	101	SQD	O7-S-C6	2.93	111.13	106.76
31	a	420	LHG	O8-C23-C24	2.93	120.77	111.83
22	B	616	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
27	A	412	SQD	O9-S-C6	2.93	111.13	106.76
22	B	610	CLA	CHB-C4A-NA	2.92	128.62	124.40
22	b	611	CLA	CHB-C4A-NA	2.92	128.62	124.40
24	a	408	PL9	C27-C28-C29	-2.92	120.94	127.62
23	b	618	BCR	C33-C5-C6	-2.92	121.30	124.48
22	c	508	CLA	CHB-C4A-NA	2.92	128.61	124.40
22	B	612	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
22	a	404	CLA	C3B-C4B-NB	-2.91	107.93	110.53
27	X	101	SQD	O9-S-C6	2.90	111.09	106.76
22	C	513	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
27	X	101	SQD	O7-S-C6	2.90	111.08	106.76
22	C	507	CLA	CHB-C4A-NA	2.90	128.58	124.40
22	c	507	CLA	CHB-C4A-NA	2.90	128.58	124.40
22	B	605	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
22	B	608	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
22	c	513	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
22	b	613	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
27	x	101	SQD	O5-C5-C4	2.89	114.91	109.70
27	x	101	SQD	O9-S-C6	2.89	111.07	106.76
22	C	512	CLA	C3B-C4B-NB	-2.89	107.95	110.53
22	C	503	CLA	C3B-C4B-NB	-2.88	107.96	110.53
22	c	503	CLA	C3B-C4B-NB	-2.88	107.96	110.53
22	c	512	CLA	C3B-C4B-NB	-2.88	107.96	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	609	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
22	b	602	CLA	C3B-C4B-NB	-2.85	107.98	110.53
22	B	604	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
22	b	605	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
22	C	513	CLA	C3B-C4B-NB	-2.85	107.99	110.53
30	d	401	PHO	C2B-C1B-NB	-2.84	107.38	109.43
22	b	606	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
27	X	101	SQD	O5-C5-C4	2.84	114.82	109.70
23	b	619	BCR	C27-C26-C25	2.83	126.53	122.70
32	b	624	LMT	C1'-O5'-C5'	-2.83	108.20	113.72
27	B	620	SQD	O48-C23-C24	2.83	120.45	111.83
22	A	405	CLA	C9-C8-C10	2.83	121.34	111.27
32	c	525	LMT	C3'-C4'-C5'	-2.82	104.67	110.93
32	Z	101	LMT	C1'-O5'-C5'	-2.82	108.21	113.72
24	a	408	PL9	C40-C39-C41	2.82	120.13	115.23
23	D	406	BCR	C27-C26-C25	2.82	126.52	122.70
23	B	617	BCR	C33-C5-C6	-2.82	121.41	124.48
22	a	404	CLA	CHB-C4A-NA	2.82	128.47	124.40
32	B	623	LMT	C1'-O5'-C5'	-2.81	108.23	113.72
22	D	405	CLA	C3B-C4B-NB	-2.81	108.02	110.53
22	d	405	CLA	C3B-C4B-NB	-2.81	108.02	110.53
22	A	404	CLA	CHB-C4A-NA	2.81	128.45	124.40
28	a	413	DGD	O6D-C1D-O3G	-2.80	103.42	110.04
27	a	411	SQD	O7-S-C6	2.80	110.94	106.76
32	z	101	LMT	C1'-O5'-C5'	-2.80	108.25	113.72
22	B	601	CLA	C3B-C4B-NB	-2.80	108.03	110.53
22	c	513	CLA	C3B-C4B-NB	-2.80	108.03	110.53
22	b	614	CLA	CHB-C4A-NA	2.80	128.44	124.40
24	A	408	PL9	C40-C39-C41	2.80	120.09	115.23
22	B	607	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
22	B	613	CLA	CHB-C4A-NA	2.80	128.44	124.40
32	C	525	LMT	C3'-C4'-C5'	-2.80	104.73	110.93
27	A	411	SQD	O7-S-C6	2.80	110.93	106.76
23	A	407	BCR	C27-C26-C25	2.79	126.48	122.70
23	a	407	BCR	C27-C26-C25	2.79	126.48	122.70
22	b	607	CLA	C3B-C4B-NB	-2.79	108.04	110.53
22	B	616	CLA	C3B-C4B-NB	-2.79	108.04	110.53
22	b	617	CLA	C3B-C4B-NB	-2.79	108.04	110.53
23	d	406	BCR	C27-C26-C25	2.79	126.47	122.70
26	c	520	LMG	O6-C1-O1	-2.79	103.46	110.04
30	D	401	PHO	C2B-C1B-NB	-2.79	107.42	109.43
28	A	413	DGD	O6D-C1D-O3G	-2.78	103.46	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	608	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
22	C	506	CLA	C3B-C4B-NB	-2.78	108.05	110.53
22	c	506	CLA	C3B-C4B-NB	-2.78	108.05	110.53
26	C	520	LMG	O6-C1-O1	-2.78	103.48	110.04
30	d	401	PHO	CMB-C2B-C3B	2.78	130.23	124.68
22	b	613	CLA	CHB-C4A-NA	2.77	128.40	124.40
22	C	511	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
22	c	511	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
23	B	618	BCR	C27-C26-C25	2.77	126.44	122.70
28	a	413	DGD	C3G-C2G-C1G	-2.77	105.33	111.78
22	B	606	CLA	C3B-C4B-NB	-2.77	108.06	110.53
24	A	408	PL9	C22-C23-C24	-2.77	121.29	127.62
32	m	101	LMT	C3'-C4'-C5'	-2.76	104.80	110.93
22	B	612	CLA	CHB-C4A-NA	2.76	128.39	124.40
23	t	102	BCR	C7-C8-C9	-2.76	122.15	126.23
32	M	102	LMT	C3'-C4'-C5'	-2.76	104.81	110.93
23	b	620	BCR	C27-C26-C25	2.76	126.44	122.70
22	C	508	CLA	C3B-C4B-NB	-2.76	108.07	110.53
22	c	508	CLA	C3B-C4B-NB	-2.76	108.07	110.53
23	T	101	BCR	C7-C8-C9	-2.76	122.16	126.23
30	D	401	PHO	CMB-C2B-C3B	2.76	130.19	124.68
26	c	524	LMG	C1-O6-C5	-2.76	108.34	113.72
23	T	101	BCR	C33-C5-C6	-2.75	121.48	124.48
23	B	619	BCR	C27-C26-C25	2.75	126.42	122.70
30	a	418	PHO	CMB-C2B-C3B	2.74	130.16	124.68
23	h	102	BCR	C24-C23-C22	-2.74	122.18	126.23
23	t	102	BCR	C33-C5-C6	-2.74	121.50	124.48
23	H	102	BCR	C24-C23-C22	-2.73	122.19	126.23
32	c	523	LMT	C4'-C3'-C2'	2.73	115.62	110.83
22	B	605	CLA	C4-C3-C5	2.73	119.96	115.23
22	b	605	CLA	C3B-C4B-NB	-2.73	108.10	110.53
30	A	418	PHO	CMB-C2B-C3B	2.72	130.12	124.68
22	C	513	CLA	CHB-C4A-NA	2.72	128.32	124.40
22	c	513	CLA	CHB-C4A-NA	2.72	128.32	124.40
22	b	606	CLA	C4-C3-C5	2.72	119.94	115.23
26	C	524	LMG	C1-O6-C5	-2.71	108.42	113.72
23	b	618	BCR	C2-C1-C6	2.71	114.38	110.44
28	c	517	DGD	O6D-C1D-O3G	-2.71	103.64	110.04
22	b	607	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
22	C	507	CLA	C3B-C4B-NB	-2.71	108.11	110.53
22	c	507	CLA	C3B-C4B-NB	-2.71	108.11	110.53
28	C	517	DGD	O6D-C1D-O3G	-2.70	103.65	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	610	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
22	b	611	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
28	h	103	DGD	CDB-CCB-CBB	-2.70	100.72	114.37
22	B	614	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
28	H	103	DGD	CDB-CCB-CBB	-2.70	100.74	114.37
24	a	408	PL9	C22-C23-C24	-2.70	121.45	127.62
22	c	510	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
22	B	604	CLA	C3B-C4B-NB	-2.69	108.13	110.53
22	C	510	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
22	d	405	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
23	B	617	BCR	C2-C1-C6	2.69	114.34	110.44
22	B	606	CLA	CHB-C4A-NA	2.68	128.27	124.40
22	b	607	CLA	CHB-C4A-NA	2.68	128.27	124.40
22	B	606	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
22	d	405	CLA	CHB-C4A-NA	2.68	128.26	124.40
31	d	409	LHG	O8-C23-C24	2.67	119.99	111.83
22	C	504	CLA	C3B-C4B-NB	-2.67	108.14	110.53
22	c	504	CLA	C3B-C4B-NB	-2.67	108.14	110.53
22	D	405	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
23	C	514	BCR	C33-C5-C6	-2.67	121.58	124.48
22	b	615	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
31	D	409	LHG	O8-C23-C24	2.67	119.96	111.83
28	C	517	DGD	CDB-CCB-CBB	-2.67	100.89	114.37
28	A	413	DGD	C3G-C2G-C1G	-2.67	105.57	111.78
22	B	604	CLA	C1-C2-C3	-2.66	121.83	126.20
22	b	605	CLA	C1-C2-C3	-2.66	121.83	126.20
22	b	602	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
22	C	505	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
22	c	505	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
28	c	517	DGD	CDB-CCB-CBB	-2.66	100.94	114.37
23	c	514	BCR	C33-C5-C6	-2.66	121.58	124.48
23	k	103	BCR	C33-C5-C6	-2.66	121.59	124.48
22	B	601	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
22	D	405	CLA	CHB-C4A-NA	2.65	128.23	124.40
35	v	201	HEC	C2A-C1A-NA	-2.65	107.77	110.32
26	D	408	LMG	O6-C1-O1	-2.65	103.79	110.04
22	a	405	CLA	CHB-C4A-NA	2.64	128.21	124.40
23	K	103	BCR	C33-C5-C6	-2.63	121.61	124.48
26	d	408	LMG	O6-C1-O1	-2.63	103.83	110.04
30	d	401	PHO	O2D-CGD-O1D	-2.63	118.73	123.85
23	K	103	BCR	C27-C26-C25	2.63	126.26	122.70
22	b	602	CLA	O2A-CGA-O1A	-2.63	117.06	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	502	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
22	B	601	CLA	O2A-CGA-O1A	-2.62	117.07	123.63
22	A	405	CLA	CHB-C4A-NA	2.62	128.18	124.40
22	C	502	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
28	H	103	DGD	O6D-C1D-O3G	-2.61	103.87	110.04
28	h	103	DGD	O6D-C1D-O3G	-2.61	103.87	110.04
22	C	506	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
22	c	506	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
35	V	201	HEC	C2A-C1A-NA	-2.61	107.81	110.32
27	b	621	SQD	O48-C23-C24	2.60	119.77	111.83
32	B	623	LMT	C3'-C4'-C5'	-2.60	105.17	110.93
32	b	624	LMT	C3'-C4'-C5'	-2.60	105.17	110.93
23	k	103	BCR	C27-C26-C25	2.60	126.22	122.70
31	d	411	LHG	O8-C23-C24	2.60	119.75	111.83
31	L	101	LHG	O8-C23-C24	2.59	119.74	111.83
22	b	602	CLA	CHB-C4A-NA	2.59	128.14	124.40
23	b	618	BCR	C29-C30-C25	2.59	114.20	110.44
23	T	101	BCR	C27-C26-C25	2.59	126.20	122.70
31	D	411	LHG	O8-C23-C24	2.59	119.73	111.83
31	a	420	LHG	C11-C10-C9	-2.59	101.29	114.37
27	B	620	SQD	O9-S-C6	2.59	110.62	106.76
30	D	401	PHO	O2D-CGD-O1D	-2.58	118.82	123.85
22	B	601	CLA	CHB-C4A-NA	2.58	128.13	124.40
22	c	510	CLA	CHB-C4A-NA	2.58	128.13	124.40
31	l	101	LHG	O8-C23-C24	2.58	119.71	111.83
23	t	102	BCR	C27-C26-C25	2.58	126.19	122.70
23	B	617	BCR	C29-C30-C25	2.58	114.19	110.44
24	d	407	PL9	C22-C23-C24	-2.58	121.72	127.62
22	C	510	CLA	CHB-C4A-NA	2.58	128.12	124.40
31	A	420	LHG	C11-C10-C9	-2.58	101.33	114.37
24	D	407	PL9	C22-C23-C24	-2.58	121.72	127.62
22	b	602	CLA	C1-C2-C3	-2.58	121.97	126.20
26	D	402	LMG	O1-C7-C8	-2.58	105.15	111.77
27	X	101	SQD	O48-C23-C24	2.57	119.67	111.83
22	b	612	CLA	C1-C2-C3	-2.57	121.99	126.20
22	B	607	CLA	CHB-C4A-NA	2.57	128.11	124.40
22	b	608	CLA	CHB-C4A-NA	2.57	128.11	124.40
26	d	402	LMG	O1-C7-C8	-2.56	105.18	111.77
22	B	601	CLA	C1-C2-C3	-2.56	122.01	126.20
23	c	514	BCR	C27-C26-C25	2.56	126.16	122.70
27	x	101	SQD	O48-C23-C24	2.55	119.61	111.83
32	M	102	LMT	C1'-O5'-C5'	-2.54	108.76	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	m	101	LMT	C1'-O5'-C5'	-2.54	108.76	113.72
24	a	408	PL9	C7-C8-C9	-2.54	122.46	126.83
22	c	508	CLA	O2D-CGD-CBD	2.53	115.66	111.23
23	C	514	BCR	C27-C26-C25	2.53	126.12	122.70
22	B	602	CLA	O2D-CGD-CBD	2.53	115.65	111.23
27	A	411	SQD	O48-C23-C24	2.53	119.54	111.83
26	H	101	LMG	O1-C7-C8	-2.52	105.28	111.77
22	B	611	CLA	C1-C2-C3	-2.52	122.06	126.20
27	a	411	SQD	O48-C23-C24	2.52	119.53	111.83
26	h	101	LMG	O1-C7-C8	-2.52	105.29	111.77
23	a	407	BCR	C2-C1-C6	2.52	114.10	110.44
23	C	515	BCR	C15-C16-C17	-2.52	118.36	123.52
23	c	514	BCR	C15-C16-C17	-2.52	118.37	123.52
22	C	508	CLA	O2D-CGD-CBD	2.52	115.63	111.23
23	A	407	BCR	C2-C1-C6	2.51	114.09	110.44
23	c	515	BCR	C15-C16-C17	-2.51	118.38	123.52
22	a	406	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
27	a	412	SQD	O48-C23-C24	2.51	119.49	111.83
23	c	514	BCR	C2-C1-C6	2.51	114.08	110.44
27	A	412	SQD	O48-C23-C24	2.51	119.47	111.83
22	C	504	CLA	CHB-C4A-NA	2.50	128.01	124.40
22	c	504	CLA	CHB-C4A-NA	2.50	128.01	124.40
22	C	501	CLA	CHB-C4A-NA	2.50	128.01	124.40
22	c	501	CLA	CHB-C4A-NA	2.50	128.01	124.40
24	d	407	PL9	C20-C19-C21	2.50	119.57	115.23
23	C	514	BCR	C2-C1-C6	2.50	114.08	110.44
22	B	615	CLA	CHB-C4A-NA	2.50	128.01	124.40
23	k	101	BCR	C33-C5-C6	-2.49	121.76	124.48
24	A	408	PL9	C7-C8-C9	-2.49	122.54	126.83
23	K	101	BCR	C33-C5-C6	-2.49	121.76	124.48
22	b	603	CLA	O2D-CGD-CBD	2.49	115.59	111.23
23	H	102	BCR	C15-C16-C17	-2.49	118.42	123.52
22	C	506	CLA	CHB-C4A-NA	2.49	127.99	124.40
22	c	506	CLA	CHB-C4A-NA	2.49	127.99	124.40
23	C	514	BCR	C15-C16-C17	-2.49	118.43	123.52
22	B	603	CLA	CHB-C4A-NA	2.49	127.99	124.40
22	b	604	CLA	CHB-C4A-NA	2.49	127.99	124.40
23	h	102	BCR	C15-C16-C17	-2.48	118.45	123.52
22	b	616	CLA	CHB-C4A-NA	2.47	127.97	124.40
22	A	406	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
26	C	524	LMG	O2-C2-C1	-2.47	104.19	110.08
23	C	515	BCR	C27-C26-C25	2.47	126.04	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	515	BCR	C27-C26-C25	2.47	126.04	122.70
23	a	407	BCR	C33-C5-C6	-2.47	121.79	124.48
23	H	102	BCR	C33-C5-C6	-2.47	121.79	124.48
28	c	518	DGD	C1D-C2D-C3D	-2.46	104.83	110.01
26	c	524	LMG	O2-C2-C1	-2.46	104.20	110.08
23	B	618	BCR	C33-C5-C6	-2.46	121.80	124.48
26	D	408	LMG	C40-C39-C38	-2.46	101.92	114.37
26	d	408	LMG	C40-C39-C38	-2.46	101.94	114.37
24	D	407	PL9	C20-C19-C21	2.46	119.49	115.23
22	B	609	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
23	h	102	BCR	C33-C5-C6	-2.46	121.81	124.48
23	C	515	BCR	C33-C5-C6	-2.45	121.81	124.48
23	c	515	BCR	C33-C5-C6	-2.45	121.81	124.48
22	C	509	CLA	CHB-C4A-NA	2.45	127.94	124.40
31	D	410	LHG	O8-C23-C24	2.45	119.31	111.83
28	C	518	DGD	C1D-C2D-C3D	-2.45	104.86	110.01
31	D	411	LHG	C11-C10-C9	-2.45	102.00	114.37
31	d	411	LHG	C11-C10-C9	-2.45	102.00	114.37
22	a	406	CLA	CHB-C4A-NA	2.45	127.93	124.40
22	b	610	CLA	O2D-CGD-O1D	-2.45	119.09	123.85
22	b	610	CLA	O1D-CGD-CBD	2.44	129.34	124.52
22	c	509	CLA	CHB-C4A-NA	2.44	127.92	124.40
31	d	410	LHG	O8-C23-C24	2.44	119.27	111.83
22	B	608	CLA	CHB-C4A-NA	2.44	127.92	124.40
22	b	609	CLA	CHB-C4A-NA	2.44	127.92	124.40
22	A	406	CLA	CHB-C4A-NA	2.43	127.91	124.40
22	C	503	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
22	c	503	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
22	B	609	CLA	O1D-CGD-CBD	2.43	129.30	124.52
26	b	625	LMG	O6-C1-O1	-2.42	104.32	110.04
22	b	612	CLA	O2D-CGD-CBD	2.42	115.47	111.23
23	A	407	BCR	C33-C5-C6	-2.42	121.84	124.48
22	c	508	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
23	b	619	BCR	C33-C5-C6	-2.42	121.84	124.48
26	A	410	LMG	O6-C1-O1	-2.42	104.33	110.04
23	D	406	BCR	C33-C5-C6	-2.42	121.85	124.48
28	C	519	DGD	CDB-CCB-CBB	-2.42	102.16	114.37
22	B	611	CLA	O2D-CGD-CBD	2.41	115.45	111.23
28	c	519	DGD	CDB-CCB-CBB	-2.41	102.17	114.37
32	C	523	LMT	C4'-C3'-C2'	2.41	115.06	110.83
26	a	410	LMG	O6-C1-O1	-2.40	104.37	110.04
34	E	105	HEM	C1B-NB-C4B	2.40	108.05	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	509	CLA	C1-C2-C3	-2.40	122.27	126.20
22	c	509	CLA	C1-C2-C3	-2.40	122.27	126.20
34	e	105	HEM	C1B-NB-C4B	2.40	108.05	105.21
26	B	624	LMG	O6-C1-O1	-2.40	104.38	110.04
31	D	410	LHG	C11-C10-C9	-2.40	102.26	114.37
22	C	508	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
26	c	524	LMG	C38-C37-C36	-2.38	102.32	114.37
27	b	621	SQD	O8-S-C6	2.38	110.57	105.97
26	C	524	LMG	C38-C37-C36	-2.38	102.33	114.37
22	b	617	CLA	CHB-C4A-NA	2.38	127.83	124.40
24	d	407	PL9	C27-C28-C29	-2.38	122.18	127.62
31	d	411	LHG	C20-C19-C18	-2.37	102.37	114.37
23	d	406	BCR	C33-C5-C6	-2.37	121.90	124.48
22	A	406	CLA	O2D-CGD-CBD	2.37	115.37	111.23
22	B	616	CLA	CHB-C4A-NA	2.37	127.82	124.40
31	D	411	LHG	C20-C19-C18	-2.37	102.40	114.37
24	D	407	PL9	C27-C28-C29	-2.37	122.21	127.62
22	a	406	CLA	O2D-CGD-CBD	2.36	115.36	111.23
27	X	101	SQD	O8-S-C6	2.36	110.52	105.97
26	b	625	LMG	C38-C37-C36	-2.36	102.46	114.37
28	H	103	DGD	C3D-C4D-C5D	-2.35	105.97	110.23
28	h	103	DGD	C3D-C4D-C5D	-2.35	105.97	110.23
28	A	413	DGD	CDB-CCB-CBB	-2.35	102.50	114.37
26	B	624	LMG	C38-C37-C36	-2.35	102.51	114.37
26	h	101	LMG	C40-C39-C38	-2.34	102.53	114.37
26	B	624	LMG	C40-C39-C38	-2.34	102.56	114.37
27	x	101	SQD	O8-S-C6	2.34	110.48	105.97
26	H	101	LMG	C40-C39-C38	-2.33	102.57	114.37
24	A	408	PL9	O2-C1-C6	2.33	124.19	120.48
24	a	408	PL9	O2-C1-C6	2.33	124.19	120.48
23	K	101	BCR	C2-C1-C6	2.33	113.82	110.44
26	b	625	LMG	C40-C39-C38	-2.33	102.59	114.37
31	d	410	LHG	C11-C10-C9	-2.32	102.63	114.37
24	a	408	PL9	C12-C13-C14	-2.32	122.31	127.62
28	a	413	DGD	CDB-CCB-CBB	-2.32	102.66	114.37
27	a	411	SQD	O8-S-C6	2.32	110.44	105.97
22	b	614	CLA	O2D-CGD-O1D	-2.32	119.34	123.85
28	c	517	DGD	C3G-C2G-C1G	-2.31	106.39	111.78
30	a	418	PHO	O2D-CGD-O1D	-2.31	119.35	123.85
22	C	509	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
22	c	509	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
27	A	411	SQD	O8-S-C6	2.31	110.43	105.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	k	101	BCR	C2-C1-C6	2.31	113.79	110.44
32	J	102	LMT	C1'-O5'-C5'	-2.31	109.22	113.72
28	C	517	DGD	C3G-C2G-C1G	-2.30	106.41	111.78
28	C	518	DGD	CDB-CCB-CBB	-2.30	102.73	114.37
28	c	518	DGD	CDB-CCB-CBB	-2.30	102.73	114.37
32	j	102	LMT	C1'-O5'-C5'	-2.30	109.23	113.72
31	D	411	LHG	C18-C17-C16	-2.29	102.77	114.37
31	d	411	LHG	C18-C17-C16	-2.29	102.77	114.37
22	C	506	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
25	B	622	STE	C3-C2-C1	-2.29	108.54	114.51
22	B	609	CLA	CHB-C4A-NA	2.28	127.69	124.40
25	b	623	STE	C3-C2-C1	-2.28	108.55	114.51
26	c	520	LMG	O1-C7-C8	-2.28	105.27	110.82
30	A	418	PHO	O2D-CGD-O1D	-2.28	119.41	123.85
22	b	610	CLA	CHB-C4A-NA	2.27	127.68	124.40
22	B	613	CLA	O2D-CGD-O1D	-2.27	119.42	123.85
22	c	506	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
26	C	520	LMG	O1-C7-C8	-2.27	105.29	110.82
30	D	401	PHO	C1-C2-C3	-2.27	122.48	126.20
23	K	101	BCR	C24-C23-C22	-2.27	122.88	126.23
23	k	101	BCR	C24-C23-C22	-2.27	122.88	126.23
30	a	418	PHO	O1D-CGD-CBD	2.27	128.16	124.72
28	c	517	DGD	O5D-C6D-C5D	-2.27	104.31	109.42
32	e	104	LMT	C1'-O5'-C5'	-2.26	109.30	113.72
31	l	101	LHG	C11-C10-C9	-2.26	102.94	114.37
31	A	420	LHG	C20-C19-C18	-2.26	102.95	114.37
24	A	408	PL9	C12-C13-C14	-2.26	122.45	127.62
34	E	105	HEM	C4D-ND-C1D	2.26	107.88	105.21
22	A	419	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
31	L	101	LHG	C11-C10-C9	-2.25	102.98	114.37
22	C	505	CLA	C1-C2-C3	-2.25	122.51	126.20
31	a	420	LHG	C20-C19-C18	-2.25	102.99	114.37
24	d	407	PL9	C12-C13-C14	-2.25	122.48	127.62
28	C	517	DGD	O5D-C6D-C5D	-2.25	104.36	109.42
22	B	604	CLA	CHB-C4A-NA	2.25	127.64	124.40
22	b	605	CLA	CHB-C4A-NA	2.25	127.64	124.40
32	E	104	LMT	C1'-O5'-C5'	-2.24	109.34	113.72
34	e	105	HEM	C3B-C4B-NB	-2.24	107.86	109.47
26	C	524	LMG	O6-C1-O1	-2.24	104.74	110.04
22	B	611	CLA	CHB-C4A-NA	2.24	127.63	124.40
22	b	612	CLA	CHB-C4A-NA	2.24	127.63	124.40
24	D	407	PL9	O2-C1-C6	2.24	124.04	120.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	407	PL9	O2-C1-C6	2.24	124.04	120.48
26	C	524	LMG	O7-C10-O9	-2.24	118.47	123.70
22	A	405	CLA	O2A-CGA-O1A	-2.24	118.04	123.63
26	C	520	LMG	O3-C3-C2	-2.23	105.11	110.38
23	b	619	BCR	C38-C26-C25	-2.23	122.05	124.48
30	d	401	PHO	C1-C2-C3	-2.23	122.54	126.20
24	D	407	PL9	C12-C13-C14	-2.23	122.52	127.62
31	A	420	LHG	C18-C17-C16	-2.23	103.09	114.37
22	c	505	CLA	C1-C2-C3	-2.23	122.54	126.20
26	c	520	LMG	O3-C3-C2	-2.23	105.12	110.38
22	a	405	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
30	A	418	PHO	O1D-CGD-CBD	2.23	128.10	124.72
28	A	413	DGD	C1D-C2D-C3D	-2.23	105.33	110.01
26	c	520	LMG	O2-C2-C1	-2.22	104.77	110.08
22	C	511	CLA	CHB-C4A-NA	2.22	127.61	124.40
31	a	420	LHG	C18-C17-C16	-2.22	103.12	114.37
34	e	105	HEM	C4D-ND-C1D	2.22	107.84	105.21
24	a	408	PL9	C37-C38-C39	-2.22	122.54	127.62
28	A	413	DGD	O6E-C1E-O5D	-2.22	104.80	110.04
22	a	419	CLA	O2D-CGD-O1D	-2.22	119.53	123.85
23	b	618	BCR	C7-C8-C9	-2.21	122.96	126.23
28	a	413	DGD	C1D-C2D-C3D	-2.21	105.35	110.01
28	a	413	DGD	O6E-C1E-O5D	-2.21	104.83	110.04
23	B	619	BCR	C38-C26-C25	-2.21	122.08	124.48
24	A	408	PL9	C37-C38-C39	-2.21	122.58	127.62
26	c	524	LMG	O7-C10-O9	-2.21	118.55	123.70
22	A	419	CLA	O2D-CGD-CBD	2.21	115.08	111.23
23	B	617	BCR	C7-C8-C9	-2.20	122.97	126.23
26	C	520	LMG	O2-C2-C1	-2.20	104.82	110.08
22	b	614	CLA	C1-C2-C3	-2.20	122.59	126.20
26	c	520	LMG	O1-C1-C2	-2.20	104.93	108.27
34	e	105	HEM	CBD-CAD-C3D	-2.20	106.45	112.53
26	a	410	LMG	O3-C3-C2	-2.20	105.19	110.38
34	E	105	HEM	CBD-CAD-C3D	-2.20	106.45	112.53
31	L	101	LHG	C20-C19-C18	-2.20	103.25	114.37
31	l	101	LHG	C20-C19-C18	-2.20	103.25	114.37
24	D	407	PL9	C7-C8-C9	-2.20	123.04	126.83
28	c	517	DGD	C4E-C3E-C2E	-2.20	106.97	110.83
31	D	409	LHG	C20-C19-C18	-2.20	103.26	114.37
24	d	407	PL9	C7-C8-C9	-2.20	123.05	126.83
22	c	501	CLA	O2D-CGD-CBD	2.20	115.07	111.23
24	A	408	PL9	O2-C1-C2	-2.19	116.84	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	E	105	HEM	C3B-C4B-NB	-2.19	107.89	109.47
28	a	413	DGD	CBB-CAB-C9B	-2.19	103.28	114.37
26	A	410	LMG	O3-C3-C2	-2.19	105.21	110.38
31	d	409	LHG	C20-C19-C18	-2.19	103.30	114.37
22	B	613	CLA	C1-C2-C3	-2.19	122.61	126.20
23	D	406	BCR	C2-C1-C6	2.19	113.61	110.44
22	D	404	CLA	O2D-CGD-CBD	2.19	115.05	111.23
22	a	419	CLA	O2D-CGD-CBD	2.19	115.05	111.23
23	d	406	BCR	C2-C1-C6	2.18	113.61	110.44
24	a	408	PL9	O2-C1-C2	-2.18	116.87	121.83
22	B	614	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
27	A	411	SQD	C3-C4-C5	2.18	114.18	110.23
28	C	517	DGD	C4E-C3E-C2E	-2.18	107.01	110.83
26	c	524	LMG	O6-C1-O1	-2.17	104.91	110.04
22	B	612	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
22	c	512	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
23	H	102	BCR	C7-C8-C9	-2.17	123.03	126.23
22	C	512	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
23	C	515	BCR	C2-C1-C6	2.16	113.58	110.44
23	c	515	BCR	C2-C1-C6	2.16	113.58	110.44
22	B	602	CLA	CHB-C4A-NA	2.16	127.52	124.40
24	d	407	PL9	C37-C38-C39	-2.16	122.67	127.62
26	C	520	LMG	O1-C1-C2	-2.16	104.99	108.27
26	b	625	LMG	O3-C3-C2	-2.16	105.28	110.38
26	c	524	LMG	O3-C3-C2	-2.16	105.28	110.38
26	d	408	LMG	O2-C2-C1	-2.16	104.93	110.08
22	d	404	CLA	O2D-CGD-CBD	2.16	115.00	111.23
24	D	407	PL9	C37-C38-C39	-2.16	122.68	127.62
26	C	524	LMG	O3-C3-C2	-2.16	105.29	110.38
22	b	603	CLA	CHB-C4A-NA	2.16	127.51	124.40
22	C	501	CLA	O2D-CGD-CBD	2.16	115.00	111.23
23	h	102	BCR	C7-C8-C9	-2.16	123.04	126.23
22	c	511	CLA	CHB-C4A-NA	2.16	127.51	124.40
22	A	419	CLA	CHD-C1D-ND	-2.15	121.77	124.80
26	d	408	LMG	C38-C37-C36	-2.15	103.48	114.37
23	B	619	BCR	C33-C5-C6	-2.15	122.14	124.48
22	B	605	CLA	O1D-CGD-CBD	2.15	128.76	124.52
22	b	613	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
22	d	404	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
27	a	411	SQD	C3-C4-C5	2.15	114.13	110.23
22	D	404	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
23	B	617	BCR	C15-C16-C17	-2.15	119.13	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	615	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
23	b	620	BCR	C38-C26-C25	-2.14	122.14	124.48
28	A	413	DGD	CBB-CAB-C9B	-2.14	103.53	114.37
26	a	410	LMG	C40-C39-C38	-2.14	103.53	114.37
23	B	617	BCR	C28-C27-C26	-2.14	110.23	114.06
26	D	408	LMG	O2-C2-C1	-2.14	104.97	110.08
26	B	624	LMG	O3-C3-C2	-2.14	105.33	110.38
22	a	419	CLA	CHD-C1D-ND	-2.14	121.79	124.80
23	b	618	BCR	C15-C16-C17	-2.14	119.15	123.52
23	b	620	BCR	C33-C5-C6	-2.13	122.16	124.48
26	b	625	LMG	C1-C2-C3	-2.13	105.53	110.01
22	c	507	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
26	A	410	LMG	C40-C39-C38	-2.13	103.61	114.37
23	b	620	BCR	C3-C4-C5	-2.13	110.27	114.06
26	D	408	LMG	C38-C37-C36	-2.12	103.63	114.37
28	C	517	DGD	CBB-CAB-C9B	-2.12	103.65	114.37
22	D	404	CLA	CHB-C4A-NA	2.12	127.46	124.40
22	d	404	CLA	CHB-C4A-NA	2.12	127.46	124.40
26	a	410	LMG	C38-C37-C36	-2.12	103.66	114.37
22	b	606	CLA	O1D-CGD-CBD	2.12	128.70	124.52
26	B	624	LMG	C1-C2-C3	-2.12	105.55	110.01
22	C	507	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
28	c	517	DGD	CBB-CAB-C9B	-2.11	103.68	114.37
28	h	103	DGD	CAB-C9B-C8B	-2.11	103.68	114.37
27	B	620	SQD	O8-S-C6	2.11	110.05	105.97
26	A	410	LMG	C38-C37-C36	-2.11	103.69	114.37
31	l	101	LHG	C27-C26-C25	-2.11	103.69	114.37
23	B	619	BCR	C3-C4-C5	-2.11	110.29	114.06
28	a	413	DGD	CFB-CEB-CDB	-2.11	103.70	114.37
22	c	512	CLA	O2D-CGD-CBD	2.11	114.92	111.23
28	H	103	DGD	CAB-C9B-C8B	-2.11	103.72	114.37
22	b	610	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
23	K	103	BCR	C15-C16-C17	-2.11	119.21	123.52
22	B	609	CLA	CED-O2D-CGD	2.10	120.69	115.92
23	h	102	BCR	C15-C14-C13	-2.10	124.33	127.28
23	C	515	BCR	C38-C26-C25	-2.10	122.19	124.48
23	c	515	BCR	C38-C26-C25	-2.10	122.19	124.48
31	L	101	LHG	C27-C26-C25	-2.10	103.74	114.37
23	h	102	BCR	C2-C1-C6	2.10	113.49	110.44
31	A	420	LHG	C5-O7-C7	-2.10	112.77	117.80
23	b	618	BCR	C28-C27-C26	-2.10	110.31	114.06
23	k	103	BCR	C15-C16-C17	-2.10	119.22	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	512	CLA	O2D-CGD-CBD	2.10	114.90	111.23
23	H	102	BCR	C15-C14-C13	-2.10	124.33	127.28
23	T	101	BCR	C15-C16-C17	-2.10	119.23	123.52
23	H	102	BCR	C2-C1-C6	2.10	113.48	110.44
28	a	413	DGD	CAB-C9B-C8B	-2.10	103.77	114.37
23	C	514	BCR	C15-C14-C13	-2.10	124.34	127.28
22	a	419	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
22	b	610	CLA	CED-O2D-CGD	2.10	120.67	115.92
31	d	410	LHG	C18-C17-C16	-2.10	103.78	114.37
23	D	406	BCR	C15-C16-C17	-2.10	119.23	123.52
22	b	614	CLA	O1D-CGD-CBD	2.09	128.65	124.52
22	C	507	CLA	O2D-CGD-CBD	2.09	114.89	111.23
26	c	520	LMG	C38-C37-C36	-2.09	103.79	114.37
22	B	609	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
22	c	511	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
22	C	501	CLA	CHD-C1D-ND	-2.09	121.86	124.80
22	c	501	CLA	CHD-C1D-ND	-2.09	121.86	124.80
22	C	503	CLA	CHB-C4A-NA	2.09	127.42	124.40
26	C	520	LMG	C38-C37-C36	-2.09	103.80	114.37
31	d	411	LHG	C27-C26-C25	-2.09	103.81	114.37
31	D	411	LHG	C27-C26-C25	-2.09	103.82	114.37
22	A	419	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
22	C	511	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
26	D	402	LMG	O7-C10-O9	-2.09	118.83	123.70
23	c	514	BCR	C15-C14-C13	-2.08	124.36	127.28
26	d	402	LMG	O7-C10-O9	-2.08	118.83	123.70
26	d	408	LMG	O1-C7-C8	-2.08	105.75	110.82
22	B	603	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
23	K	101	BCR	C15-C16-C17	-2.08	119.26	123.52
23	k	101	BCR	C15-C16-C17	-2.08	119.26	123.52
23	d	406	BCR	C15-C16-C17	-2.08	119.26	123.52
22	c	503	CLA	CHB-C4A-NA	2.08	127.40	124.40
31	D	409	LHG	C27-C26-C25	-2.08	103.86	114.37
31	d	409	LHG	C27-C26-C25	-2.08	103.86	114.37
23	t	102	BCR	C15-C16-C17	-2.08	119.27	123.52
26	a	410	LMG	O2-C2-C1	-2.08	105.12	110.08
31	d	409	LHG	C11-C10-C9	-2.08	103.87	114.37
24	d	407	PL9	C32-C33-C34	-2.08	122.87	127.62
23	B	618	BCR	C38-C26-C25	-2.08	122.22	124.48
22	c	507	CLA	O2D-CGD-CBD	2.08	114.86	111.23
31	D	409	LHG	C11-C10-C9	-2.08	103.88	114.37
24	a	408	PL9	C20-C19-C21	2.08	118.83	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	513	CLA	O2D-CGD-CBD	2.07	114.86	111.23
24	D	407	PL9	C32-C33-C34	-2.07	122.88	127.62
22	B	614	CLA	C1-C2-C3	-2.07	122.80	126.20
34	E	105	HEM	CBA-CAA-C2A	-2.07	106.80	112.53
22	C	513	CLA	O2D-CGD-CBD	2.07	114.85	111.23
22	B	608	CLA	O2D-CGD-CBD	2.07	114.85	111.23
28	C	519	DGD	O3E-C3E-C2E	-2.07	105.50	110.38
22	B	604	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
22	D	405	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
28	a	413	DGD	O2D-C2D-C1D	-2.07	105.14	110.08
26	A	410	LMG	O2-C2-C1	-2.07	105.15	110.08
22	b	604	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
34	E	105	HEM	C3B-C2B-C1B	2.07	107.96	106.41
34	e	105	HEM	C3B-C2B-C1B	2.07	107.96	106.41
28	A	413	DGD	CAB-C9B-C8B	-2.06	103.94	114.37
26	D	408	LMG	O1-C7-C8	-2.06	105.80	110.82
34	e	105	HEM	CBA-CAA-C2A	-2.06	106.83	112.53
22	d	405	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
22	b	605	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
28	c	519	DGD	O3E-C3E-C2E	-2.06	105.52	110.38
24	A	408	PL9	C20-C19-C21	2.06	118.80	115.23
23	B	618	BCR	C15-C16-C17	-2.06	119.31	123.52
31	a	420	LHG	C5-O7-C7	-2.06	112.87	117.80
28	C	519	DGD	CBB-CAB-C9B	-2.06	103.98	114.37
31	A	420	LHG	C27-C26-C25	-2.06	103.98	114.37
23	H	102	BCR	C28-C27-C26	-2.05	110.39	114.06
22	b	610	CLA	C1-C2-C3	-2.05	122.83	126.20
28	c	518	DGD	CAB-C9B-C8B	-2.05	104.01	114.37
28	c	519	DGD	CBB-CAB-C9B	-2.05	104.01	114.37
28	a	413	DGD	O3G-C1D-C2D	-2.05	105.16	108.27
22	B	602	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
22	b	603	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
24	D	407	PL9	O1-C4-C3	-2.05	118.57	120.73
24	d	407	PL9	O1-C4-C3	-2.05	118.57	120.73
28	a	413	DGD	C5B-C4B-C3B	-2.05	104.02	114.37
22	B	605	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
22	b	606	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
31	a	420	LHG	C27-C26-C25	-2.04	104.04	114.37
22	B	604	CLA	O2D-CGD-CBD	2.04	114.80	111.23
22	b	605	CLA	O2D-CGD-CBD	2.04	114.80	111.23
28	A	413	DGD	CFB-CEB-CDB	-2.04	104.04	114.37
28	C	518	DGD	CAB-C9B-C8B	-2.04	104.06	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	616	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
22	C	513	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
22	c	513	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
22	B	609	CLA	C1-C2-C3	-2.04	122.86	126.20
28	A	413	DGD	C5B-C4B-C3B	-2.04	104.06	114.37
22	b	609	CLA	O2D-CGD-CBD	2.04	114.79	111.23
22	b	612	CLA	CHD-C1D-ND	-2.04	121.94	124.80
28	A	413	DGD	O2D-C2D-C1D	-2.04	105.22	110.08
22	B	613	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
22	b	614	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
26	c	524	LMG	C40-C39-C38	-2.03	104.09	114.37
22	C	503	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
22	B	613	CLA	O1D-CGD-CBD	2.03	128.53	124.52
22	b	617	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
22	c	503	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
23	t	102	BCR	C38-C26-C25	-2.03	122.27	124.48
23	h	102	BCR	C28-C27-C26	-2.03	110.44	114.06
26	C	524	LMG	C40-C39-C38	-2.03	104.12	114.37
31	D	410	LHG	C18-C17-C16	-2.02	104.13	114.37
22	b	612	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
23	T	101	BCR	C38-C26-C25	-2.02	122.28	124.48
28	H	103	DGD	C1D-C2D-C3D	-2.02	105.76	110.01
28	h	103	DGD	C1D-C2D-C3D	-2.02	105.76	110.01
27	A	412	SQD	C1-O5-C5	-2.02	109.78	113.72
22	B	611	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
23	H	102	BCR	C29-C30-C25	2.02	113.37	110.44
22	B	605	CLA	CHB-C4A-NA	2.02	127.31	124.40
22	b	606	CLA	CHB-C4A-NA	2.02	127.31	124.40
23	b	620	BCR	C29-C30-C25	2.01	113.36	110.44
22	D	405	CLA	CHD-C1D-ND	-2.01	121.97	124.80
26	d	408	LMG	C1-O6-C5	-2.01	109.79	113.72
23	B	618	BCR	C24-C23-C22	-2.01	123.26	126.23
23	b	619	BCR	C15-C16-C17	-2.01	119.41	123.52
32	B	623	LMT	O1'-C1'-C2'	2.01	111.33	108.27
30	a	418	PHO	OBD-CAD-CBD	-2.01	122.88	125.82
26	D	408	LMG	C1-O6-C5	-2.01	109.80	113.72
26	b	625	LMG	O7-C10-O9	-2.01	119.01	123.70
32	c	525	LMT	C1'-O5'-C5'	-2.01	109.80	113.72
26	B	624	LMG	O7-C10-O9	-2.01	119.02	123.70
27	a	412	SQD	C1-O5-C5	-2.00	109.81	113.72
23	k	103	BCR	C7-C8-C9	-2.00	123.27	126.23
22	B	611	CLA	CHD-C1D-ND	-2.00	121.99	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	C	525	LMT	C1'-O5'-C5'	-2.00	109.81	113.72
32	b	624	LMT	O1'-C1'-C2'	2.00	111.31	108.27

All (56) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	404	CLA	ND
22	A	405	CLA	ND
22	A	406	CLA	ND
22	A	419	CLA	ND
22	B	601	CLA	ND
22	B	602	CLA	ND
22	B	603	CLA	ND
22	B	604	CLA	ND
22	B	606	CLA	ND
22	B	607	CLA	ND
22	B	608	CLA	ND
22	B	610	CLA	ND
22	B	611	CLA	ND
22	B	612	CLA	ND
22	B	613	CLA	ND
22	B	614	CLA	ND
22	B	615	CLA	ND
22	B	616	CLA	ND
22	C	501	CLA	ND
22	C	504	CLA	ND
22	C	505	CLA	ND
22	C	506	CLA	ND
22	C	507	CLA	ND
22	C	509	CLA	ND
22	C	510	CLA	ND
22	C	511	CLA	ND
22	C	512	CLA	ND
22	C	513	CLA	ND
22	a	404	CLA	ND
22	a	405	CLA	ND
22	a	406	CLA	ND
22	a	419	CLA	ND
22	b	602	CLA	ND
22	b	603	CLA	ND
22	b	604	CLA	ND
22	b	605	CLA	ND

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Mol	Chain	Res	Type	Atom
22	b	607	CLA	ND
22	b	608	CLA	ND
22	b	609	CLA	ND
22	b	611	CLA	ND
22	b	612	CLA	ND
22	b	613	CLA	ND
22	b	614	CLA	ND
22	b	615	CLA	ND
22	b	616	CLA	ND
22	b	617	CLA	ND
22	c	501	CLA	ND
22	c	504	CLA	ND
22	c	505	CLA	ND
22	c	506	CLA	ND
22	c	507	CLA	ND
22	c	509	CLA	ND
22	c	510	CLA	ND
22	c	511	CLA	ND
22	c	512	CLA	ND
22	c	513	CLA	ND

All (1520) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	406	CLA	C2-C3-C5-C6
22	A	406	CLA	C4-C3-C5-C6
22	B	601	CLA	C1A-C2A-CAA-CBA
22	B	601	CLA	C3A-C2A-CAA-CBA
22	B	614	CLA	CAD-CBD-CGD-O1D
22	B	614	CLA	CAD-CBD-CGD-O2D
22	C	507	CLA	CHA-CBD-CGD-O1D
22	C	507	CLA	CHA-CBD-CGD-O2D
22	a	406	CLA	C2-C3-C5-C6
22	a	406	CLA	C4-C3-C5-C6
22	b	602	CLA	C1A-C2A-CAA-CBA
22	b	602	CLA	C3A-C2A-CAA-CBA
22	b	615	CLA	CAD-CBD-CGD-O1D
22	b	615	CLA	CAD-CBD-CGD-O2D
22	b	615	CLA	C11-C12-C13-C15
22	c	507	CLA	CHA-CBD-CGD-O1D
22	c	507	CLA	CHA-CBD-CGD-O2D
23	H	102	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
23	h	102	BCR	C16-C17-C18-C36
24	A	408	PL9	C22-C23-C24-C25
24	A	408	PL9	C27-C28-C29-C30
24	A	408	PL9	C27-C28-C29-C31
24	A	408	PL9	C32-C33-C34-C36
24	A	408	PL9	C37-C38-C39-C40
24	D	407	PL9	C37-C38-C39-C41
24	a	408	PL9	C22-C23-C24-C25
24	a	408	PL9	C27-C28-C29-C30
24	a	408	PL9	C27-C28-C29-C31
24	a	408	PL9	C32-C33-C34-C36
24	a	408	PL9	C37-C38-C39-C40
24	d	407	PL9	C37-C38-C39-C41
26	A	410	LMG	O6-C1-O1-C7
26	A	410	LMG	O1-C7-C8-O7
26	A	410	LMG	O9-C10-O7-C8
26	C	524	LMG	O9-C10-O7-C8
26	C	524	LMG	C11-C10-O7-C8
26	a	410	LMG	O6-C1-O1-C7
26	a	410	LMG	O1-C7-C8-O7
26	a	410	LMG	O9-C10-O7-C8
26	c	524	LMG	O9-C10-O7-C8
26	c	524	LMG	C11-C10-O7-C8
27	B	620	SQD	O49-C7-O47-C45
27	B	620	SQD	C8-C7-O47-C45
27	B	620	SQD	O5-C5-C6-S
27	X	101	SQD	C45-C44-O6-C1
27	b	621	SQD	O5-C1-O6-C44
27	b	621	SQD	C8-C7-O47-C45
27	b	621	SQD	O5-C5-C6-S
27	x	101	SQD	C45-C44-O6-C1
28	A	413	DGD	O1A-C1A-O1G-C1G
28	A	413	DGD	C2B-C1B-O2G-C2G
28	a	413	DGD	O1A-C1A-O1G-C1G
28	a	413	DGD	C2B-C1B-O2G-C2G
31	A	420	LHG	O1-C1-C2-C3
31	A	420	LHG	C3-O3-P-O5
31	A	420	LHG	C3-O3-P-O6
31	D	409	LHG	O1-C1-C2-C3
31	D	409	LHG	O2-C2-C3-O3
31	D	409	LHG	C3-O3-P-O5
31	D	409	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
31	D	409	LHG	C4-O6-P-O4
31	a	420	LHG	O1-C1-C2-C3
31	a	420	LHG	C3-O3-P-O5
31	a	420	LHG	C3-O3-P-O6
31	d	409	LHG	O1-C1-C2-C3
31	d	409	LHG	O2-C2-C3-O3
31	d	409	LHG	C3-O3-P-O5
31	d	409	LHG	C4-O6-P-O3
31	d	409	LHG	C4-O6-P-O4
35	V	201	HEC	C2B-C3B-CAB-CBB
35	V	201	HEC	C4B-C3B-CAB-CBB
35	V	201	HEC	C2C-C3C-CAC-CBC
35	V	201	HEC	C4C-C3C-CAC-CBC
35	v	201	HEC	C2B-C3B-CAB-CBB
35	v	201	HEC	C4B-C3B-CAB-CBB
35	v	201	HEC	C2C-C3C-CAC-CBC
35	v	201	HEC	C4C-C3C-CAC-CBC
22	B	601	CLA	O1A-CGA-O2A-C1
22	B	616	CLA	O1A-CGA-O2A-C1
22	b	602	CLA	O1A-CGA-O2A-C1
22	b	617	CLA	O1A-CGA-O2A-C1
22	B	601	CLA	CBA-CGA-O2A-C1
22	b	602	CLA	CBA-CGA-O2A-C1
28	A	413	DGD	C2A-C1A-O1G-C1G
28	a	413	DGD	C2A-C1A-O1G-C1G
26	C	524	LMG	O10-C28-O8-C9
26	c	524	LMG	O10-C28-O8-C9
27	X	101	SQD	O10-C23-O48-C46
27	x	101	SQD	O10-C23-O48-C46
22	b	602	CLA	CBD-CGD-O2D-CED
27	b	621	SQD	O49-C7-O47-C45
22	C	512	CLA	C3-C5-C6-C7
22	c	512	CLA	C3-C5-C6-C7
27	X	101	SQD	C44-C45-C46-O48
27	x	101	SQD	C44-C45-C46-O48
22	B	616	CLA	CBA-CGA-O2A-C1
22	b	617	CLA	CBA-CGA-O2A-C1
26	C	524	LMG	C29-C28-O8-C9
26	c	524	LMG	C29-C28-O8-C9
22	B	601	CLA	CBD-CGD-O2D-CED
22	C	506	CLA	CBD-CGD-O2D-CED
22	c	506	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	A	410	LMG	C11-C10-O7-C8
26	a	410	LMG	C11-C10-O7-C8
22	B	605	CLA	C4-C3-C5-C6
22	b	606	CLA	C4-C3-C5-C6
24	A	408	PL9	C38-C39-C41-C42
24	a	408	PL9	C38-C39-C41-C42
32	Z	101	LMT	O5'-C5'-C6'-O6'
32	z	101	LMT	O5'-C5'-C6'-O6'
26	C	520	LMG	C29-C28-O8-C9
26	c	520	LMG	C29-C28-O8-C9
27	X	101	SQD	C24-C23-O48-C46
27	x	101	SQD	C24-C23-O48-C46
24	A	408	PL9	C32-C33-C34-C35
24	a	408	PL9	C32-C33-C34-C35
24	A	408	PL9	C22-C23-C24-C26
24	A	408	PL9	C37-C38-C39-C41
24	a	408	PL9	C22-C23-C24-C26
24	a	408	PL9	C37-C38-C39-C41
26	c	524	LMG	O6-C5-C6-O5
32	Z	101	LMT	C4B-C5B-C6B-O6B
32	z	101	LMT	C4B-C5B-C6B-O6B
26	C	524	LMG	O6-C5-C6-O5
26	H	101	LMG	C11-C10-O7-C8
26	h	101	LMG	C11-C10-O7-C8
32	Z	101	LMT	C4'-C5'-C6'-O6'
32	z	101	LMT	C4'-C5'-C6'-O6'
22	B	605	CLA	C2-C3-C5-C6
22	b	606	CLA	C2-C3-C5-C6
24	A	408	PL9	C24-C26-C27-C28
24	A	408	PL9	C34-C36-C37-C38
24	D	407	PL9	C39-C41-C42-C43
24	a	408	PL9	C24-C26-C27-C28
24	a	408	PL9	C34-C36-C37-C38
24	d	407	PL9	C39-C41-C42-C43
32	Z	101	LMT	O5B-C5B-C6B-O6B
32	z	101	LMT	O5B-C5B-C6B-O6B
26	C	524	LMG	C4-C5-C6-O5
26	c	524	LMG	C4-C5-C6-O5
27	B	620	SQD	O5-C1-O6-C44
32	Z	101	LMT	O5'-C1'-O1'-C1
32	z	101	LMT	O5'-C1'-O1'-C1
24	a	408	PL9	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
27	B	620	SQD	C24-C23-O48-C46
27	b	621	SQD	C24-C23-O48-C46
22	B	603	CLA	CBD-CGD-O2D-CED
22	b	604	CLA	CBD-CGD-O2D-CED
27	b	621	SQD	O10-C23-O48-C46
32	J	102	LMT	O5'-C5'-C6'-O6'
32	j	102	LMT	O5'-C5'-C6'-O6'
27	B	620	SQD	O10-C23-O48-C46
22	b	602	CLA	O1D-CGD-O2D-CED
25	A	415	STE	C13-C14-C15-C16
25	a	415	STE	C13-C14-C15-C16
31	D	409	LHG	C32-C33-C34-C35
31	a	420	LHG	C30-C31-C32-C33
31	d	409	LHG	C32-C33-C34-C35
22	B	601	CLA	O1D-CGD-O2D-CED
32	J	102	LMT	C4'-C5'-C6'-O6'
32	j	102	LMT	C4'-C5'-C6'-O6'
22	A	405	CLA	C11-C10-C8-C9
22	B	601	CLA	C11-C12-C13-C14
22	B	604	CLA	C6-C7-C8-C9
22	C	503	CLA	C11-C10-C8-C9
22	C	509	CLA	C6-C7-C8-C9
22	C	512	CLA	C11-C10-C8-C9
22	D	405	CLA	C14-C13-C15-C16
22	b	602	CLA	C11-C12-C13-C14
22	b	605	CLA	C6-C7-C8-C9
22	b	615	CLA	C11-C10-C8-C9
22	c	503	CLA	C11-C10-C8-C9
22	c	509	CLA	C6-C7-C8-C9
22	c	512	CLA	C11-C10-C8-C9
22	d	405	CLA	C14-C13-C15-C16
27	B	620	SQD	C2-C1-O6-C44
28	C	518	DGD	C1A-C2A-C3A-C4A
22	C	506	CLA	O1D-CGD-O2D-CED
22	c	506	CLA	O1D-CGD-O2D-CED
28	c	518	DGD	C1A-C2A-C3A-C4A
32	E	104	LMT	O5'-C5'-C6'-O6'
32	e	104	LMT	O5'-C5'-C6'-O6'
22	B	608	CLA	C15-C16-C17-C18
22	b	609	CLA	C15-C16-C17-C18
22	b	615	CLA	C5-C6-C7-C8
31	a	420	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
22	B	609	CLA	CBD-CGD-O2D-CED
22	C	504	CLA	CBD-CGD-O2D-CED
22	b	610	CLA	CBD-CGD-O2D-CED
22	c	504	CLA	CBD-CGD-O2D-CED
22	B	614	CLA	C11-C12-C13-C15
22	B	615	CLA	C6-C7-C8-C10
22	D	404	CLA	C12-C13-C15-C16
22	b	616	CLA	C6-C7-C8-C10
22	d	404	CLA	C12-C13-C15-C16
31	A	420	LHG	C7-C8-C9-C10
31	a	420	LHG	C7-C8-C9-C10
28	a	413	DGD	O1B-C1B-O2G-C2G
32	C	525	LMT	C4B-C5B-C6B-O6B
32	c	525	LMT	C4B-C5B-C6B-O6B
26	B	624	LMG	C28-C29-C30-C31
22	B	606	CLA	C2A-CAA-CBA-CGA
22	b	607	CLA	C2A-CAA-CBA-CGA
22	B	614	CLA	C5-C6-C7-C8
26	A	410	LMG	C10-C11-C12-C13
26	a	410	LMG	C10-C11-C12-C13
26	b	625	LMG	C28-C29-C30-C31
26	C	520	LMG	O10-C28-O8-C9
26	c	520	LMG	O10-C28-O8-C9
22	B	604	CLA	CBD-CGD-O2D-CED
22	b	605	CLA	CBD-CGD-O2D-CED
32	B	623	LMT	C4'-C5'-C6'-O6'
32	b	624	LMT	C4'-C5'-C6'-O6'
22	B	616	CLA	C8-C10-C11-C12
22	C	512	CLA	C13-C15-C16-C17
22	b	617	CLA	C8-C10-C11-C12
22	c	512	CLA	C13-C15-C16-C17
31	A	420	LHG	O2-C2-C3-O3
31	a	420	LHG	O2-C2-C3-O3
32	Z	101	LMT	O1'-C1-C2-C3
32	z	101	LMT	O1'-C1-C2-C3
28	A	413	DGD	O1B-C1B-O2G-C2G
22	C	505	CLA	C15-C16-C17-C18
22	C	513	CLA	C5-C6-C7-C8
22	c	505	CLA	C15-C16-C17-C18
22	c	513	CLA	C5-C6-C7-C8
22	B	604	CLA	C5-C6-C7-C8
22	b	605	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	d	404	CLA	C15-C16-C17-C18
25	a	421	STE	C1-C2-C3-C4
24	A	408	PL9	C31-C32-C33-C34
31	A	420	LHG	C1-C2-C3-O3
31	D	409	LHG	C1-C2-C3-O3
31	a	420	LHG	C1-C2-C3-O3
31	d	409	LHG	C1-C2-C3-O3
22	B	605	CLA	C15-C16-C17-C18
22	b	606	CLA	C15-C16-C17-C18
25	A	416	STE	C12-C13-C14-C15
25	a	416	STE	C12-C13-C14-C15
26	H	101	LMG	C28-C29-C30-C31
26	h	101	LMG	C28-C29-C30-C31
22	C	503	CLA	C5-C6-C7-C8
22	D	404	CLA	C15-C16-C17-C18
22	c	503	CLA	C5-C6-C7-C8
27	A	412	SQD	C24-C23-O48-C46
27	a	412	SQD	C24-C23-O48-C46
32	Z	101	LMT	C2'-C1'-O1'-C1
32	z	101	LMT	C2'-C1'-O1'-C1
22	B	601	CLA	C10-C11-C12-C13
22	b	602	CLA	C10-C11-C12-C13
25	A	421	STE	C1-C2-C3-C4
27	B	620	SQD	C23-C24-C25-C26
22	b	607	CLA	C16-C17-C18-C19
23	H	102	BCR	C20-C21-C22-C37
23	T	101	BCR	C20-C21-C22-C37
23	h	102	BCR	C20-C21-C22-C37
23	t	102	BCR	C20-C21-C22-C37
23	H	102	BCR	C37-C22-C23-C24
23	b	619	BCR	C36-C18-C19-C20
23	h	102	BCR	C37-C22-C23-C24
26	D	402	LMG	O10-C28-O8-C9
26	d	402	LMG	O10-C28-O8-C9
22	C	512	CLA	C2A-CAA-CBA-CGA
22	c	512	CLA	C2A-CAA-CBA-CGA
31	D	410	LHG	O1-C1-C2-C3
31	d	410	LHG	O1-C1-C2-C3
26	C	524	LMG	C9-C8-O7-C10
26	c	524	LMG	C9-C8-O7-C10
27	B	620	SQD	C46-C45-O47-C7
27	b	621	SQD	C46-C45-O47-C7

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Mol	Chain	Res	Type	Atoms
31	l	101	LHG	C32-C33-C34-C35
22	C	513	CLA	C16-C17-C18-C20
31	L	101	LHG	C32-C33-C34-C35
32	B	623	LMT	O5'-C5'-C6'-O6'
32	b	624	LMT	O5'-C5'-C6'-O6'
23	H	102	BCR	C16-C17-C18-C19
23	h	102	BCR	C16-C17-C18-C19
22	C	513	CLA	C16-C17-C18-C19
22	c	513	CLA	C16-C17-C18-C20
25	D	412	STE	C5-C6-C7-C8
25	J	101	STE	C10-C11-C12-C13
25	d	412	STE	C5-C6-C7-C8
26	C	520	LMG	C35-C36-C37-C38
28	C	518	DGD	C6A-C7A-C8A-C9A
28	H	103	DGD	CBA-CCA-CDA-CEA
28	c	518	DGD	C6A-C7A-C8A-C9A
25	b	601	STE	C6-C7-C8-C9
25	j	101	STE	C10-C11-C12-C13
26	C	520	LMG	C33-C34-C35-C36
26	c	520	LMG	C33-C34-C35-C36
26	h	101	LMG	C33-C34-C35-C36
28	C	518	DGD	C4B-C5B-C6B-C7B
28	c	518	DGD	C4B-C5B-C6B-C7B
28	c	519	DGD	C9A-CAA-CBA-CCA
28	h	103	DGD	CBA-CCA-CDA-CEA
31	L	101	LHG	C30-C31-C32-C33
31	l	101	LHG	C30-C31-C32-C33
32	z	101	LMT	C3-C4-C5-C6
25	B	625	STE	C6-C7-C8-C9
27	A	411	SQD	C14-C15-C16-C17
28	C	519	DGD	C8A-C9A-CAA-CBA
28	C	519	DGD	C9A-CAA-CBA-CCA
28	c	519	DGD	C8A-C9A-CAA-CBA
32	Z	101	LMT	C3-C4-C5-C6
25	C	516	STE	C5-C6-C7-C8
25	a	416	STE	C14-C15-C16-C17
25	b	622	STE	C11-C12-C13-C14
25	c	516	STE	C5-C6-C7-C8
25	e	102	STE	C14-C15-C16-C17
26	c	520	LMG	C35-C36-C37-C38
27	A	411	SQD	C29-C30-C31-C32
27	a	411	SQD	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
28	C	518	DGD	C5B-C6B-C7B-C8B
28	C	519	DGD	C5A-C6A-C7A-C8A
28	H	103	DGD	C6B-C7B-C8B-C9B
28	a	413	DGD	CEA-CFA-CGA-CHA
28	c	519	DGD	C5A-C6A-C7A-C8A
28	h	103	DGD	C6B-C7B-C8B-C9B
31	a	420	LHG	C33-C34-C35-C36
31	A	420	LHG	O1-C1-C2-O2
25	B	621	STE	C11-C12-C13-C14
25	E	102	STE	C14-C15-C16-C17
25	T	102	STE	C6-C7-C8-C9
26	H	101	LMG	C33-C34-C35-C36
28	A	413	DGD	CDB-CEB-CFB-CGB
28	c	518	DGD	C5B-C6B-C7B-C8B
26	A	410	LMG	C16-C17-C18-C19
26	A	410	LMG	C29-C30-C31-C32
26	a	410	LMG	C29-C30-C31-C32
32	J	102	LMT	C4-C5-C6-C7
32	j	102	LMT	C4-C5-C6-C7
28	C	517	DGD	O6E-C5E-C6E-O5E
28	c	517	DGD	O6E-C5E-C6E-O5E
22	c	513	CLA	C16-C17-C18-C19
25	A	416	STE	C14-C15-C16-C17
25	c	521	STE	C4-C5-C6-C7
26	a	410	LMG	C16-C17-C18-C19
31	L	101	LHG	C14-C15-C16-C17
31	l	101	LHG	C14-C15-C16-C17
25	I	101	STE	C4-C5-C6-C7
25	i	101	STE	C4-C5-C6-C7
26	D	408	LMG	C18-C19-C20-C21
28	C	518	DGD	C6B-C7B-C8B-C9B
28	h	103	DGD	C9B-CAB-CBB-CCB
22	c	512	CLA	C11-C10-C8-C7
25	C	521	STE	C4-C5-C6-C7
28	H	103	DGD	C9B-CAB-CBB-CCB
28	c	518	DGD	C6B-C7B-C8B-C9B
26	D	402	LMG	C28-C29-C30-C31
27	X	101	SQD	O6-C44-C45-C46
27	x	101	SQD	O6-C44-C45-C46
26	d	408	LMG	C18-C19-C20-C21
26	d	408	LMG	C30-C31-C32-C33
27	B	620	SQD	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
27	b	621	SQD	C17-C18-C19-C20
27	A	412	SQD	O10-C23-O48-C46
27	a	412	SQD	O10-C23-O48-C46
26	D	408	LMG	C30-C31-C32-C33
27	B	620	SQD	C31-C32-C33-C34
28	A	413	DGD	O6E-C5E-C6E-O5E
26	d	408	LMG	C16-C17-C18-C19
22	B	603	CLA	O1D-CGD-O2D-CED
22	b	604	CLA	O1D-CGD-O2D-CED
22	B	601	CLA	C16-C17-C18-C20
22	b	602	CLA	C16-C17-C18-C20
28	a	413	DGD	O6E-C5E-C6E-O5E
26	A	410	LMG	C31-C32-C33-C34
26	D	408	LMG	C16-C17-C18-C19
27	b	621	SQD	C15-C16-C17-C18
27	x	101	SQD	C33-C34-C35-C36
28	A	413	DGD	CCB-CDB-CEB-CFB
26	A	410	LMG	C33-C34-C35-C36
26	a	410	LMG	C31-C32-C33-C34
26	a	410	LMG	C33-C34-C35-C36
27	A	411	SQD	C16-C17-C18-C19
31	L	101	LHG	C10-C11-C12-C13
31	l	101	LHG	C29-C30-C31-C32
27	X	101	SQD	C33-C34-C35-C36
28	a	413	DGD	CDA-CEA-CFA-CGA
31	L	101	LHG	C29-C30-C31-C32
31	l	101	LHG	C10-C11-C12-C13
26	d	402	LMG	C28-C29-C30-C31
25	t	101	STE	C12-C13-C14-C15
26	H	101	LMG	C37-C38-C39-C40
27	a	411	SQD	C16-C17-C18-C19
27	b	621	SQD	C13-C14-C15-C16
28	C	519	DGD	C9B-CAB-CBB-CCB
28	H	103	DGD	C4B-C5B-C6B-C7B
28	c	519	DGD	C9B-CAB-CBB-CCB
28	h	103	DGD	C4B-C5B-C6B-C7B
27	a	411	SQD	C29-C30-C31-C32
28	h	103	DGD	C9A-CAA-CBA-CCA
26	d	408	LMG	C32-C33-C34-C35
26	H	101	LMG	C11-C12-C13-C14
26	h	101	LMG	C37-C38-C39-C40
28	C	517	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
28	c	517	DGD	C4B-C5B-C6B-C7B
32	E	104	LMT	C4-C5-C6-C7
32	e	104	LMT	C4-C5-C6-C7
23	H	102	BCR	C23-C24-C25-C26
23	H	102	BCR	C23-C24-C25-C30
23	K	103	BCR	C1-C6-C7-C8
23	K	103	BCR	C5-C6-C7-C8
23	h	102	BCR	C23-C24-C25-C26
23	h	102	BCR	C23-C24-C25-C30
23	k	103	BCR	C1-C6-C7-C8
23	k	103	BCR	C5-C6-C7-C8
26	c	524	LMG	C35-C36-C37-C38
28	H	103	DGD	C9A-CAA-CBA-CCA
26	C	520	LMG	C11-C10-O7-C8
26	c	520	LMG	C11-C10-O7-C8
26	C	524	LMG	C35-C36-C37-C38
26	D	408	LMG	C32-C33-C34-C35
26	D	408	LMG	C35-C36-C37-C38
27	b	621	SQD	C16-C17-C18-C19
25	C	516	STE	C2-C3-C4-C5
25	c	516	STE	C2-C3-C4-C5
31	A	420	LHG	C26-C27-C28-C29
26	C	520	LMG	C38-C39-C40-C41
26	H	101	LMG	C35-C36-C37-C38
26	d	408	LMG	C35-C36-C37-C38
26	h	101	LMG	C35-C36-C37-C38
27	X	101	SQD	C25-C26-C27-C28
27	a	412	SQD	C11-C12-C13-C14
27	x	101	SQD	C25-C26-C27-C28
27	B	620	SQD	C27-C28-C29-C30
31	A	420	LHG	C32-C33-C34-C35
26	H	101	LMG	O9-C10-O7-C8
26	h	101	LMG	O9-C10-O7-C8
26	h	101	LMG	C11-C12-C13-C14
27	b	621	SQD	C29-C30-C31-C32
28	H	103	DGD	C7A-C8A-C9A-CAA
31	D	410	LHG	C29-C30-C31-C32
32	C	525	LMT	C2-C3-C4-C5
32	c	525	LMT	C2-C3-C4-C5
25	I	101	STE	C3-C4-C5-C6
25	a	415	STE	C12-C13-C14-C15
25	i	101	STE	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
26	H	101	LMG	C38-C39-C40-C41
26	c	520	LMG	C38-C39-C40-C41
26	h	101	LMG	C38-C39-C40-C41
27	A	411	SQD	C31-C32-C33-C34
27	A	412	SQD	C9-C10-C11-C12
28	h	103	DGD	C7A-C8A-C9A-CAA
31	d	410	LHG	C29-C30-C31-C32
22	C	513	CLA	CBA-CGA-O2A-C1
22	c	513	CLA	CBA-CGA-O2A-C1
26	C	524	LMG	C29-C30-C31-C32
27	a	412	SQD	C26-C27-C28-C29
25	T	102	STE	C3-C4-C5-C6
26	a	410	LMG	C38-C39-C40-C41
26	c	524	LMG	C29-C30-C31-C32
27	A	411	SQD	C33-C34-C35-C36
28	A	413	DGD	C3B-C4B-C5B-C6B
28	C	519	DGD	C4A-C5A-C6A-C7A
28	c	519	DGD	C4A-C5A-C6A-C7A
28	c	519	DGD	CBB-CCB-CDB-CEB
31	A	420	LHG	C33-C34-C35-C36
28	C	518	DGD	O6E-C1E-O5D-C6D
28	c	518	DGD	O6E-C1E-O5D-C6D
27	A	412	SQD	C11-C12-C13-C14
27	A	412	SQD	C32-C33-C34-C35
27	B	620	SQD	C33-C34-C35-C36
27	a	411	SQD	C31-C32-C33-C34
28	C	519	DGD	CBB-CCB-CDB-CEB
28	C	518	DGD	C2E-C1E-O5D-C6D
28	c	518	DGD	C2E-C1E-O5D-C6D
25	a	415	STE	C9-C10-C11-C12
25	c	521	STE	C6-C7-C8-C9
27	a	411	SQD	C33-C34-C35-C36
25	C	521	STE	C6-C7-C8-C9
28	C	519	DGD	C2A-C3A-C4A-C5A
32	B	623	LMT	C3-C4-C5-C6
25	A	409	STE	C4-C5-C6-C7
25	a	409	STE	C4-C5-C6-C7
26	A	410	LMG	C38-C39-C40-C41
27	a	412	SQD	C9-C10-C11-C12
28	a	413	DGD	C2A-C3A-C4A-C5A
32	b	624	LMT	C3-C4-C5-C6
22	b	607	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
26	C	520	LMG	C14-C15-C16-C17
28	c	519	DGD	C2A-C3A-C4A-C5A
26	C	524	LMG	C33-C34-C35-C36
26	D	408	LMG	C38-C39-C40-C41
26	c	520	LMG	C14-C15-C16-C17
26	d	408	LMG	C38-C39-C40-C41
27	B	620	SQD	C13-C14-C15-C16
26	c	524	LMG	C33-C34-C35-C36
28	a	413	DGD	C3B-C4B-C5B-C6B
28	C	518	DGD	C8A-C9A-CAA-CBA
28	c	518	DGD	C8A-C9A-CAA-CBA
26	c	524	LMG	C8-C7-O1-C1
22	B	606	CLA	C16-C17-C18-C19
22	B	606	CLA	C16-C17-C18-C20
26	C	520	LMG	C37-C38-C39-C40
26	c	520	LMG	C37-C38-C39-C40
28	A	413	DGD	C2A-C3A-C4A-C5A
25	A	421	STE	C4-C5-C6-C7
25	E	103	STE	C14-C15-C16-C17
25	a	421	STE	C4-C5-C6-C7
25	e	103	STE	C14-C15-C16-C17
26	C	524	LMG	C37-C38-C39-C40
26	c	524	LMG	C37-C38-C39-C40
31	d	410	LHG	C13-C14-C15-C16
22	C	513	CLA	C10-C11-C12-C13
22	c	513	CLA	C10-C11-C12-C13
26	H	101	LMG	C13-C14-C15-C16
32	E	104	LMT	C11-C10-C9-C8
32	e	104	LMT	C11-C10-C9-C8
31	A	420	LHG	C24-C25-C26-C27
25	b	623	STE	C4-C5-C6-C7
28	h	103	DGD	CAA-CBA-CCA-CDA
28	C	517	DGD	C1A-C2A-C3A-C4A
28	c	517	DGD	C1A-C2A-C3A-C4A
28	C	517	DGD	C2B-C3B-C4B-C5B
28	H	103	DGD	CAA-CBA-CCA-CDA
26	A	410	LMG	C32-C33-C34-C35
27	a	412	SQD	C33-C34-C35-C36
27	b	621	SQD	C10-C11-C12-C13
22	B	601	CLA	C16-C17-C18-C19
22	b	602	CLA	C16-C17-C18-C19
26	B	624	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
31	L	101	LHG	C27-C28-C29-C30
26	A	410	LMG	C30-C31-C32-C33
26	a	410	LMG	C32-C33-C34-C35
26	b	625	LMG	C38-C39-C40-C41
28	c	517	DGD	C2B-C3B-C4B-C5B
31	a	420	LHG	C31-C32-C33-C34
31	l	101	LHG	C27-C28-C29-C30
31	D	411	LHG	C7-C8-C9-C10
31	d	411	LHG	C7-C8-C9-C10
22	C	509	CLA	C13-C15-C16-C17
25	B	621	STE	C9-C10-C11-C12
25	b	622	STE	C9-C10-C11-C12
26	H	101	LMG	C14-C15-C16-C17
26	a	410	LMG	C30-C31-C32-C33
26	D	408	LMG	O6-C5-C6-O5
26	d	408	LMG	O6-C5-C6-O5
32	C	525	LMT	O5B-C5B-C6B-O6B
26	A	410	LMG	O7-C8-C9-O8
27	B	620	SQD	O6-C44-C45-O47
25	B	622	STE	C4-C5-C6-C7
25	t	101	STE	C10-C11-C12-C13
26	h	101	LMG	C14-C15-C16-C17
27	X	101	SQD	C31-C32-C33-C34
32	c	525	LMT	O5B-C5B-C6B-O6B
26	B	624	LMG	C17-C18-C19-C20
26	D	402	LMG	C33-C34-C35-C36
26	b	625	LMG	C17-C18-C19-C20
26	d	402	LMG	C33-C34-C35-C36
26	h	101	LMG	C13-C14-C15-C16
27	A	411	SQD	C30-C31-C32-C33
27	B	620	SQD	C9-C10-C11-C12
27	a	411	SQD	C30-C31-C32-C33
22	c	509	CLA	C13-C15-C16-C17
25	t	101	STE	C6-C7-C8-C9
27	x	101	SQD	C31-C32-C33-C34
28	a	413	DGD	CAA-CBA-CCA-CDA
31	D	411	LHG	C29-C30-C31-C32
22	C	506	CLA	C15-C16-C17-C18
22	c	506	CLA	C15-C16-C17-C18
25	m	102	STE	C4-C5-C6-C7
27	B	620	SQD	C32-C33-C34-C35
27	a	411	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
24	D	407	PL9	C37-C38-C39-C40
24	d	407	PL9	C37-C38-C39-C40
27	A	411	SQD	C12-C13-C14-C15
31	a	420	LHG	C32-C33-C34-C35
31	d	411	LHG	C29-C30-C31-C32
25	M	101	STE	C4-C5-C6-C7
27	A	411	SQD	C32-C33-C34-C35
25	E	101	STE	C6-C7-C8-C9
27	a	411	SQD	C32-C33-C34-C35
31	d	410	LHG	C11-C12-C13-C14
25	K	102	STE	C11-C10-C9-C8
25	B	622	STE	C3-C4-C5-C6
25	e	101	STE	C6-C7-C8-C9
26	D	402	LMG	C32-C33-C34-C35
26	d	402	LMG	C32-C33-C34-C35
31	D	409	LHG	O1-C1-C2-O2
31	d	409	LHG	O1-C1-C2-O2
22	c	513	CLA	O1A-CGA-O2A-C1
28	A	413	DGD	CEB-CFB-CGB-CHB
25	B	622	STE	C2-C3-C4-C5
25	i	101	STE	C5-C6-C7-C8
22	C	503	CLA	C1A-C2A-CAA-CBA
22	c	503	CLA	C1A-C2A-CAA-CBA
25	I	101	STE	C5-C6-C7-C8
26	H	101	LMG	C39-C40-C41-C42
28	A	413	DGD	C9A-CAA-CBA-CCA
31	L	101	LHG	C9-C10-C11-C12
31	l	101	LHG	C9-C10-C11-C12
22	A	404	CLA	C2C-C3C-CAC-CBC
22	a	404	CLA	C2C-C3C-CAC-CBC
25	d	412	STE	C2-C3-C4-C5
31	a	420	LHG	C28-C29-C30-C31
22	C	513	CLA	O1A-CGA-O2A-C1
25	A	415	STE	C12-C13-C14-C15
26	c	520	LMG	C17-C18-C19-C20
26	d	408	LMG	C15-C16-C17-C18
26	h	101	LMG	C39-C40-C41-C42
27	A	412	SQD	C17-C18-C19-C20
31	L	101	LHG	O6-C4-C5-C6
31	l	101	LHG	O6-C4-C5-C6
25	T	102	STE	C5-C6-C7-C8
26	B	624	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
26	D	408	LMG	C36-C37-C38-C39
27	B	620	SQD	C34-C35-C36-C37
22	B	601	CLA	C11-C10-C8-C7
22	B	614	CLA	C12-C13-C15-C16
22	C	512	CLA	C11-C10-C8-C7
22	b	602	CLA	C11-C10-C8-C7
25	a	421	STE	C3-C4-C5-C6
26	C	520	LMG	C18-C19-C20-C21
26	D	408	LMG	C15-C16-C17-C18
31	A	420	LHG	C31-C32-C33-C34
22	A	419	CLA	C2C-C3C-CAC-CBC
22	a	419	CLA	C2C-C3C-CAC-CBC
25	D	412	STE	C2-C3-C4-C5
26	C	520	LMG	C17-C18-C19-C20
26	c	520	LMG	C18-C19-C20-C21
28	a	413	DGD	C5B-C6B-C7B-C8B
24	a	408	PL9	C13-C14-C16-C17
24	A	408	PL9	C47-C48-C49-C51
24	a	408	PL9	C47-C48-C49-C51
26	D	408	LMG	C39-C40-C41-C42
26	a	410	LMG	C18-C19-C20-C21
26	b	625	LMG	C30-C31-C32-C33
27	x	101	SQD	C26-C27-C28-C29
22	B	601	CLA	C11-C10-C8-C9
22	B	614	CLA	C14-C13-C15-C16
22	C	506	CLA	C14-C13-C15-C16
22	D	404	CLA	C14-C13-C15-C16
22	b	602	CLA	C11-C10-C8-C9
22	c	506	CLA	C14-C13-C15-C16
22	c	512	CLA	C14-C13-C15-C16
25	E	103	STE	C9-C10-C11-C12
25	e	103	STE	C9-C10-C11-C12
26	A	410	LMG	C18-C19-C20-C21
26	d	408	LMG	C36-C37-C38-C39
26	d	408	LMG	C39-C40-C41-C42
31	d	411	LHG	C24-C25-C26-C27
22	B	609	CLA	O1D-CGD-O2D-CED
22	b	610	CLA	O1D-CGD-O2D-CED
31	D	411	LHG	C24-C25-C26-C27
27	X	101	SQD	C26-C27-C28-C29
26	D	408	LMG	C28-C29-C30-C31
26	d	408	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
26	A	410	LMG	O1-C7-C8-C9
26	C	520	LMG	O1-C7-C8-C9
26	a	410	LMG	O1-C7-C8-C9
26	c	520	LMG	O1-C7-C8-C9
25	T	102	STE	C9-C10-C11-C12
27	a	412	SQD	C17-C18-C19-C20
28	C	519	DGD	C2B-C3B-C4B-C5B
28	c	519	DGD	C2B-C3B-C4B-C5B
22	B	609	CLA	C15-C16-C17-C18
22	B	614	CLA	C13-C15-C16-C17
22	b	610	CLA	C15-C16-C17-C18
25	A	421	STE	C3-C4-C5-C6
27	b	621	SQD	C12-C13-C14-C15
31	L	101	LHG	C34-C35-C36-C37
22	C	507	CLA	C16-C17-C18-C20
22	c	507	CLA	C16-C17-C18-C20
31	l	101	LHG	C34-C35-C36-C37
25	C	516	STE	C6-C7-C8-C9
25	c	516	STE	C6-C7-C8-C9
25	C	516	STE	C7-C8-C9-C10
25	c	516	STE	C7-C8-C9-C10
28	A	413	DGD	C5B-C6B-C7B-C8B
31	d	410	LHG	C15-C16-C17-C18
23	D	406	BCR	C20-C21-C22-C37
28	C	517	DGD	C6A-C7A-C8A-C9A
28	c	517	DGD	C6A-C7A-C8A-C9A
24	D	407	PL9	C45-C44-C46-C47
24	d	407	PL9	C45-C44-C46-C47
31	a	420	LHG	C26-C27-C28-C29
22	d	405	CLA	C10-C11-C12-C13
25	K	102	STE	C12-C13-C14-C15
27	A	411	SQD	C13-C14-C15-C16
32	j	102	LMT	C3-C4-C5-C6
26	B	624	LMG	C15-C16-C17-C18
27	a	411	SQD	C13-C14-C15-C16
32	E	104	LMT	C7-C8-C9-C10
32	J	102	LMT	C3-C4-C5-C6
32	e	104	LMT	C7-C8-C9-C10
26	B	624	LMG	C36-C37-C38-C39
26	b	625	LMG	C36-C37-C38-C39
28	c	519	DGD	CAB-CBB-CCB-CDB
32	z	101	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	b	623	STE	C2-C3-C4-C5
26	D	408	LMG	C14-C15-C16-C17
26	d	408	LMG	C14-C15-C16-C17
28	C	519	DGD	CAB-CBB-CCB-CDB
28	a	413	DGD	C7A-C8A-C9A-CAA
32	Z	101	LMT	C4-C5-C6-C7
28	H	103	DGD	CDB-CEB-CFB-CGB
28	h	103	DGD	CDB-CEB-CFB-CGB
22	D	405	CLA	C10-C11-C12-C13
26	b	625	LMG	C15-C16-C17-C18
27	a	412	SQD	C30-C31-C32-C33
27	A	412	SQD	C26-C27-C28-C29
25	t	101	STE	C13-C14-C15-C16
31	D	409	LHG	C34-C35-C36-C37
31	d	409	LHG	C11-C10-C9-C8
31	d	409	LHG	C34-C35-C36-C37
22	a	406	CLA	C5-C6-C7-C8
25	t	101	STE	C4-C5-C6-C7
27	A	411	SQD	C11-C12-C13-C14
27	A	412	SQD	C30-C31-C32-C33
27	a	411	SQD	C11-C12-C13-C14
31	D	409	LHG	C11-C10-C9-C8
22	c	507	CLA	C16-C17-C18-C19
22	A	406	CLA	C5-C6-C7-C8
27	A	411	SQD	C9-C10-C11-C12
31	d	411	LHG	C27-C28-C29-C30
25	T	102	STE	C2-C3-C4-C5
27	a	411	SQD	C9-C10-C11-C12
28	A	413	DGD	C6B-C7B-C8B-C9B
32	E	104	LMT	C6-C7-C8-C9
32	e	104	LMT	C6-C7-C8-C9
26	a	410	LMG	O7-C8-C9-O8
25	a	416	STE	C11-C10-C9-C8
28	a	413	DGD	C8B-C9B-CAB-CBB
31	D	411	LHG	C27-C28-C29-C30
22	C	504	CLA	O1D-CGD-O2D-CED
22	c	504	CLA	O1D-CGD-O2D-CED
25	A	416	STE	C11-C10-C9-C8
26	D	402	LMG	C36-C37-C38-C39
26	d	402	LMG	C36-C37-C38-C39
25	A	415	STE	C9-C10-C11-C12
27	A	412	SQD	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
22	c	504	CLA	C11-C12-C13-C14
25	J	101	STE	C5-C6-C7-C8
22	C	507	CLA	C16-C17-C18-C19
22	C	504	CLA	C11-C12-C13-C14
26	A	410	LMG	C34-C35-C36-C37
27	A	412	SQD	C31-C32-C33-C34
26	D	402	LMG	C29-C28-O8-C9
26	d	402	LMG	C29-C28-O8-C9
25	c	521	STE	C5-C6-C7-C8
26	B	624	LMG	C14-C15-C16-C17
26	b	625	LMG	C14-C15-C16-C17
28	A	413	DGD	C6A-C7A-C8A-C9A
26	b	625	LMG	C29-C30-C31-C32
27	b	621	SQD	C11-C10-C9-C8
26	C	524	LMG	C28-C29-C30-C31
26	c	524	LMG	C28-C29-C30-C31
31	A	420	LHG	C34-C35-C36-C37
26	D	408	LMG	C40-C41-C42-C43
22	c	512	CLA	C8-C10-C11-C12
28	a	413	DGD	CEB-CFB-CGB-CHB
32	B	623	LMT	C11-C10-C9-C8
32	b	624	LMT	C11-C10-C9-C8
26	d	408	LMG	C40-C41-C42-C43
25	j	101	STE	C5-C6-C7-C8
26	a	410	LMG	C34-C35-C36-C37
32	z	101	LMT	C2-C3-C4-C5
25	C	521	STE	C5-C6-C7-C8
25	E	103	STE	C13-C14-C15-C16
25	e	103	STE	C13-C14-C15-C16
26	B	624	LMG	C18-C19-C20-C21
26	B	624	LMG	C29-C30-C31-C32
26	b	625	LMG	C18-C19-C20-C21
31	A	420	LHG	C17-C18-C19-C20
22	B	603	CLA	C11-C10-C8-C9
22	B	614	CLA	C11-C10-C8-C9
22	B	614	CLA	C11-C12-C13-C14
22	B	615	CLA	C6-C7-C8-C9
22	C	506	CLA	C6-C7-C8-C9
22	b	604	CLA	C11-C10-C8-C9
22	b	616	CLA	C6-C7-C8-C9
22	c	506	CLA	C6-C7-C8-C9
22	d	404	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	C	512	CLA	C8-C10-C11-C12
31	D	410	LHG	C35-C36-C37-C38
27	a	412	SQD	C31-C32-C33-C34
32	Z	101	LMT	C2-C3-C4-C5
25	c	521	STE	C2-C3-C4-C5
28	A	413	DGD	C8A-C9A-CAA-CBA
31	a	420	LHG	C17-C18-C19-C20
22	B	603	CLA	C11-C10-C8-C7
22	C	506	CLA	C6-C7-C8-C10
22	C	506	CLA	C12-C13-C15-C16
22	C	507	CLA	C11-C10-C8-C7
22	C	507	CLA	C11-C12-C13-C15
22	C	512	CLA	C12-C13-C15-C16
22	D	405	CLA	C12-C13-C15-C16
22	b	604	CLA	C11-C10-C8-C7
22	c	506	CLA	C6-C7-C8-C10
22	c	506	CLA	C12-C13-C15-C16
22	c	507	CLA	C11-C10-C8-C7
22	c	507	CLA	C11-C12-C13-C15
22	c	512	CLA	C12-C13-C15-C16
22	d	405	CLA	C12-C13-C15-C16
26	C	520	LMG	C36-C37-C38-C39
26	c	520	LMG	C36-C37-C38-C39
31	A	420	LHG	C11-C10-C9-C8
22	d	405	CLA	C16-C17-C18-C20
28	a	413	DGD	CFA-CGA-CHA-CIA
31	d	410	LHG	C35-C36-C37-C38
25	D	412	STE	C11-C10-C9-C8
28	C	519	DGD	CAA-CBA-CCA-CDA
28	c	519	DGD	CAA-CBA-CCA-CDA
22	C	509	CLA	C8-C10-C11-C12
22	b	608	CLA	C15-C16-C17-C18
22	c	509	CLA	C8-C10-C11-C12
25	E	102	STE	C7-C8-C9-C10
25	d	412	STE	C11-C10-C9-C8
22	B	601	CLA	C15-C16-C17-C18
22	B	607	CLA	C15-C16-C17-C18
22	b	602	CLA	C15-C16-C17-C18
22	B	616	CLA	C11-C12-C13-C14
25	A	421	STE	C6-C7-C8-C9
25	e	102	STE	C7-C8-C9-C10
28	H	103	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
28	h	103	DGD	C7B-C8B-C9B-CAB
28	a	413	DGD	C6B-C7B-C8B-C9B
31	a	420	LHG	C11-C10-C9-C8
31	a	420	LHG	C24-C25-C26-C27
26	A	410	LMG	C7-C8-C9-O8
26	a	410	LMG	C7-C8-C9-O8
27	B	620	SQD	O6-C44-C45-C46
22	B	616	CLA	C11-C12-C13-C15
22	D	405	CLA	C16-C17-C18-C20
22	b	617	CLA	C11-C12-C13-C14
22	b	617	CLA	C11-C12-C13-C15
22	C	509	CLA	C10-C11-C12-C13
22	c	509	CLA	C10-C11-C12-C13
32	J	102	LMT	O1'-C1-C2-C3
32	j	102	LMT	O1'-C1-C2-C3
25	a	421	STE	C6-C7-C8-C9
32	j	102	LMT	C1-C2-C3-C4
32	J	102	LMT	C1-C2-C3-C4
32	e	104	LMT	C4'-C5'-C6'-O6'
25	D	413	STE	C10-C11-C12-C13
25	d	413	STE	C10-C11-C12-C13
27	B	620	SQD	C10-C11-C12-C13
32	E	104	LMT	C4'-C5'-C6'-O6'
23	D	406	BCR	C23-C24-C25-C26
23	D	406	BCR	C23-C24-C25-C30
23	d	406	BCR	C23-C24-C25-C26
23	d	406	BCR	C23-C24-C25-C30
28	C	518	DGD	C2B-C3B-C4B-C5B
25	C	521	STE	C2-C3-C4-C5
26	b	625	LMG	C19-C20-C21-C22
28	c	518	DGD	C2B-C3B-C4B-C5B
24	A	408	PL9	C4-C3-C7-C8
24	a	408	PL9	C4-C3-C7-C8
26	B	624	LMG	C19-C20-C21-C22
25	b	622	STE	C2-C3-C4-C5
24	A	408	PL9	C15-C14-C16-C17
25	t	101	STE	C3-C4-C5-C6
31	L	101	LHG	C12-C13-C14-C15
31	l	101	LHG	C12-C13-C14-C15
32	B	623	LMT	C7-C8-C9-C10
32	b	624	LMT	C7-C8-C9-C10
24	A	408	PL9	C13-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
24	A	408	PL9	C33-C34-C36-C37
24	D	407	PL9	C43-C44-C46-C47
24	a	408	PL9	C33-C34-C36-C37
24	d	407	PL9	C43-C44-C46-C47
25	B	621	STE	C2-C3-C4-C5
25	t	101	STE	C11-C10-C9-C8
26	C	520	LMG	C28-C29-C30-C31
26	c	520	LMG	C28-C29-C30-C31
22	B	604	CLA	O1D-CGD-O2D-CED
22	b	605	CLA	O1D-CGD-O2D-CED
26	C	524	LMG	C38-C39-C40-C41
28	c	519	DGD	C3B-C4B-C5B-C6B
22	C	507	CLA	C11-C12-C13-C14
22	C	512	CLA	C14-C13-C15-C16
22	c	507	CLA	C11-C12-C13-C14
26	c	524	LMG	C38-C39-C40-C41
28	C	519	DGD	C3B-C4B-C5B-C6B
26	D	402	LMG	C16-C17-C18-C19
26	d	402	LMG	C16-C17-C18-C19
25	C	521	STE	C3-C4-C5-C6
25	M	101	STE	C7-C8-C9-C10
25	m	102	STE	C7-C8-C9-C10
25	E	102	STE	C15-C16-C17-C18
25	e	102	STE	C15-C16-C17-C18
27	X	101	SQD	C30-C31-C32-C33
25	m	102	STE	C5-C6-C7-C8
25	A	409	STE	C5-C6-C7-C8
25	c	521	STE	C3-C4-C5-C6
32	c	523	LMT	C1-C2-C3-C4
25	a	409	STE	C5-C6-C7-C8
23	B	619	BCR	C20-C21-C22-C37
23	b	619	BCR	C20-C21-C22-C37
23	b	620	BCR	C20-C21-C22-C37
23	d	406	BCR	C20-C21-C22-C37
25	a	409	STE	C6-C7-C8-C9
32	C	523	LMT	C1-C2-C3-C4
25	E	103	STE	C2-C3-C4-C5
25	e	103	STE	C2-C3-C4-C5
22	b	612	CLA	C13-C15-C16-C17
26	c	520	LMG	C39-C40-C41-C42
27	B	620	SQD	C28-C29-C30-C31
22	B	613	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	B	615	CLA	C11-C12-C13-C15
22	B	616	CLA	C6-C7-C8-C10
22	C	509	CLA	C6-C7-C8-C10
22	b	616	CLA	C11-C12-C13-C15
22	b	617	CLA	C6-C7-C8-C10
22	c	509	CLA	C6-C7-C8-C10
25	M	101	STE	C5-C6-C7-C8
25	c	516	STE	C11-C10-C9-C8
26	C	520	LMG	C39-C40-C41-C42
26	b	625	LMG	C33-C34-C35-C36
27	x	101	SQD	C30-C31-C32-C33
22	B	611	CLA	C13-C15-C16-C17
25	k	102	STE	C11-C12-C13-C14
26	B	624	LMG	C33-C34-C35-C36
25	A	409	STE	C6-C7-C8-C9
26	C	524	LMG	C8-C7-O1-C1
28	C	518	DGD	C2G-C3G-O3G-C1D
28	C	518	DGD	C5D-C6D-O5D-C1E
28	c	518	DGD	C2G-C3G-O3G-C1D
28	c	518	DGD	C5D-C6D-O5D-C1E
28	A	413	DGD	C4A-C5A-C6A-C7A
28	C	519	DGD	C1B-C2B-C3B-C4B
22	b	615	CLA	C13-C15-C16-C17
25	C	516	STE	C11-C10-C9-C8
25	I	101	STE	C6-C7-C8-C9
25	b	623	STE	C5-C6-C7-C8
32	j	102	LMT	C7-C8-C9-C10
25	i	101	STE	C6-C7-C8-C9
32	J	102	LMT	C7-C8-C9-C10
22	C	512	CLA	O2A-C1-C2-C3
22	c	512	CLA	O2A-C1-C2-C3
32	E	104	LMT	C5-C6-C7-C8
28	c	519	DGD	C1B-C2B-C3B-C4B
32	e	104	LMT	C5-C6-C7-C8
27	b	621	SQD	C30-C31-C32-C33
27	b	621	SQD	C27-C28-C29-C30
32	C	525	LMT	C6-C7-C8-C9
28	C	517	DGD	CAA-CBA-CCA-CDA
25	I	101	STE	C12-C13-C14-C15
28	c	517	DGD	CAA-CBA-CCA-CDA
31	L	101	LHG	O6-C4-C5-O7
31	l	101	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
26	B	624	LMG	C31-C32-C33-C34
26	d	408	LMG	C22-C23-C24-C25
26	C	520	LMG	C7-C8-C9-O8
26	c	520	LMG	C7-C8-C9-O8
27	A	412	SQD	C8-C7-O47-C45
22	D	405	CLA	C16-C17-C18-C19
22	d	405	CLA	C16-C17-C18-C19
32	c	525	LMT	C6-C7-C8-C9
25	K	102	STE	C10-C11-C12-C13
24	A	408	PL9	C35-C34-C36-C37
26	b	625	LMG	C31-C32-C33-C34
28	C	517	DGD	CBA-CCA-CDA-CEA
28	c	517	DGD	CBA-CCA-CDA-CEA
26	C	520	LMG	O7-C8-C9-O8
26	c	520	LMG	O7-C8-C9-O8
22	b	615	CLA	C11-C12-C13-C14
25	A	421	STE	C2-C3-C4-C5
28	C	517	DGD	C5A-C6A-C7A-C8A
28	c	517	DGD	C5A-C6A-C7A-C8A
31	D	411	LHG	C33-C34-C35-C36
25	k	102	STE	C10-C11-C12-C13
28	a	413	DGD	CCA-CDA-CEA-CFA
31	d	411	LHG	C33-C34-C35-C36
32	c	523	LMT	C5-C6-C7-C8
22	B	609	CLA	C13-C15-C16-C17
22	b	610	CLA	C13-C15-C16-C17
31	D	410	LHG	C15-C16-C17-C18
25	a	421	STE	C2-C3-C4-C5
28	c	517	DGD	CCA-CDA-CEA-CFA
32	C	523	LMT	C5-C6-C7-C8
28	C	517	DGD	CCA-CDA-CEA-CFA
27	a	412	SQD	C8-C7-O47-C45
25	b	623	STE	C3-C4-C5-C6
27	X	101	SQD	C29-C30-C31-C32
27	b	621	SQD	C9-C10-C11-C12
26	A	410	LMG	C2-C1-O1-C7
26	a	410	LMG	C2-C1-O1-C7
22	a	406	CLA	CBA-CGA-O2A-C1
27	A	412	SQD	C7-C8-C9-C10
26	H	101	LMG	C15-C16-C17-C18
27	x	101	SQD	C29-C30-C31-C32
22	C	506	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	c	506	CLA	C4-C3-C5-C6
25	B	621	STE	C6-C7-C8-C9
25	b	622	STE	C6-C7-C8-C9
22	A	406	CLA	CBA-CGA-O2A-C1
22	c	505	CLA	C13-C15-C16-C17
26	h	101	LMG	C15-C16-C17-C18
22	C	505	CLA	C13-C15-C16-C17
25	i	101	STE	C12-C13-C14-C15
27	B	620	SQD	C29-C30-C31-C32
25	t	101	STE	C11-C12-C13-C14
28	A	413	DGD	CDA-CEA-CFA-CGA
22	A	404	CLA	C4C-C3C-CAC-CBC
22	a	404	CLA	C4C-C3C-CAC-CBC
27	b	621	SQD	C24-C25-C26-C27
28	C	517	DGD	C4D-C5D-C6D-O5D
28	c	517	DGD	C4D-C5D-C6D-O5D
25	a	415	STE	C11-C10-C9-C8
27	a	412	SQD	O49-C7-O47-C45
26	A	410	LMG	C15-C16-C17-C18
25	E	102	STE	C9-C10-C11-C12
26	a	410	LMG	C15-C16-C17-C18
22	B	601	CLA	C12-C13-C15-C16
22	B	603	CLA	C6-C7-C8-C10
22	B	604	CLA	C6-C7-C8-C10
22	B	606	CLA	C11-C10-C8-C7
22	C	504	CLA	C6-C7-C8-C10
22	b	602	CLA	C12-C13-C15-C16
22	b	604	CLA	C6-C7-C8-C10
22	b	605	CLA	C6-C7-C8-C10
22	b	614	CLA	C12-C13-C15-C16
22	c	504	CLA	C6-C7-C8-C10
22	C	510	CLA	C16-C17-C18-C20
22	c	510	CLA	C16-C17-C18-C20
27	a	412	SQD	C7-C8-C9-C10
28	C	517	DGD	C5B-C6B-C7B-C8B
28	A	413	DGD	C4B-C5B-C6B-C7B
22	A	406	CLA	O1A-CGA-O2A-C1
22	a	406	CLA	O1A-CGA-O2A-C1
31	D	410	LHG	C2-C3-O3-P
31	d	410	LHG	C2-C3-O3-P
28	c	517	DGD	C5B-C6B-C7B-C8B
24	a	408	PL9	C35-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
26	D	408	LMG	C22-C23-C24-C25
26	B	624	LMG	C20-C21-C22-C23
26	b	625	LMG	C20-C21-C22-C23
27	A	412	SQD	O49-C7-O47-C45
28	C	517	DGD	O6D-C5D-C6D-O5D
24	a	408	PL9	C47-C48-C49-C50
25	e	102	STE	C11-C10-C9-C8
28	c	517	DGD	O6D-C5D-C6D-O5D
26	c	520	LMG	O1-C7-C8-O7
28	a	413	DGD	CCB-CDB-CEB-CFB
32	M	102	LMT	C11-C10-C9-C8
25	B	625	STE	C7-C8-C9-C10
27	B	620	SQD	C18-C19-C20-C21
28	a	413	DGD	C4B-C5B-C6B-C7B
26	C	524	LMG	C7-C8-C9-O8
26	c	524	LMG	C7-C8-C9-O8
25	E	102	STE	C11-C10-C9-C8
25	e	102	STE	C9-C10-C11-C12
22	B	608	CLA	C13-C15-C16-C17
22	b	609	CLA	C13-C15-C16-C17
28	A	413	DGD	O6D-C5D-C6D-O5D
22	B	605	CLA	CAD-CBD-CGD-O2D
22	C	502	CLA	CAD-CBD-CGD-O2D
22	b	606	CLA	CAD-CBD-CGD-O2D
22	c	502	CLA	CAD-CBD-CGD-O2D
22	A	419	CLA	C4C-C3C-CAC-CBC
22	a	419	CLA	C4C-C3C-CAC-CBC
22	C	502	CLA	C16-C17-C18-C19
22	c	502	CLA	C16-C17-C18-C19
27	B	620	SQD	C35-C36-C37-C38
28	A	413	DGD	C4D-C5D-C6D-O5D
28	a	413	DGD	C4D-C5D-C6D-O5D
32	m	101	LMT	C11-C10-C9-C8
22	C	510	CLA	C8-C10-C11-C12
22	c	510	CLA	C8-C10-C11-C12
27	B	620	SQD	C24-C25-C26-C27
25	b	601	STE	C7-C8-C9-C10
27	a	412	SQD	C32-C33-C34-C35
28	a	413	DGD	O6D-C5D-C6D-O5D
22	B	605	CLA	CAD-CBD-CGD-O1D
22	C	502	CLA	CAD-CBD-CGD-O1D
22	b	606	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	c	502	CLA	CAD-CBD-CGD-O1D
31	A	420	LHG	C3-O3-P-O4
31	D	409	LHG	C4-O6-P-O5
31	D	411	LHG	C3-O3-P-O4
31	L	101	LHG	C4-O6-P-O5
31	a	420	LHG	C3-O3-P-O4
31	d	409	LHG	C4-O6-P-O5
31	d	411	LHG	C3-O3-P-O4
31	l	101	LHG	C4-O6-P-O5
23	B	617	BCR	C1-C6-C7-C8
23	b	618	BCR	C1-C6-C7-C8
27	a	412	SQD	C27-C28-C29-C30
28	a	413	DGD	C4A-C5A-C6A-C7A
22	B	601	CLA	C8-C10-C11-C12
22	b	602	CLA	C8-C10-C11-C12
26	H	101	LMG	C9-C8-O7-C10
26	h	101	LMG	C9-C8-O7-C10
26	C	520	LMG	C10-C11-C12-C13
22	B	606	CLA	C10-C11-C12-C13
26	d	408	LMG	C20-C21-C22-C23
31	d	411	LHG	C11-C12-C13-C14
22	B	616	CLA	C6-C7-C8-C9
22	C	507	CLA	C11-C10-C8-C9
22	C	513	CLA	C11-C12-C13-C14
22	b	617	CLA	C6-C7-C8-C9
22	c	507	CLA	C11-C10-C8-C9
22	c	513	CLA	C11-C12-C13-C14
24	A	408	PL9	C47-C48-C49-C50
22	B	601	CLA	C6-C7-C8-C10
22	B	604	CLA	C11-C12-C13-C15
22	B	606	CLA	C11-C12-C13-C15
22	C	503	CLA	C6-C7-C8-C10
22	C	513	CLA	C11-C12-C13-C15
22	b	602	CLA	C6-C7-C8-C10
22	b	605	CLA	C11-C12-C13-C15
22	c	503	CLA	C6-C7-C8-C10
22	c	513	CLA	C11-C12-C13-C15
31	D	411	LHG	C11-C12-C13-C14
26	c	520	LMG	C10-C11-C12-C13
26	H	101	LMG	C19-C20-C21-C22
26	h	101	LMG	C19-C20-C21-C22
31	d	410	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
22	D	404	CLA	C2C-C3C-CAC-CBC
22	d	404	CLA	C2C-C3C-CAC-CBC
25	K	102	STE	C11-C12-C13-C14
26	A	410	LMG	C13-C14-C15-C16
26	a	410	LMG	C13-C14-C15-C16
25	k	102	STE	C9-C10-C11-C12
28	C	517	DGD	O1B-C1B-O2G-C2G
28	c	517	DGD	O1B-C1B-O2G-C2G
31	d	410	LHG	C33-C34-C35-C36
26	C	520	LMG	O1-C7-C8-O7
25	A	409	STE	C3-C4-C5-C6
26	D	408	LMG	C20-C21-C22-C23
22	C	502	CLA	C16-C17-C18-C20
22	c	502	CLA	C16-C17-C18-C20
25	a	409	STE	C3-C4-C5-C6
27	A	411	SQD	C23-C24-C25-C26
32	C	525	LMT	C4-C5-C6-C7
32	c	525	LMT	C4-C5-C6-C7
31	A	420	LHG	O8-C23-C24-C25
25	k	102	STE	C14-C15-C16-C17
28	A	413	DGD	C8B-C9B-CAB-CBB
22	C	505	CLA	C8-C10-C11-C12
22	c	505	CLA	C8-C10-C11-C12
22	c	508	CLA	C15-C16-C17-C18
28	A	413	DGD	O2G-C1B-C2B-C3B
28	a	413	DGD	O2G-C1B-C2B-C3B
26	H	101	LMG	C40-C41-C42-C43
26	h	101	LMG	C40-C41-C42-C43
27	A	412	SQD	C27-C28-C29-C30
28	c	518	DGD	C3A-C4A-C5A-C6A
31	a	420	LHG	O8-C23-C24-C25
28	C	517	DGD	C5D-C6D-O5D-C1E
28	c	517	DGD	C5D-C6D-O5D-C1E
26	a	410	LMG	C14-C15-C16-C17
28	H	103	DGD	CCA-CDA-CEA-CFA
22	C	501	CLA	C2A-CAA-CBA-CGA
22	c	501	CLA	C2A-CAA-CBA-CGA
26	A	410	LMG	C14-C15-C16-C17
22	C	512	CLA	C4-C3-C5-C6
24	D	407	PL9	C40-C39-C41-C42
24	d	407	PL9	C40-C39-C41-C42
22	C	506	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	c	506	CLA	C2-C3-C5-C6
25	k	102	STE	C15-C16-C17-C18
28	C	518	DGD	C3A-C4A-C5A-C6A
22	C	508	CLA	C15-C16-C17-C18
31	D	410	LHG	C34-C35-C36-C37
22	B	601	CLA	C6-C7-C8-C9
22	B	603	CLA	C6-C7-C8-C9
22	B	606	CLA	C11-C10-C8-C9
22	C	504	CLA	C6-C7-C8-C9
22	b	602	CLA	C6-C7-C8-C9
22	b	604	CLA	C6-C7-C8-C9
22	b	615	CLA	C14-C13-C15-C16
22	c	504	CLA	C6-C7-C8-C9
22	D	404	CLA	C4B-C3B-CAB-CBB
22	d	404	CLA	C4B-C3B-CAB-CBB
28	A	413	DGD	CEA-CFA-CGA-CHA
22	b	615	CLA	C16-C17-C18-C19
25	D	412	STE	C1-C2-C3-C4
22	c	512	CLA	C4-C3-C5-C6
28	h	103	DGD	CCA-CDA-CEA-CFA
26	H	101	LMG	C30-C31-C32-C33
28	A	413	DGD	CCA-CDA-CEA-CFA
28	c	518	DGD	C7B-C8B-C9B-CAB
22	b	615	CLA	C12-C13-C15-C16
28	C	518	DGD	C7B-C8B-C9B-CAB
31	D	411	LHG	C11-C10-C9-C8
31	d	411	LHG	C11-C10-C9-C8
25	A	416	STE	C9-C10-C11-C12
31	a	420	LHG	C24-C23-O8-C6
25	a	416	STE	C9-C10-C11-C12
25	d	412	STE	C1-C2-C3-C4
26	A	410	LMG	C11-C12-C13-C14
25	A	409	STE	C2-C3-C4-C5
25	C	516	STE	C4-C5-C6-C7
23	B	618	BCR	C20-C21-C22-C37
26	C	524	LMG	C34-C35-C36-C37
26	c	524	LMG	C34-C35-C36-C37
27	A	411	SQD	O49-C7-O47-C45
26	a	410	LMG	C11-C12-C13-C14
27	b	621	SQD	C14-C15-C16-C17
22	A	405	CLA	C10-C11-C12-C13
25	K	102	STE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	a	409	STE	C2-C3-C4-C5
25	c	516	STE	C4-C5-C6-C7
22	B	615	CLA	C4-C3-C5-C6
22	b	616	CLA	C4-C3-C5-C6
24	a	408	PL9	C15-C14-C16-C17
30	A	418	PHO	C4-C3-C5-C6
30	a	418	PHO	C4-C3-C5-C6
22	B	612	CLA	C3-C5-C6-C7
22	b	613	CLA	C3-C5-C6-C7
22	B	601	CLA	C14-C13-C15-C16
22	B	611	CLA	C11-C12-C13-C14
22	C	505	CLA	C11-C12-C13-C14
22	b	602	CLA	C14-C13-C15-C16
22	b	612	CLA	C11-C12-C13-C14
22	c	505	CLA	C11-C12-C13-C14
28	H	103	DGD	C5B-C6B-C7B-C8B
28	h	103	DGD	C5B-C6B-C7B-C8B
32	J	102	LMT	C6-C7-C8-C9
32	j	102	LMT	C6-C7-C8-C9
26	A	410	LMG	C9-C8-O7-C10
26	a	410	LMG	C9-C8-O7-C10
27	a	411	SQD	O49-C7-O47-C45
28	C	519	DGD	C6A-C7A-C8A-C9A
31	A	420	LHG	C24-C23-O8-C6
28	c	519	DGD	C6A-C7A-C8A-C9A
22	B	603	CLA	C2A-CAA-CBA-CGA
22	b	604	CLA	C2A-CAA-CBA-CGA
22	B	613	CLA	C15-C16-C17-C18
25	b	601	STE	C9-C10-C11-C12
32	M	102	LMT	C3-C4-C5-C6
25	c	522	STE	C12-C13-C14-C15
26	h	101	LMG	C30-C31-C32-C33
28	A	413	DGD	CAB-CBB-CCB-CDB
23	B	617	BCR	C5-C6-C7-C8
23	b	618	BCR	C5-C6-C7-C8
25	E	103	STE	O2-C1-C2-C3
25	e	103	STE	O2-C1-C2-C3
25	C	522	STE	C12-C13-C14-C15
31	D	410	LHG	C33-C34-C35-C36
25	E	103	STE	O1-C1-C2-C3
27	b	621	SQD	C11-C12-C13-C14
25	e	103	STE	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
32	m	101	LMT	O5'-C5'-C6'-O6'
22	C	503	CLA	C11-C10-C8-C7
22	b	607	CLA	C11-C10-C8-C7
22	c	503	CLA	C11-C10-C8-C7
32	M	102	LMT	O5'-C5'-C6'-O6'
32	m	101	LMT	C3-C4-C5-C6
31	A	420	LHG	C23-C24-C25-C26
26	C	524	LMG	O7-C8-C9-O8
27	A	412	SQD	O6-C44-C45-O47
27	a	412	SQD	O6-C44-C45-O47
25	B	625	STE	C9-C10-C11-C12
27	A	412	SQD	C15-C16-C17-C18
22	b	607	CLA	C10-C11-C12-C13
22	B	601	CLA	C4-C3-C5-C6
22	b	602	CLA	C4-C3-C5-C6
22	B	615	CLA	C2-C3-C5-C6
22	b	616	CLA	C2-C3-C5-C6
22	b	614	CLA	C15-C16-C17-C18
27	A	411	SQD	C27-C28-C29-C30
26	D	402	LMG	C35-C36-C37-C38
35	v	201	HEC	CAD-CBD-CGD-O1D
28	C	517	DGD	C8A-C9A-CAA-CBA
28	c	517	DGD	C8A-C9A-CAA-CBA
35	V	201	HEC	CAD-CBD-CGD-O1D
22	b	616	CLA	C5-C6-C7-C8
22	A	405	CLA	C11-C12-C13-C14
22	B	615	CLA	C5-C6-C7-C8
28	h	103	DGD	O1A-C1A-O1G-C1G
28	C	519	DGD	O6D-C5D-C6D-O5D
28	c	519	DGD	O6D-C5D-C6D-O5D
24	A	408	PL9	C29-C31-C32-C33
24	a	408	PL9	C29-C31-C32-C33
28	H	103	DGD	O1A-C1A-O1G-C1G
25	d	412	STE	O1-C1-C2-C3
31	D	410	LHG	O1-C1-C2-O2
31	d	410	LHG	O1-C1-C2-O2
25	D	412	STE	O2-C1-C2-C3
22	c	506	CLA	C16-C17-C18-C20
27	a	411	SQD	C27-C28-C29-C30
25	D	412	STE	O1-C1-C2-C3
25	d	412	STE	O2-C1-C2-C3
22	B	614	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	C	506	CLA	C16-C17-C18-C20
31	D	411	LHG	C1-C2-C3-O3
31	d	411	LHG	C1-C2-C3-O3
28	H	103	DGD	O2G-C1B-C2B-C3B
25	t	101	STE	O2-C1-C2-C3
31	D	409	LHG	O6-C4-C5-C6
31	d	409	LHG	O6-C4-C5-C6
26	c	524	LMG	O7-C8-C9-O8
28	a	413	DGD	O2G-C2G-C3G-O3G
25	E	101	STE	C7-C8-C9-C10
30	a	418	PHO	C2-C3-C5-C6
26	d	402	LMG	C35-C36-C37-C38
25	e	101	STE	C7-C8-C9-C10
25	e	102	STE	C10-C11-C12-C13
26	c	520	LMG	C30-C31-C32-C33
32	B	623	LMT	C9-C10-C11-C12
32	b	624	LMT	C9-C10-C11-C12
28	h	103	DGD	O2G-C1B-C2B-C3B
22	C	510	CLA	C6-C7-C8-C9
22	c	510	CLA	C6-C7-C8-C9
26	A	410	LMG	C12-C13-C14-C15
26	C	520	LMG	C30-C31-C32-C33
31	a	420	LHG	C14-C15-C16-C17
26	a	410	LMG	C12-C13-C14-C15
25	c	521	STE	O2-C1-C2-C3
22	B	602	CLA	C16-C17-C18-C20
22	b	603	CLA	C16-C17-C18-C20
30	A	418	PHO	C2-C3-C5-C6
25	B	621	STE	C1-C2-C3-C4
22	b	607	CLA	C13-C15-C16-C17
25	C	521	STE	O2-C1-C2-C3
25	E	101	STE	O2-C1-C2-C3
25	e	101	STE	O2-C1-C2-C3
27	A	412	SQD	C24-C25-C26-C27
31	A	420	LHG	C35-C36-C37-C38
25	b	622	STE	C1-C2-C3-C4
25	C	516	STE	C9-C10-C11-C12
25	c	516	STE	C9-C10-C11-C12
25	E	101	STE	O1-C1-C2-C3
25	e	101	STE	O1-C1-C2-C3
25	t	101	STE	O1-C1-C2-C3
31	a	420	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
27	a	412	SQD	C24-C25-C26-C27
28	a	413	DGD	C1G-C2G-C3G-O3G
22	B	608	CLA	O1A-CGA-O2A-C1
22	b	609	CLA	O1A-CGA-O2A-C1
22	C	506	CLA	C13-C15-C16-C17
25	C	521	STE	O1-C1-C2-C3
25	I	101	STE	C2-C3-C4-C5
25	i	101	STE	C2-C3-C4-C5
27	B	620	SQD	C16-C17-C18-C19
25	c	521	STE	O1-C1-C2-C3
22	c	506	CLA	C13-C15-C16-C17
27	B	620	SQD	C14-C15-C16-C17
32	c	525	LMT	C3-C4-C5-C6
22	a	405	CLA	C2C-C3C-CAC-CBC
32	C	525	LMT	C11-C10-C9-C8
31	A	420	LHG	C14-C15-C16-C17
22	B	611	CLA	C14-C13-C15-C16
22	B	615	CLA	C11-C12-C13-C14
22	b	612	CLA	C14-C13-C15-C16
22	b	616	CLA	C11-C12-C13-C14
22	b	614	CLA	C16-C17-C18-C20
22	A	405	CLA	C2C-C3C-CAC-CBC
22	C	510	CLA	CAA-CBA-CGA-O2A
27	A	411	SQD	O47-C7-C8-C9
27	a	411	SQD	O47-C7-C8-C9
31	a	420	LHG	C27-C28-C29-C30
28	C	518	DGD	C4A-C5A-C6A-C7A
28	c	518	DGD	C4A-C5A-C6A-C7A
32	Z	101	LMT	C7-C8-C9-C10
32	c	525	LMT	C11-C10-C9-C8
22	c	510	CLA	CAA-CBA-CGA-O2A
28	C	519	DGD	O1G-C1A-C2A-C3A
28	c	519	DGD	O1G-C1A-C2A-C3A
22	B	613	CLA	C16-C17-C18-C20
22	B	601	CLA	C11-C12-C13-C15
22	C	505	CLA	C12-C13-C15-C16
22	C	510	CLA	C6-C7-C8-C10
22	b	602	CLA	C11-C12-C13-C15
22	c	505	CLA	C12-C13-C15-C16
22	c	510	CLA	C6-C7-C8-C10
32	C	525	LMT	C3-C4-C5-C6
26	A	410	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
26	a	410	LMG	C19-C20-C21-C22
35	v	201	HEC	CAD-CBD-CGD-O2D
22	D	404	CLA	C2B-C3B-CAB-CBB
22	d	404	CLA	C2B-C3B-CAB-CBB
23	T	101	BCR	C1-C6-C7-C8
23	T	101	BCR	C5-C6-C7-C8
23	b	619	BCR	C23-C24-C25-C30
23	t	102	BCR	C1-C6-C7-C8
23	t	102	BCR	C5-C6-C7-C8
32	z	101	LMT	C7-C8-C9-C10
26	b	625	LMG	C16-C17-C18-C19
27	a	411	SQD	C23-C24-C25-C26
28	c	517	DGD	C2A-C3A-C4A-C5A
25	a	416	STE	C15-C16-C17-C18
22	b	602	CLA	CAA-CBA-CGA-O2A
28	C	518	DGD	O6D-C1D-O3G-C3G
28	c	518	DGD	O6D-C1D-O3G-C3G
28	C	517	DGD	C2A-C3A-C4A-C5A
31	l	101	LHG	C17-C18-C19-C20
31	A	420	LHG	C15-C16-C17-C18
31	L	101	LHG	C17-C18-C19-C20
22	b	603	CLA	C16-C17-C18-C19
22	B	601	CLA	CAA-CBA-CGA-O2A
24	D	407	PL9	C13-C14-C16-C17
24	d	407	PL9	C13-C14-C16-C17
26	B	624	LMG	C16-C17-C18-C19
22	B	614	CLA	C2A-CAA-CBA-CGA
27	A	411	SQD	C8-C7-O47-C45
27	a	411	SQD	C8-C7-O47-C45
31	A	420	LHG	C8-C7-O7-C5
26	D	408	LMG	C10-C11-C12-C13
25	A	416	STE	C15-C16-C17-C18
35	V	201	HEC	CAD-CBD-CGD-O2D
22	B	602	CLA	C16-C17-C18-C19
22	B	612	CLA	C13-C15-C16-C17
22	b	613	CLA	C13-C15-C16-C17
26	H	101	LMG	C32-C33-C34-C35
31	D	410	LHG	C32-C33-C34-C35
25	E	103	STE	C11-C10-C9-C8
25	e	103	STE	C11-C10-C9-C8
25	a	415	STE	C10-C11-C12-C13
27	B	620	SQD	C4-C5-C6-S

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Mol	Chain	Res	Type	Atoms
28	H	103	DGD	C3B-C4B-C5B-C6B
28	h	103	DGD	C3B-C4B-C5B-C6B
32	c	525	LMT	C5'-C4'-O1B-C1B
26	d	408	LMG	C10-C11-C12-C13
27	a	412	SQD	C15-C16-C17-C18
31	a	420	LHG	C15-C16-C17-C18
22	C	512	CLA	C2-C3-C5-C6
22	c	512	CLA	C2-C3-C5-C6
25	E	103	STE	C5-C6-C7-C8
25	e	103	STE	C5-C6-C7-C8
22	b	615	CLA	C2A-CAA-CBA-CGA
25	B	622	STE	O1-C1-C2-C3
27	a	412	SQD	O47-C7-C8-C9
26	B	624	LMG	C10-C11-C12-C13
32	E	104	LMT	C2-C1-O1'-C1'
32	e	104	LMT	C2-C1-O1'-C1'
32	C	525	LMT	C5'-C4'-O1B-C1B
25	B	622	STE	O2-C1-C2-C3
22	B	605	CLA	C14-C13-C15-C16
22	b	606	CLA	C14-C13-C15-C16
22	b	607	CLA	C11-C10-C8-C9
27	A	412	SQD	O47-C7-C8-C9
31	L	101	LHG	C16-C17-C18-C19
32	E	104	LMT	C1-C2-C3-C4
32	e	104	LMT	C1-C2-C3-C4
31	l	101	LHG	C16-C17-C18-C19
22	B	605	CLA	C4B-C3B-CAB-CBB
26	b	625	LMG	C10-C11-C12-C13
23	H	102	BCR	C22-C23-C24-C25
23	h	102	BCR	C22-C23-C24-C25
26	C	524	LMG	O6-C1-O1-C7
26	c	524	LMG	O6-C1-O1-C7
28	A	413	DGD	O2G-C2G-C3G-O3G
23	H	102	BCR	C15-C16-C17-C18
22	B	608	CLA	CBA-CGA-O2A-C1
22	b	609	CLA	CBA-CGA-O2A-C1
31	L	101	LHG	O7-C7-C8-C9
31	l	101	LHG	O7-C7-C8-C9
22	B	604	CLA	C13-C15-C16-C17
27	B	620	SQD	C25-C26-C27-C28
32	J	102	LMT	C5-C6-C7-C8
32	j	102	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	B	607	CLA	C16-C17-C18-C20
22	B	609	CLA	C16-C17-C18-C19
22	b	608	CLA	C16-C17-C18-C20
22	b	610	CLA	C16-C17-C18-C19
31	a	420	LHG	C8-C7-O7-C5
28	A	413	DGD	CAA-CBA-CCA-CDA
27	A	411	SQD	C5-C6-S-O7
27	a	411	SQD	C5-C6-S-O7
22	b	605	CLA	C13-C15-C16-C17
22	C	506	CLA	C11-C10-C8-C7
22	C	513	CLA	C11-C10-C8-C7
22	b	607	CLA	C11-C12-C13-C15
22	b	615	CLA	C11-C10-C8-C7
22	c	506	CLA	C11-C10-C8-C7
22	B	608	CLA	C2A-CAA-CBA-CGA
22	b	609	CLA	C2A-CAA-CBA-CGA
26	C	524	LMG	O8-C28-C29-C30
26	h	101	LMG	O9-C10-C11-C12
27	A	411	SQD	O49-C7-C8-C9
27	a	411	SQD	O49-C7-C8-C9
22	A	405	CLA	C11-C12-C13-C15
32	Z	101	LMT	C5-C6-C7-C8
25	A	414	STE	C11-C12-C13-C14
22	b	602	CLA	CAA-CBA-CGA-O1A
26	B	624	LMG	C35-C36-C37-C38
22	B	601	CLA	CAA-CBA-CGA-O1A
26	H	101	LMG	O9-C10-C11-C12
28	C	517	DGD	O1B-C1B-C2B-C3B
28	c	517	DGD	O1B-C1B-C2B-C3B
22	B	606	CLA	C11-C12-C13-C14
22	B	613	CLA	C14-C13-C15-C16
22	C	506	CLA	C11-C10-C8-C9
22	b	614	CLA	C14-C13-C15-C16
22	c	506	CLA	C11-C10-C8-C9
26	c	524	LMG	O8-C28-C29-C30
22	B	603	CLA	C5-C6-C7-C8
23	h	102	BCR	C15-C16-C17-C18
22	b	604	CLA	C5-C6-C7-C8
32	z	101	LMT	C5-C6-C7-C8
25	a	414	STE	C11-C12-C13-C14
22	C	510	CLA	CAA-CBA-CGA-O1A
26	c	524	LMG	O10-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
27	a	412	SQD	O49-C7-C8-C9
26	b	625	LMG	C35-C36-C37-C38
22	B	612	CLA	C8-C10-C11-C12
22	b	613	CLA	C8-C10-C11-C12
26	C	524	LMG	O10-C28-C29-C30
27	A	412	SQD	O49-C7-C8-C9
25	B	625	STE	C12-C13-C14-C15
28	A	413	DGD	C2G-C3G-O3G-C1D
28	a	413	DGD	C2G-C3G-O3G-C1D
22	b	613	CLA	O1A-CGA-O2A-C1
22	b	613	CLA	CAA-CBA-CGA-O2A
28	C	517	DGD	C7A-C8A-C9A-CAA
22	c	510	CLA	CAA-CBA-CGA-O1A
28	c	517	DGD	C7A-C8A-C9A-CAA
22	C	512	CLA	C15-C16-C17-C18
22	B	612	CLA	CAA-CBA-CGA-O2A
22	B	612	CLA	O1A-CGA-O2A-C1
22	B	616	CLA	CAD-CBD-CGD-O2D
22	b	617	CLA	CAD-CBD-CGD-O2D
27	x	101	SQD	C32-C33-C34-C35
32	J	102	LMT	O5'-C1'-O1'-C1
32	j	102	LMT	O5'-C1'-O1'-C1
22	a	405	CLA	C4C-C3C-CAC-CBC
25	c	516	STE	C3-C4-C5-C6
22	B	613	CLA	CAA-CBA-CGA-O2A
22	b	614	CLA	CAA-CBA-CGA-O2A
31	D	410	LHG	O8-C23-C24-C25
31	d	410	LHG	O8-C23-C24-C25
27	X	101	SQD	C32-C33-C34-C35
22	A	405	CLA	C4C-C3C-CAC-CBC
26	B	624	LMG	O8-C28-C29-C30
25	b	623	STE	O1-C1-C2-C3

There are no ring outliers.

146 monomers are involved in 325 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	a	412	SQD	5	0
23	b	618	BCR	3	0
25	B	621	STE	1	0
25	j	101	STE	1	0
24	D	407	PL9	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	C	518	DGD	2	0
27	B	620	SQD	3	0
22	C	512	CLA	4	0
22	b	616	CLA	2	0
26	H	101	LMG	6	0
23	H	102	BCR	6	0
22	c	509	CLA	3	0
28	a	413	DGD	10	0
35	v	201	HEC	1	0
22	B	604	CLA	1	0
31	d	411	LHG	1	0
31	D	409	LHG	2	0
23	k	103	BCR	3	0
23	b	619	BCR	5	0
25	d	412	STE	2	0
24	A	408	PL9	10	0
22	A	405	CLA	1	0
25	A	416	STE	1	0
22	a	419	CLA	1	0
22	c	512	CLA	4	0
26	D	402	LMG	1	0
32	j	102	LMT	2	0
25	t	101	STE	1	0
22	C	505	CLA	3	0
32	C	523	LMT	2	0
27	A	411	SQD	2	0
23	B	619	BCR	1	0
24	d	407	PL9	1	0
25	a	409	STE	1	0
23	K	101	BCR	1	0
22	B	605	CLA	1	0
22	b	603	CLA	3	0
22	B	609	CLA	3	0
22	a	406	CLA	1	0
22	b	617	CLA	1	0
23	D	406	BCR	5	0
25	e	102	STE	2	0
27	X	101	SQD	3	0
31	d	410	LHG	4	0
31	A	420	LHG	1	0
23	a	407	BCR	2	0
22	D	405	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	612	CLA	2	0
22	B	602	CLA	3	0
28	c	518	DGD	1	0
25	b	623	STE	1	0
26	h	101	LMG	6	0
23	C	515	BCR	5	0
24	a	408	PL9	12	0
27	b	621	SQD	3	0
25	B	622	STE	2	0
26	d	408	LMG	1	0
25	a	415	STE	2	0
22	A	419	CLA	1	0
25	k	102	STE	1	0
22	B	616	CLA	1	0
22	c	510	CLA	1	0
23	c	515	BCR	4	0
22	b	613	CLA	2	0
22	B	607	CLA	1	0
22	D	404	CLA	2	0
26	c	524	LMG	5	0
34	E	105	HEM	6	0
22	c	513	CLA	4	0
22	b	610	CLA	3	0
22	C	501	CLA	3	0
22	b	615	CLA	1	0
23	h	102	BCR	7	0
26	d	402	LMG	1	0
22	B	613	CLA	1	0
30	A	418	PHO	1	0
23	A	407	BCR	4	0
32	J	102	LMT	2	0
34	e	105	HEM	6	0
26	D	408	LMG	1	0
28	A	413	DGD	6	0
23	B	618	BCR	6	0
22	B	615	CLA	2	0
22	B	606	CLA	2	0
31	D	411	LHG	1	0
25	a	421	STE	2	0
22	b	608	CLA	1	0
26	B	624	LMG	1	0
26	a	410	LMG	1	0

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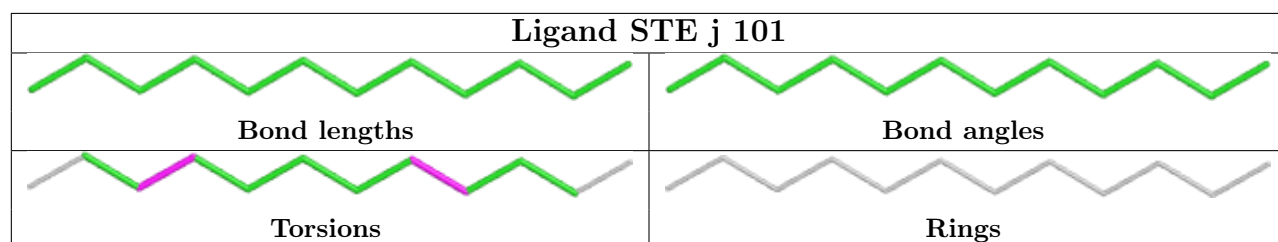
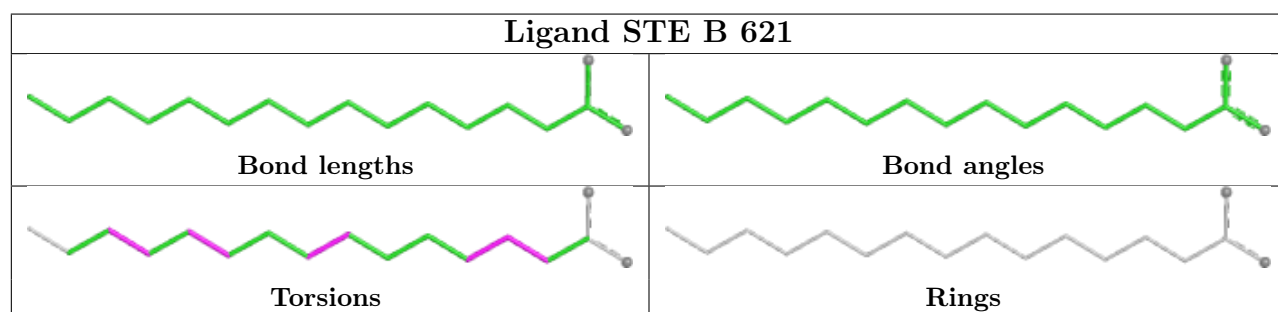
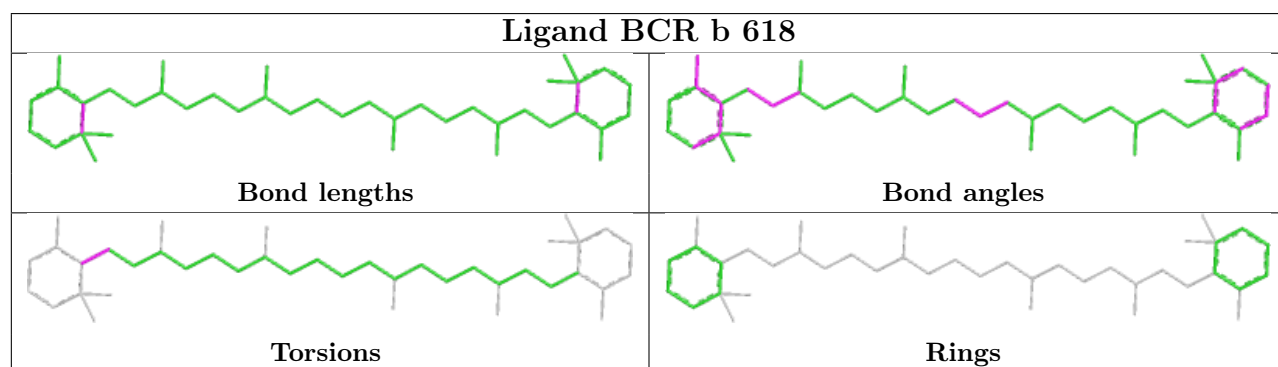
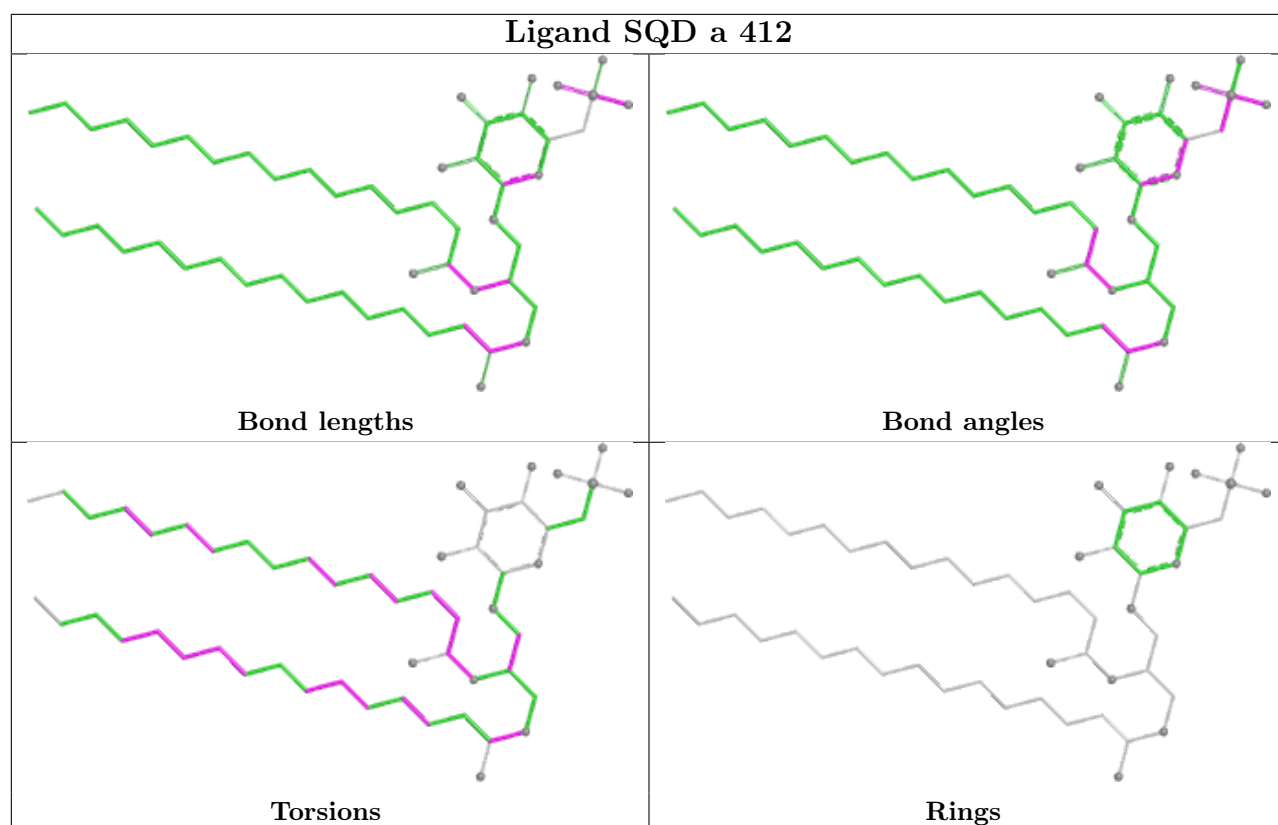
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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22	C	509	CLA	3	0
25	A	421	STE	1	0
27	A	412	SQD	2	0
22	a	404	CLA	2	0
22	C	511	CLA	3	0
23	K	103	BCR	4	0
22	b	607	CLA	5	0
22	c	501	CLA	2	0
23	T	101	BCR	7	0
32	z	101	LMT	3	0
23	t	102	BCR	11	0
25	J	101	STE	1	0
31	d	409	LHG	2	0
26	c	520	LMG	1	0
22	B	608	CLA	2	0
22	b	602	CLA	4	0
23	k	101	BCR	2	0
31	a	420	LHG	1	0
27	x	101	SQD	3	0
31	D	410	LHG	2	0
22	b	614	CLA	1	0
25	A	415	STE	1	0
23	C	514	BCR	2	0
22	B	614	CLA	1	0
22	C	502	CLA	1	0
22	C	508	CLA	3	0
26	C	524	LMG	6	0
22	c	505	CLA	3	0
32	Z	101	LMT	3	0
23	c	514	BCR	3	0
23	d	406	BCR	4	0
35	V	201	HEC	1	0
26	A	410	LMG	1	0
25	D	412	STE	2	0
22	C	510	CLA	1	0
23	B	617	BCR	3	0
32	E	104	LMT	1	0
25	E	102	STE	2	0
25	b	622	STE	1	0
22	a	405	CLA	1	0

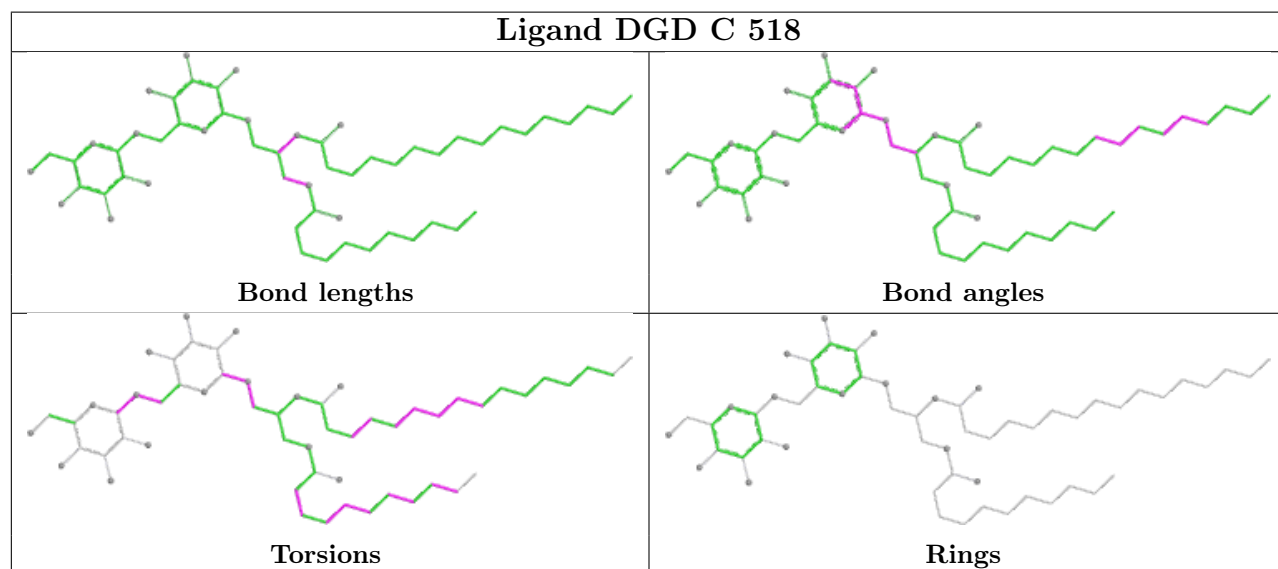
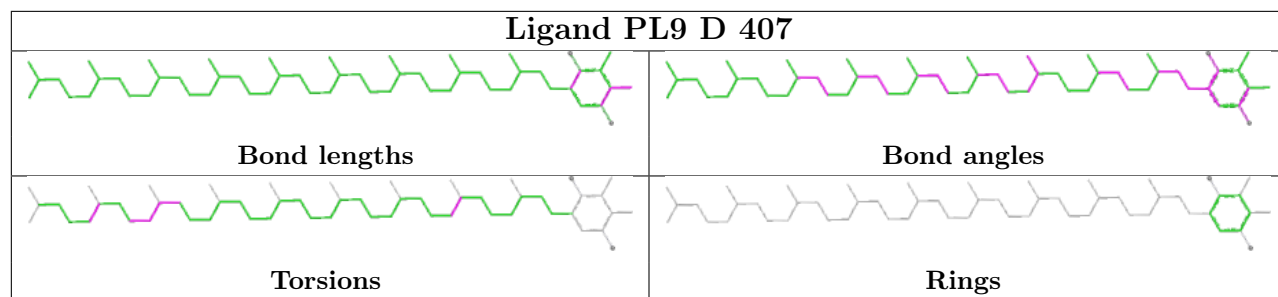
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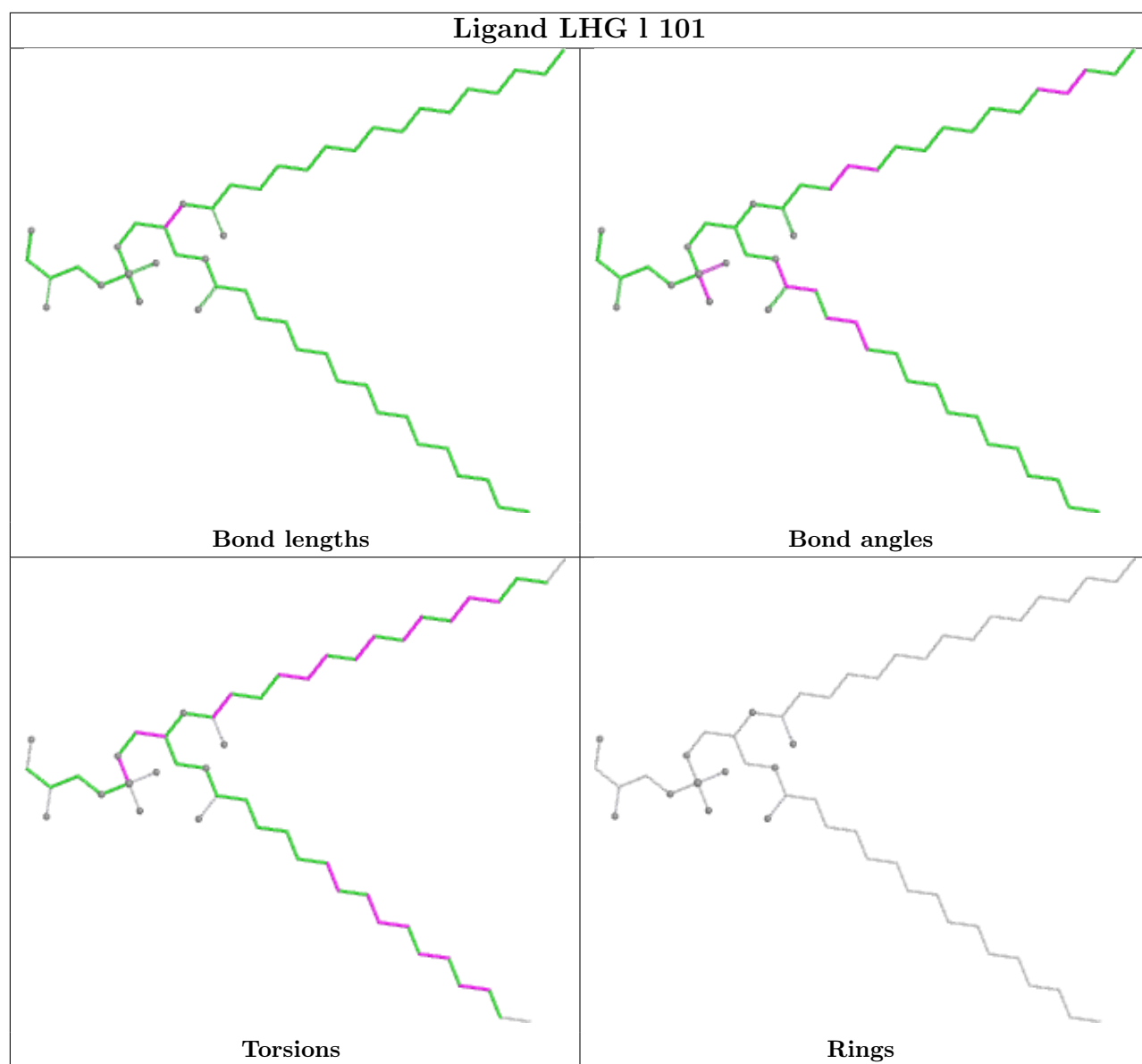
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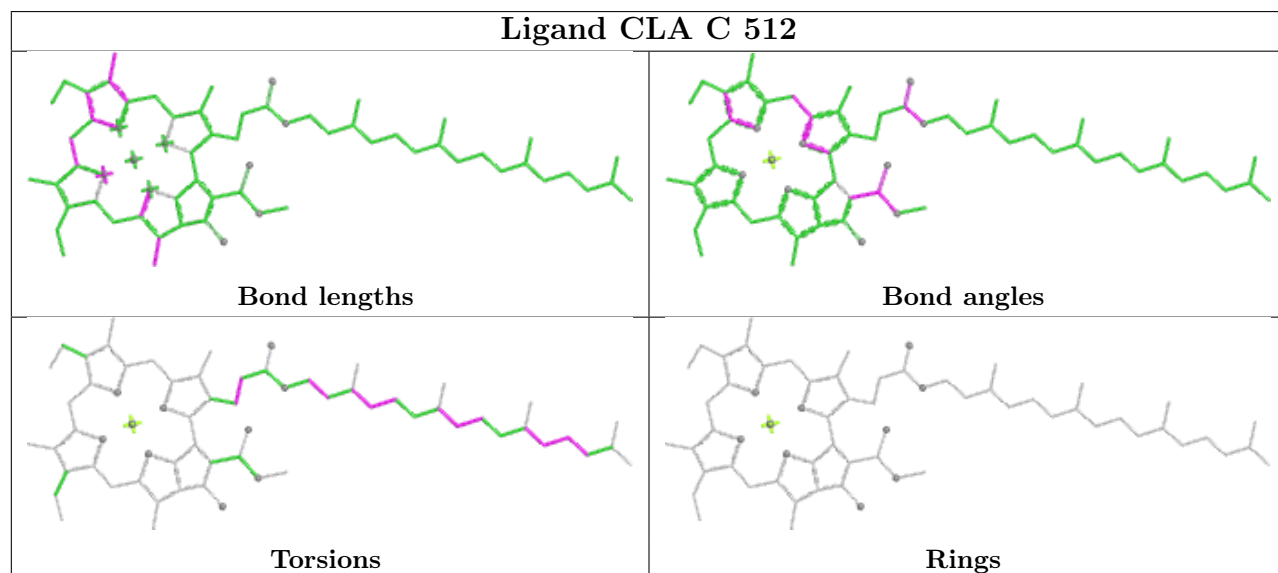
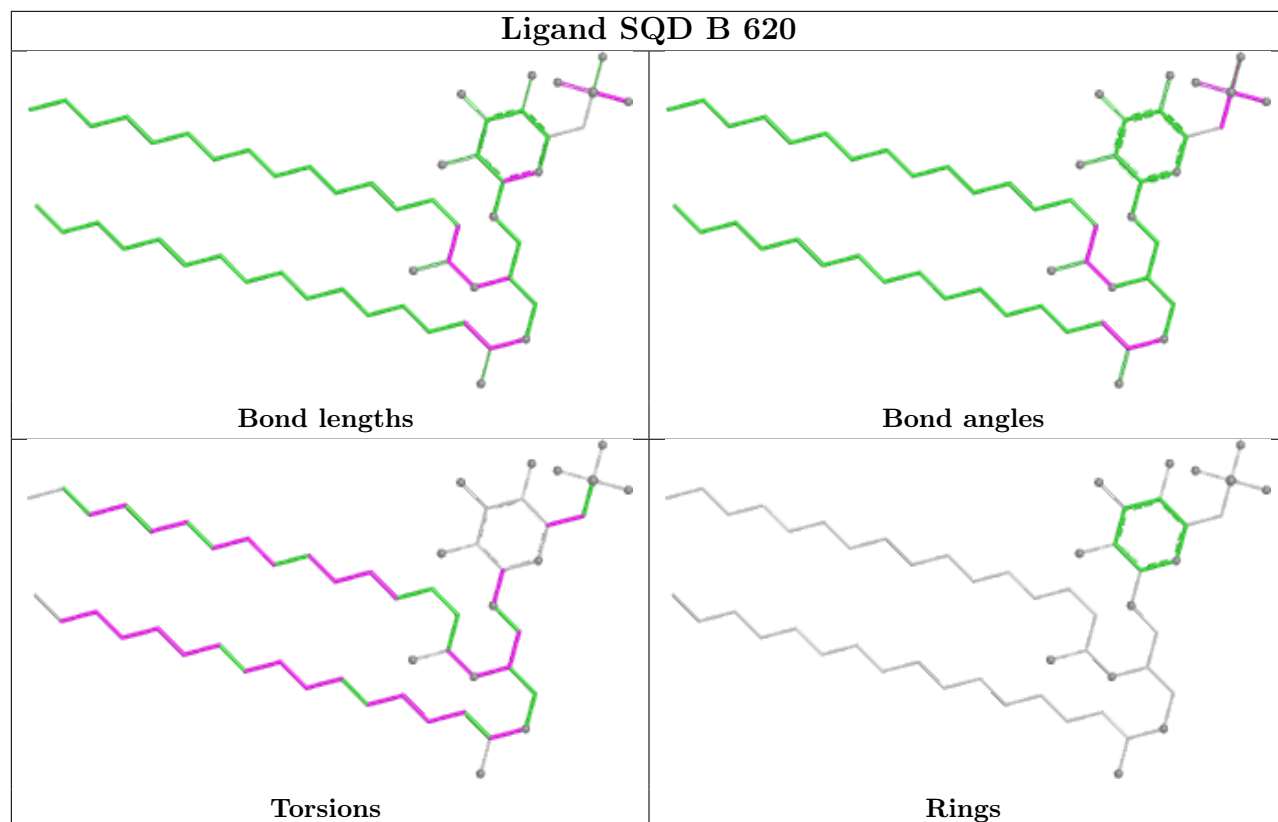
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	c	511	CLA	3	0
26	C	520	LMG	1	0
22	C	513	CLA	5	0
22	b	609	CLA	2	0
25	a	416	STE	1	0
22	c	502	CLA	1	0
22	d	404	CLA	1	0
22	b	606	CLA	1	0
22	c	508	CLA	4	0
25	A	409	STE	1	0
27	a	411	SQD	3	0
32	c	523	LMT	2	0
22	B	601	CLA	5	0
26	b	625	LMG	1	0
22	A	406	CLA	1	0

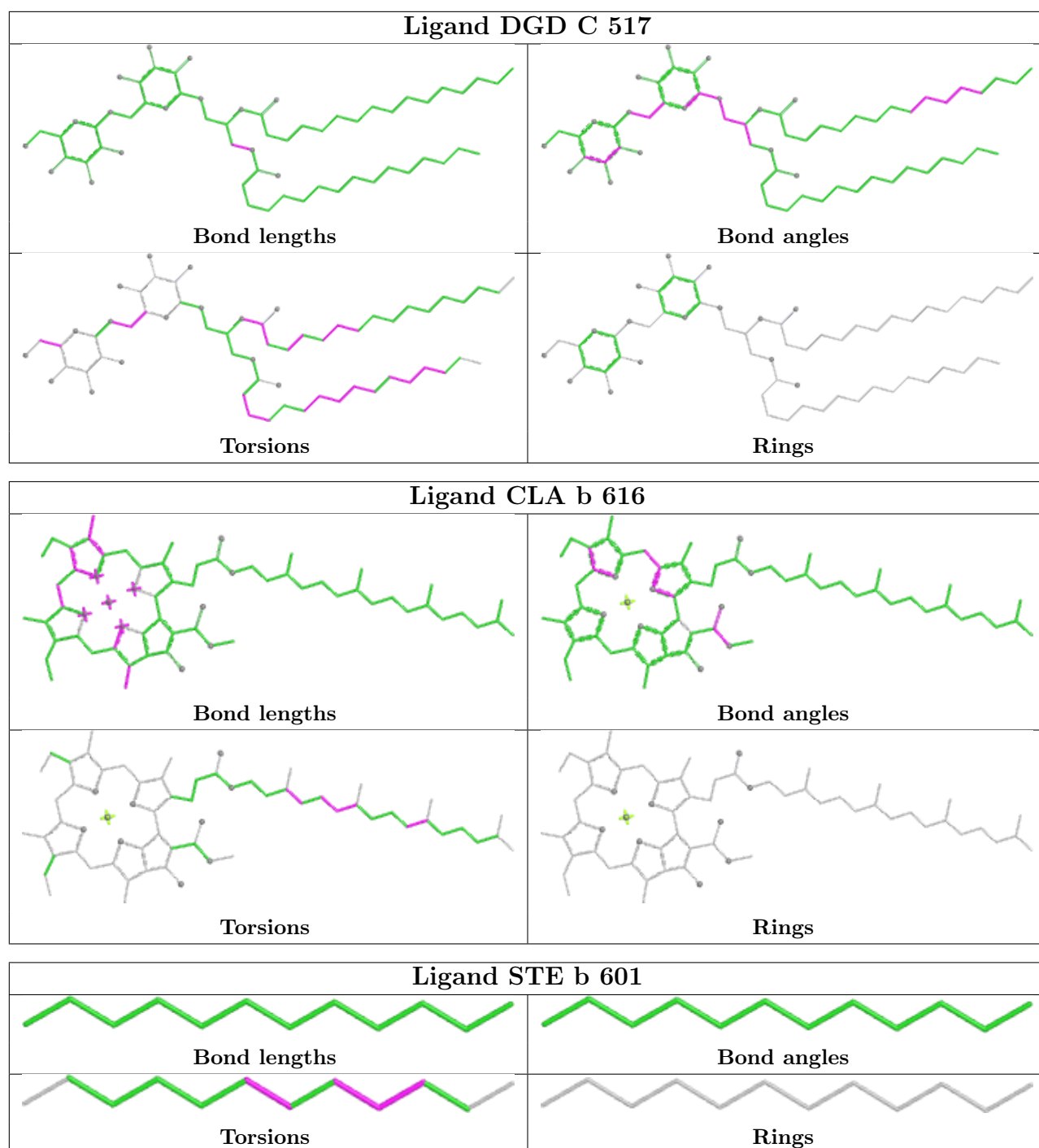
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

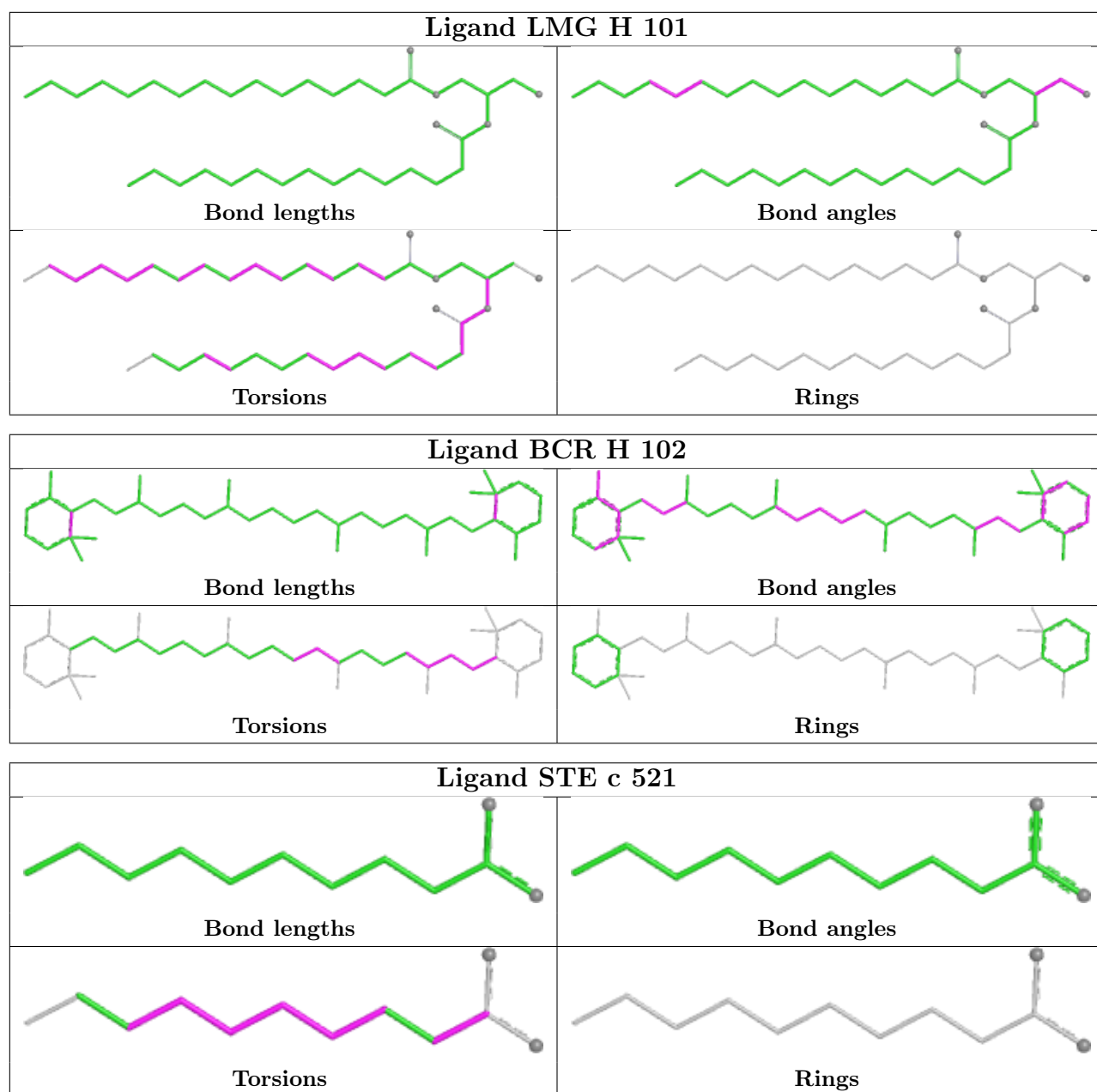


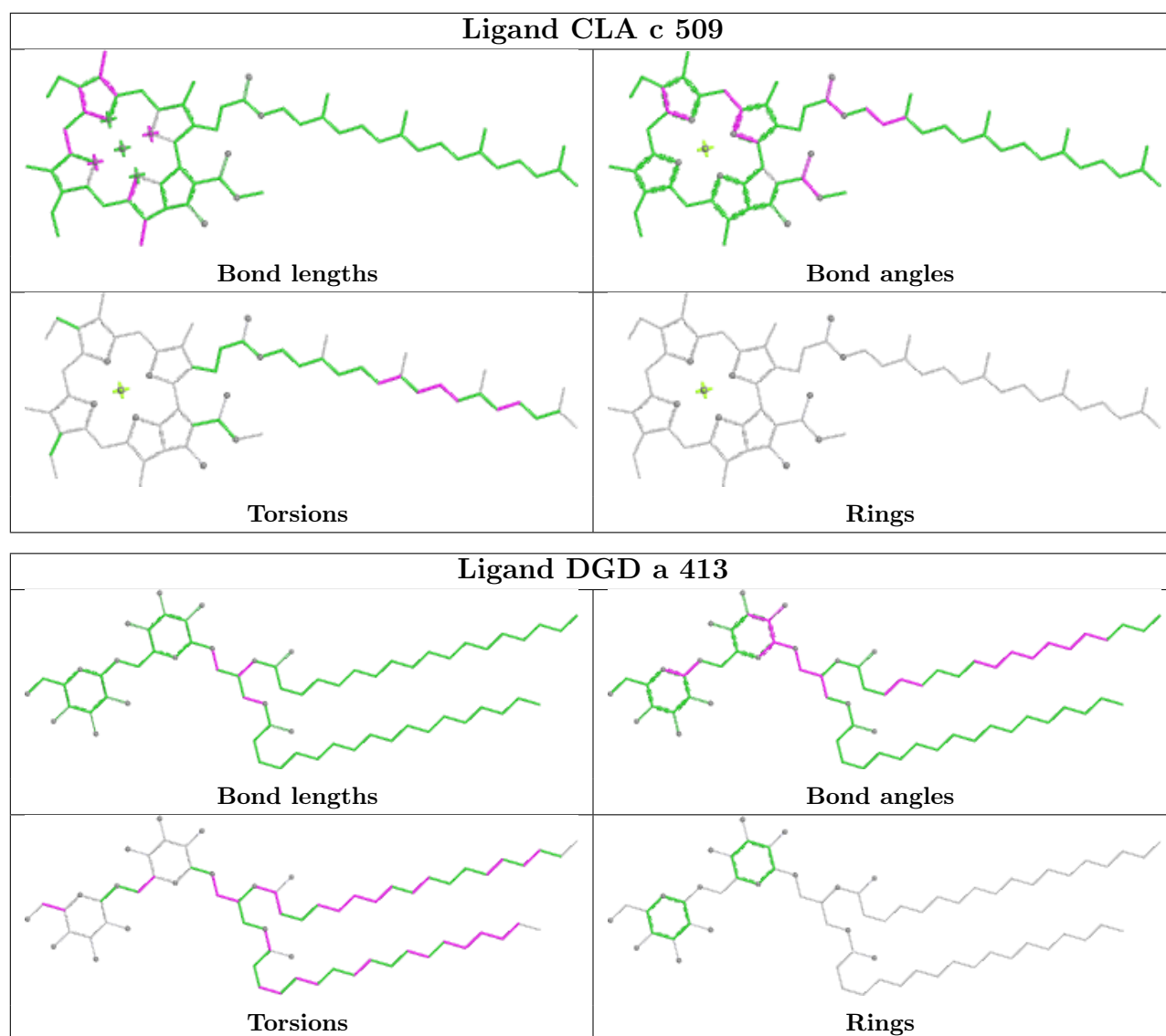




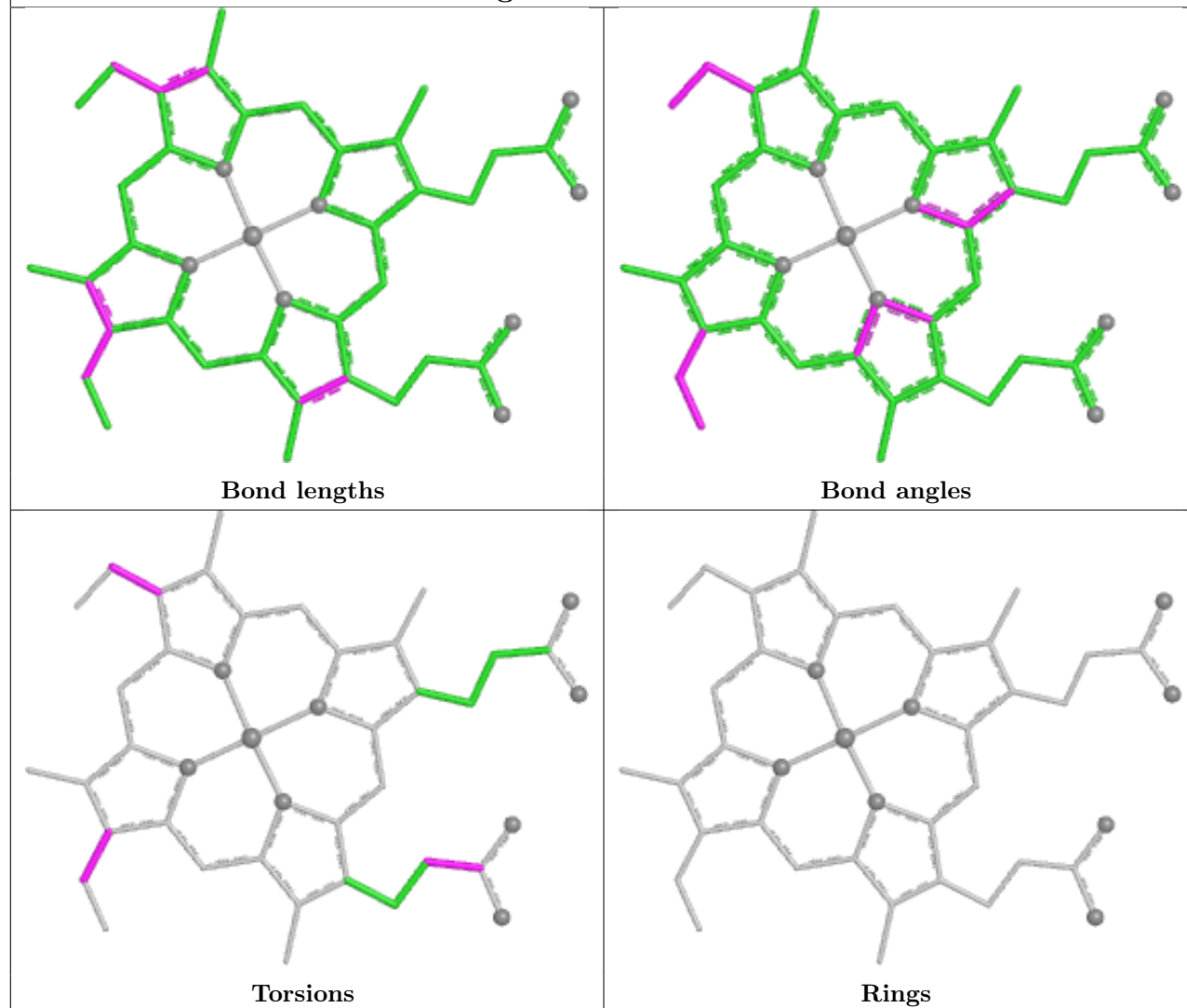




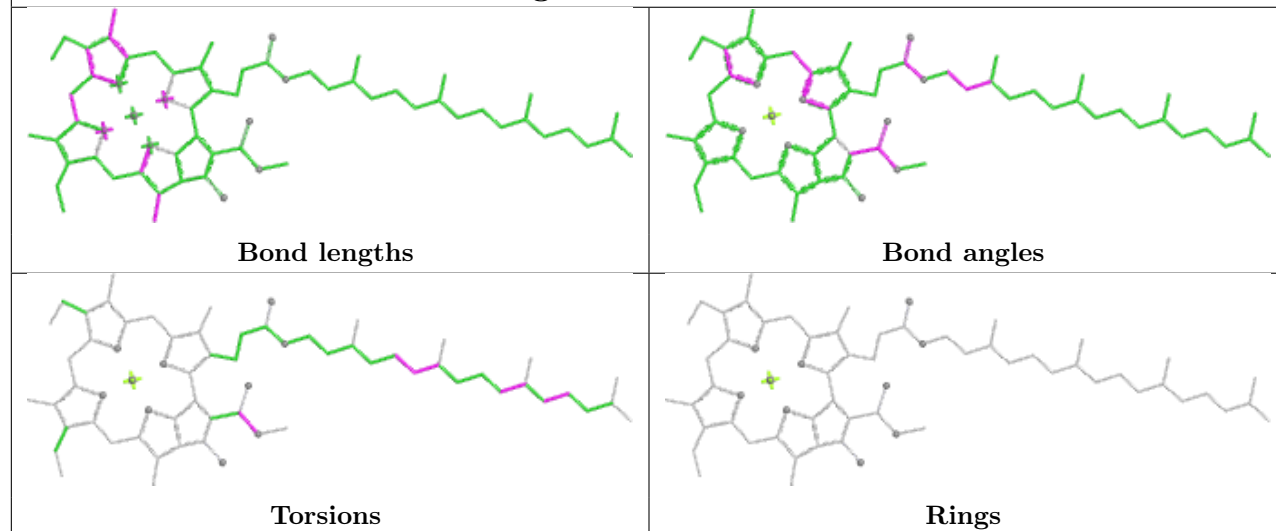


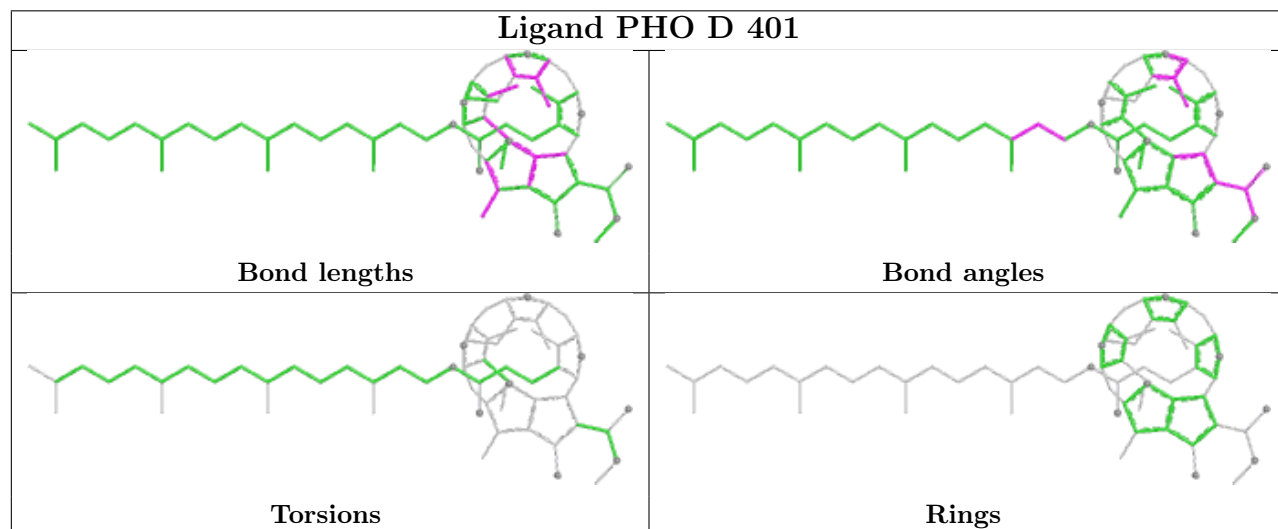
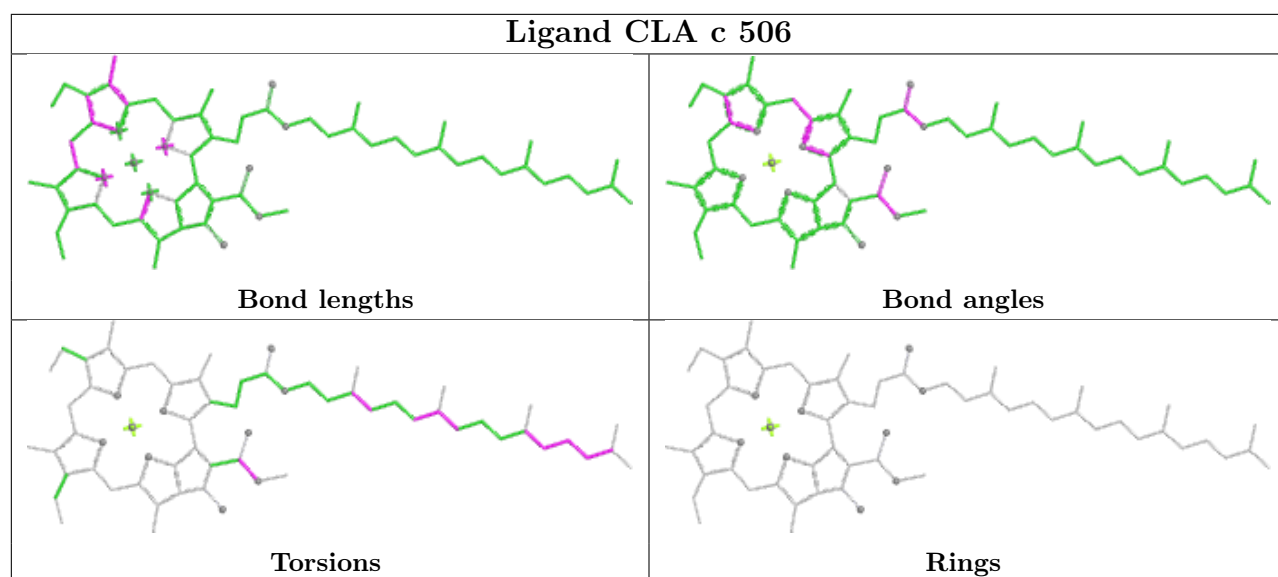


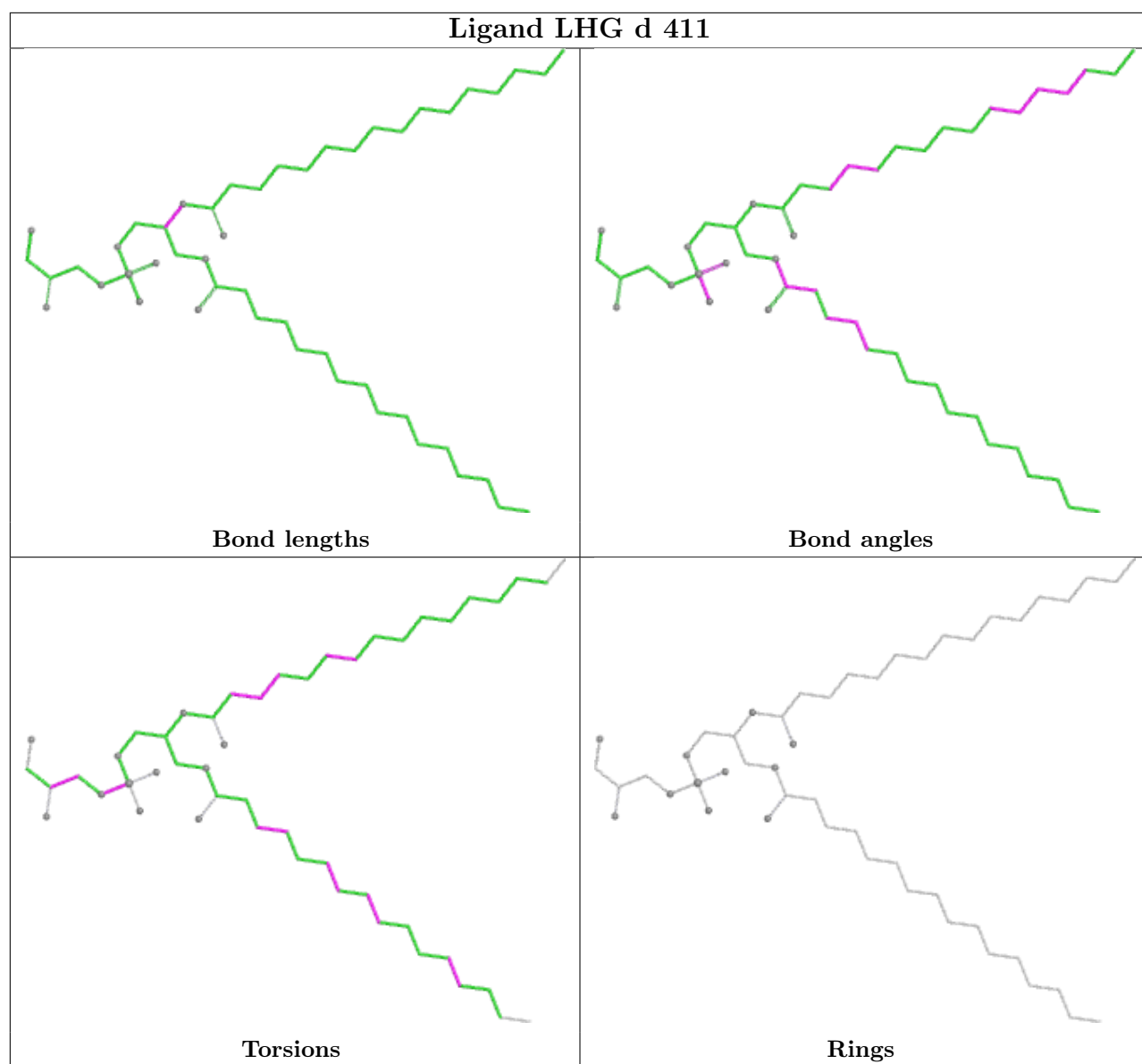
Ligand HEC v 201

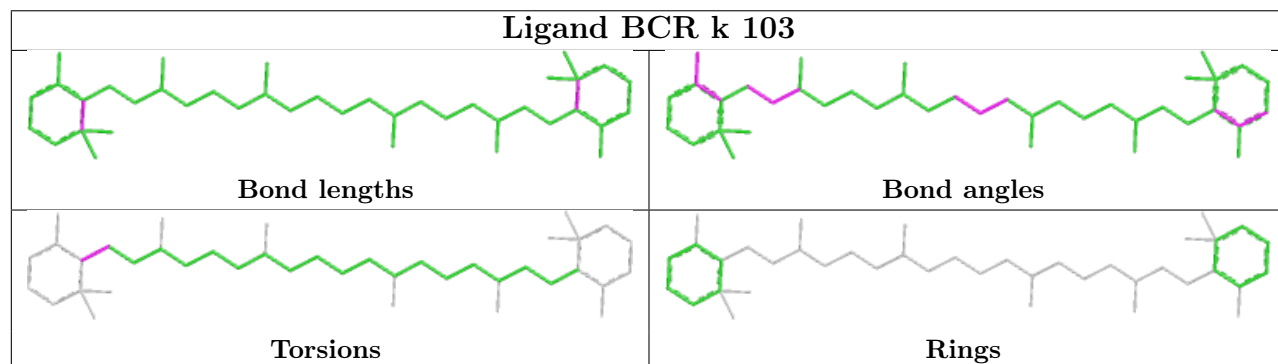
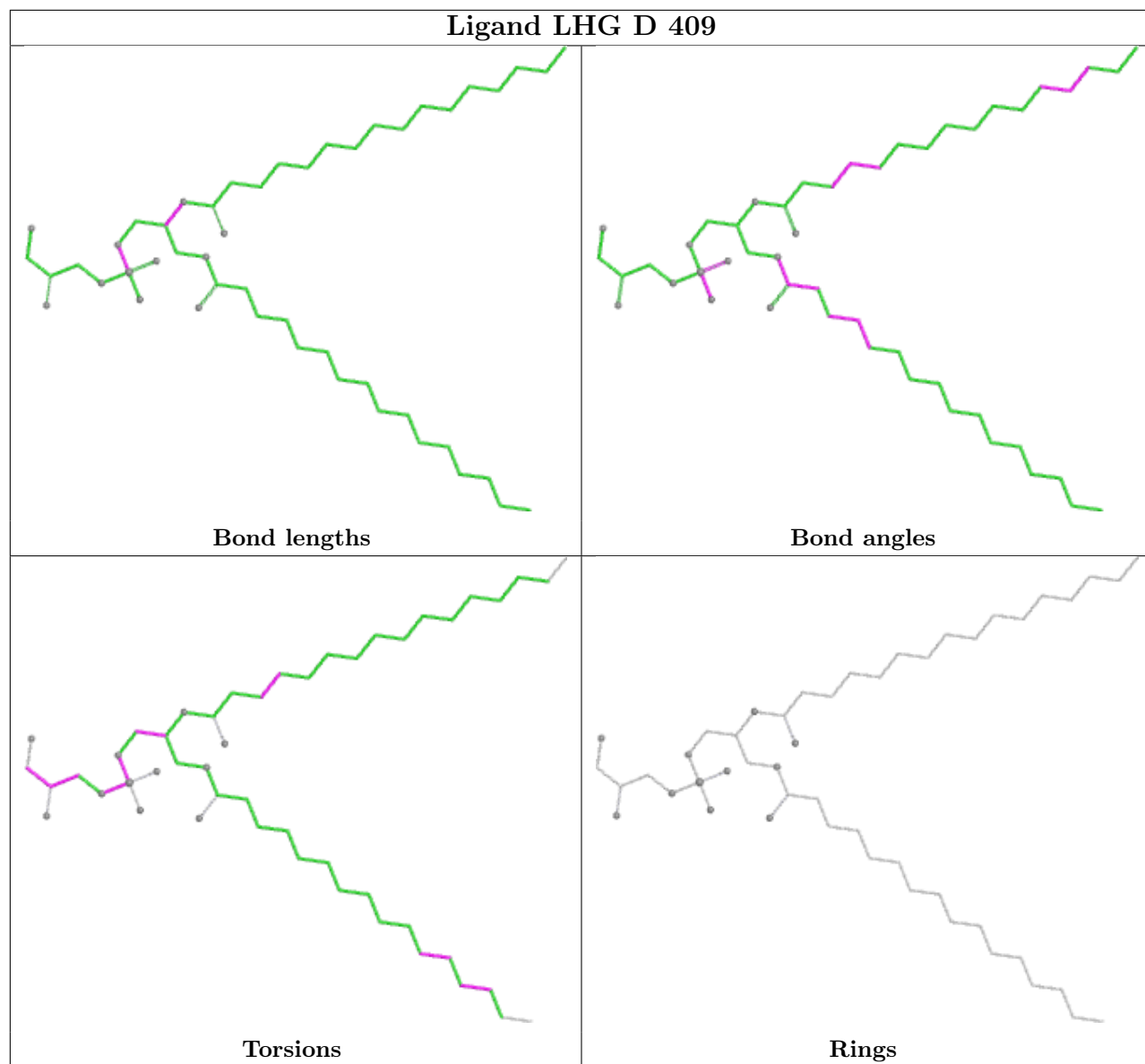


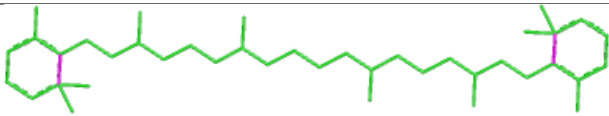
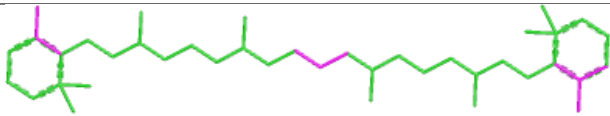
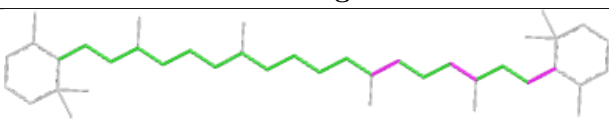
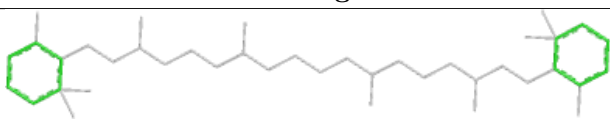
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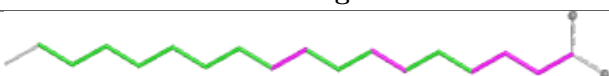
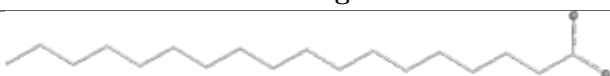


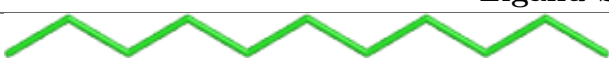
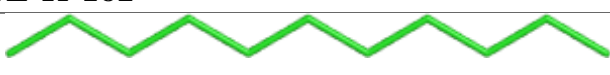


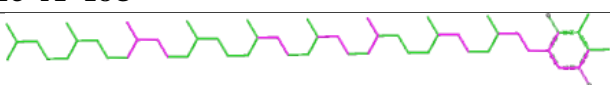
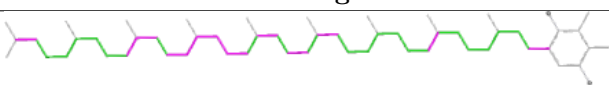
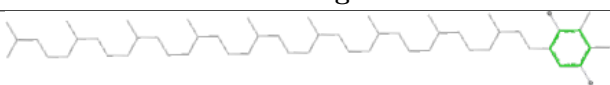


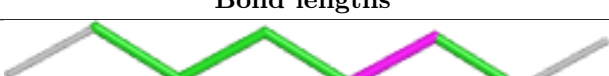


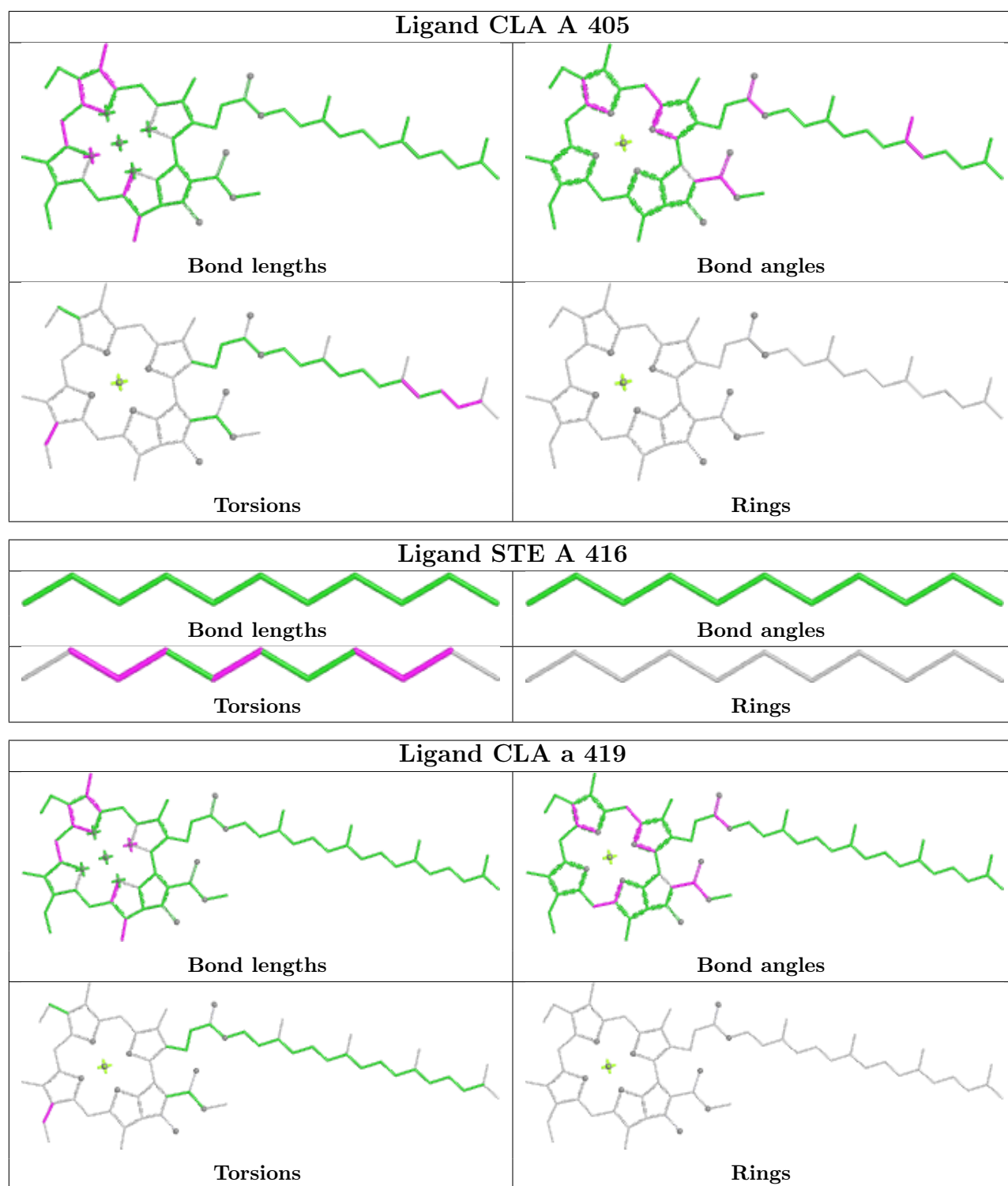
Ligand BCR b 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

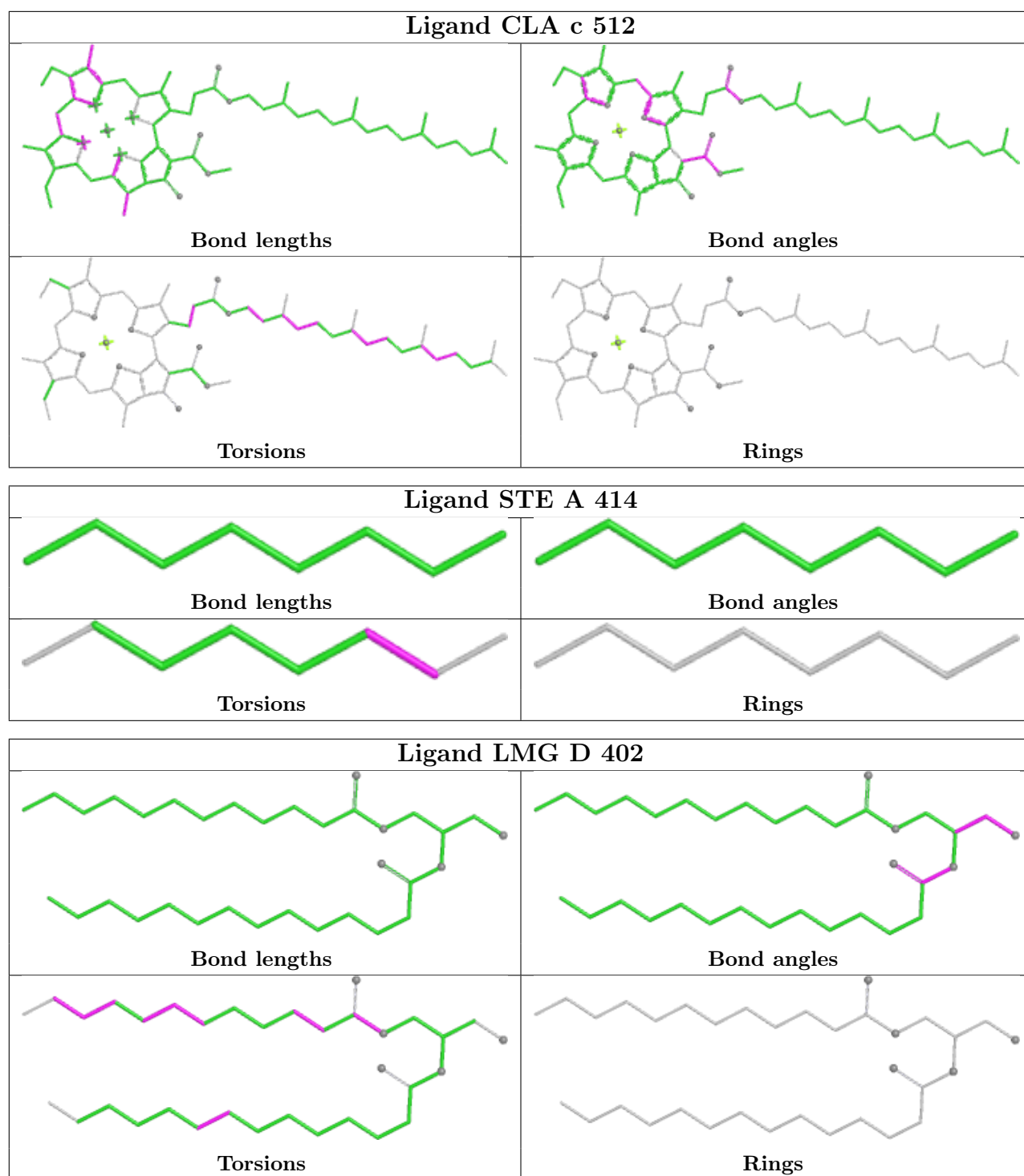
Ligand STE d 412	
	
Bond lengths	Bond angles
	
Torsions	Rings

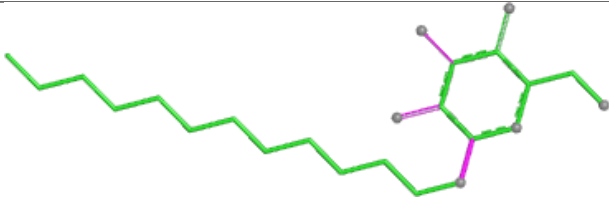
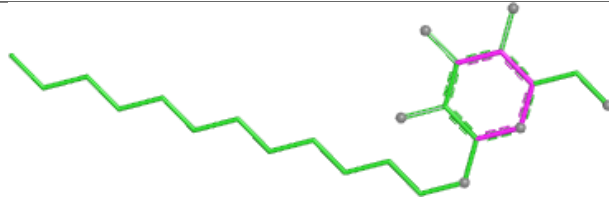
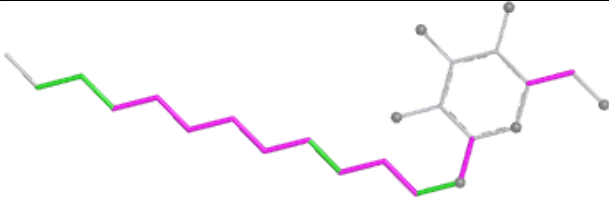
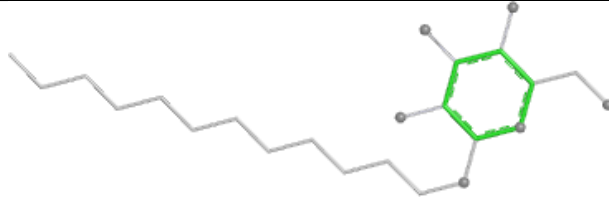
Ligand STE K 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

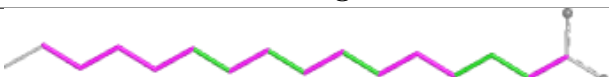
Ligand PL9 A 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

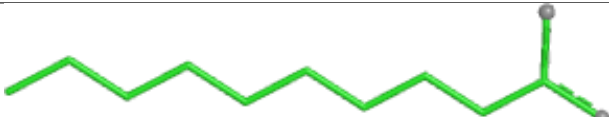
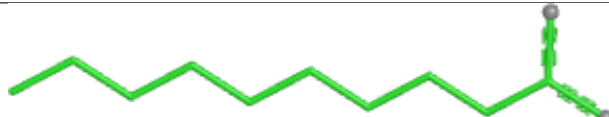
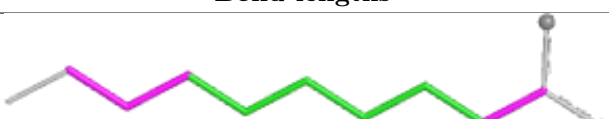
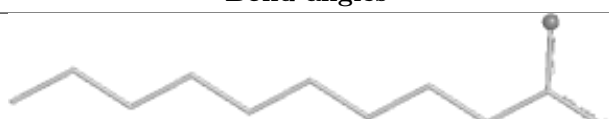
Ligand STE C 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

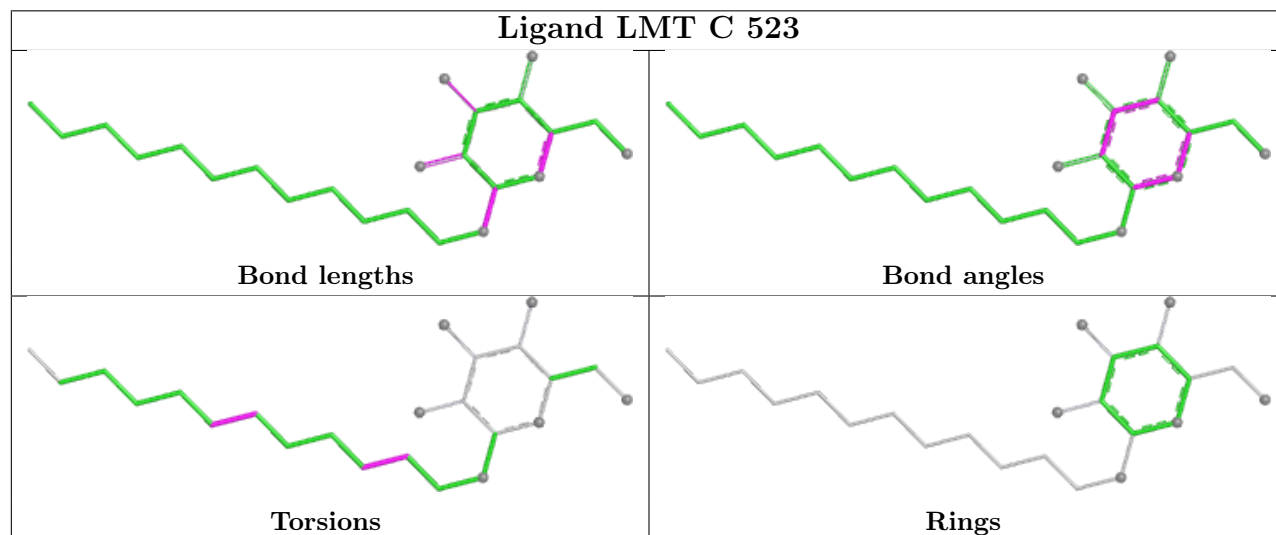
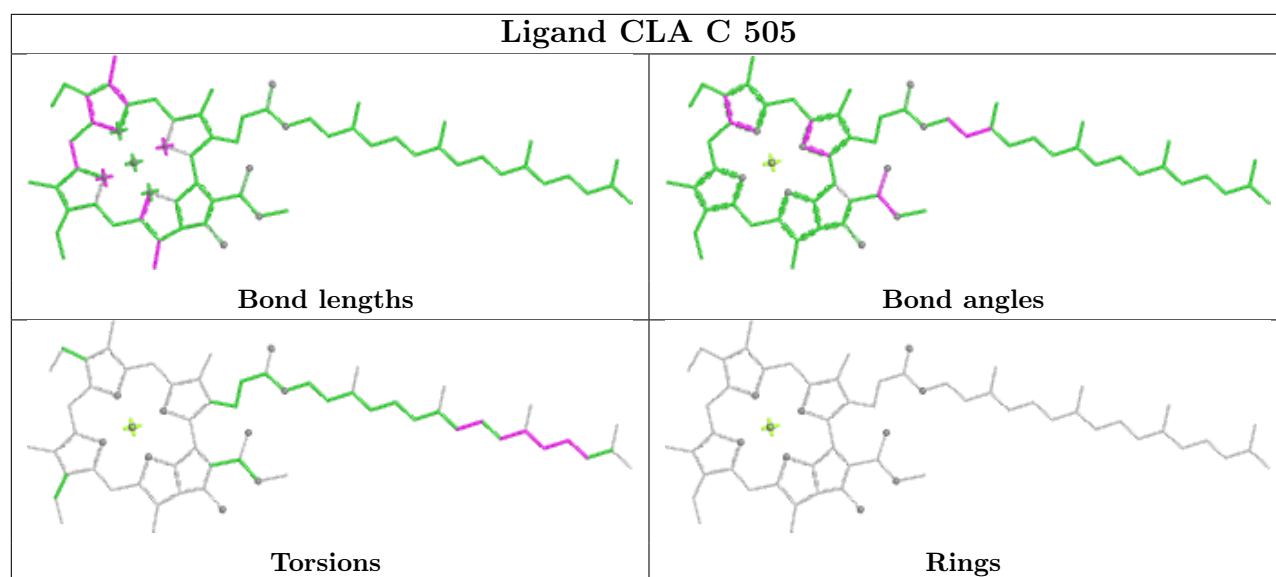


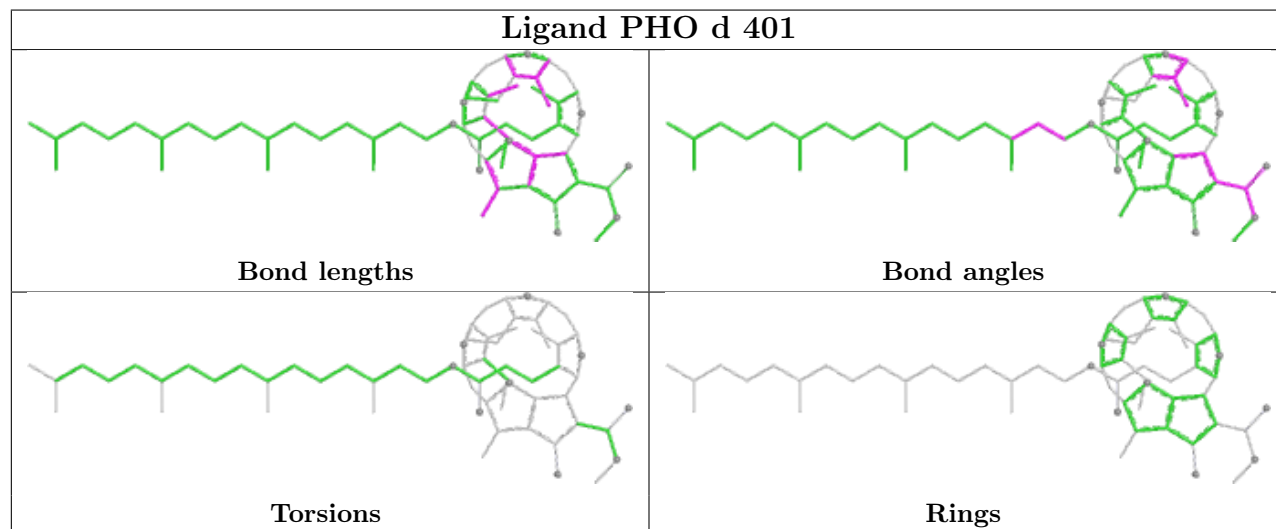
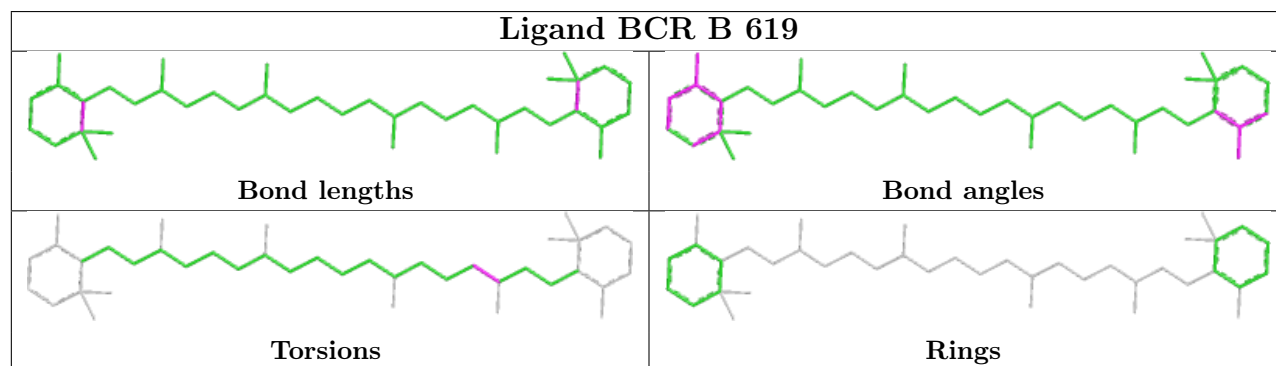
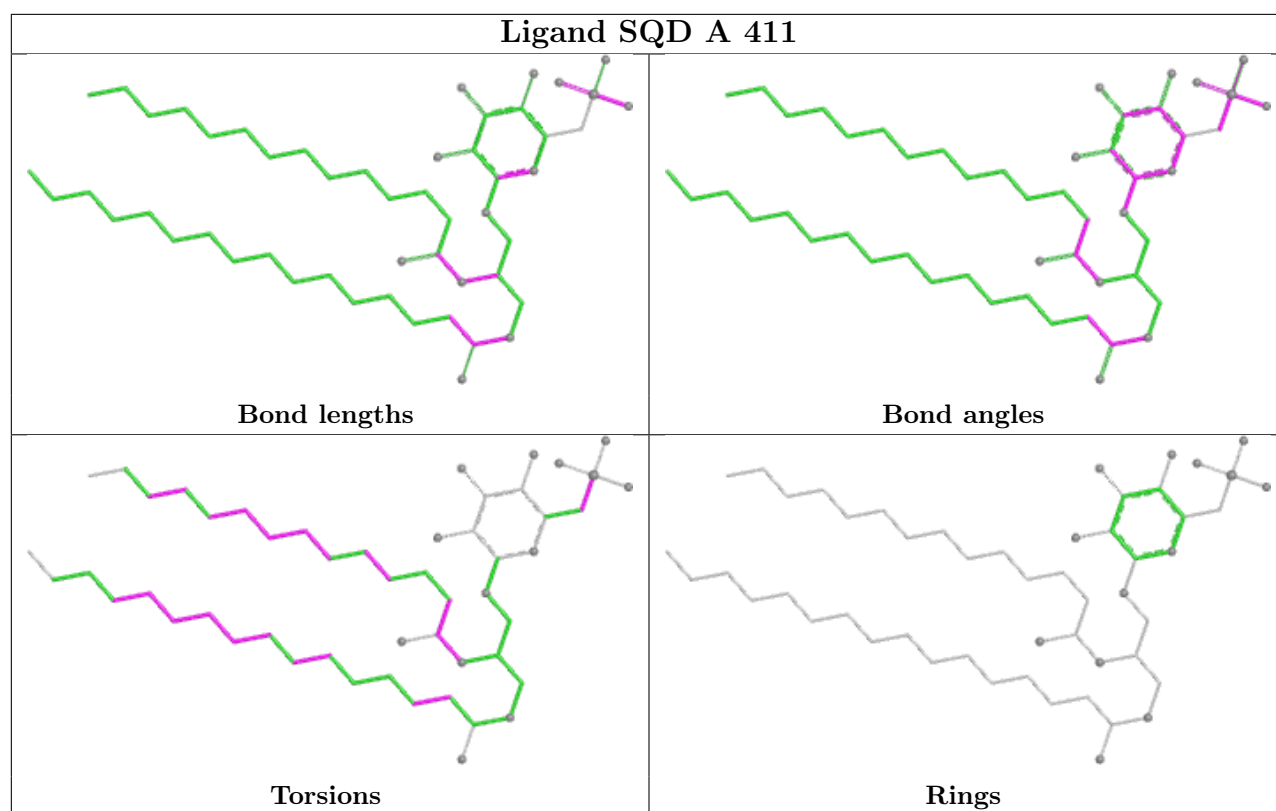


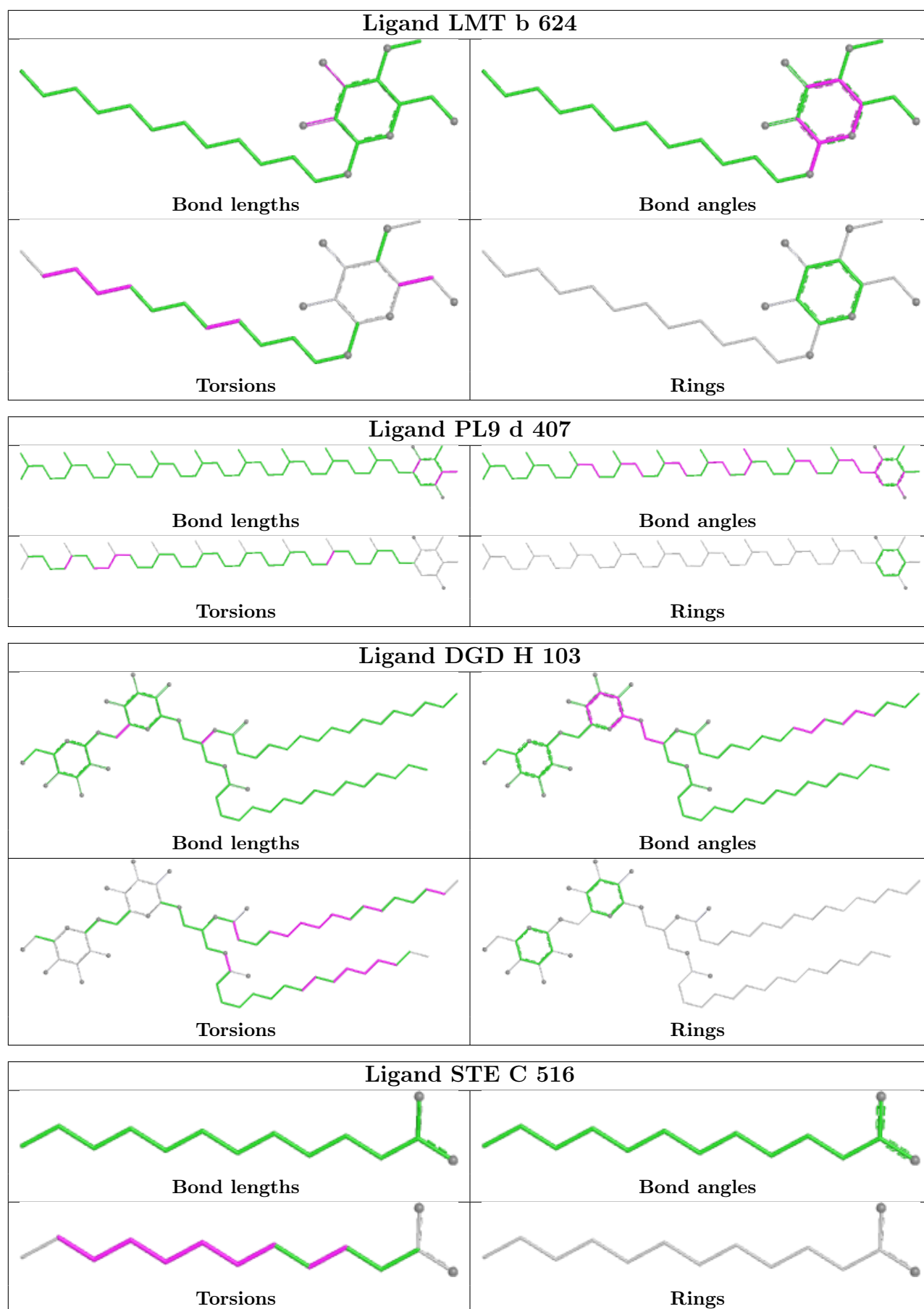
Ligand LMT j 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

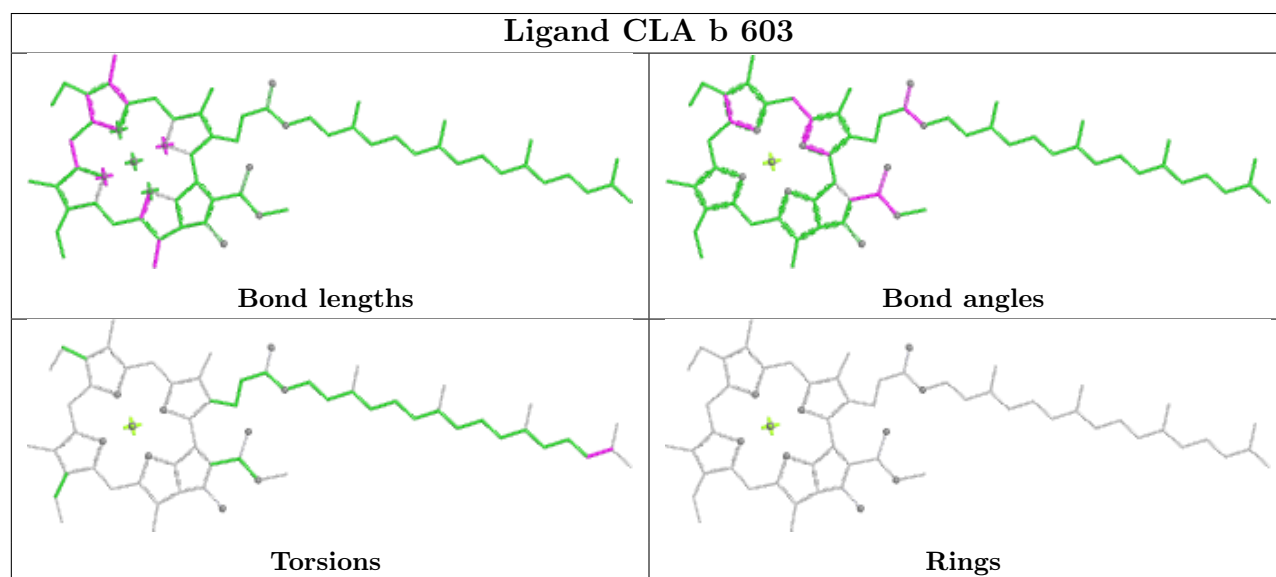
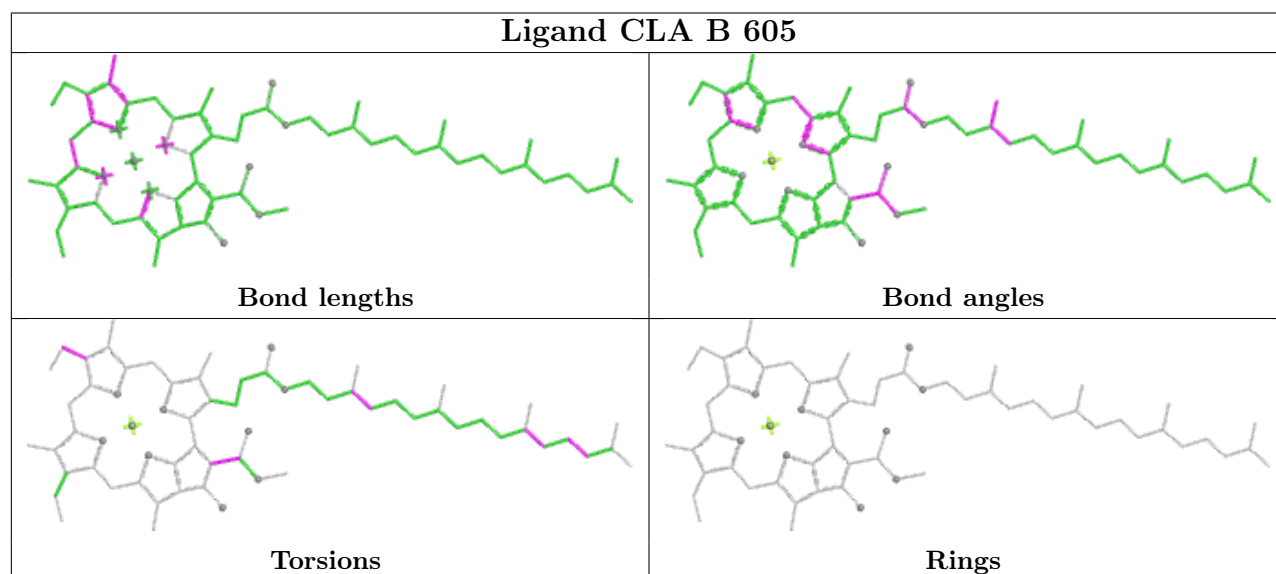
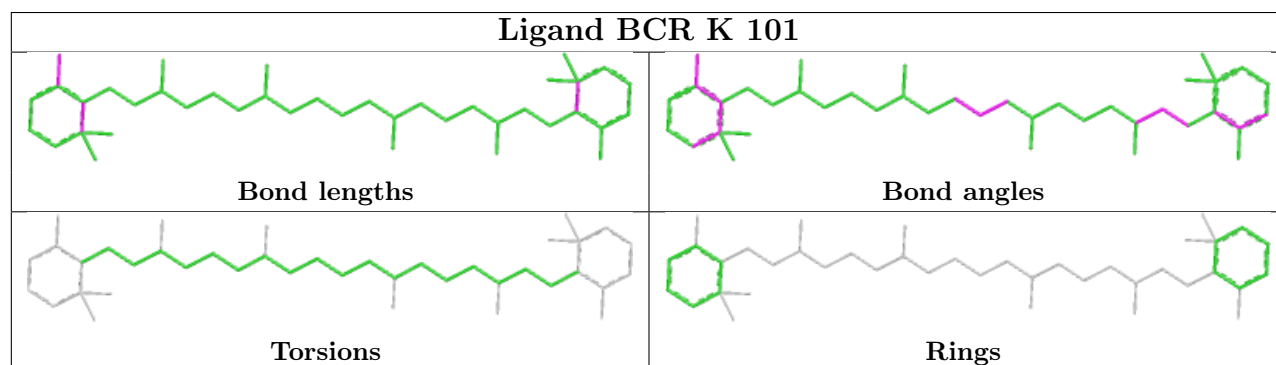
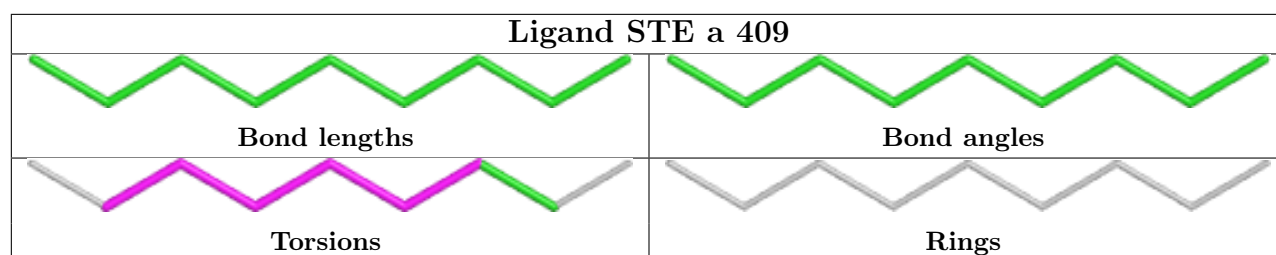
Ligand STE t 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

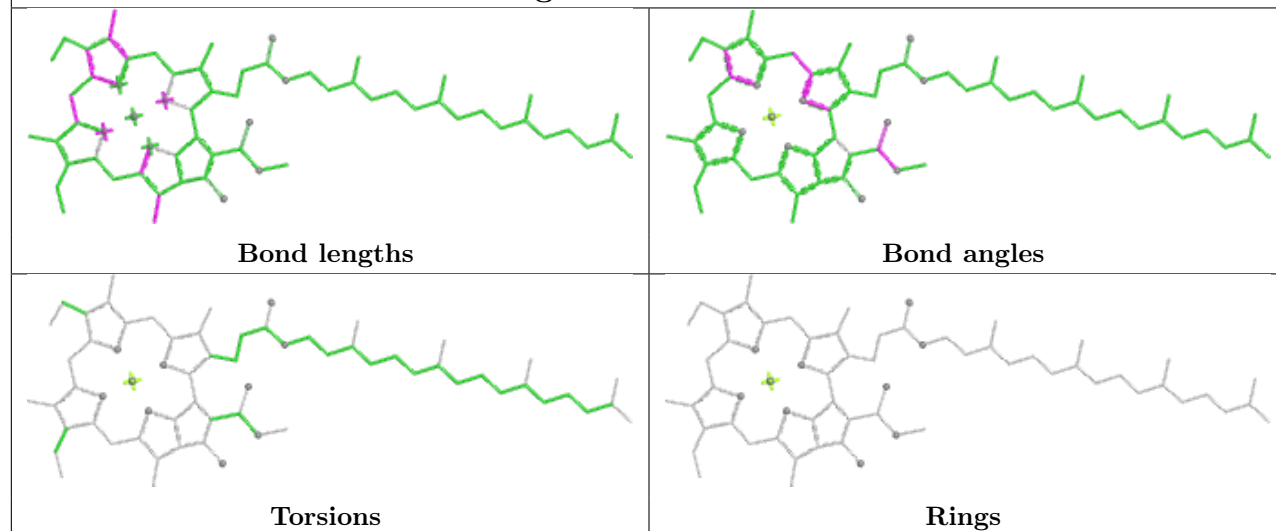
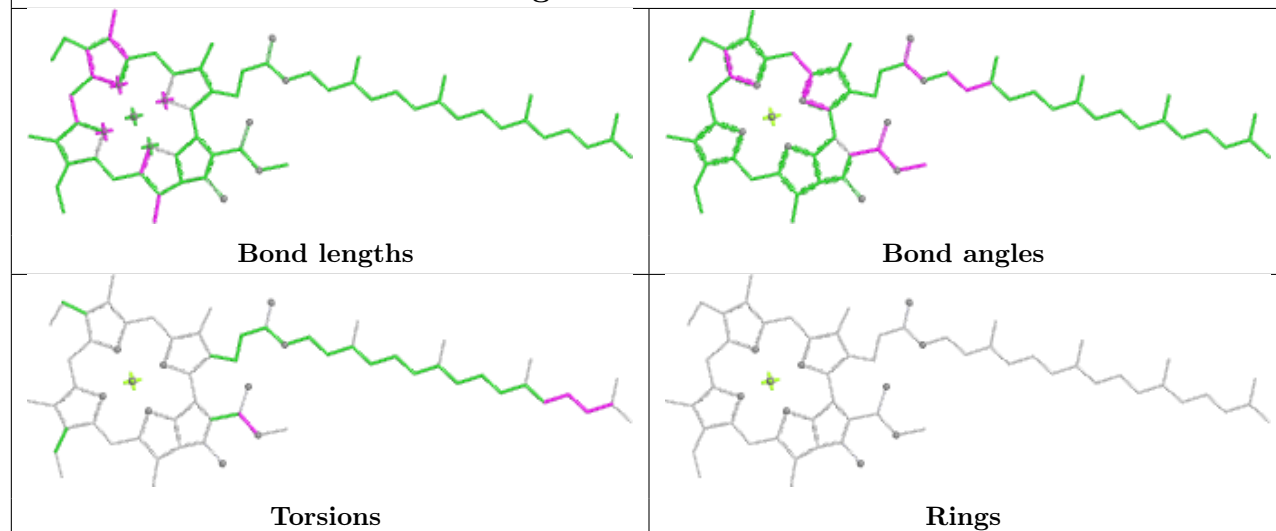
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Bond lengths	Bond angles
	
Torsions	Rings

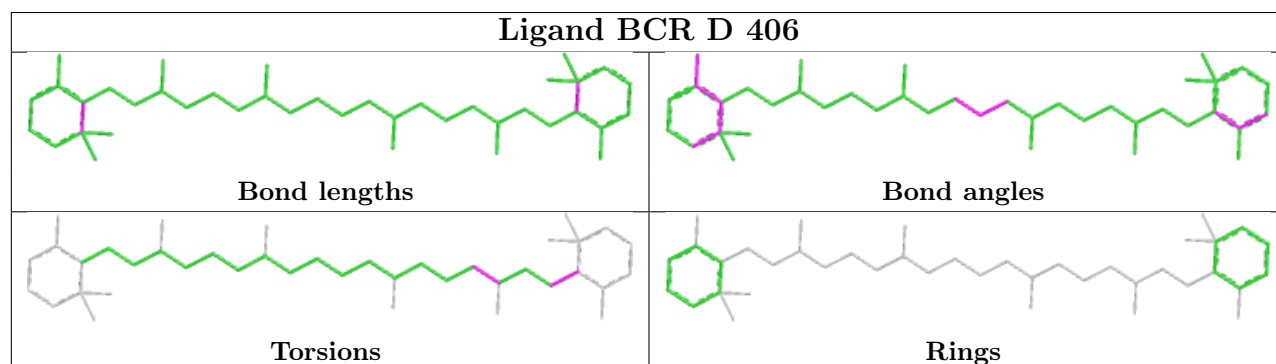
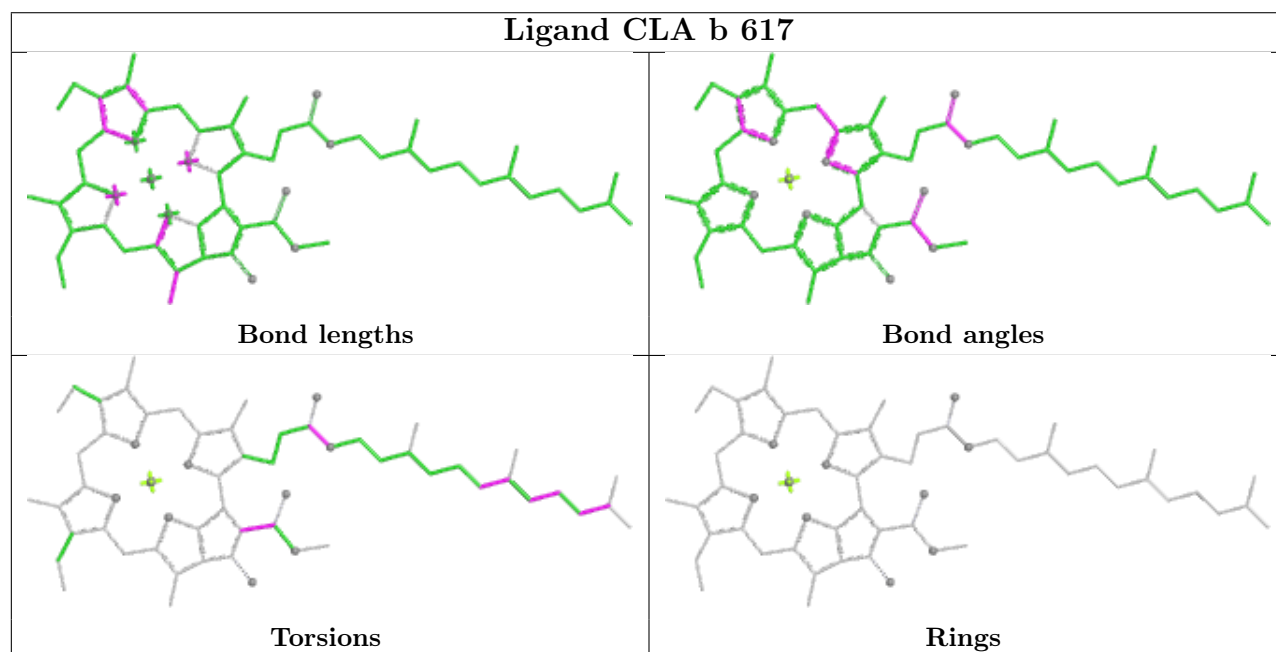
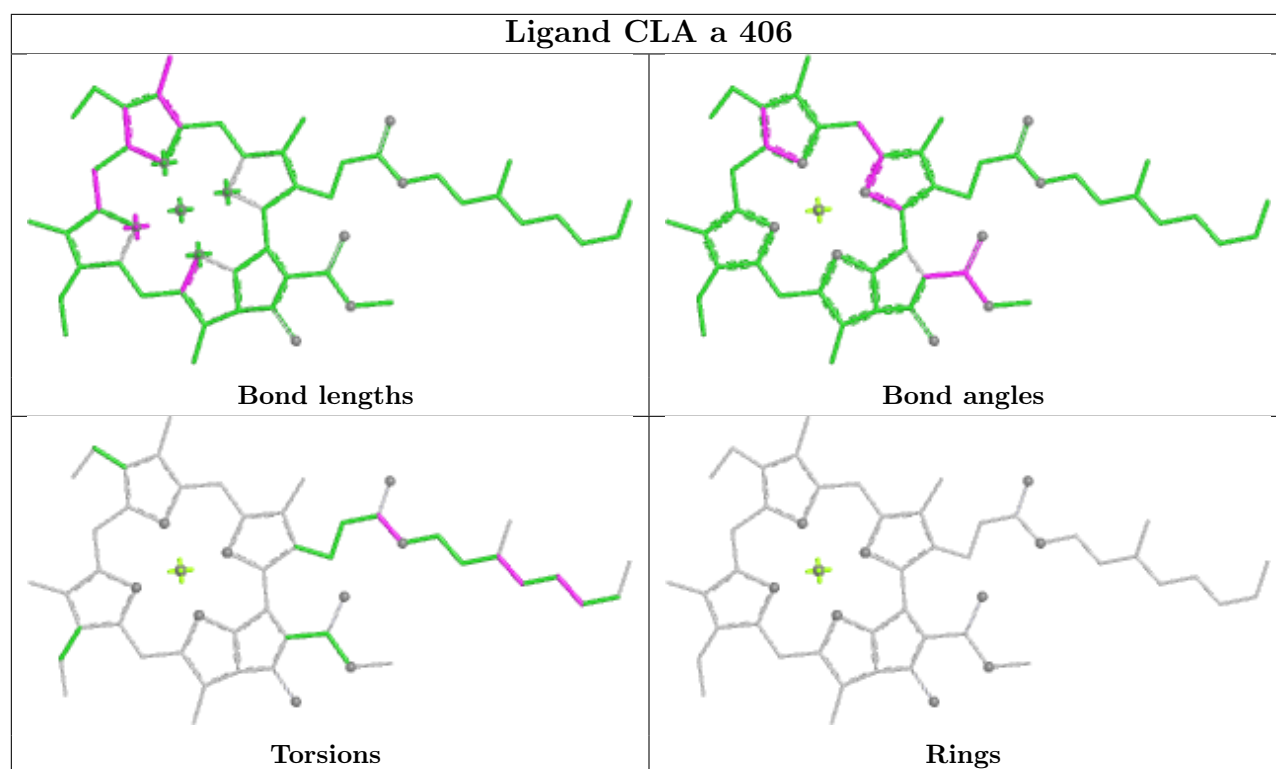


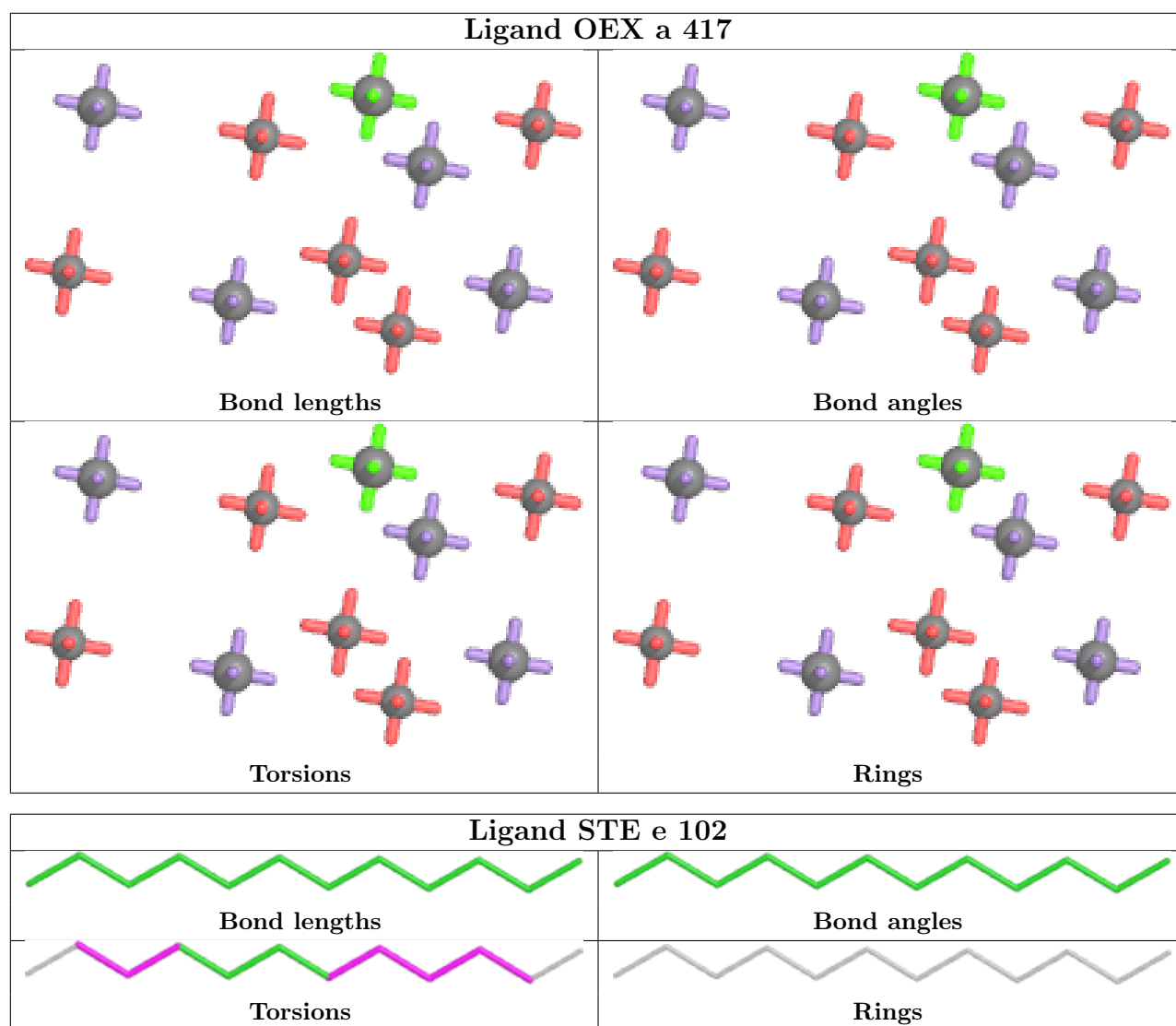


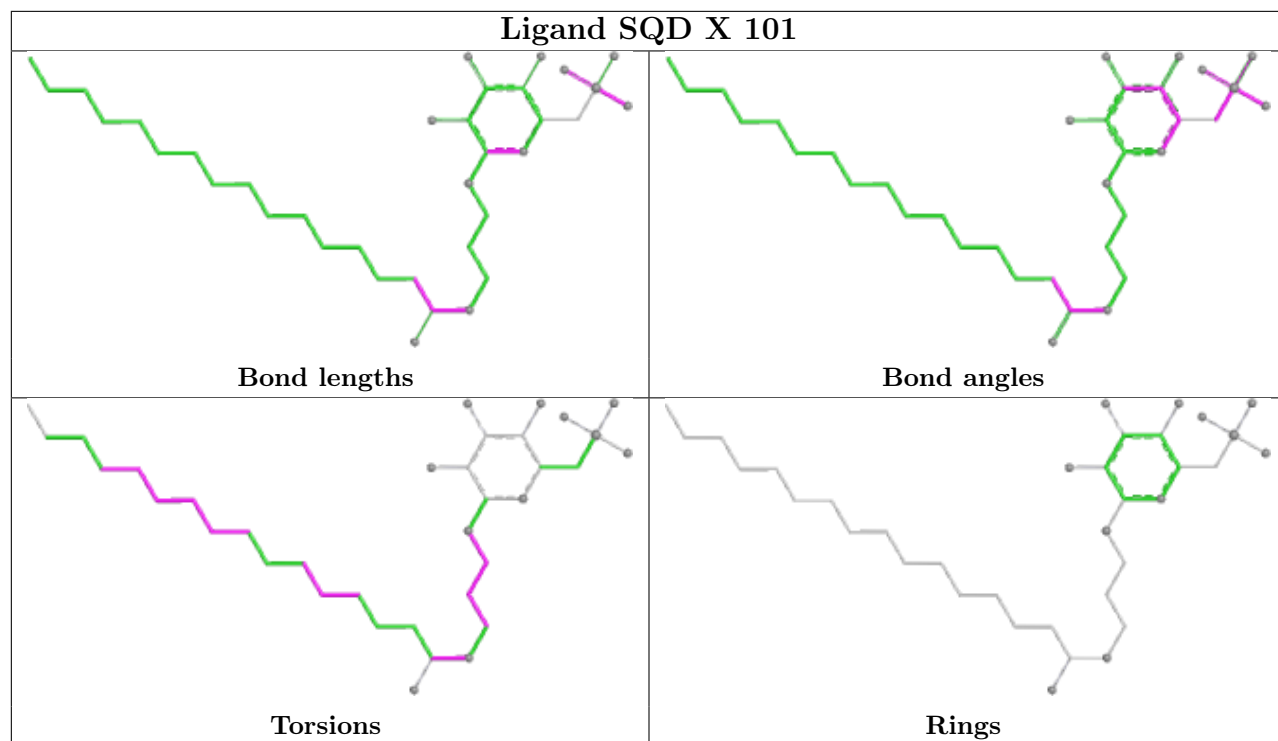


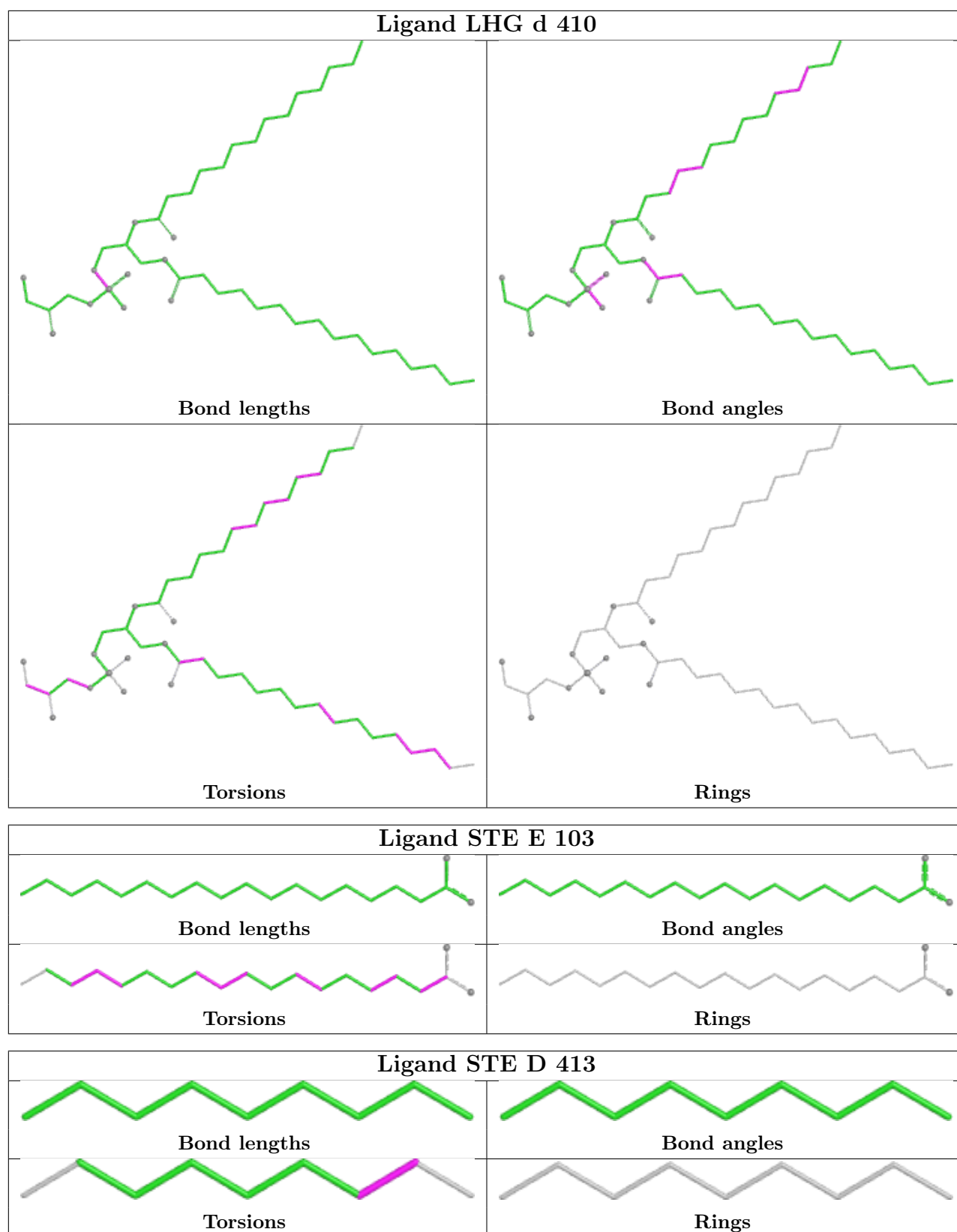


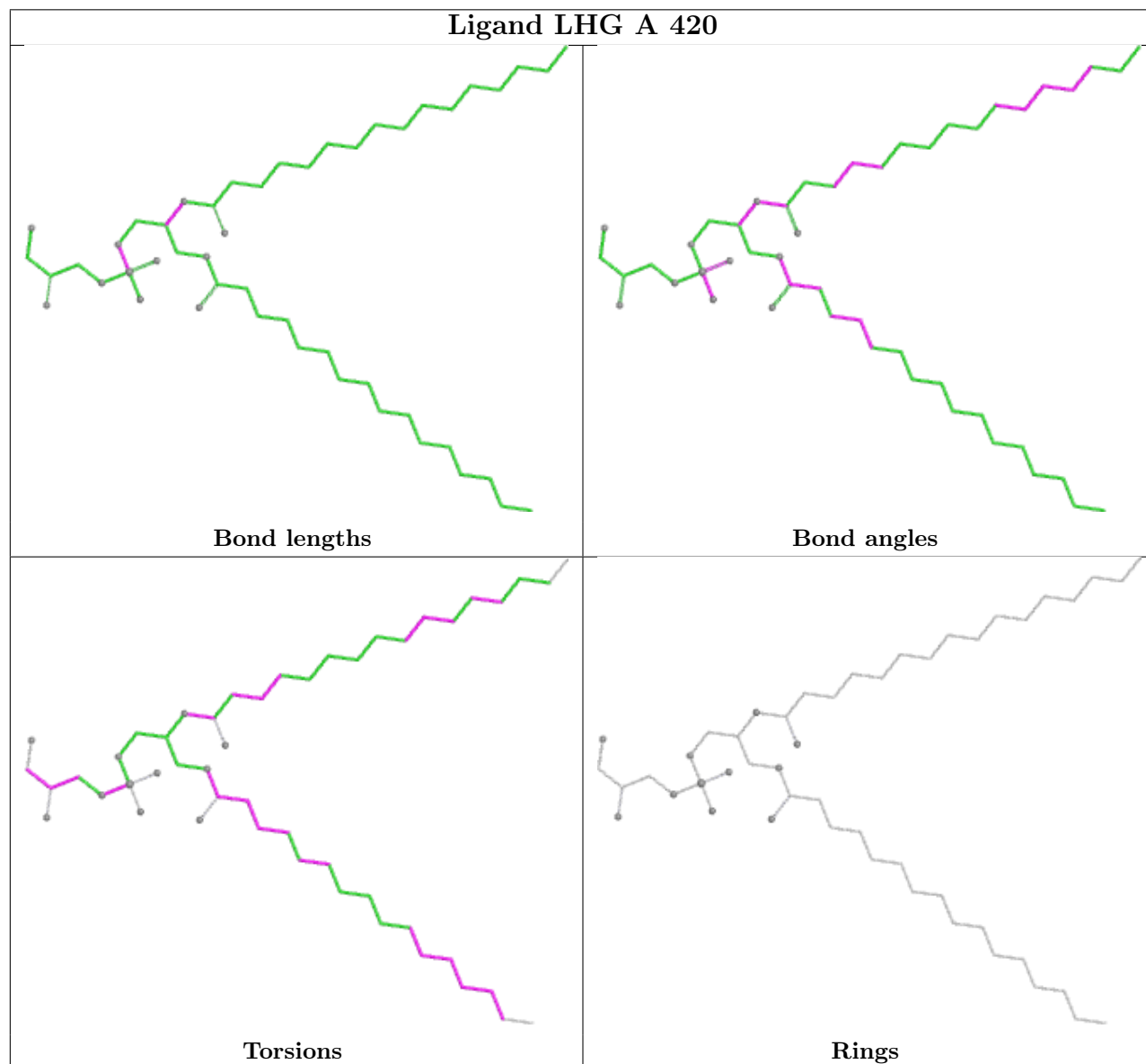
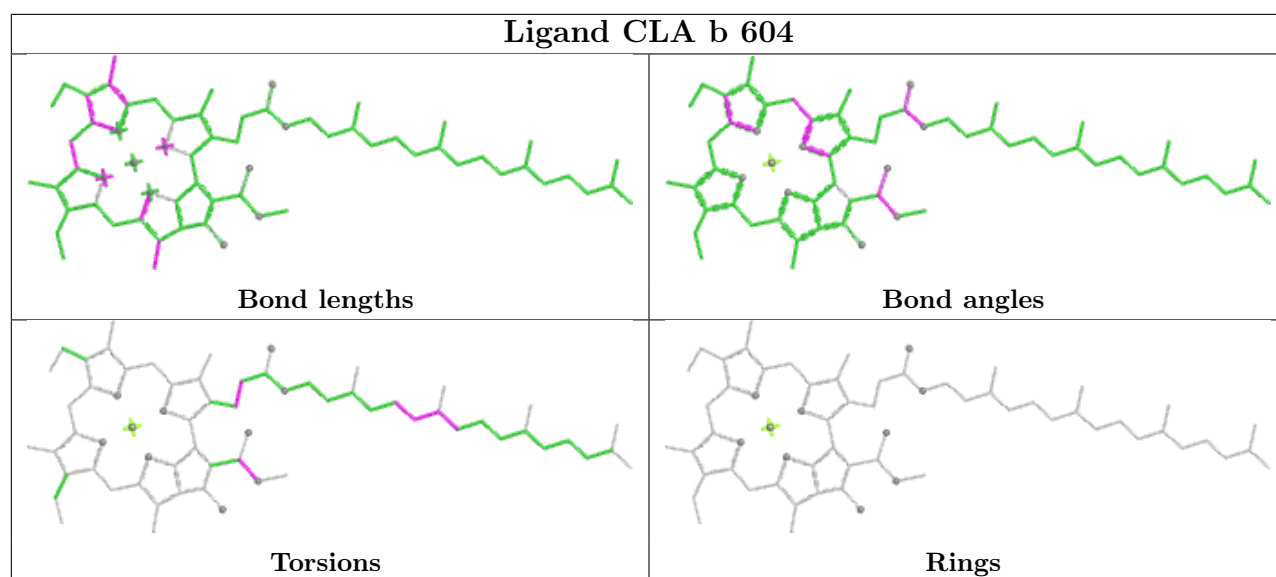
Ligand CLA b 611**Ligand CLA B 609**

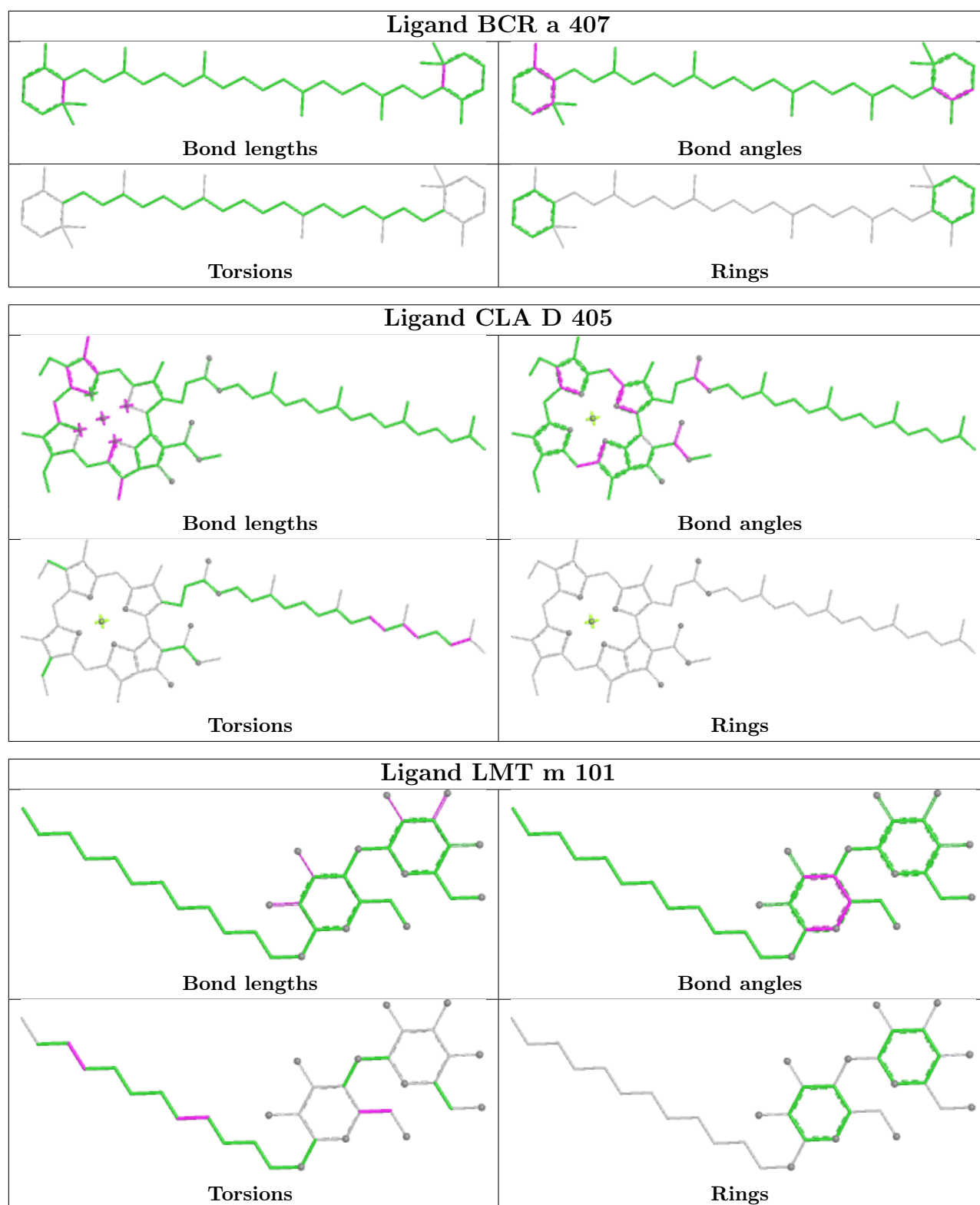


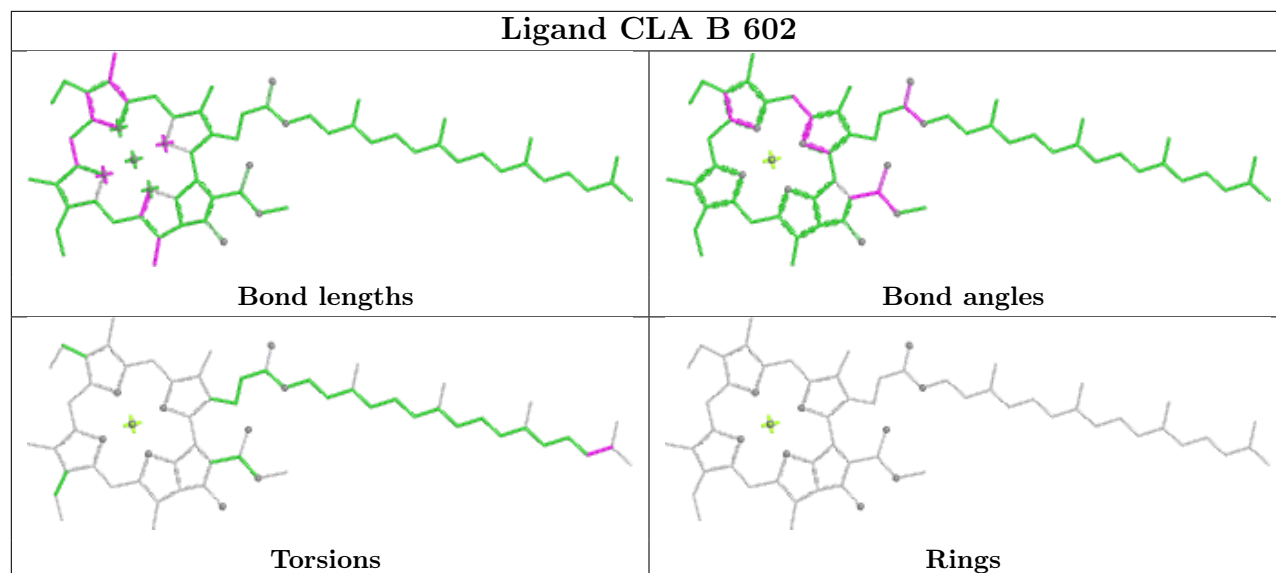
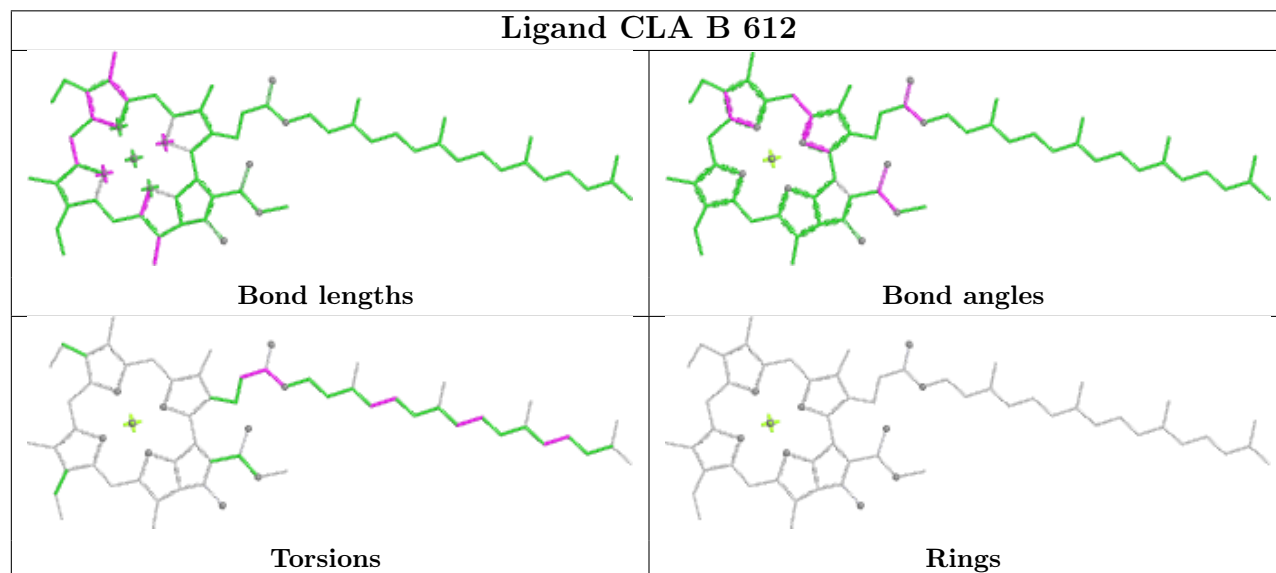
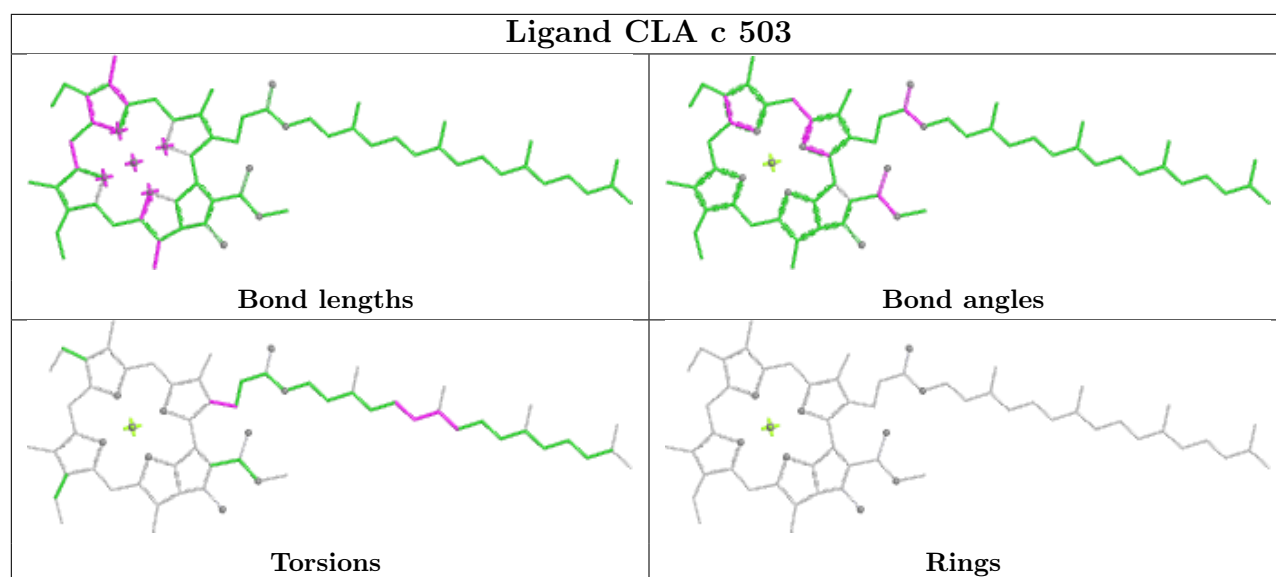


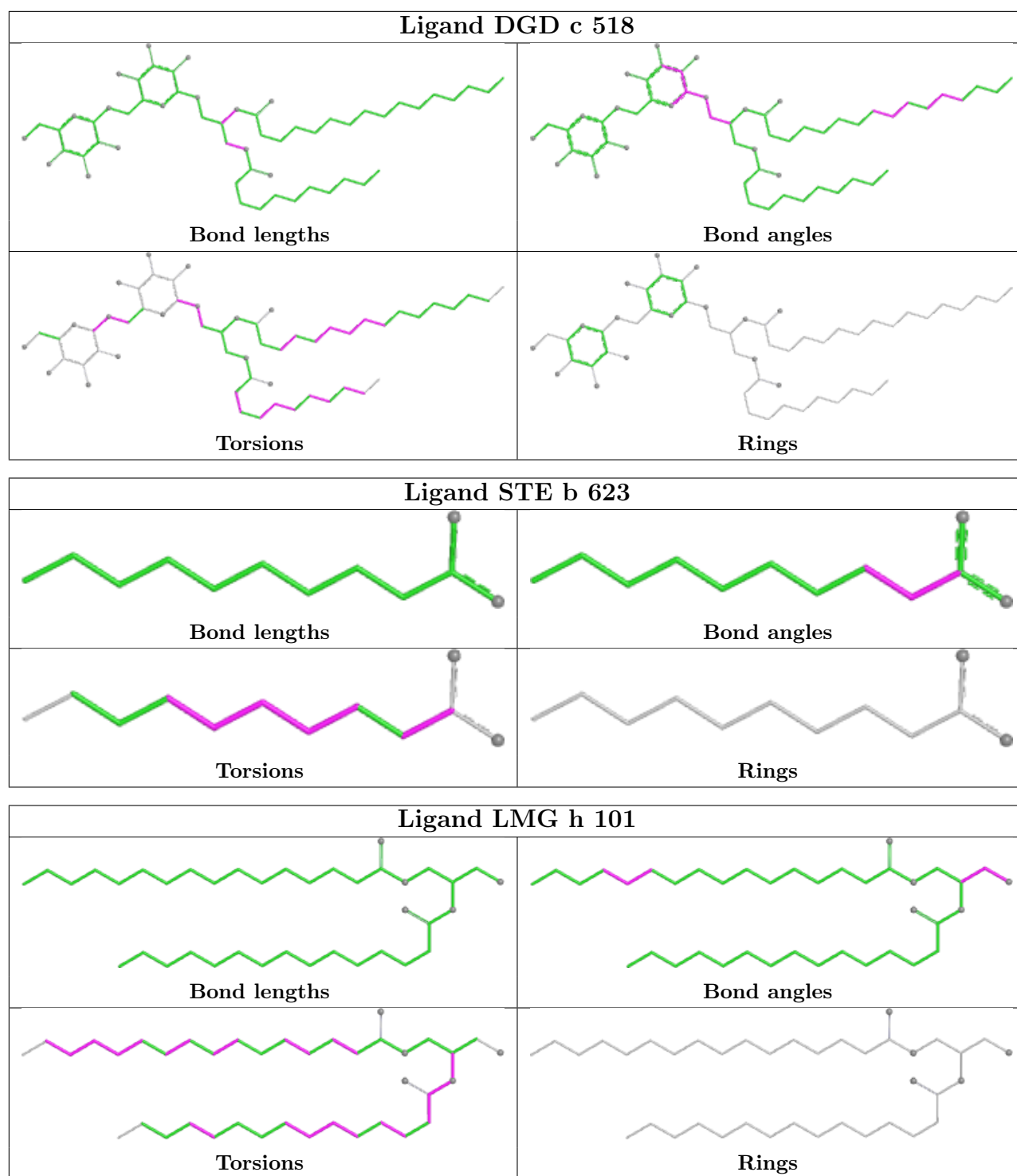


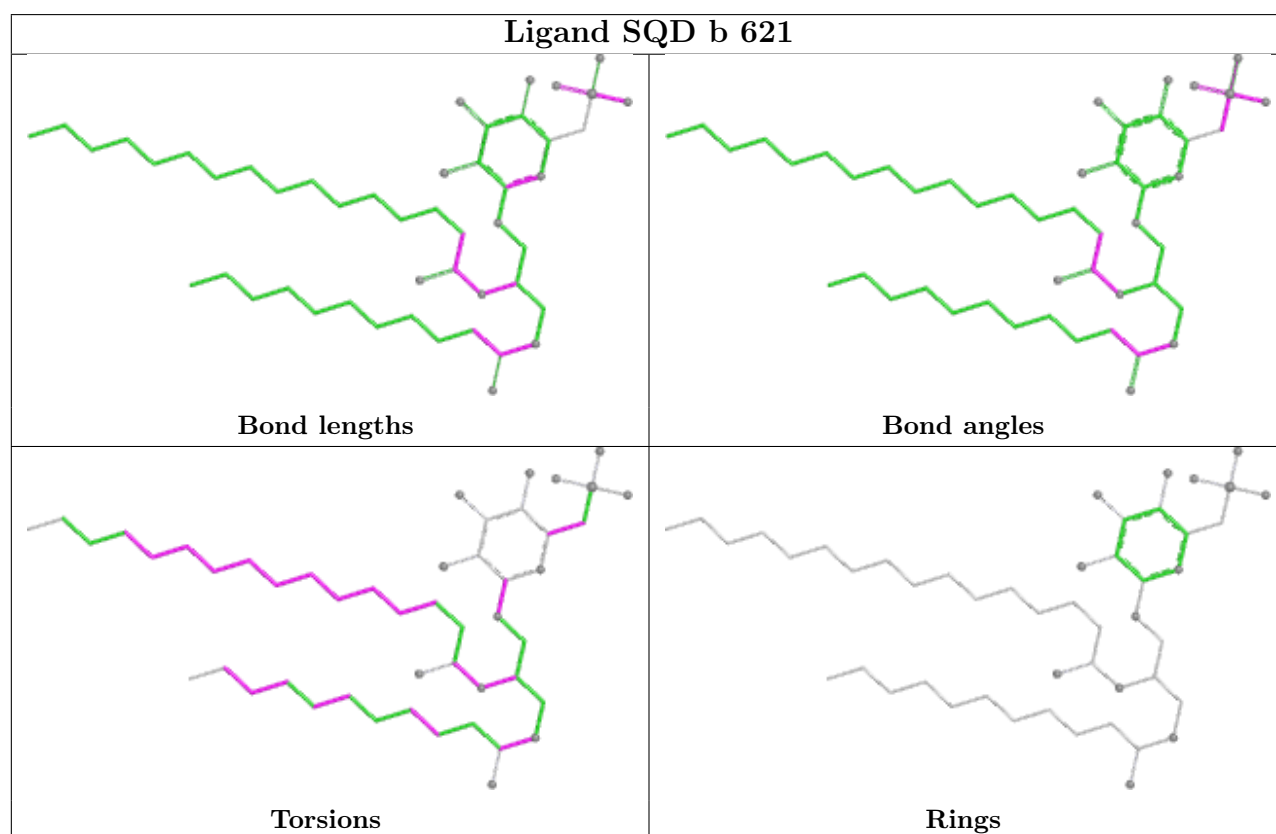
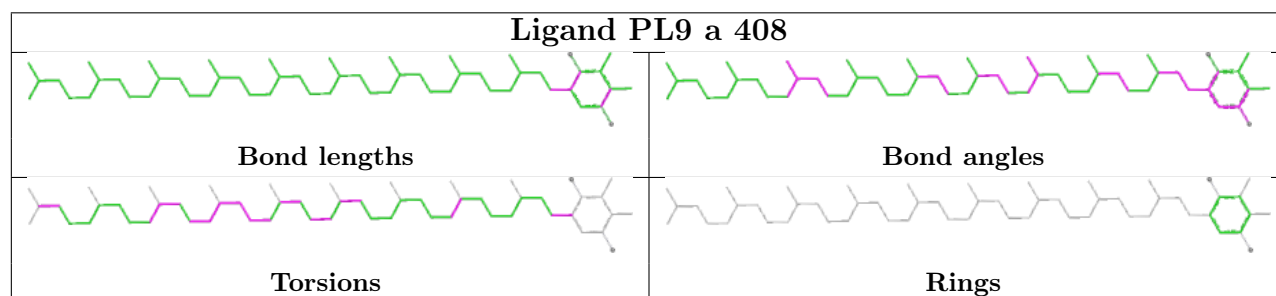
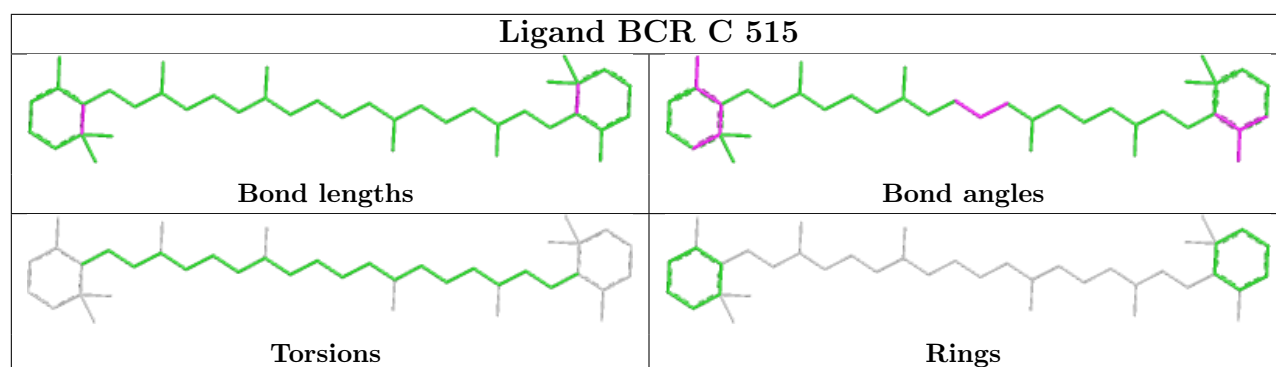


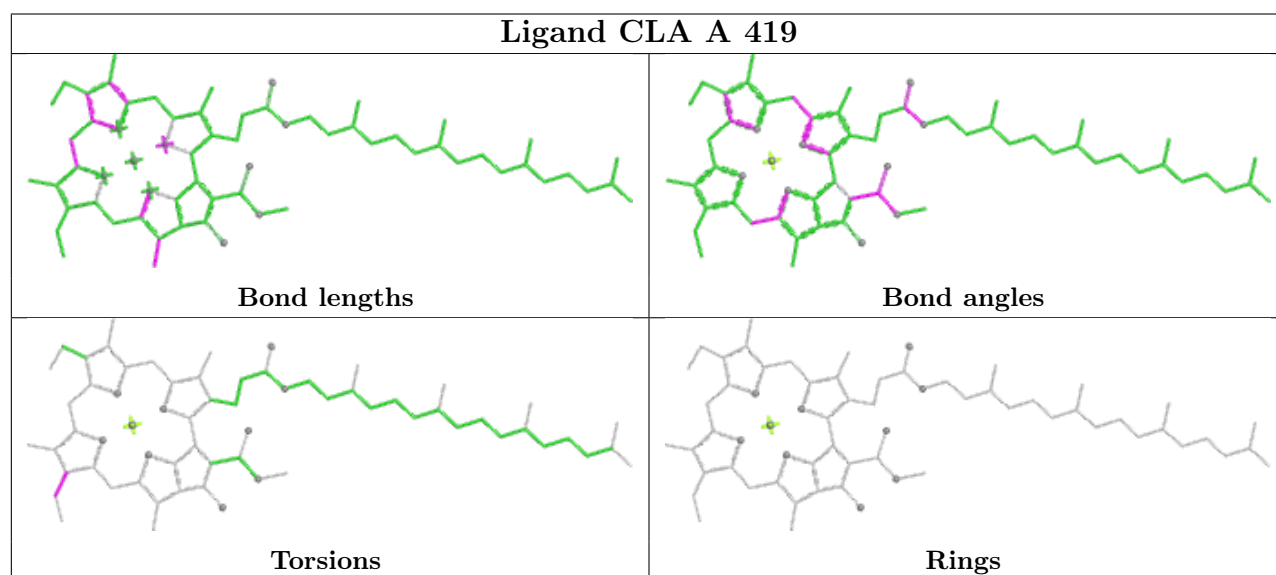
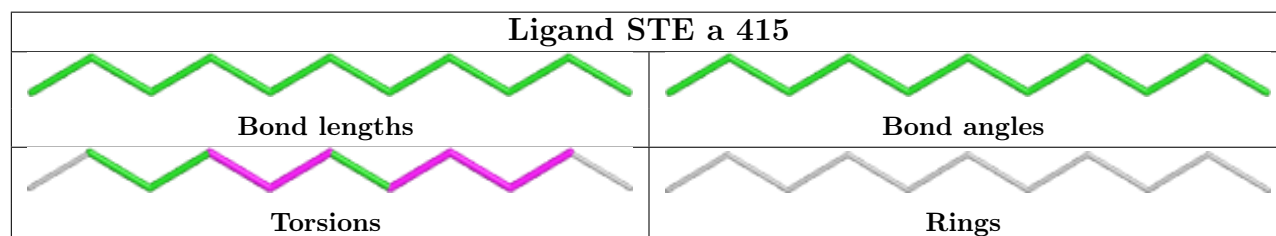
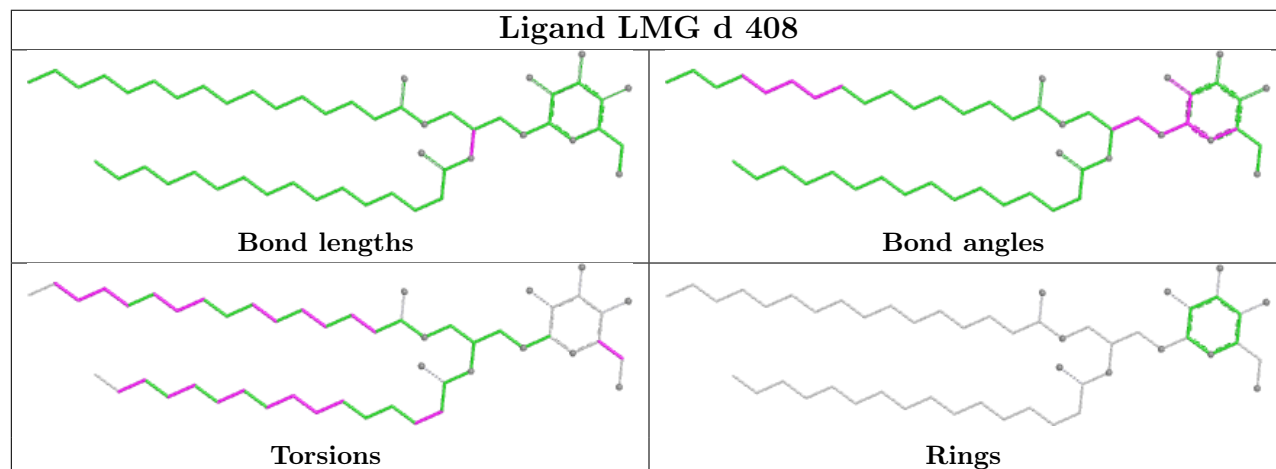
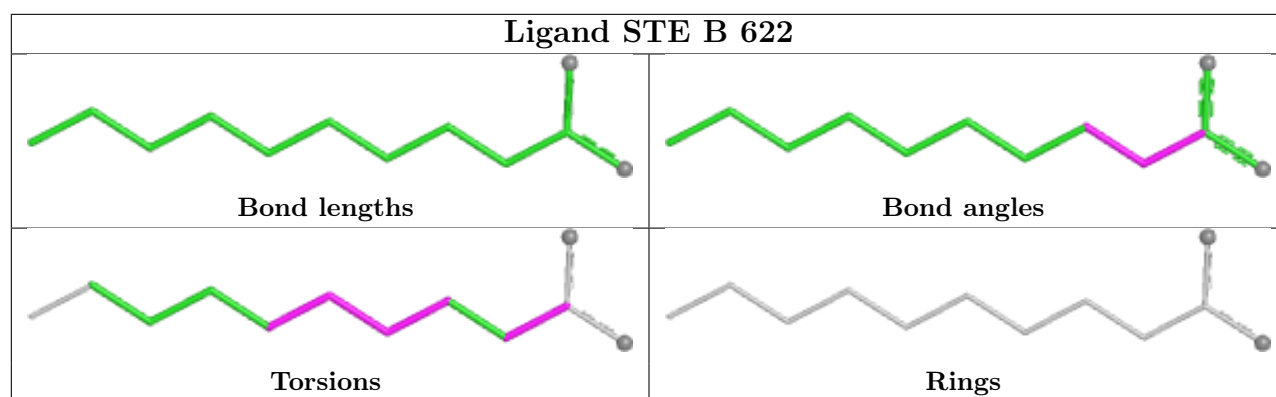


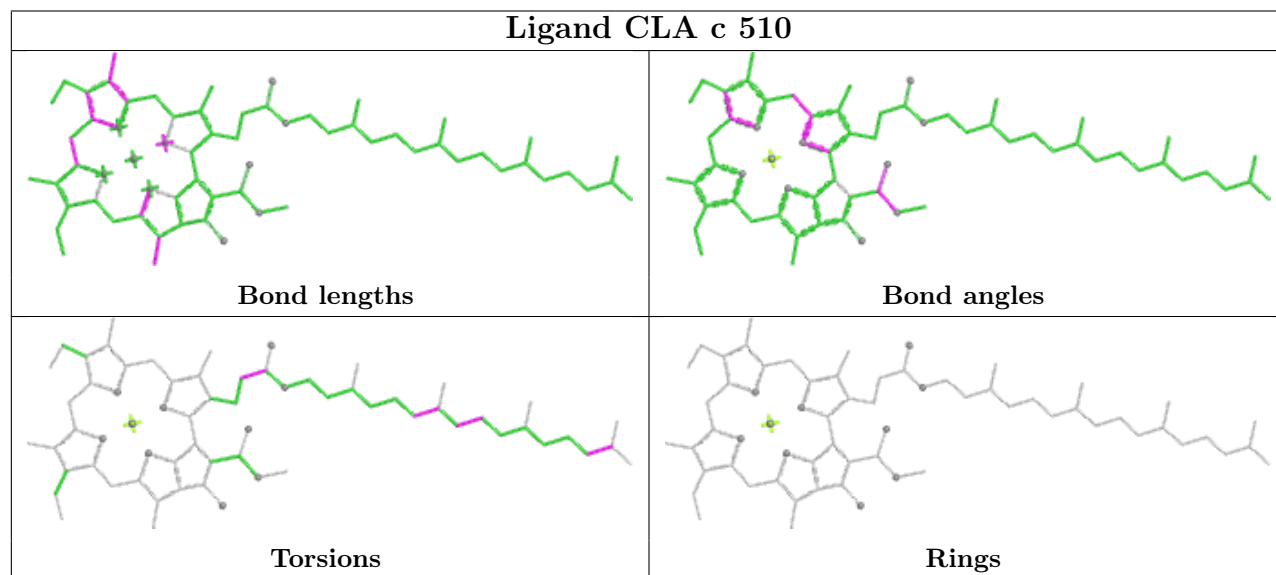
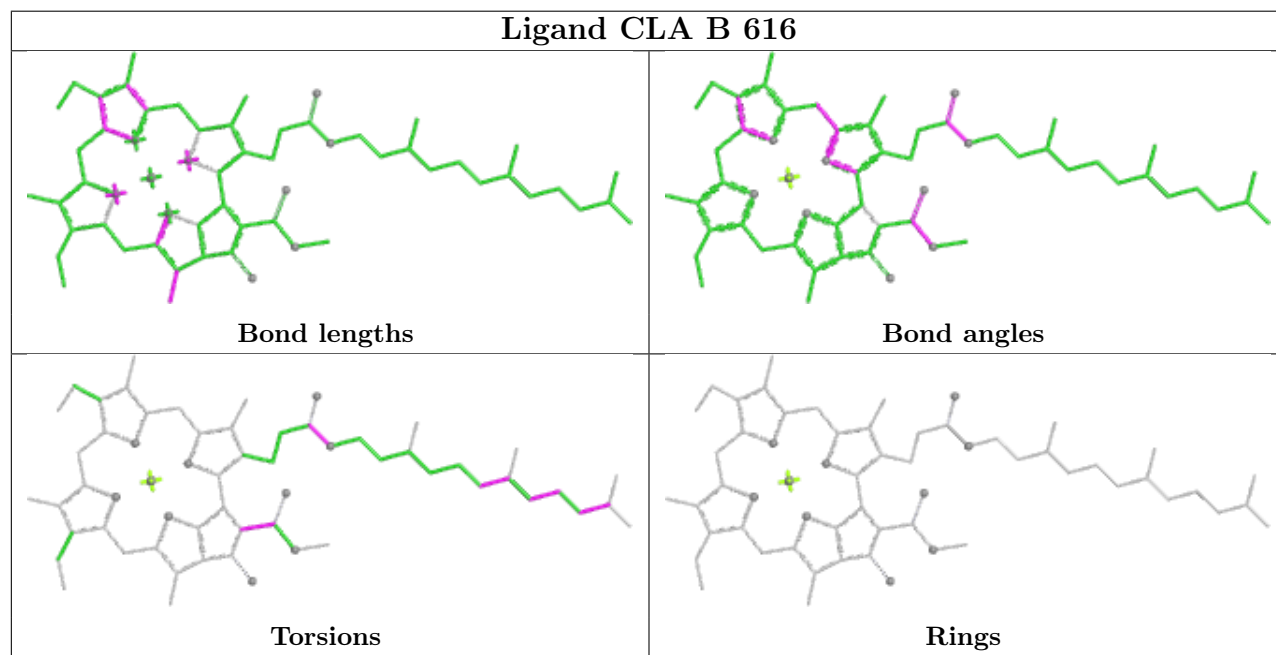
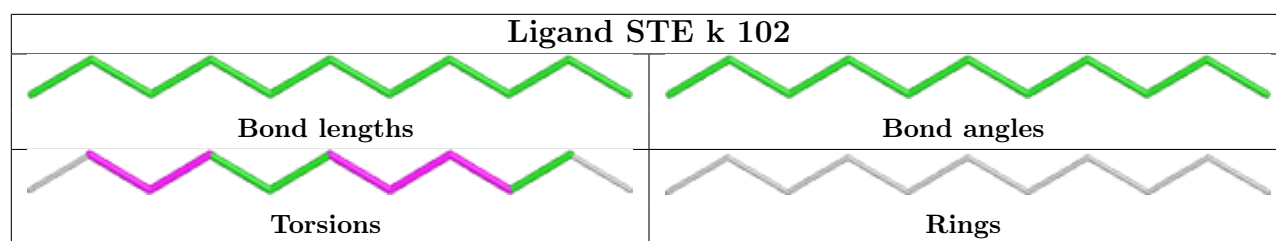


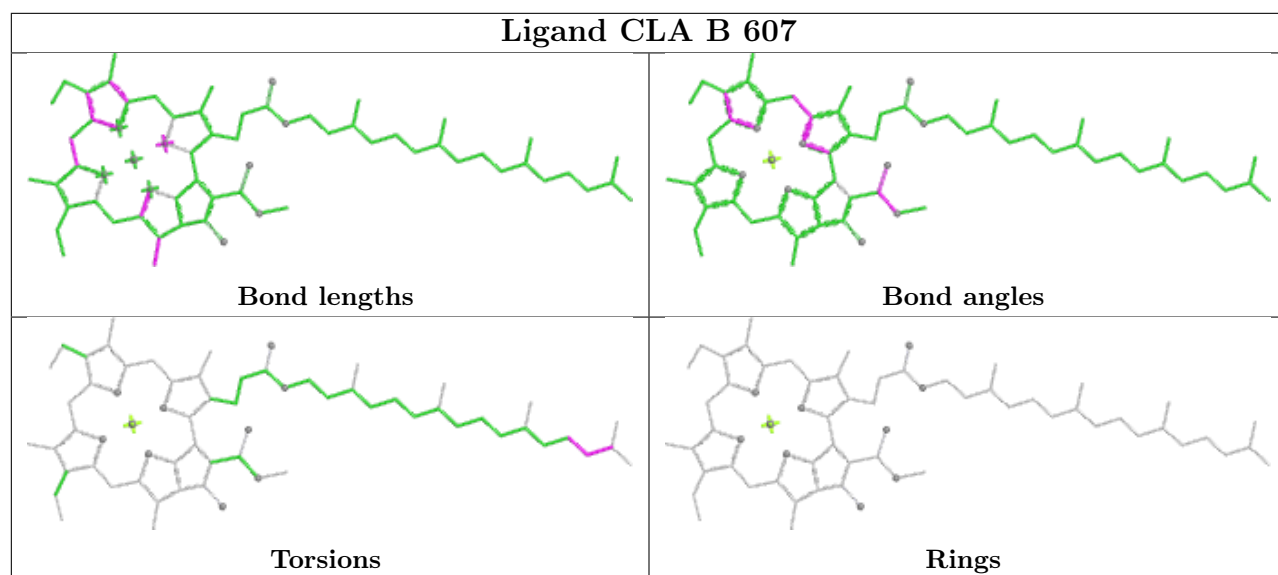
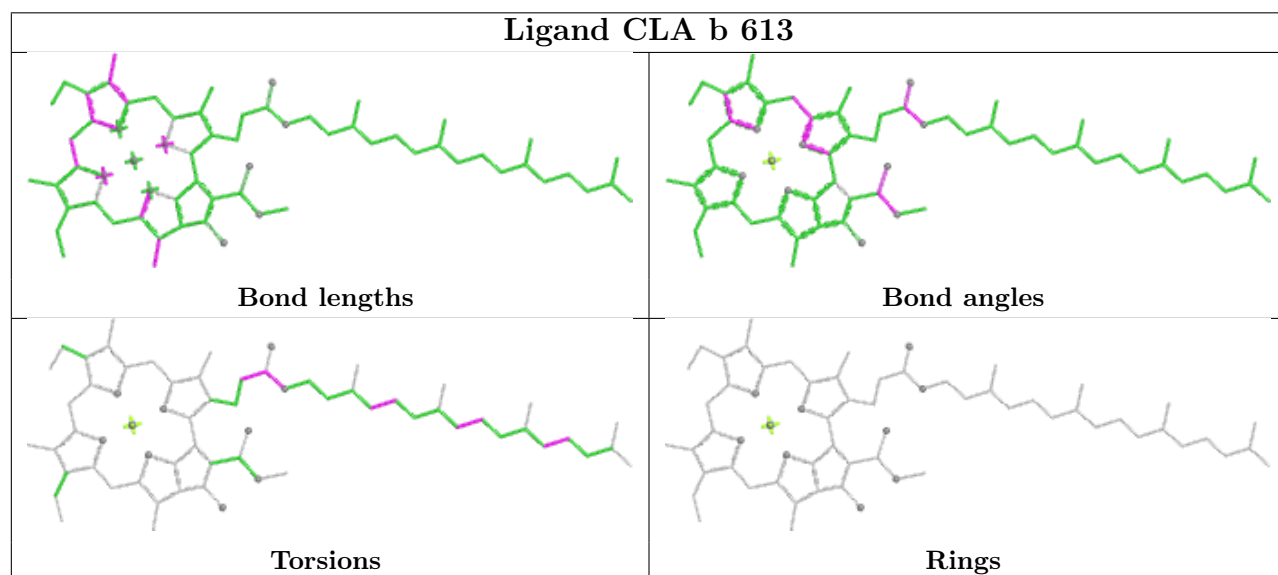
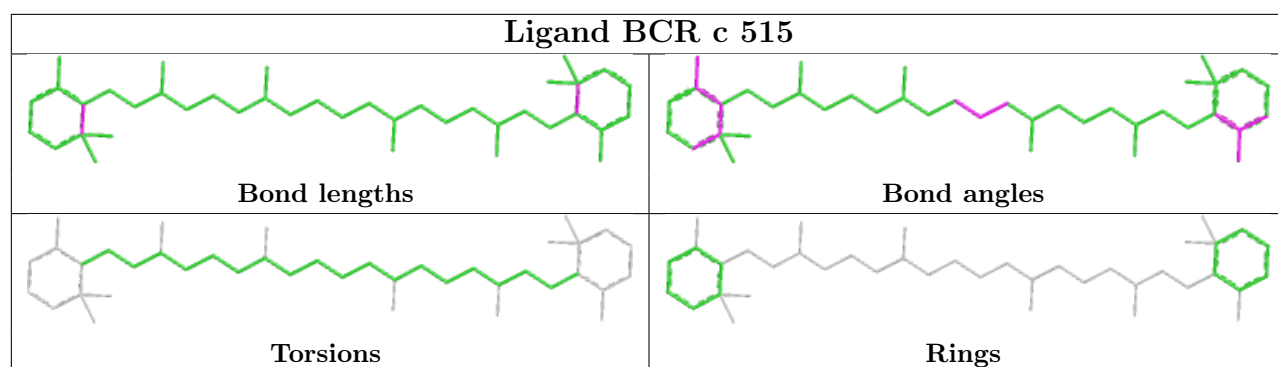


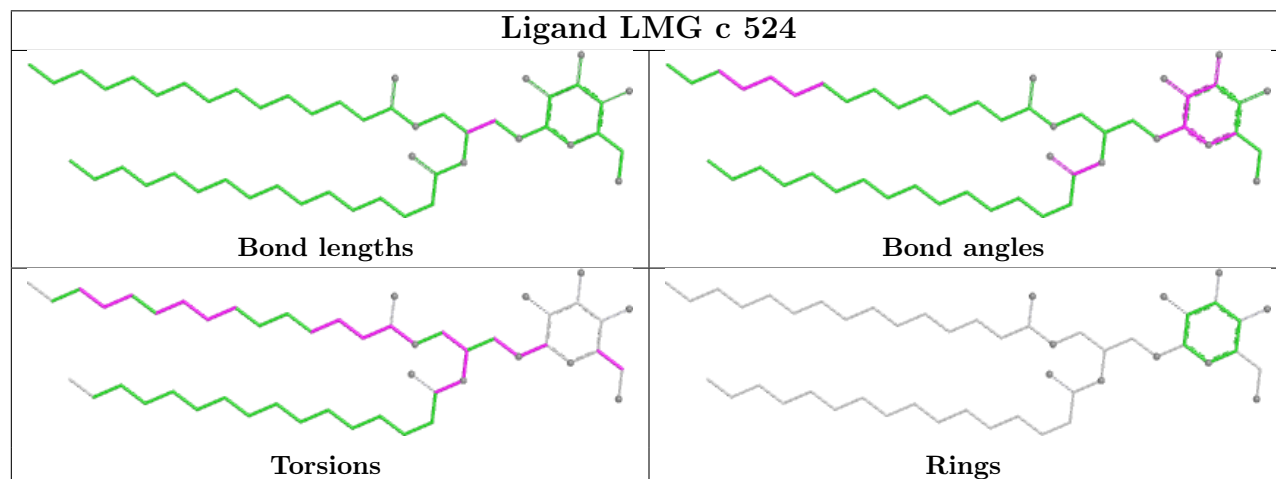
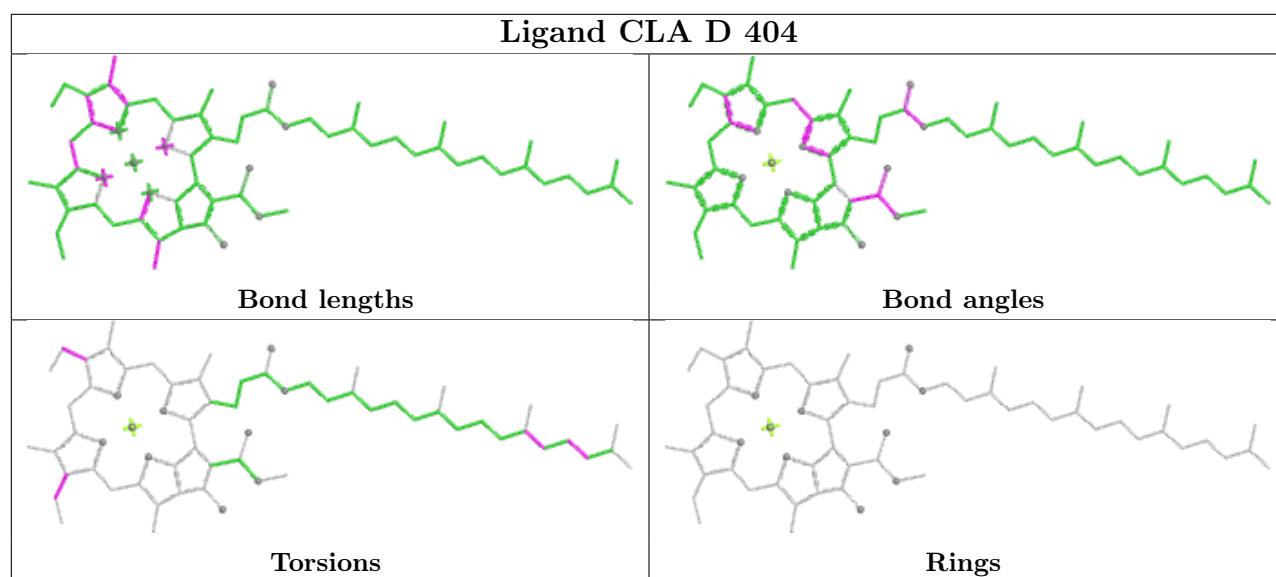


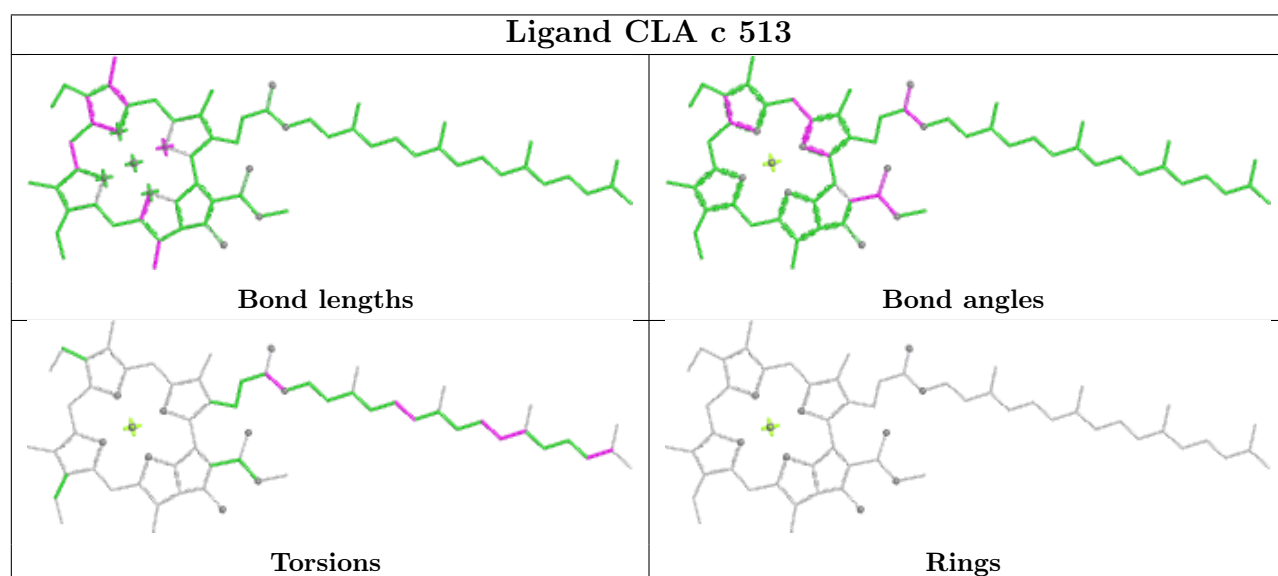
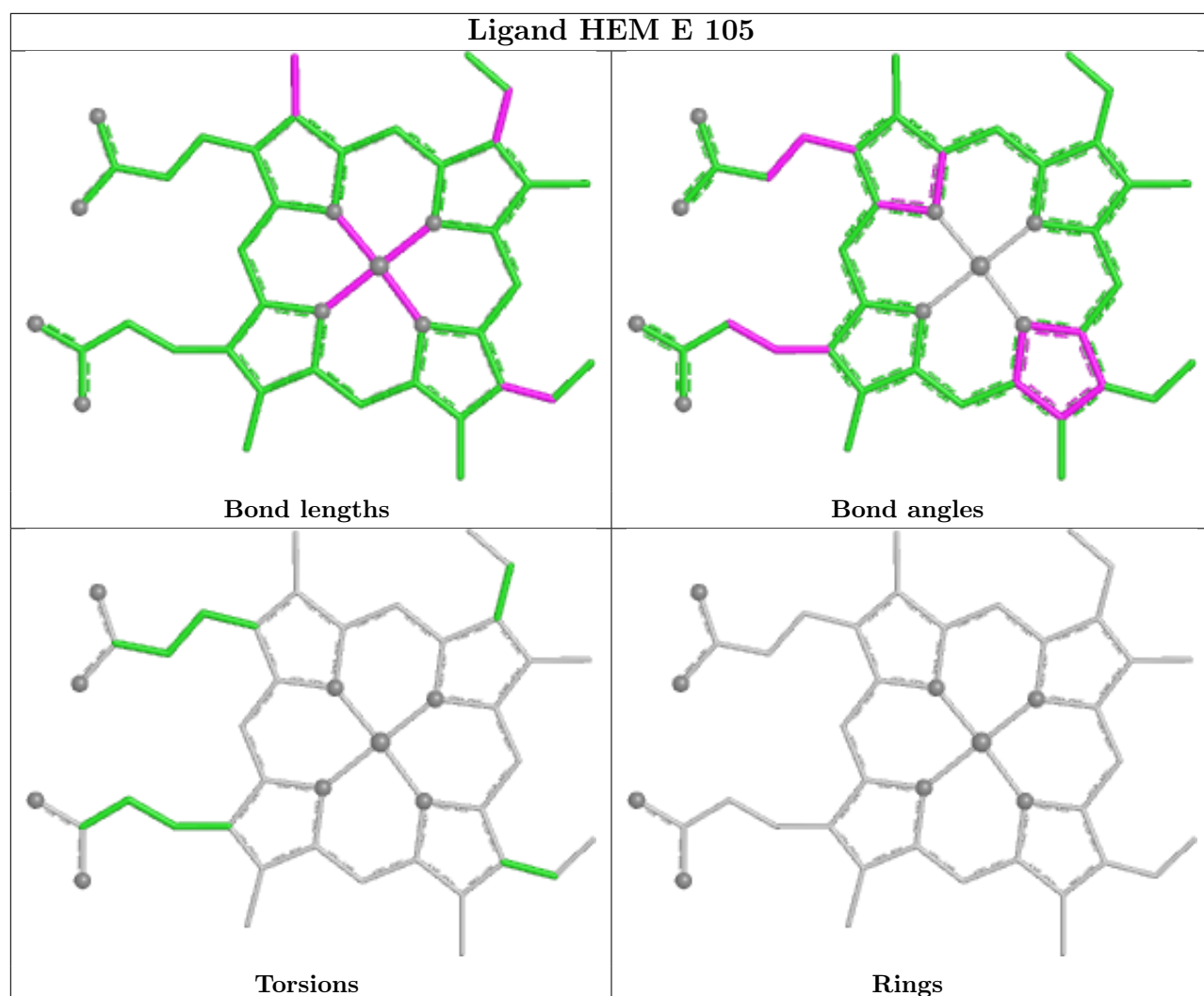


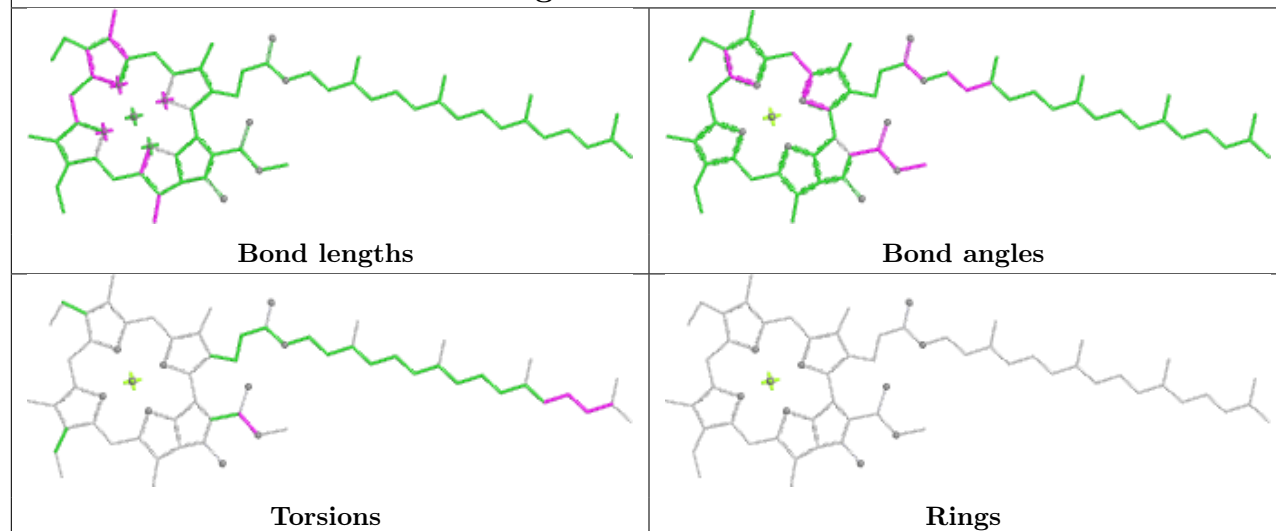
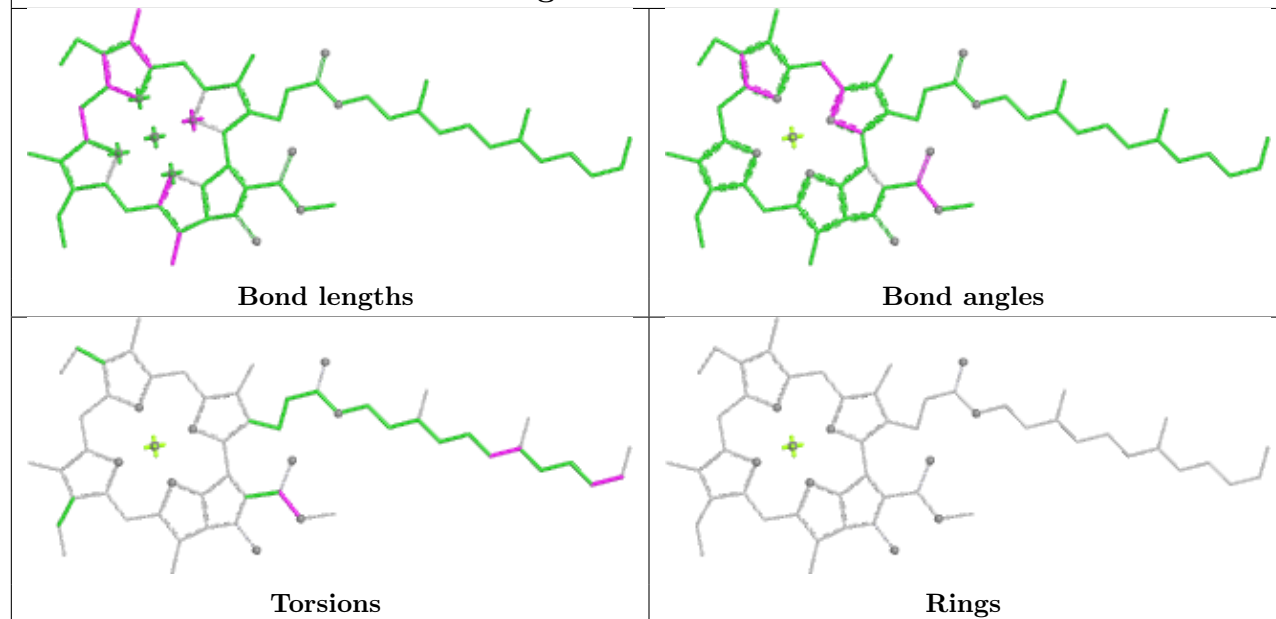


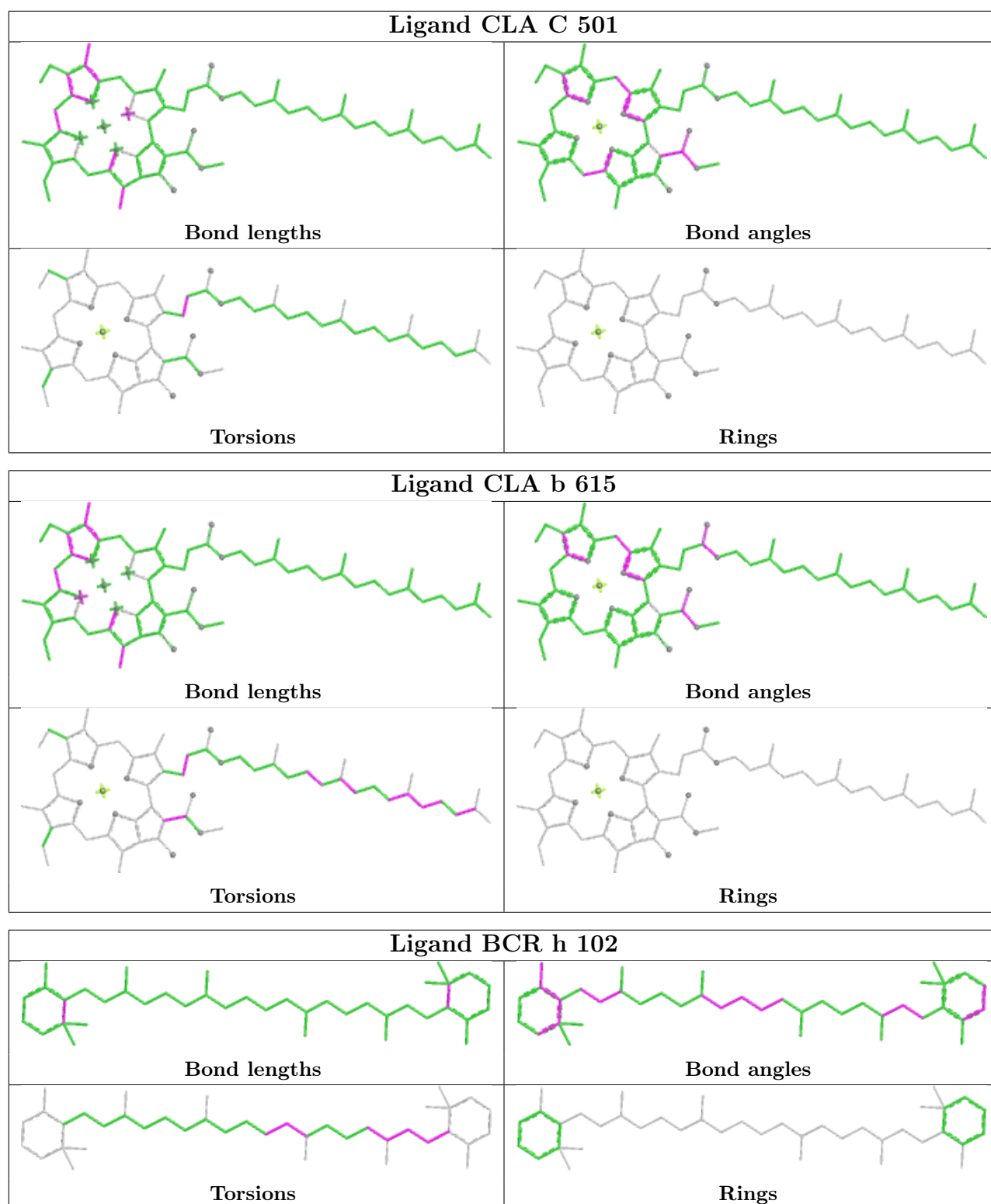


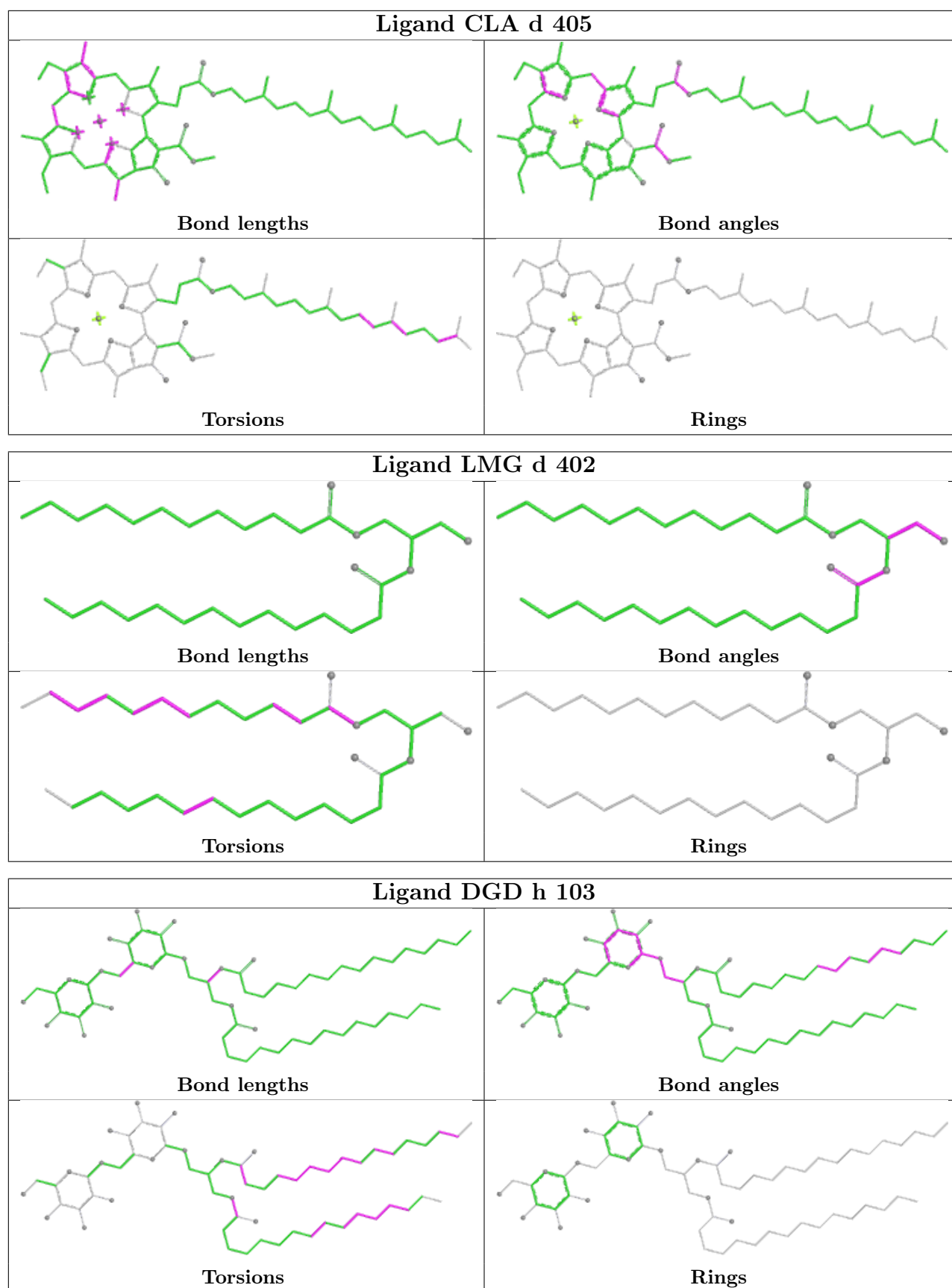


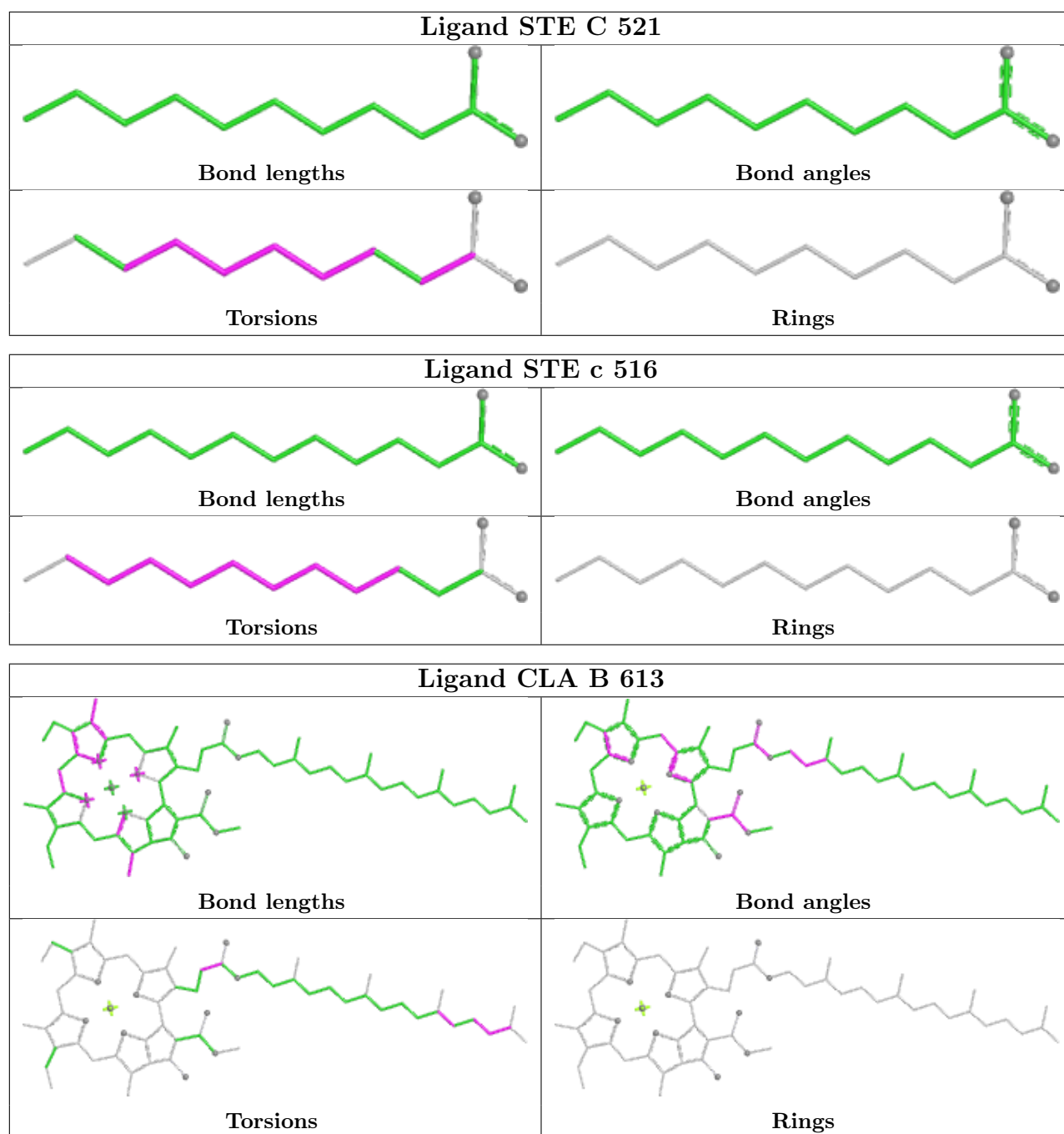


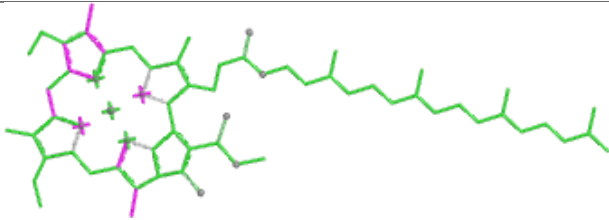
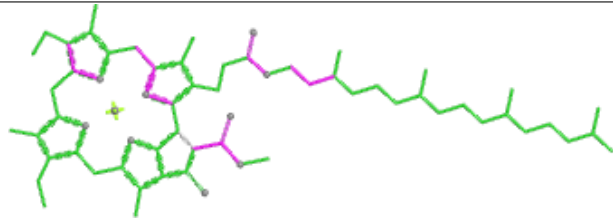
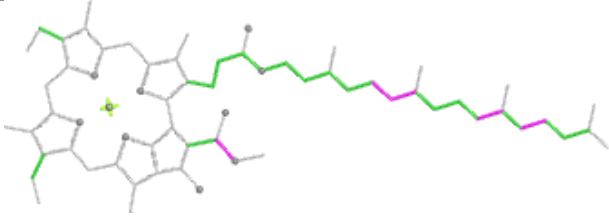
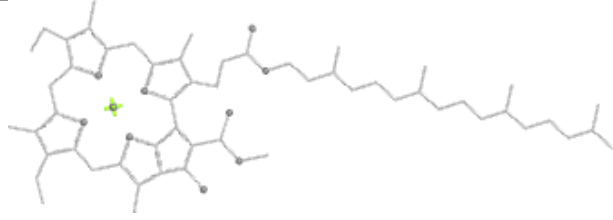


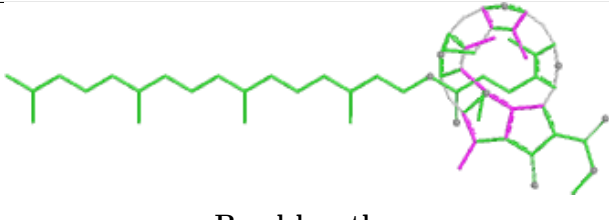
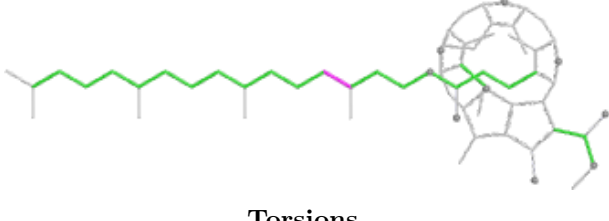
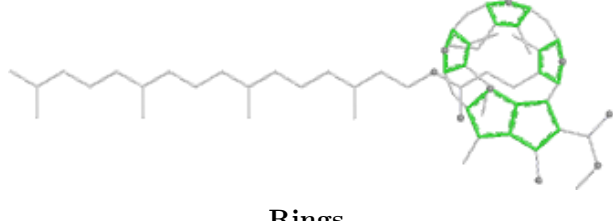
Ligand CLA b 610**Ligand CLA c 504**



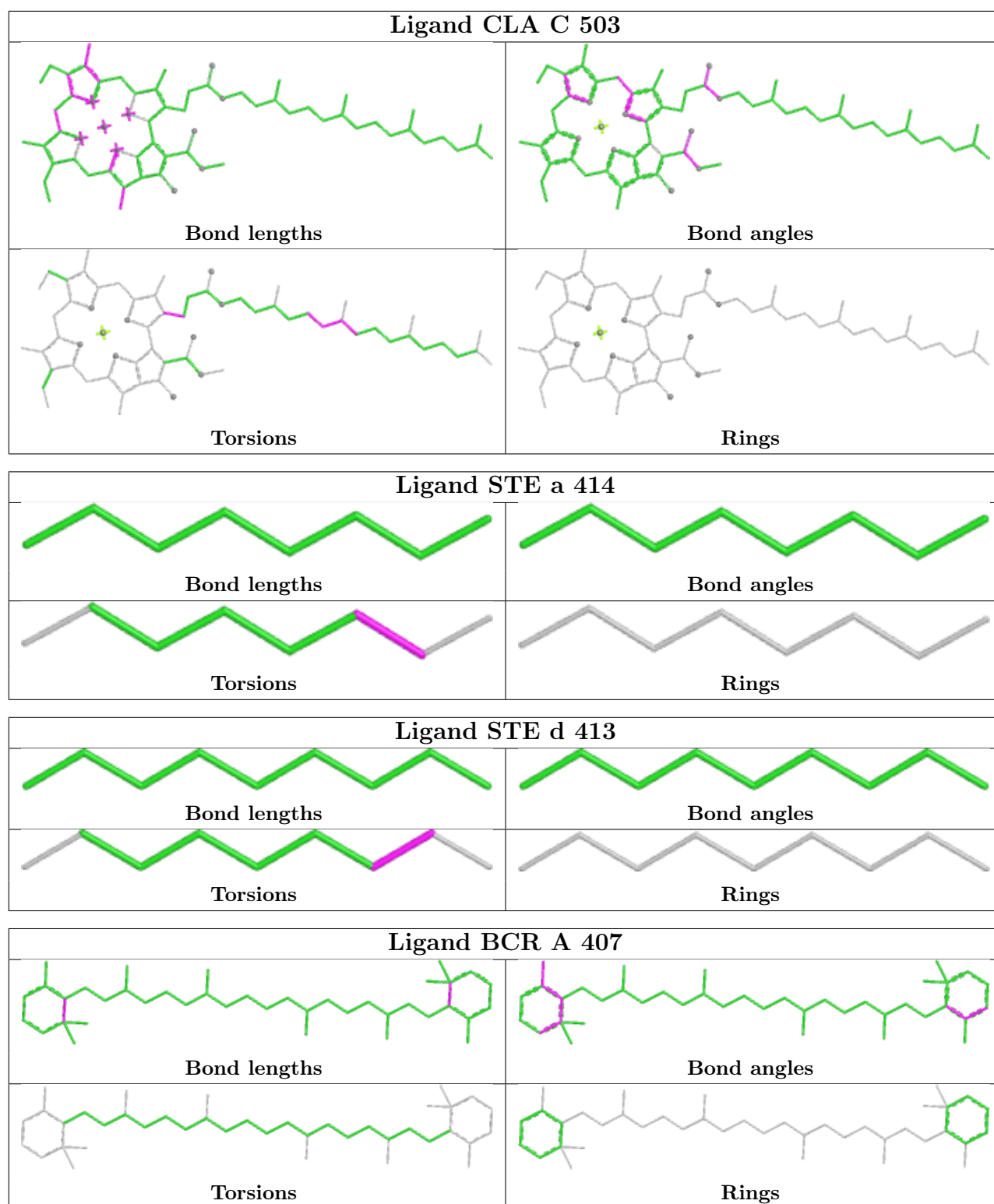


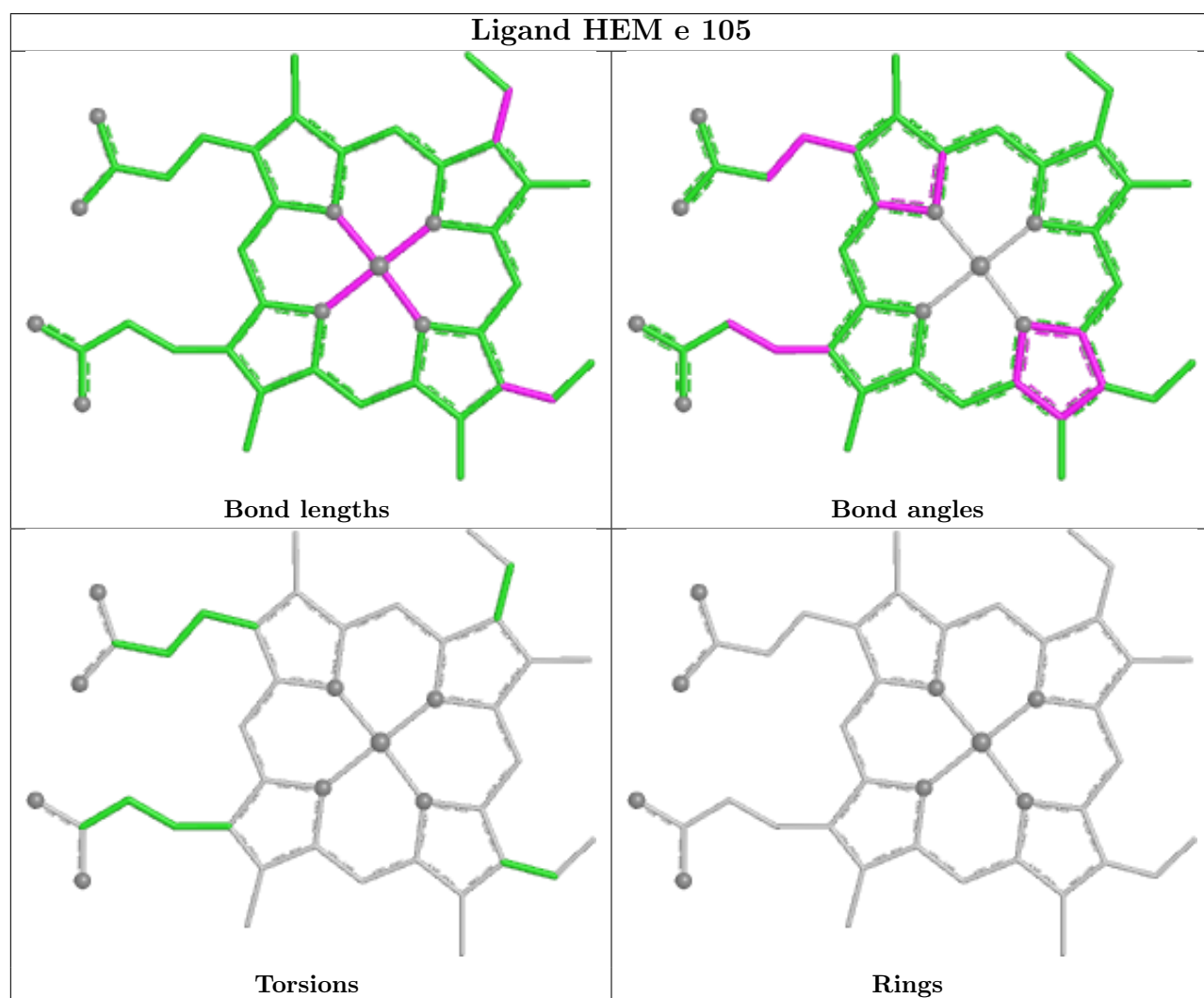
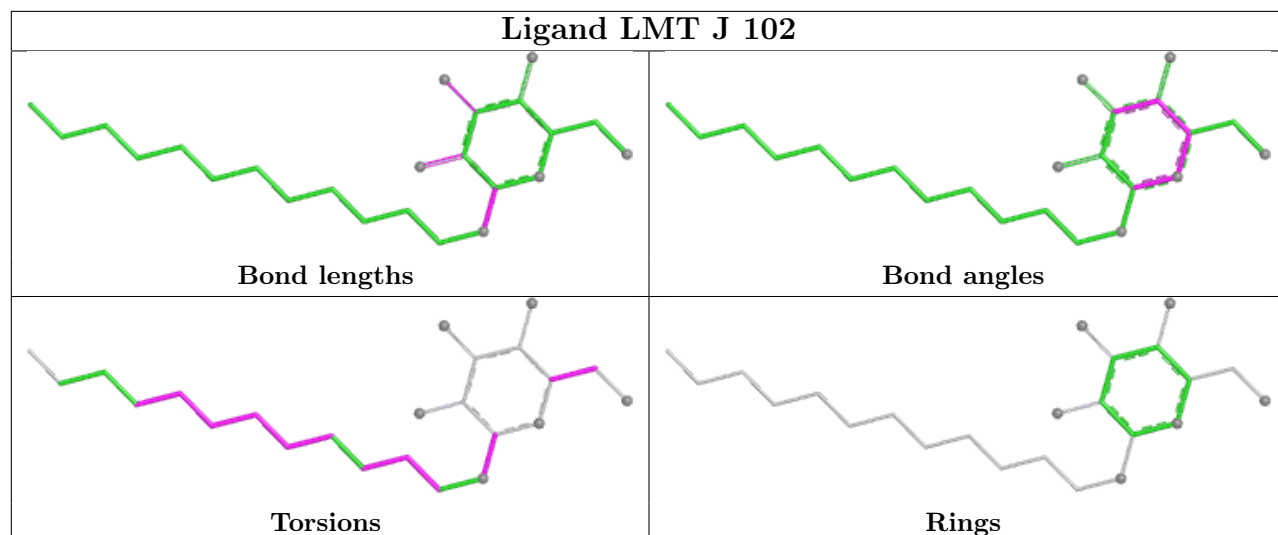


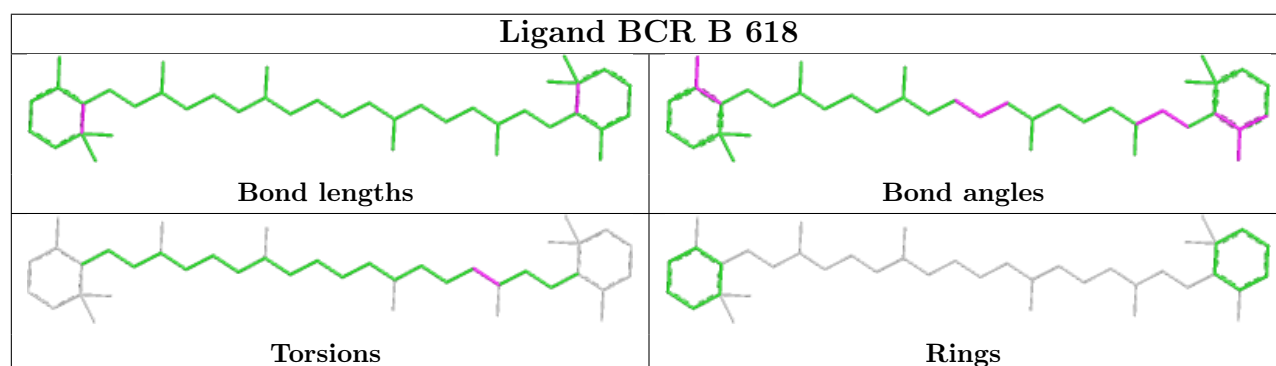
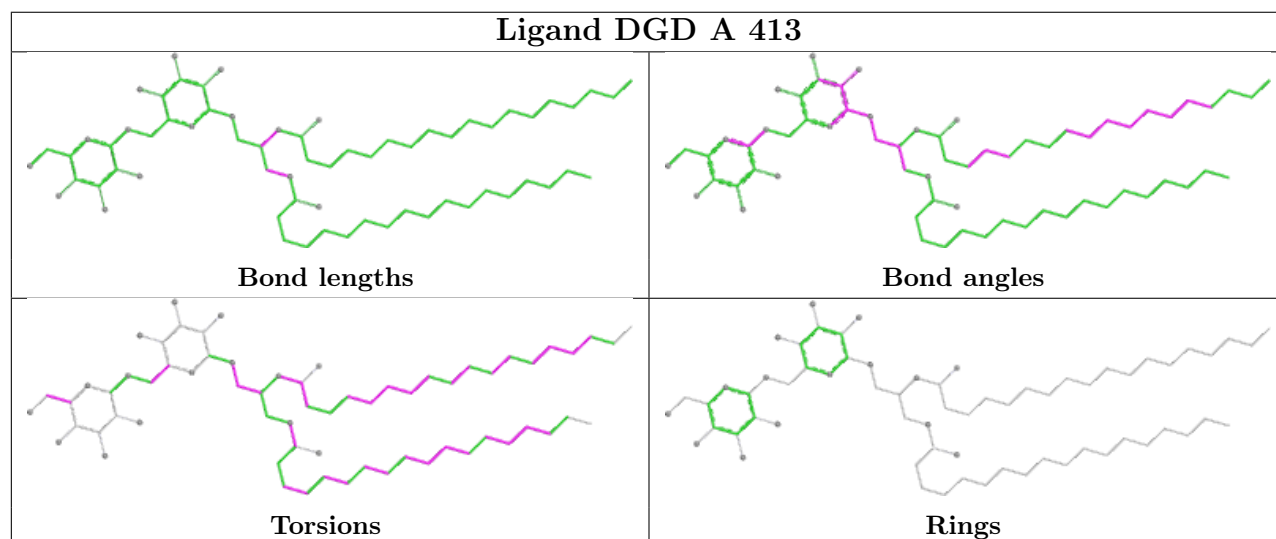
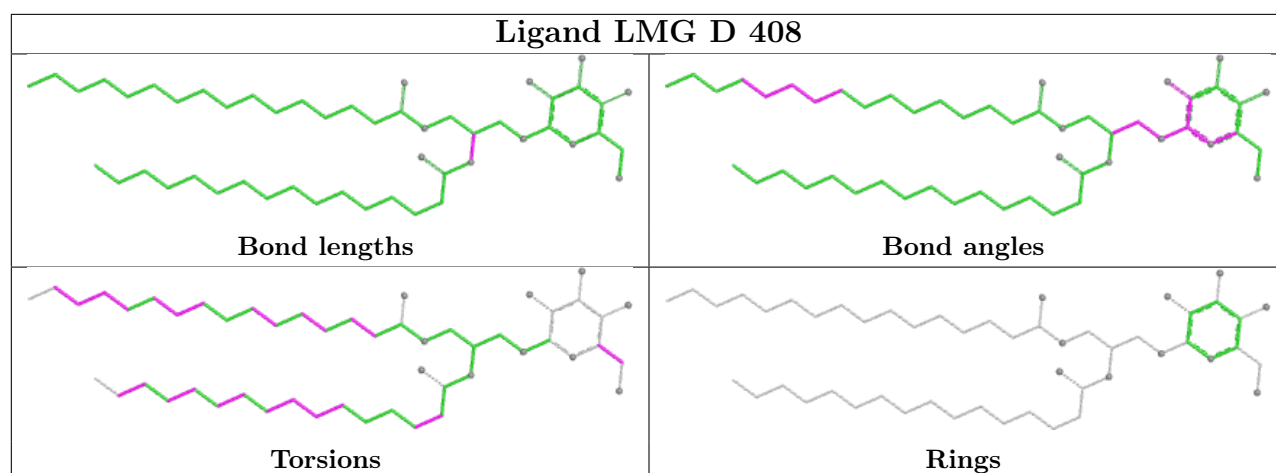
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Bond lengths	Bond angles
	
Torsions	Rings

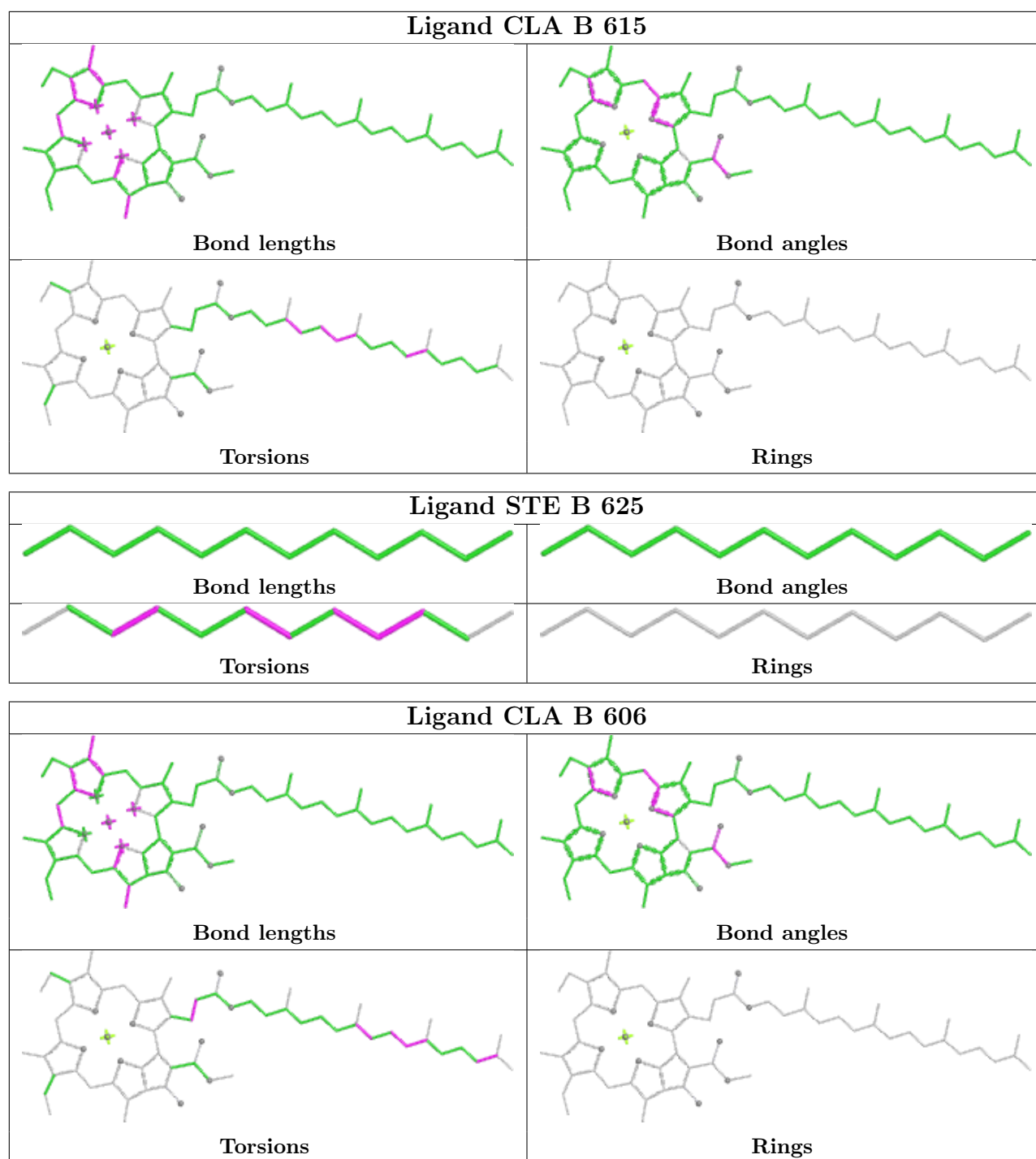
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Bond lengths	Bond angles
	
Torsions	Rings

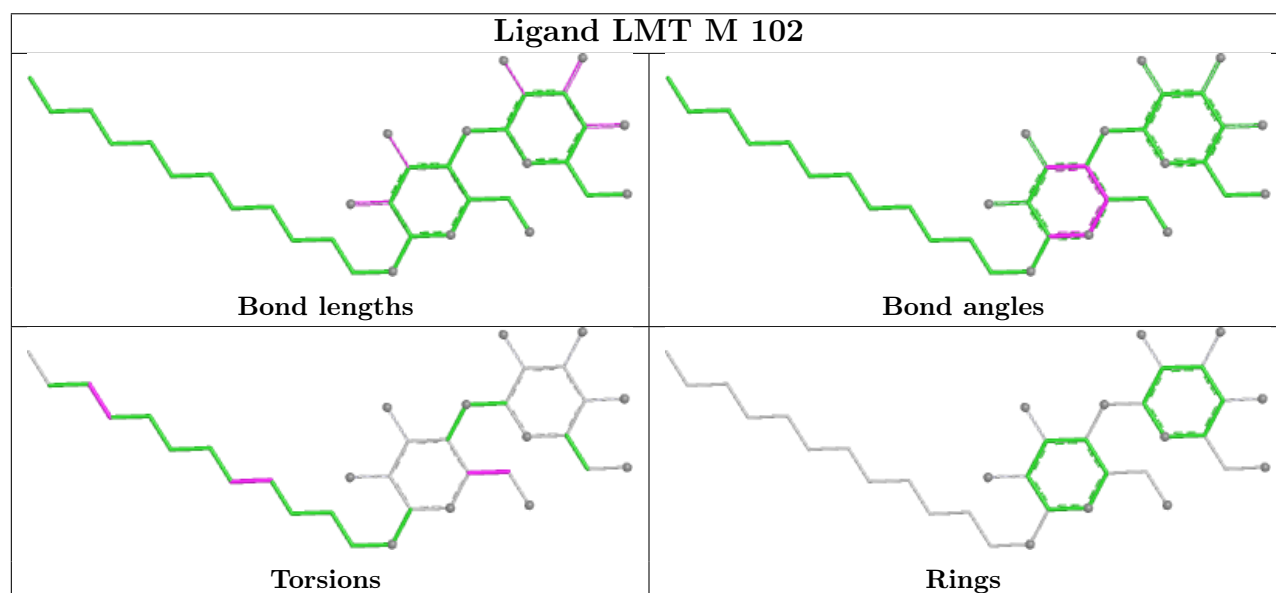
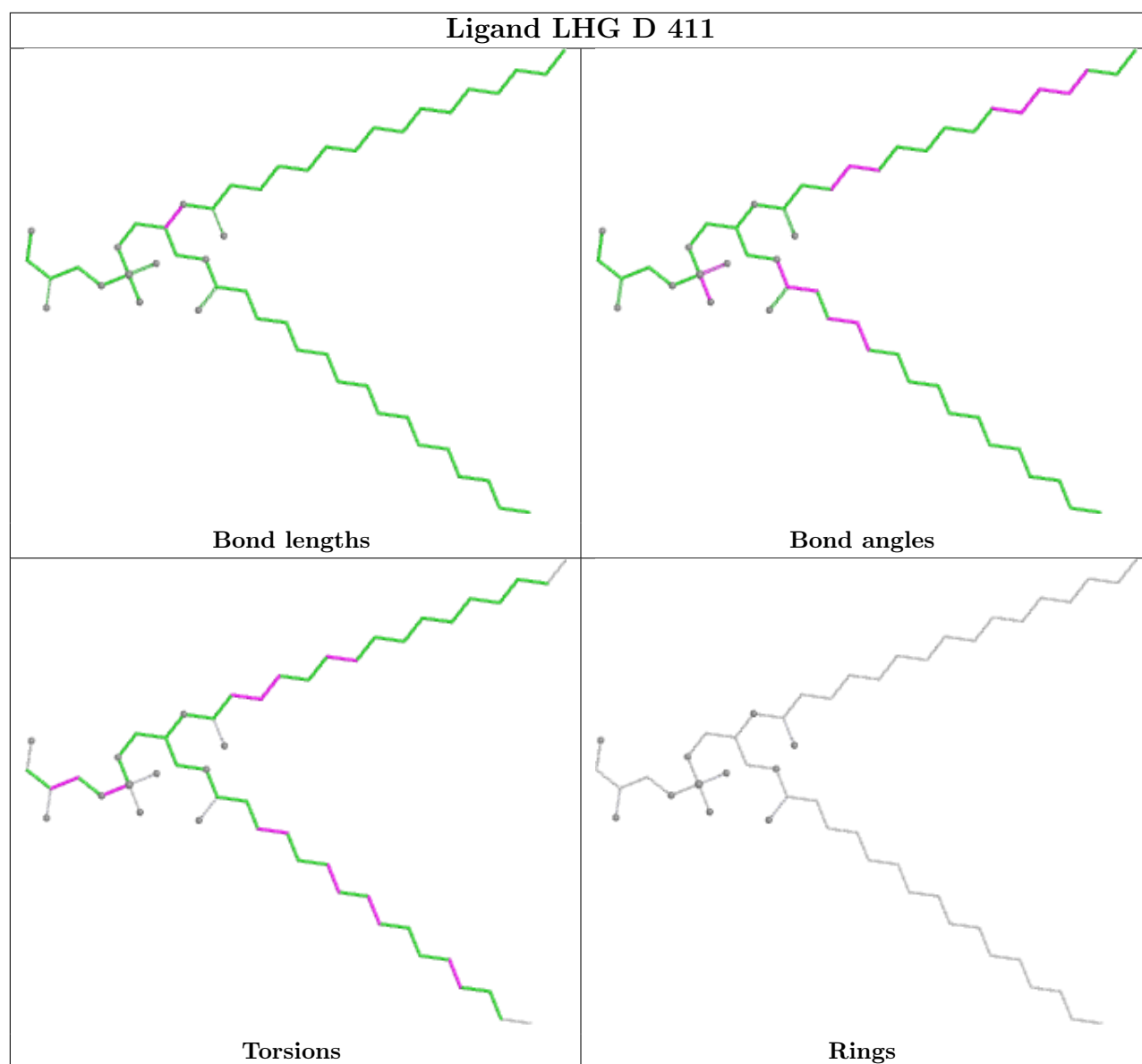
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Bond lengths	Bond angles
	
Torsions	Rings

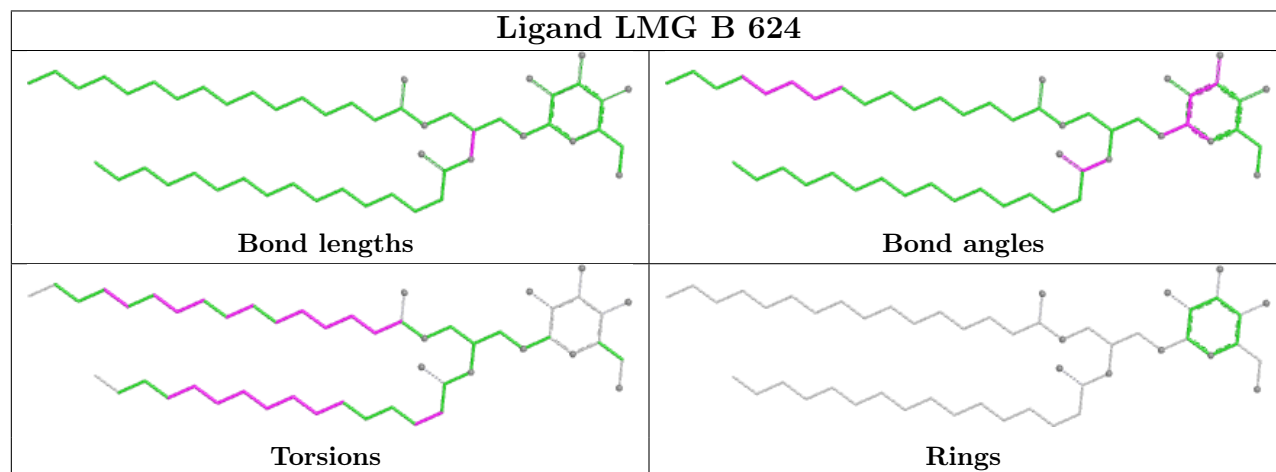
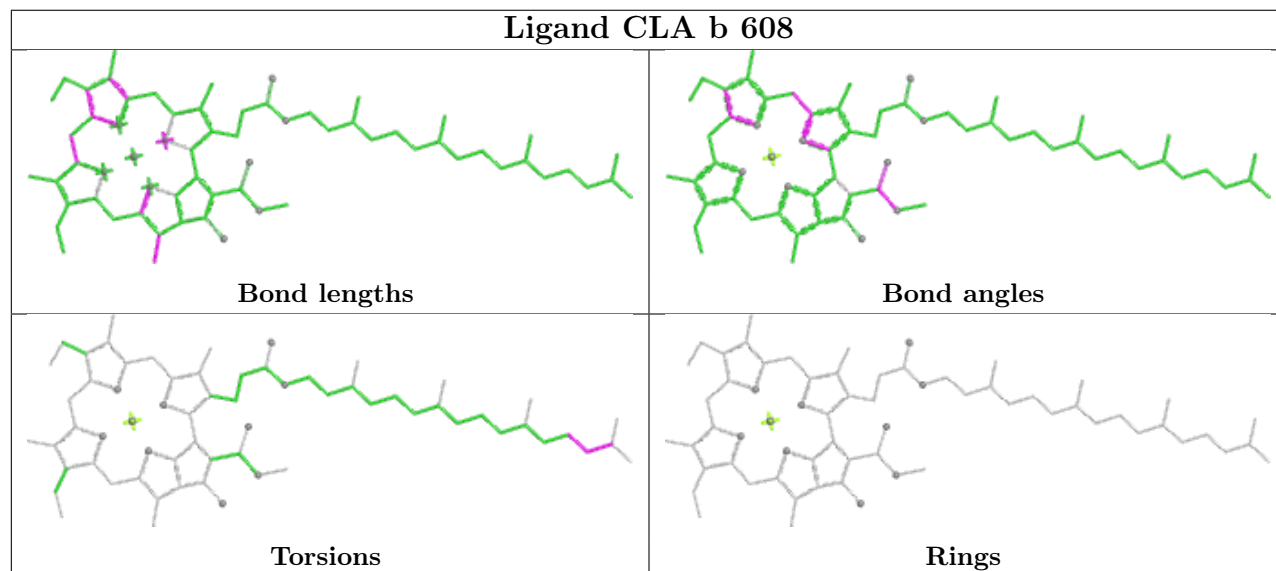
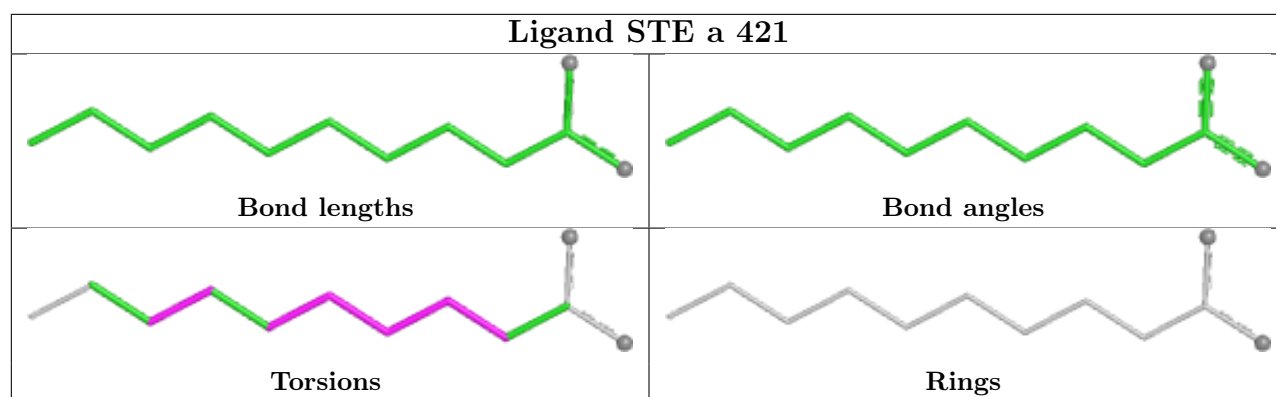


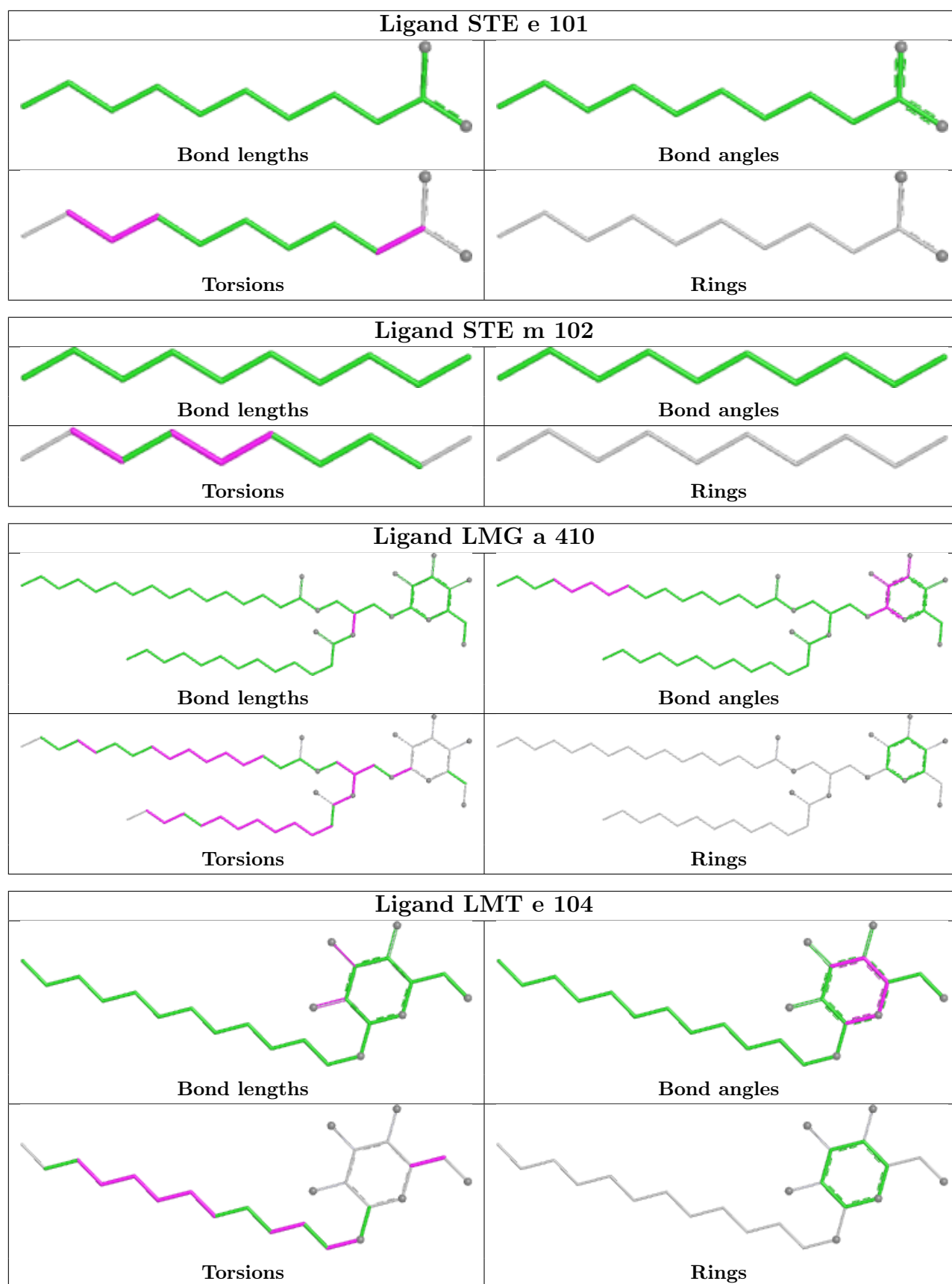


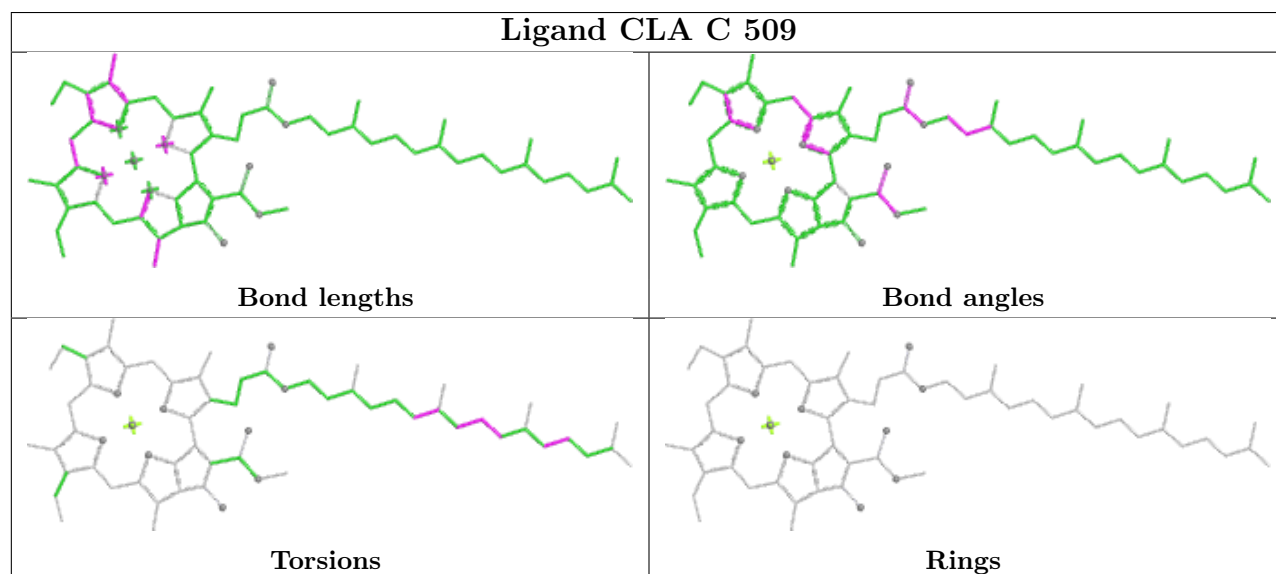
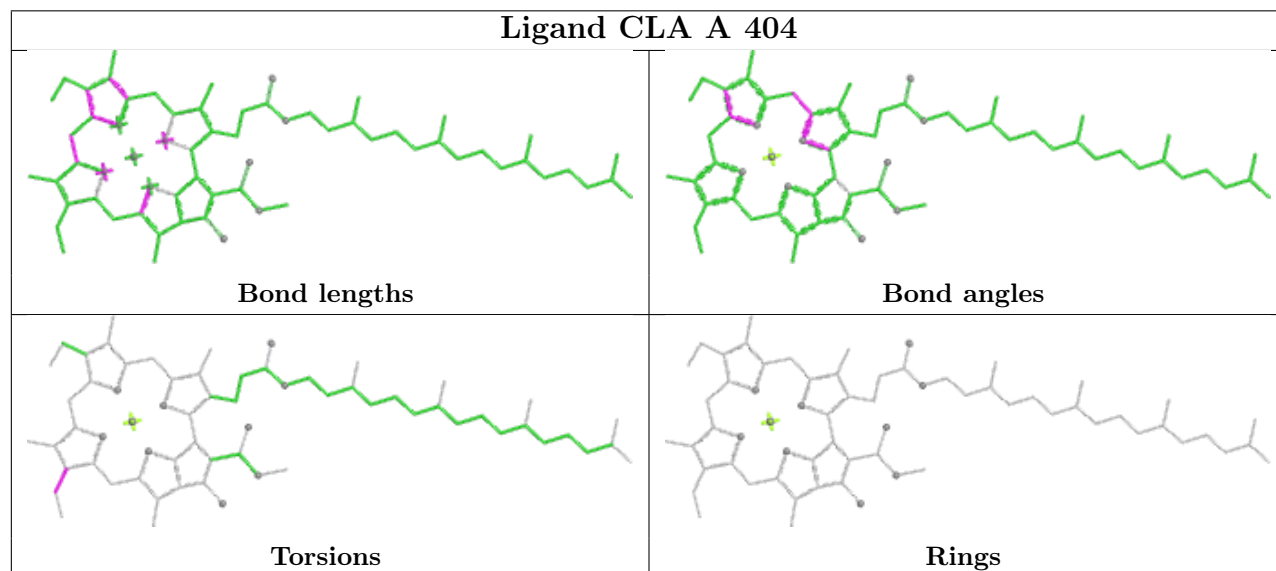
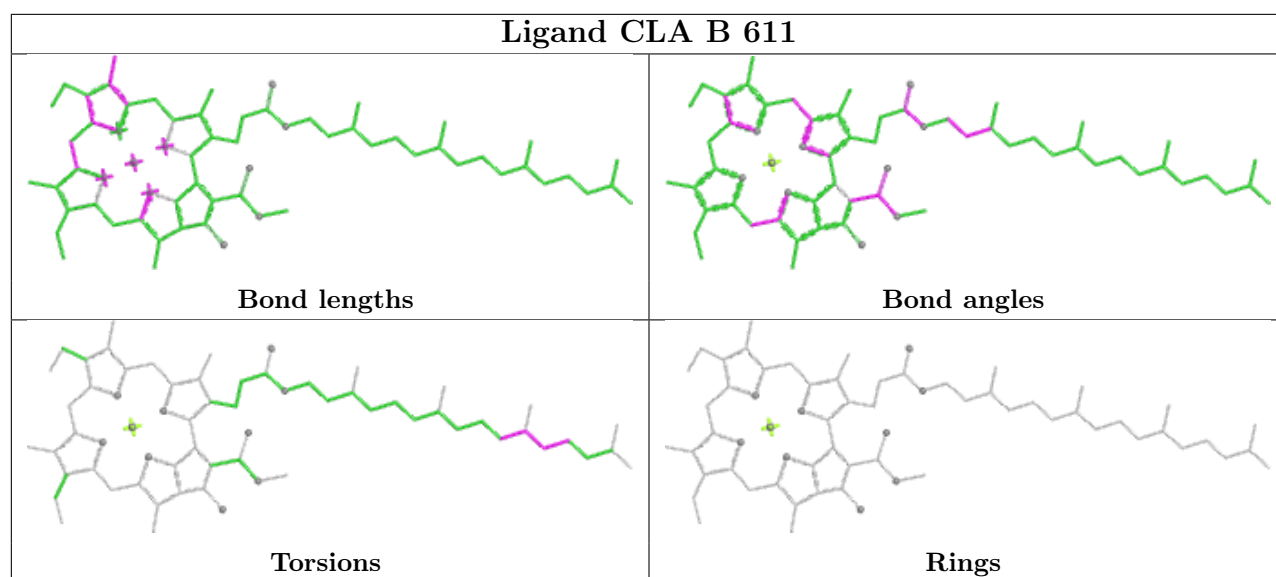


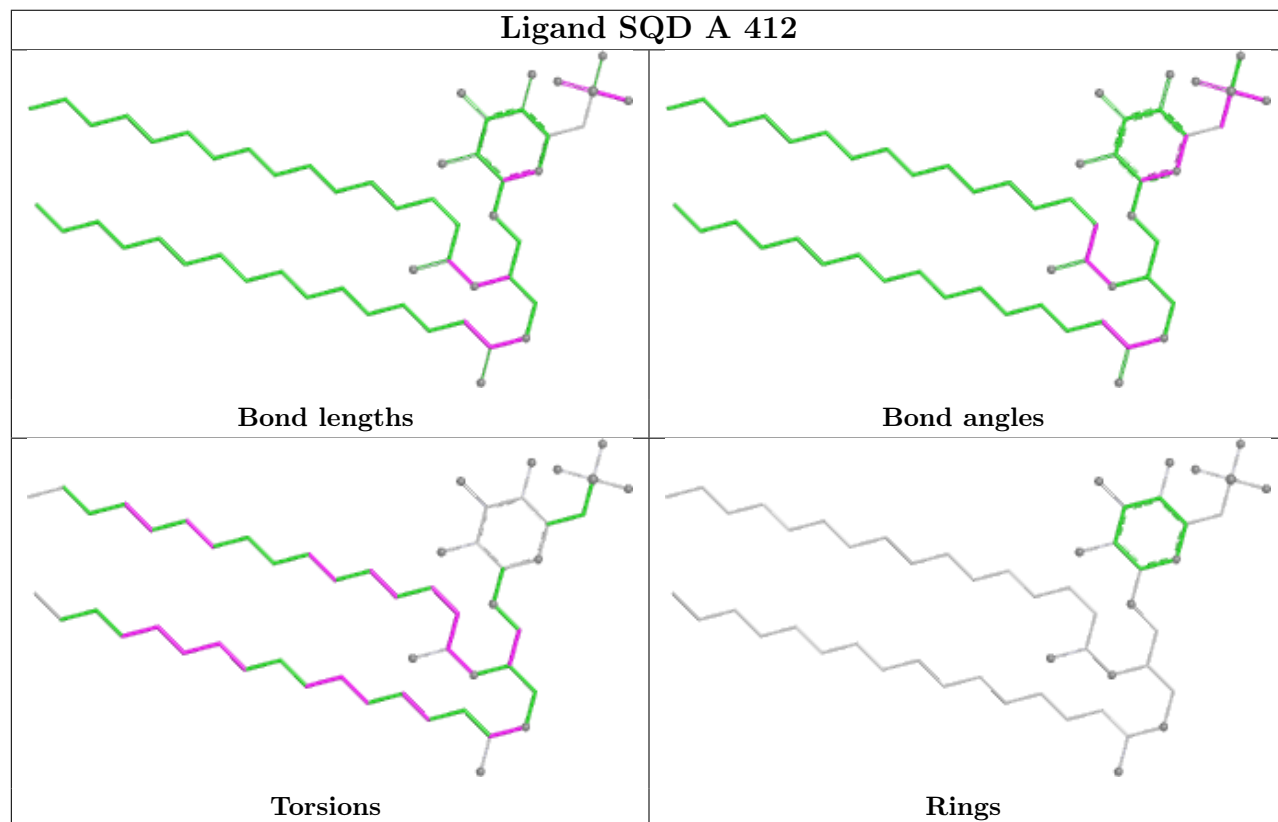
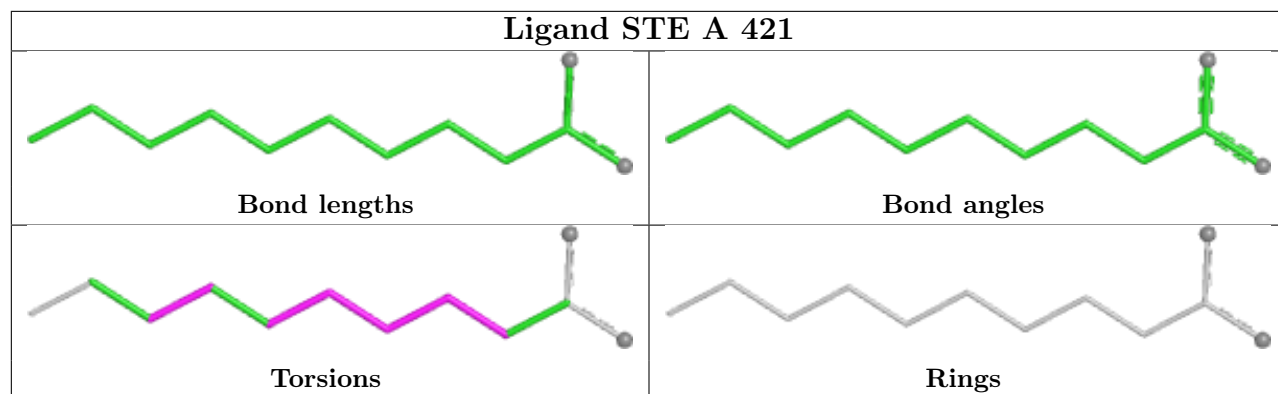


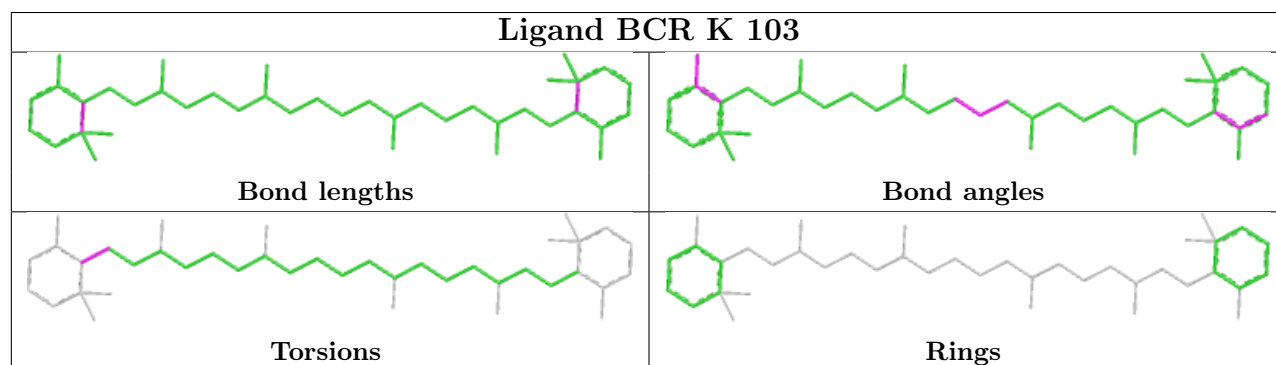
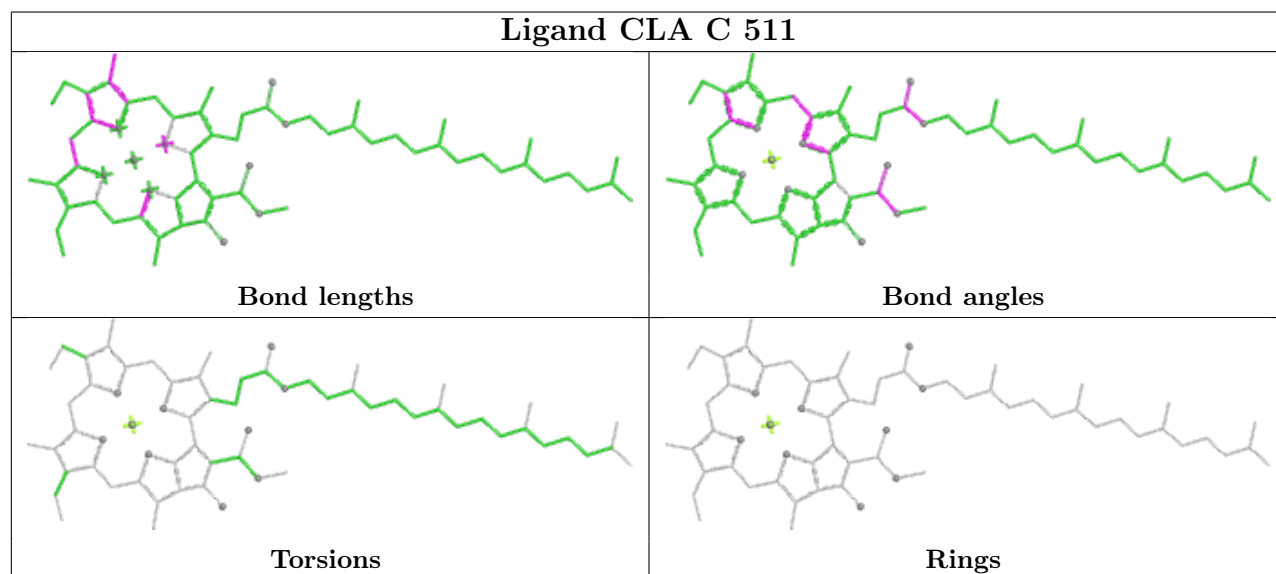
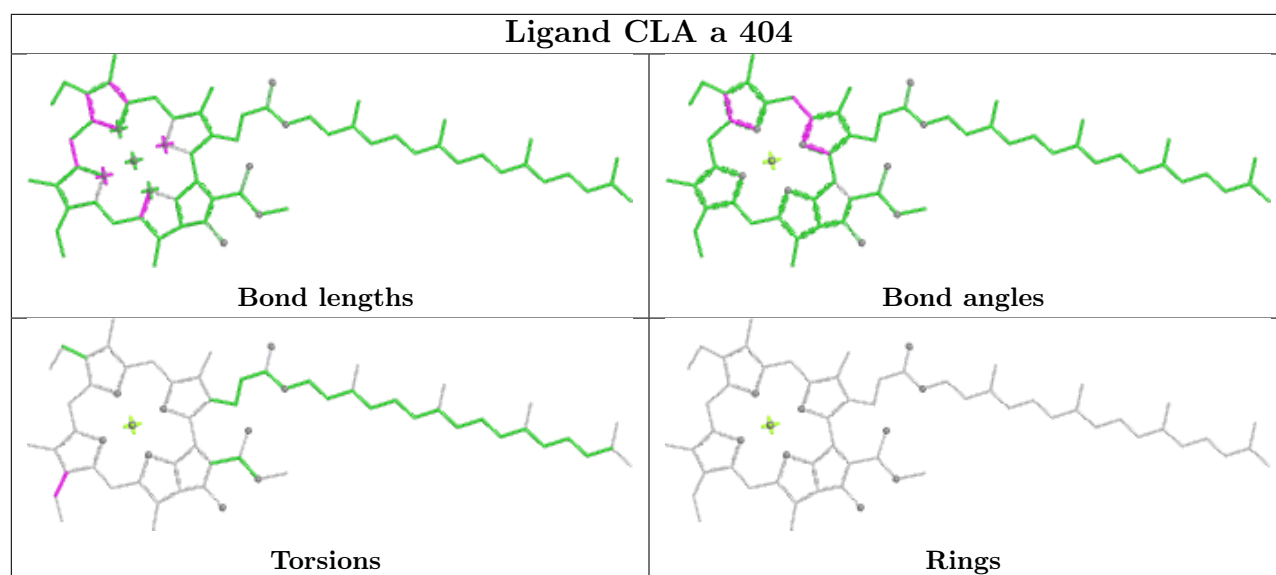


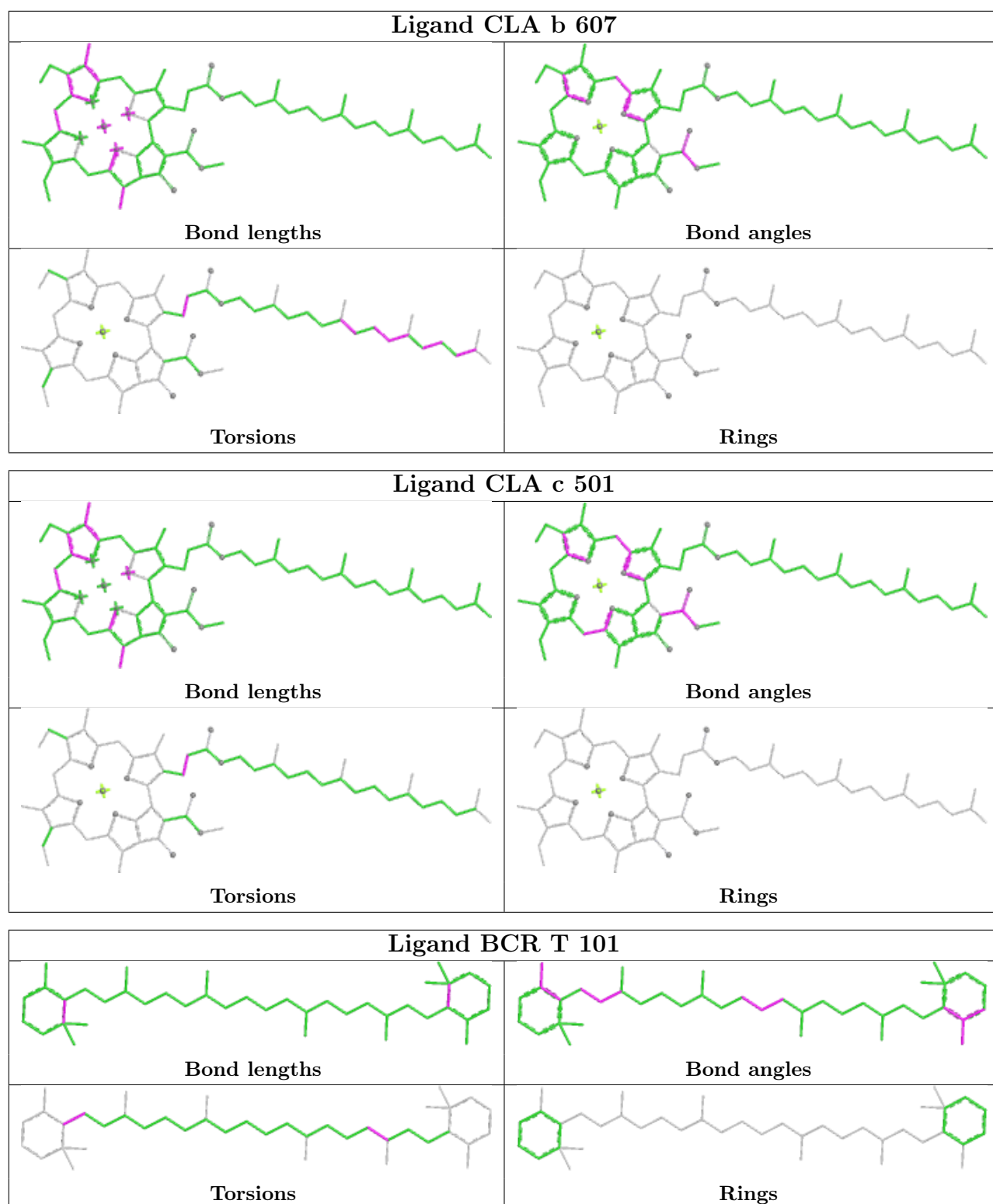


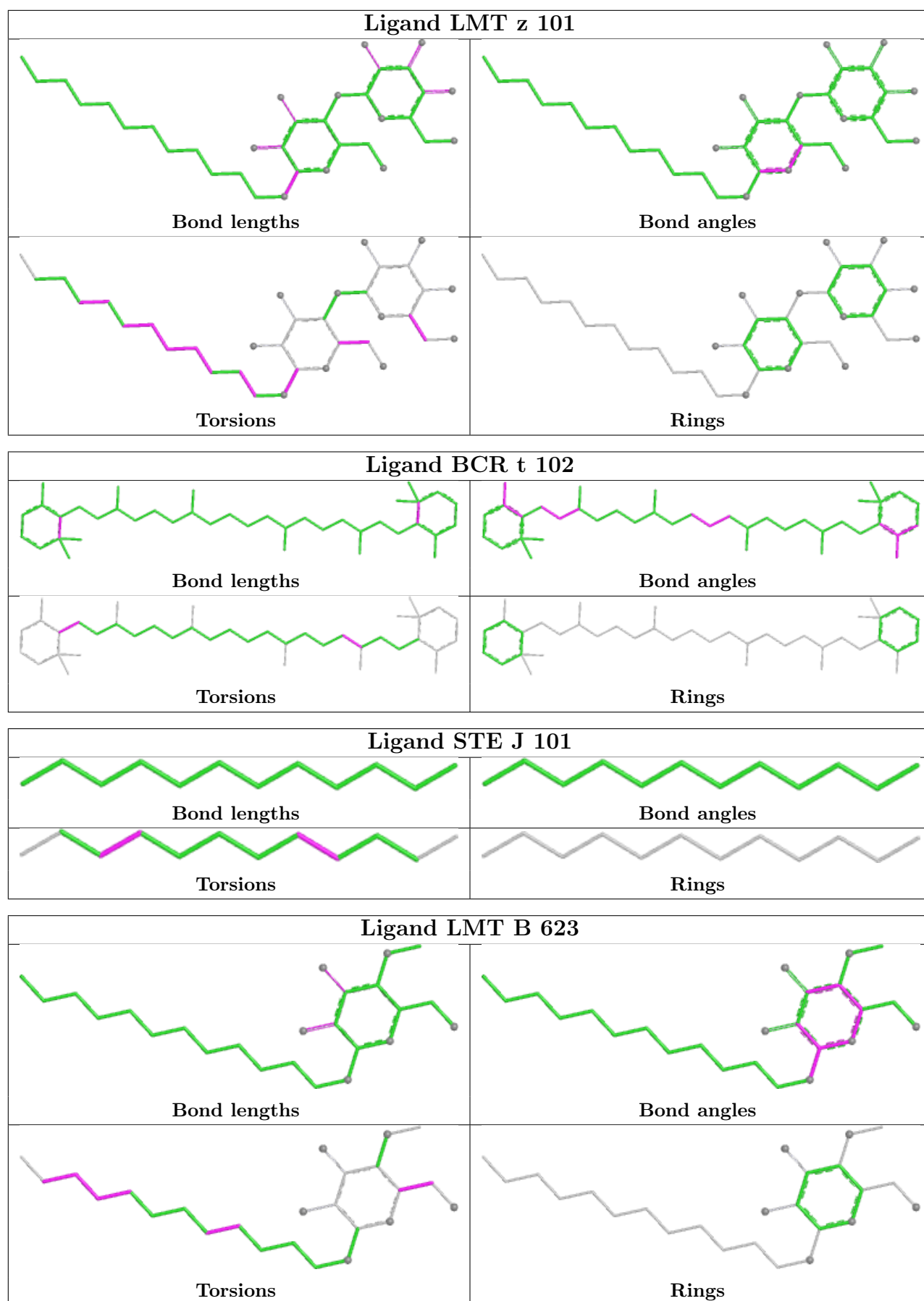


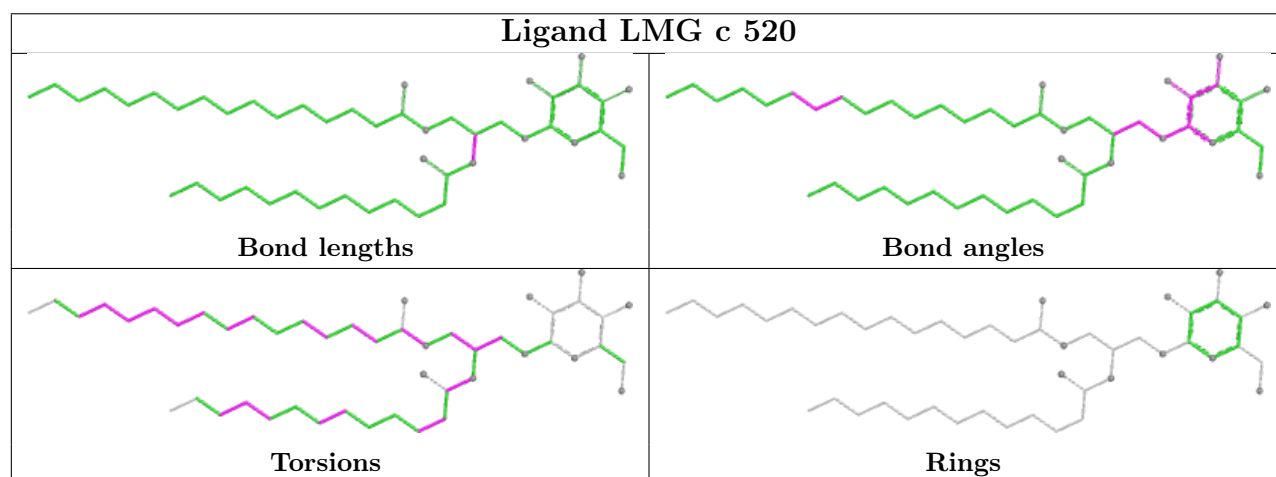
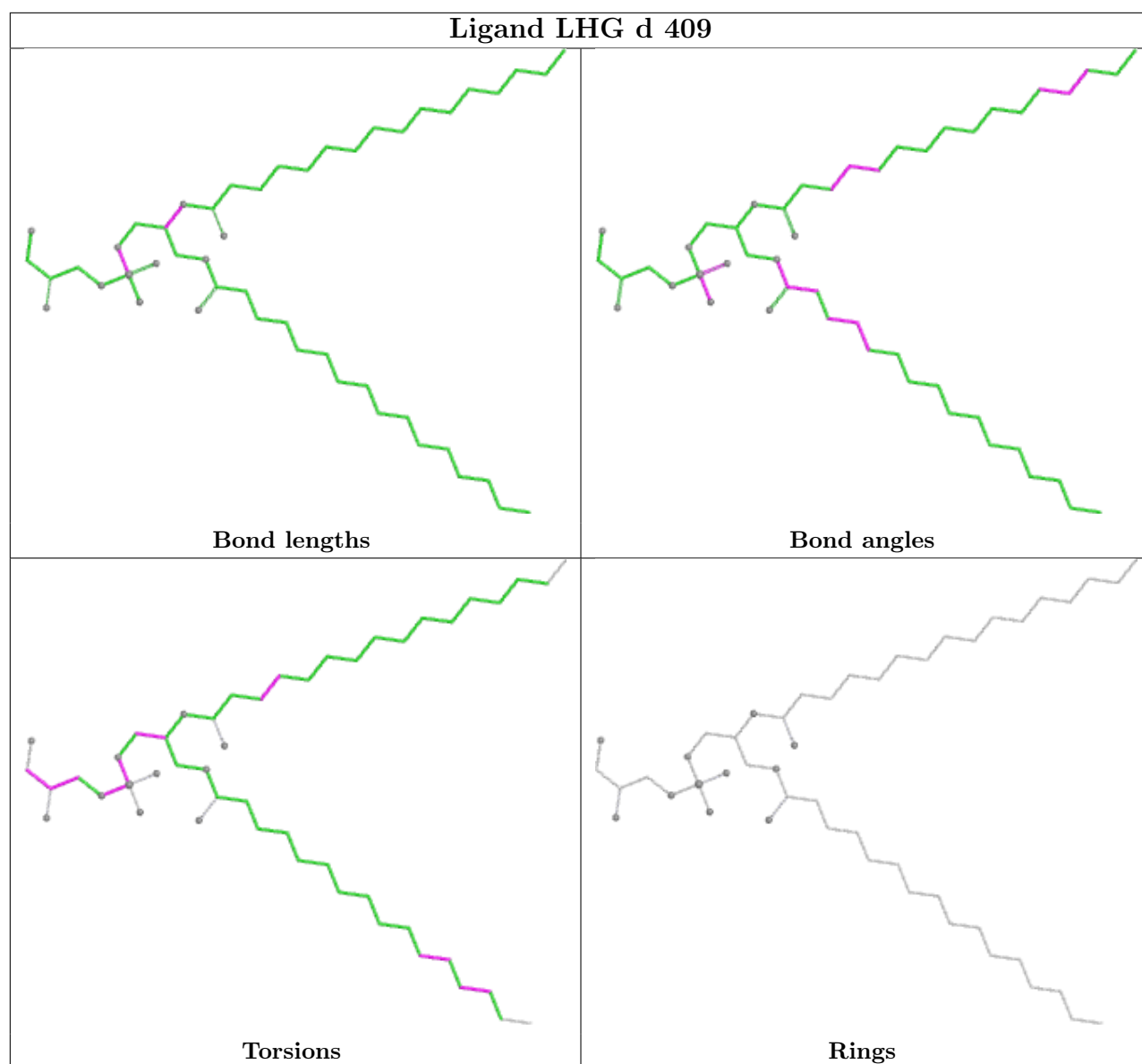


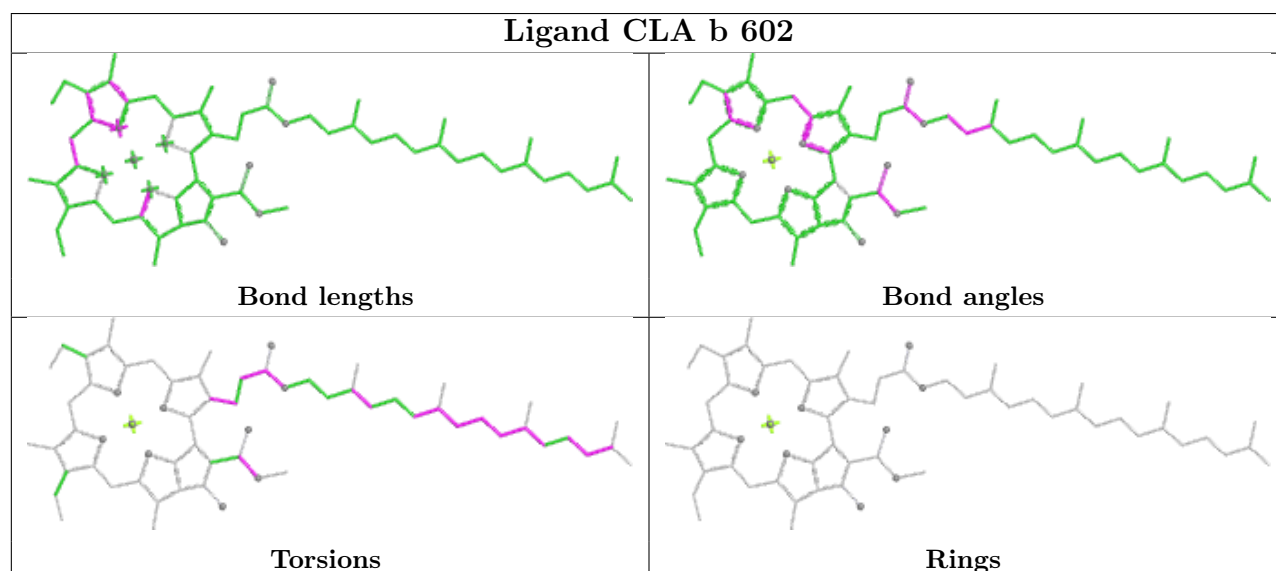
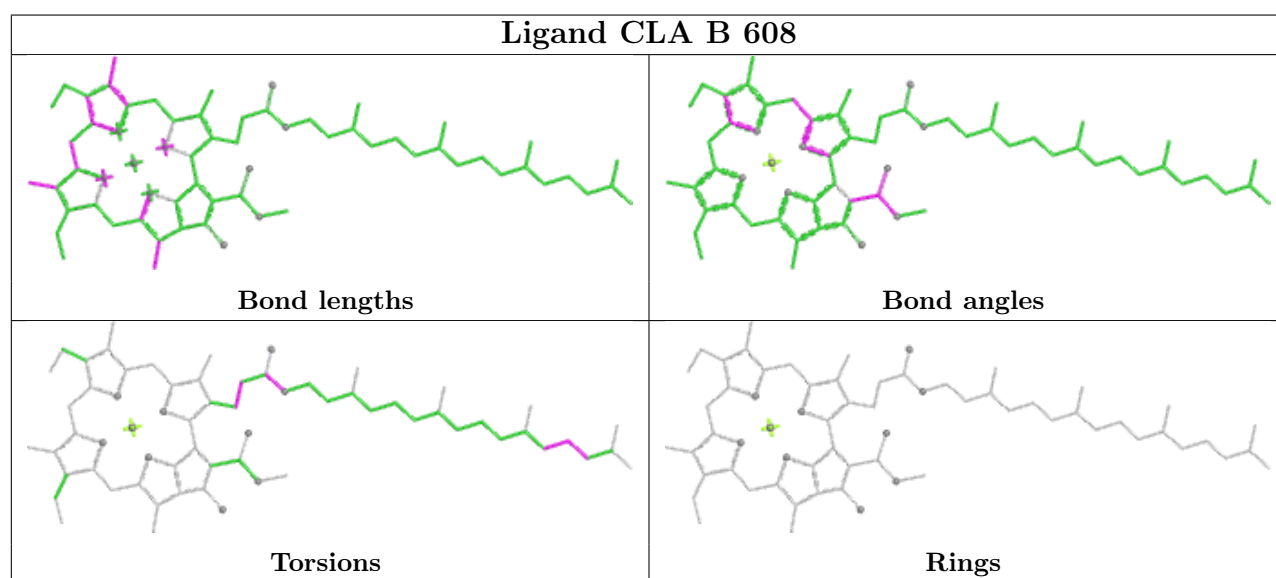
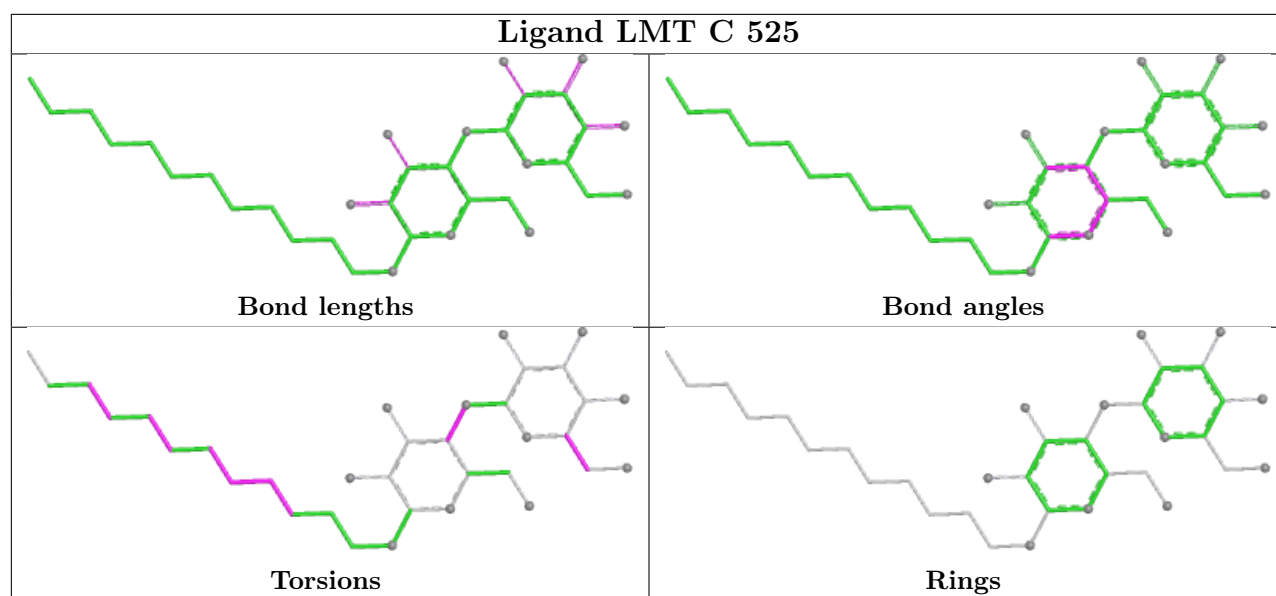


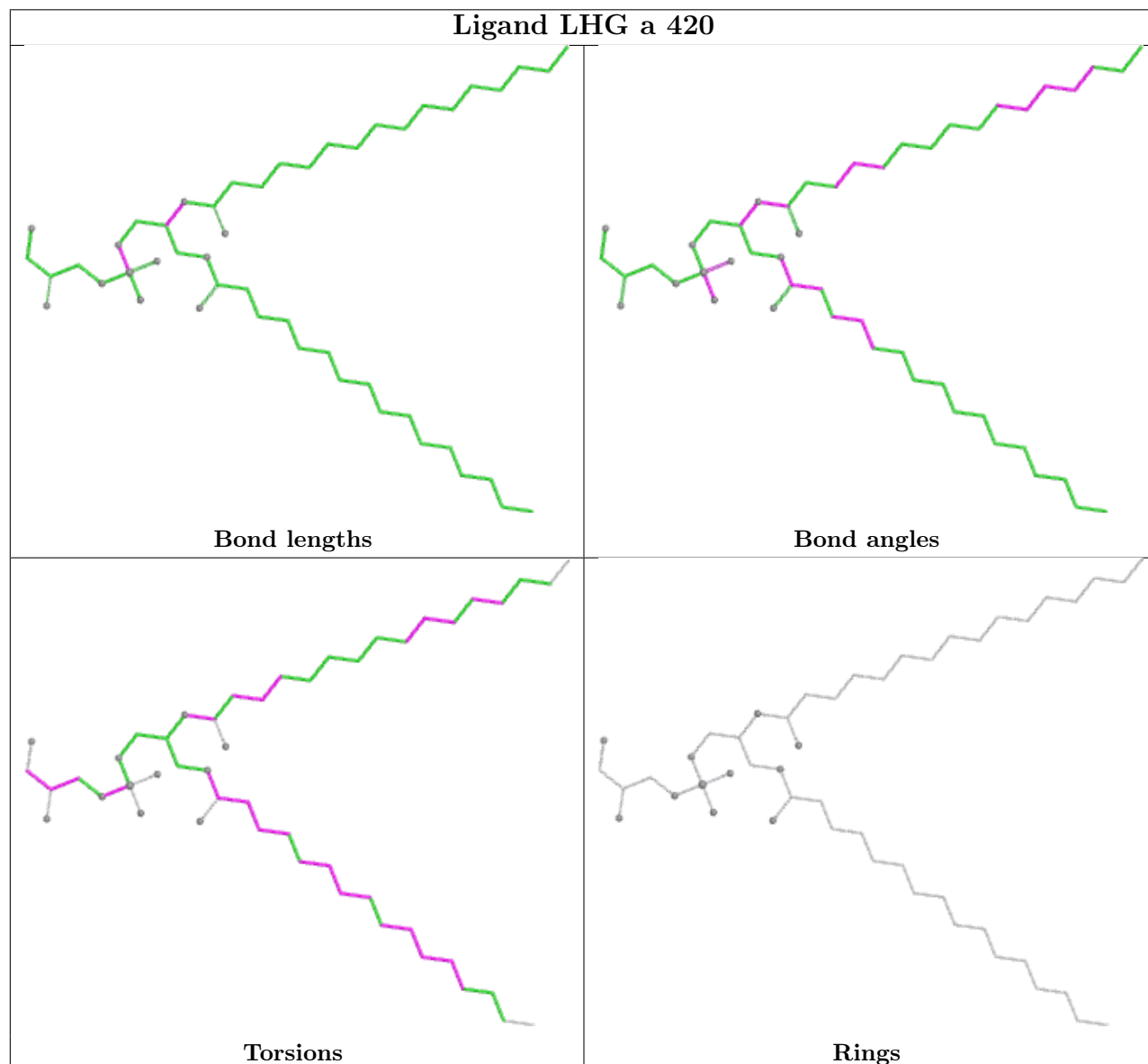
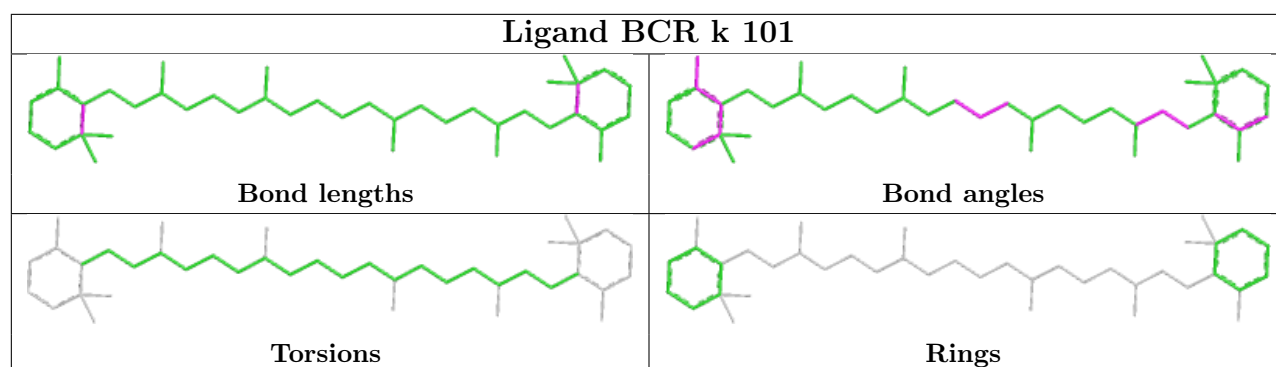


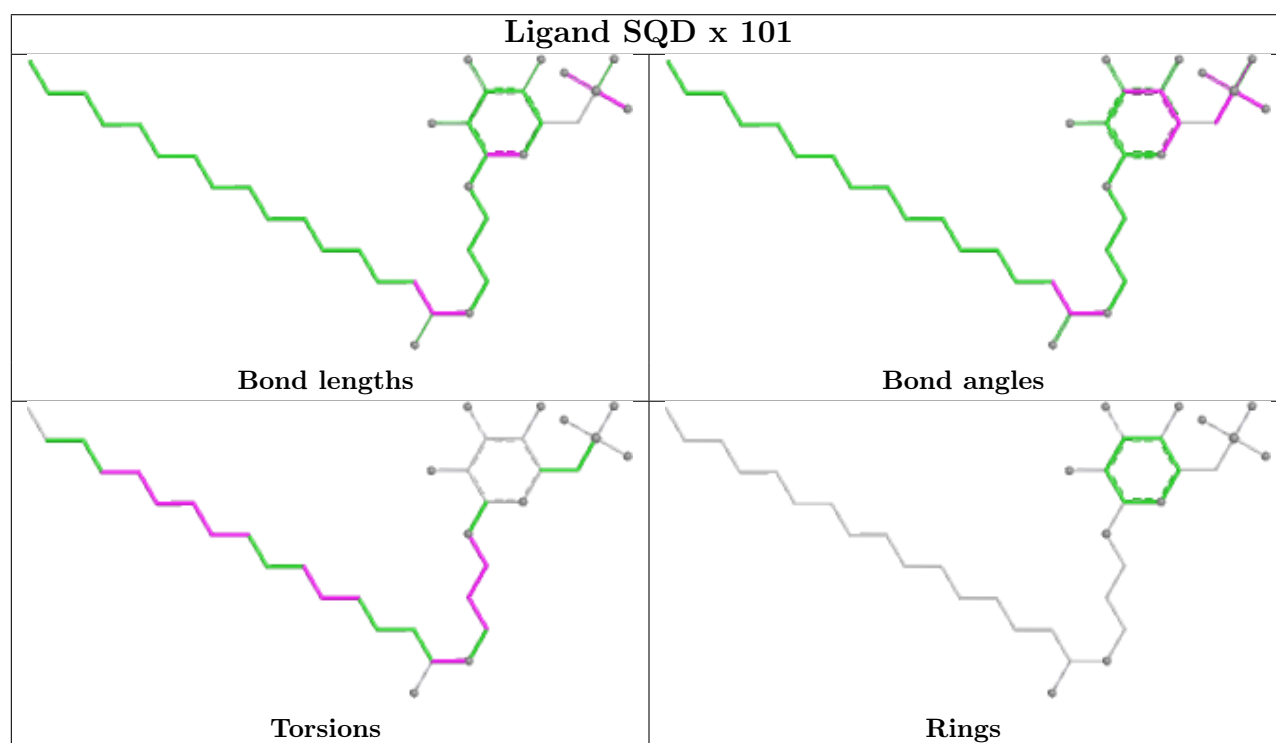
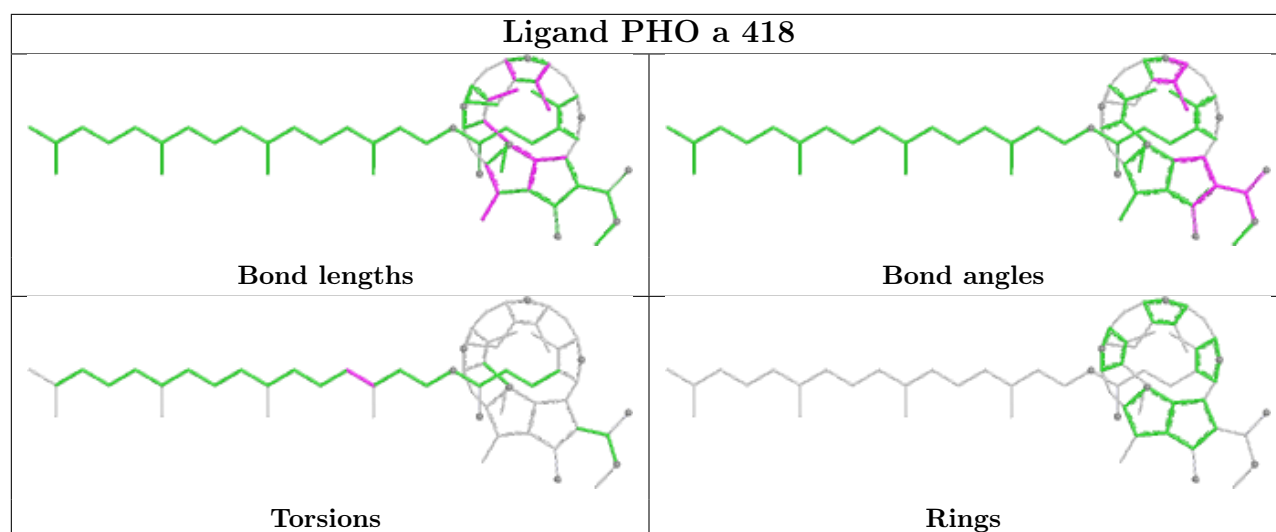


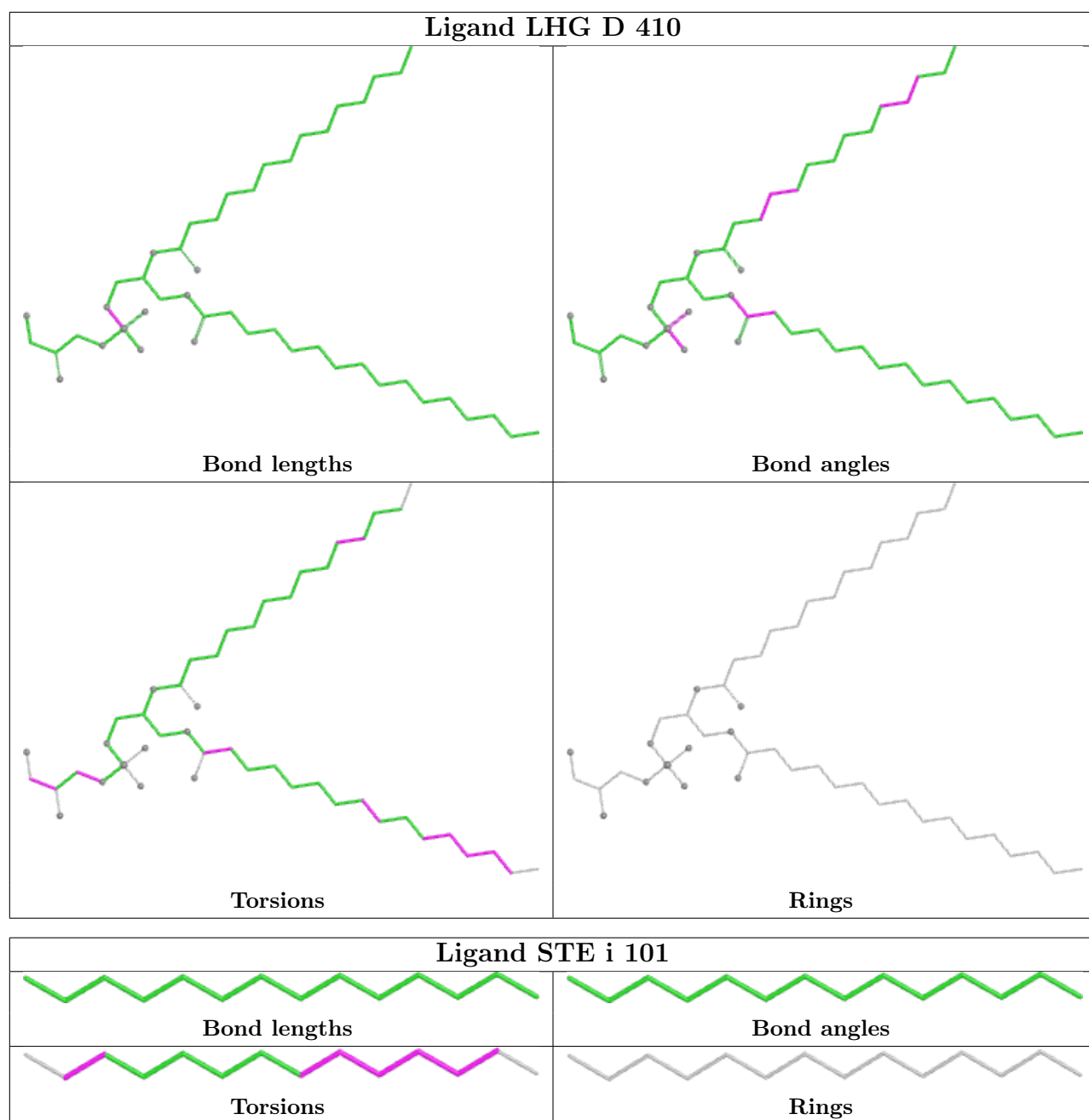


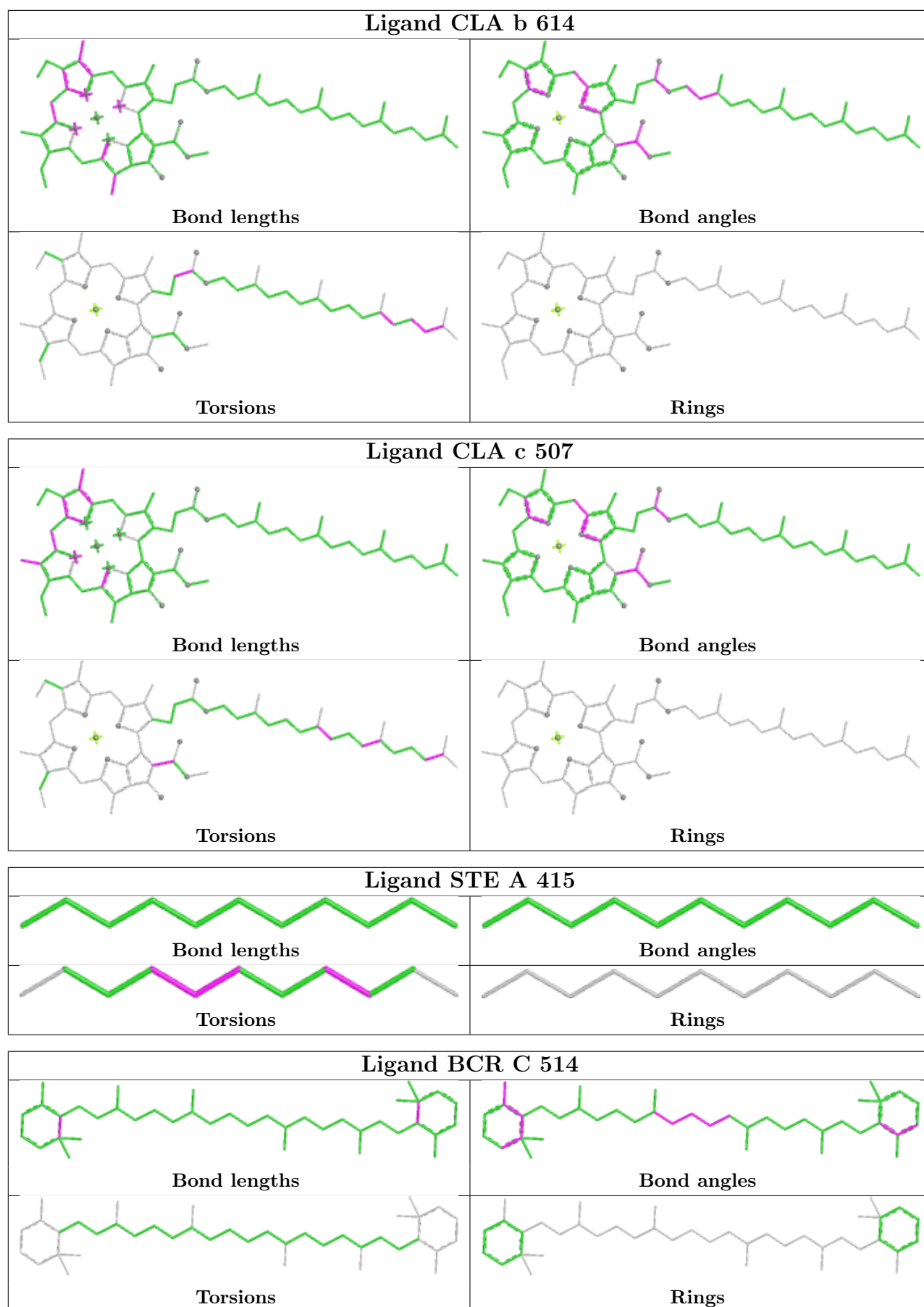


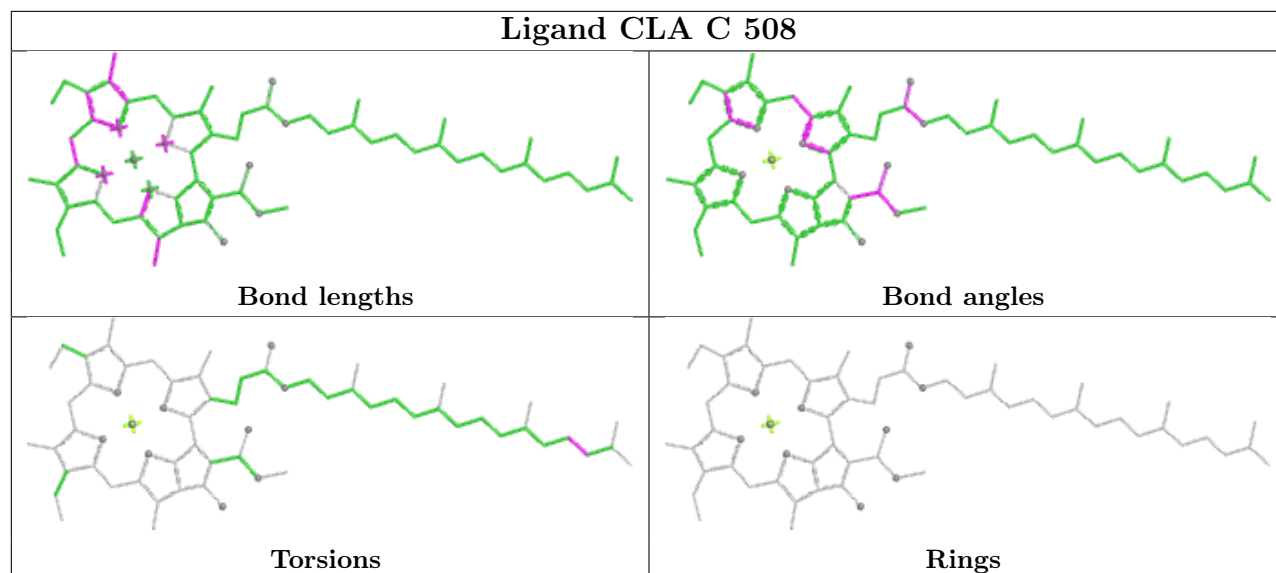
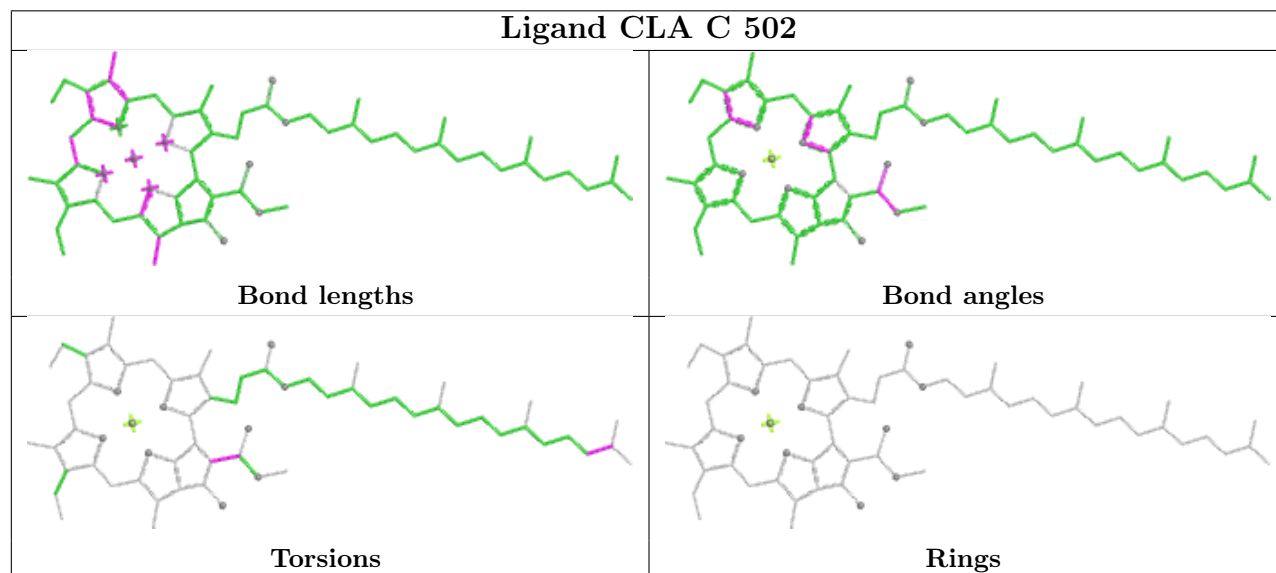
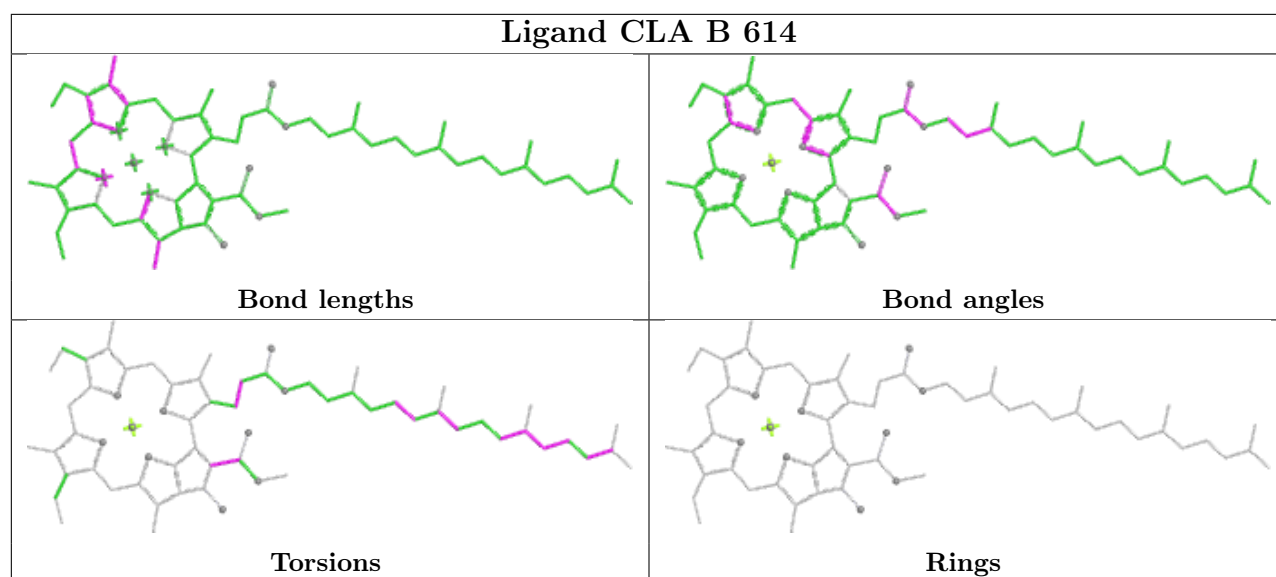


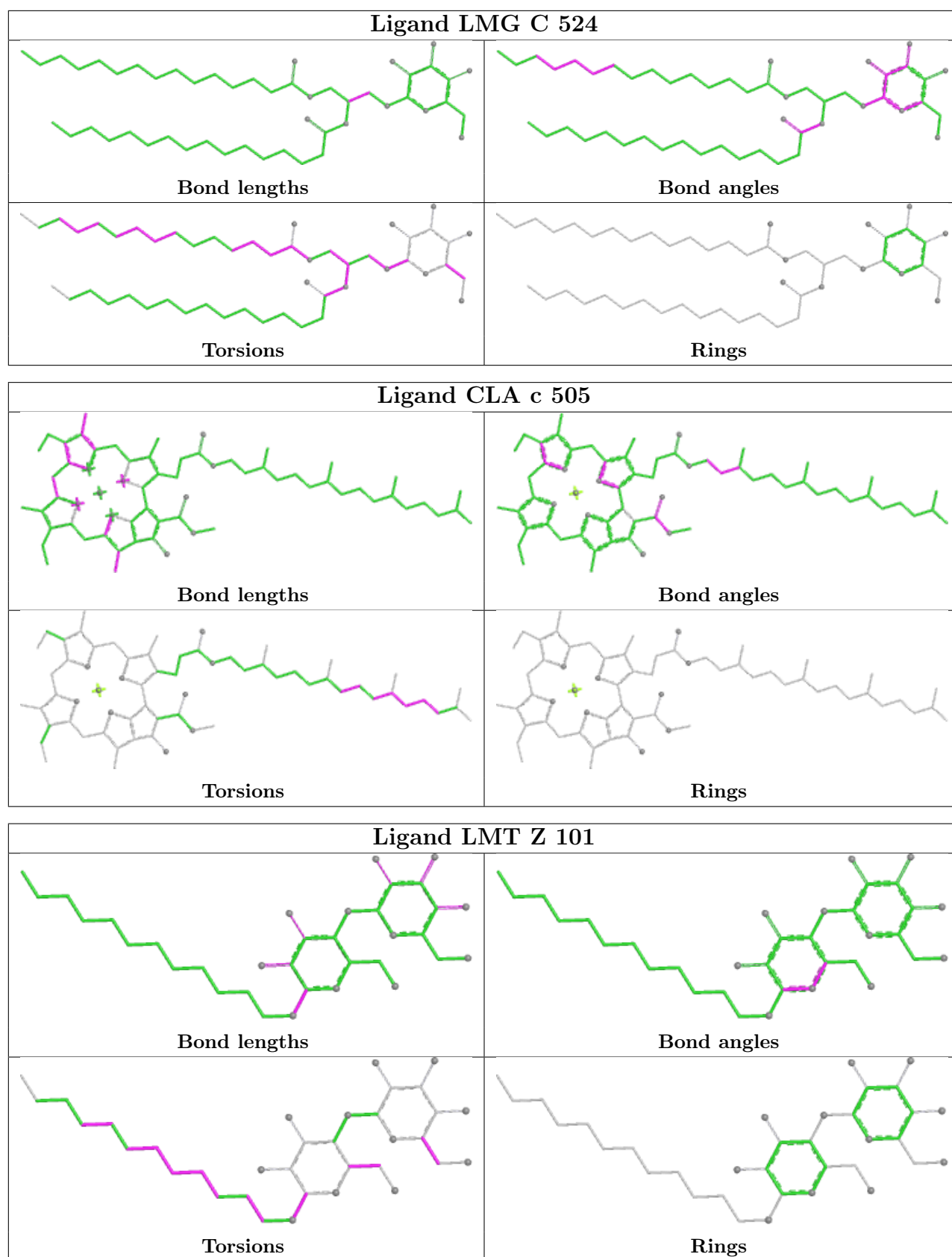


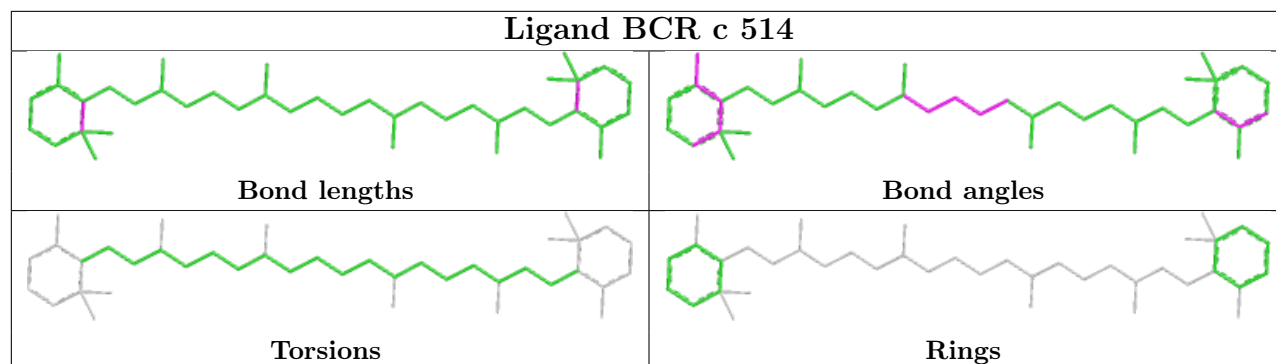
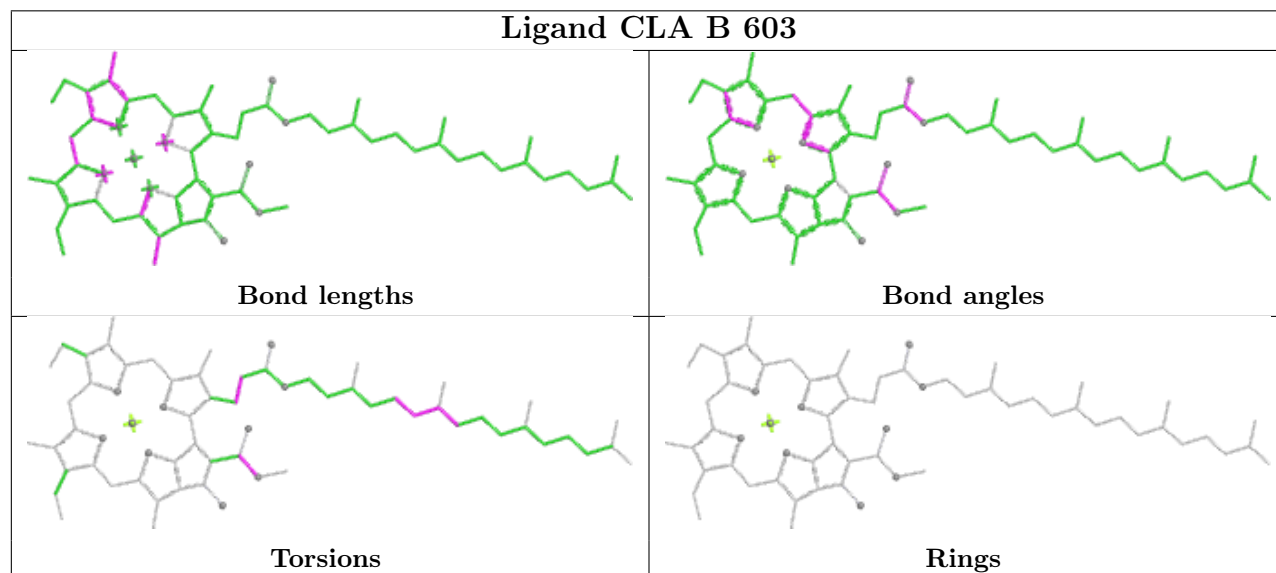
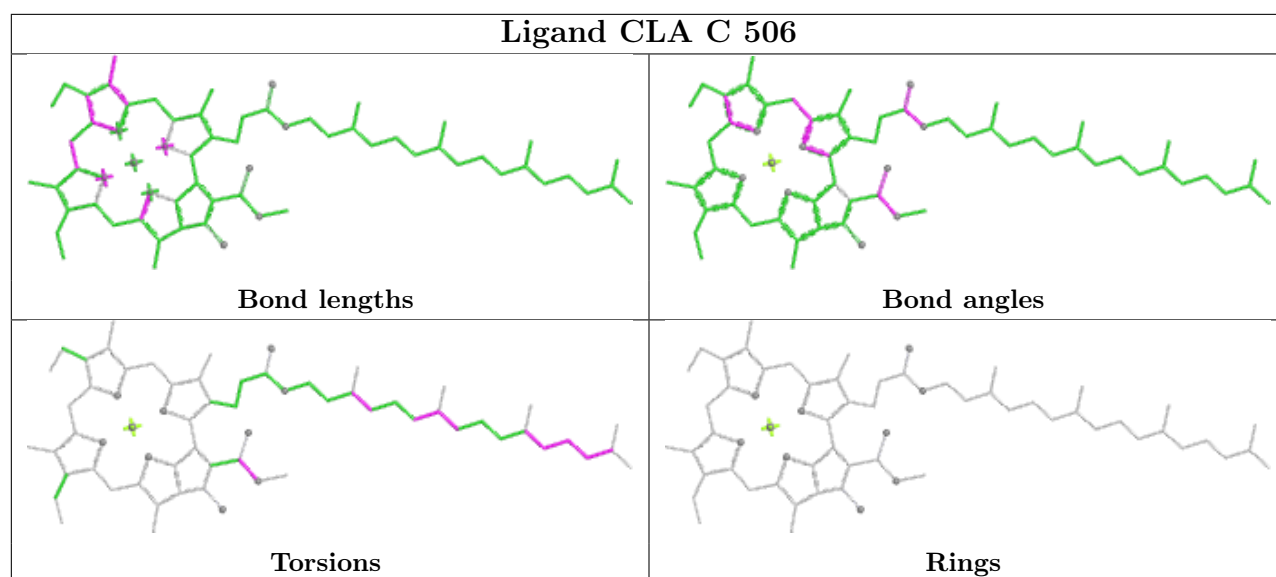


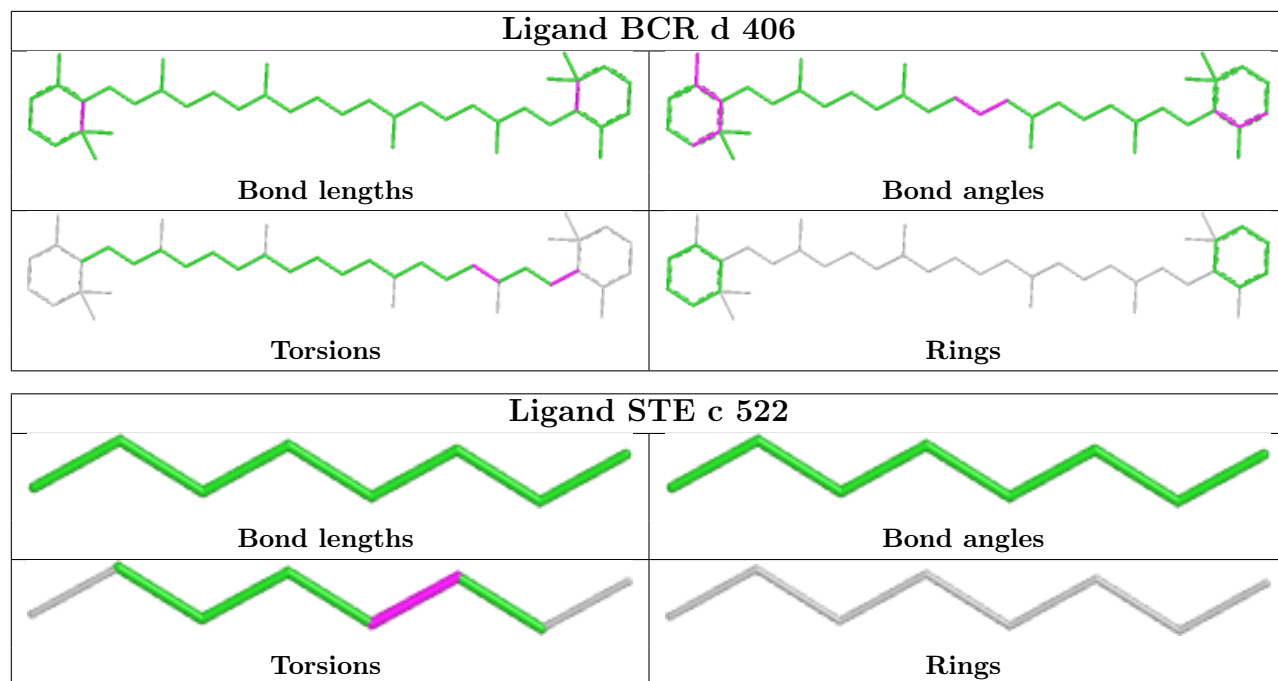


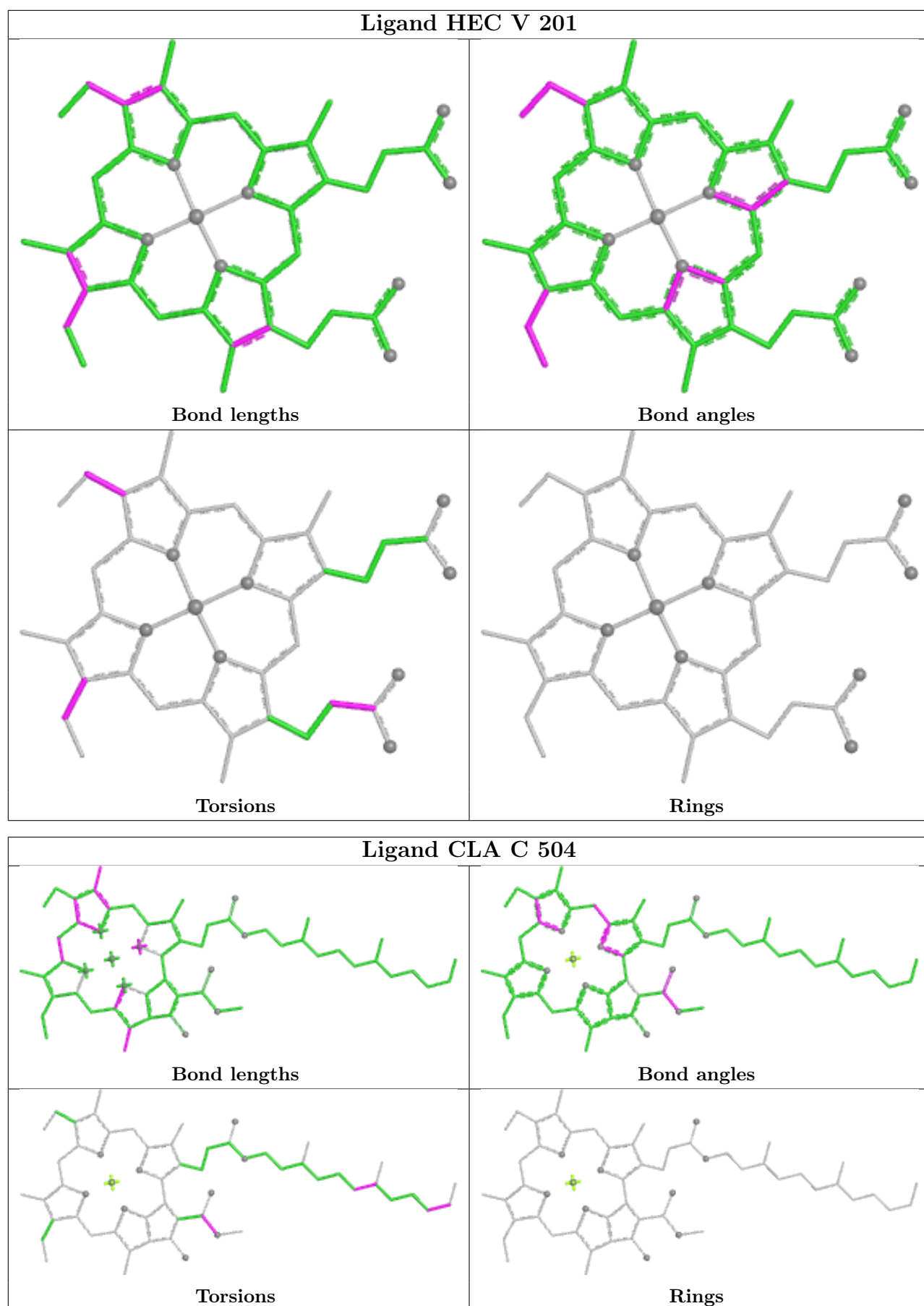


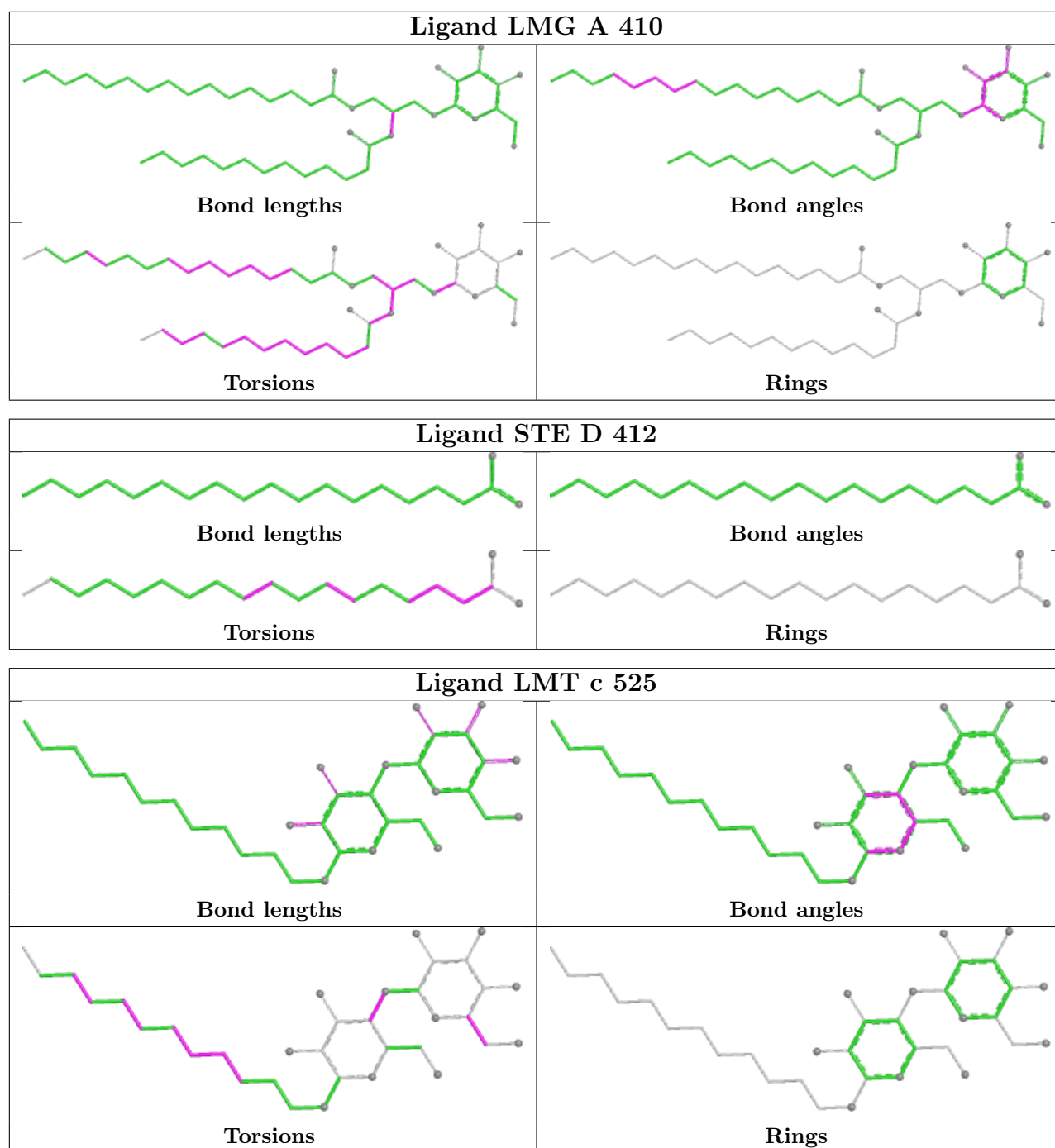


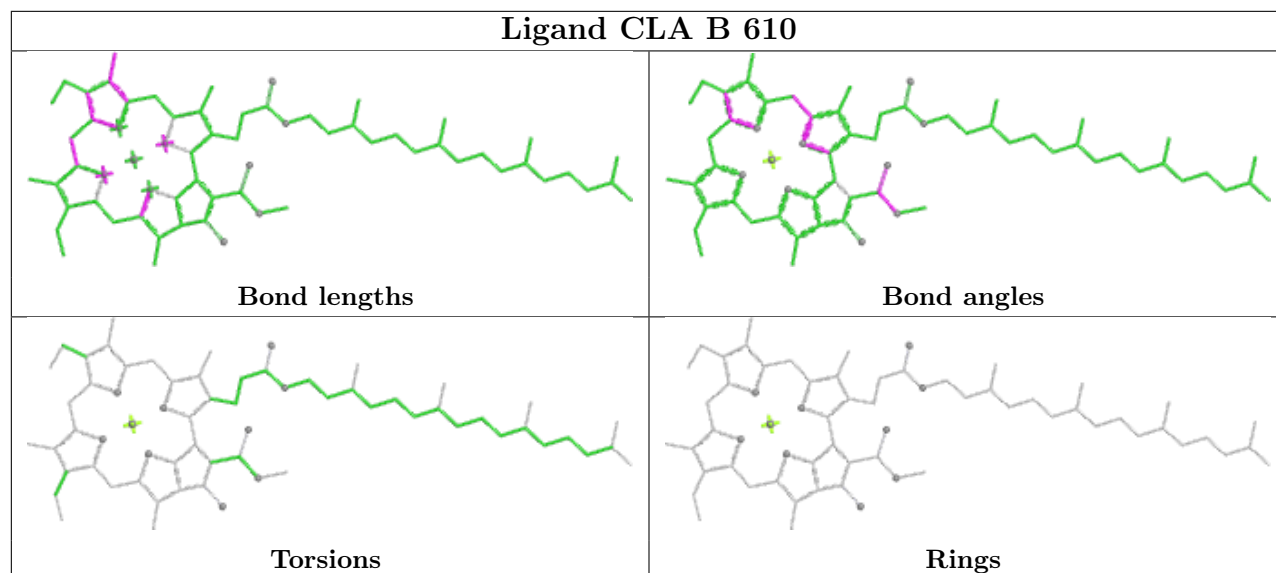
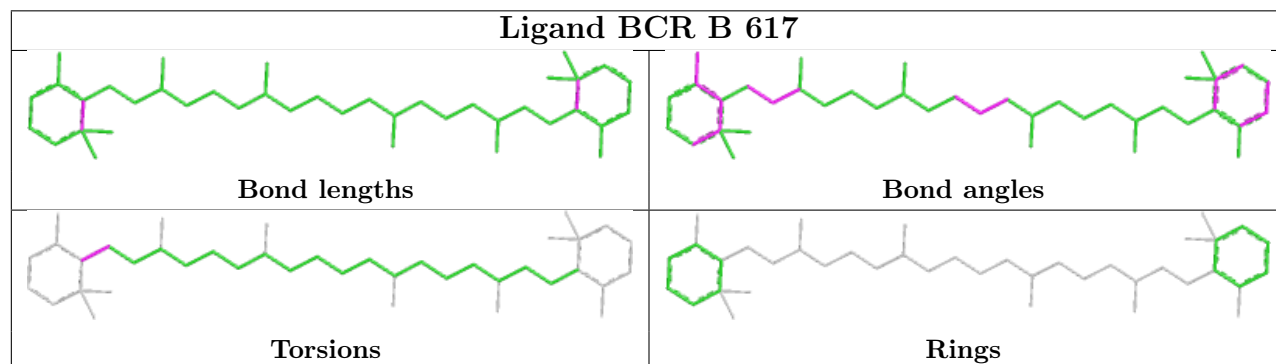
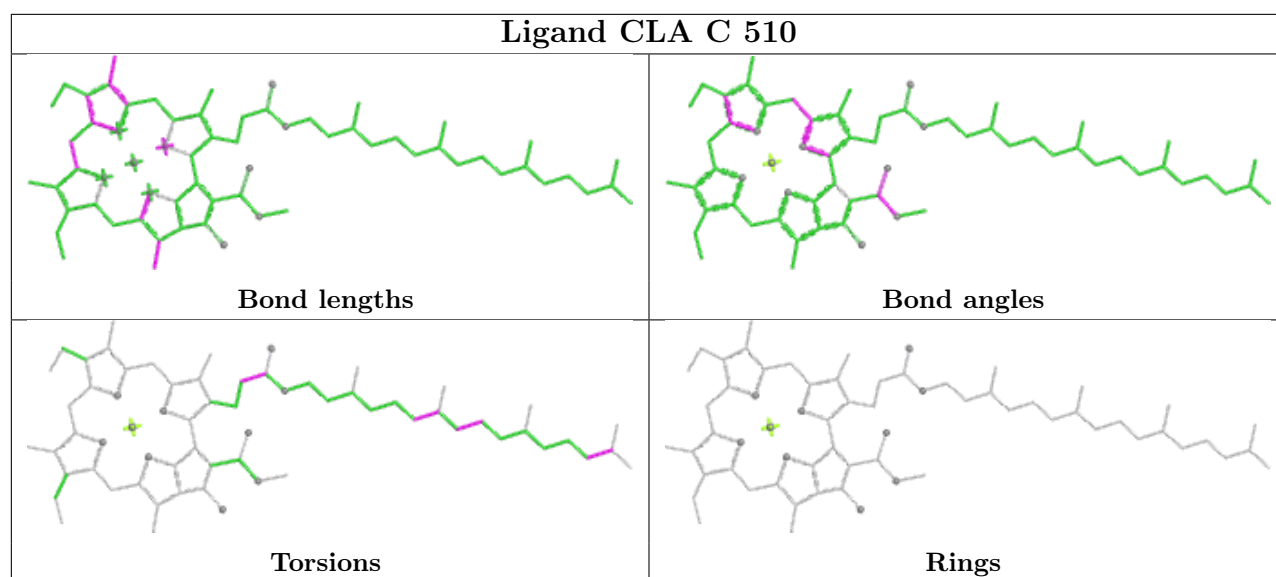


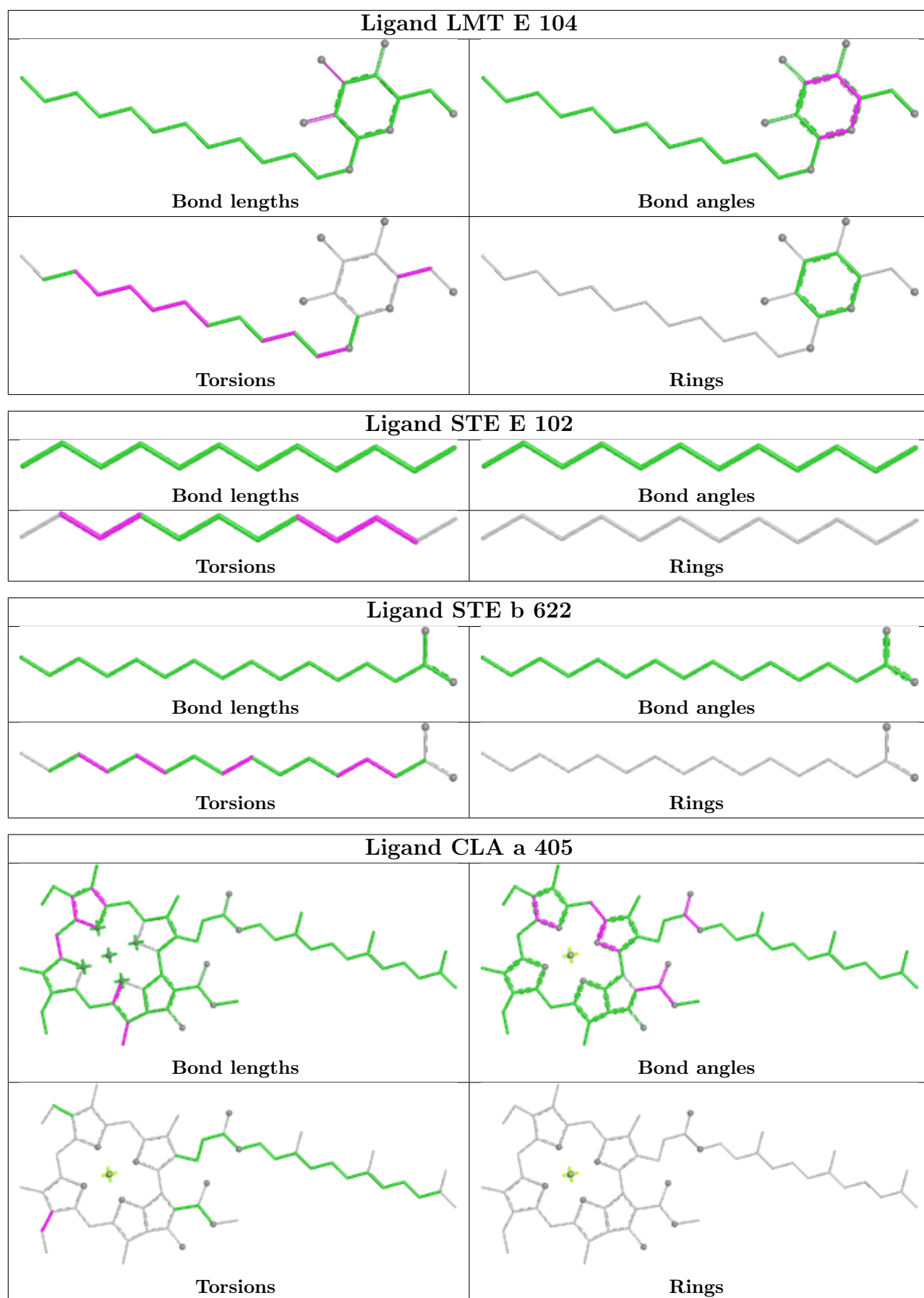


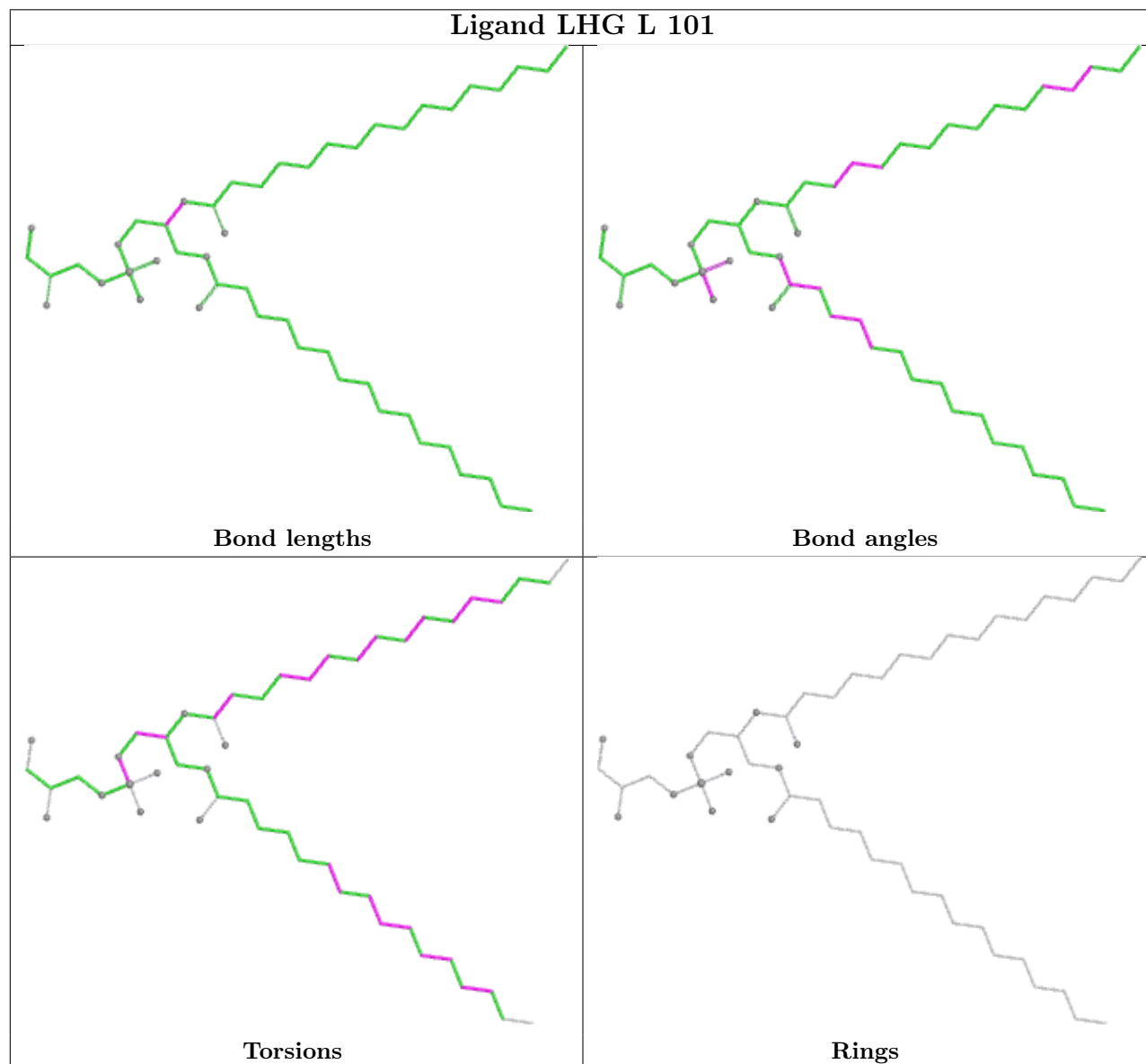
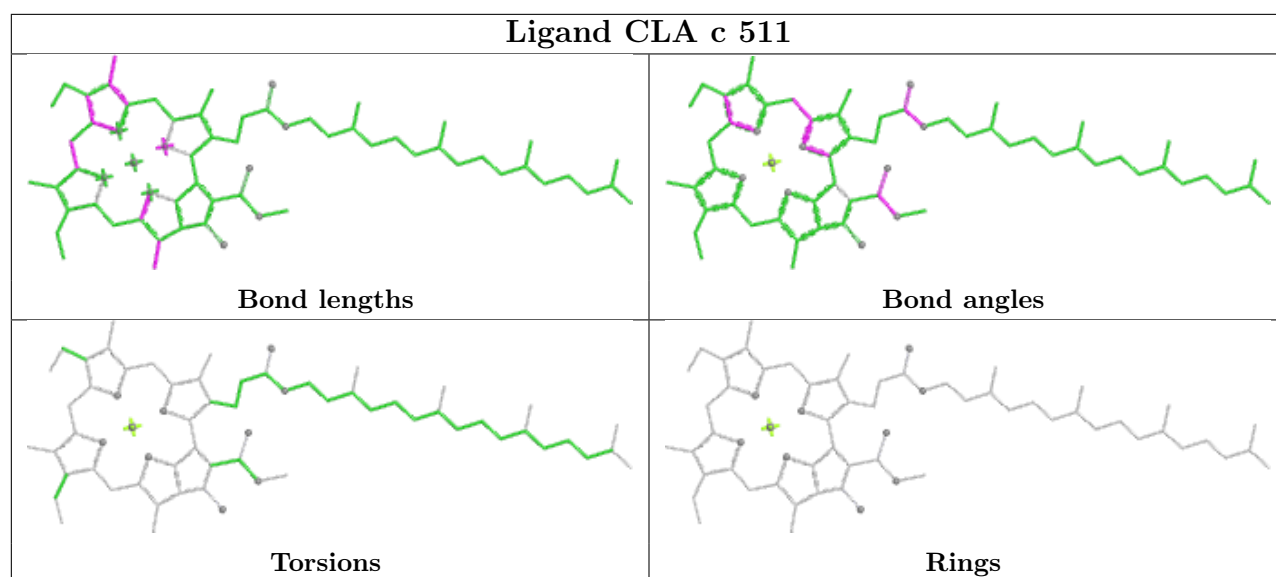


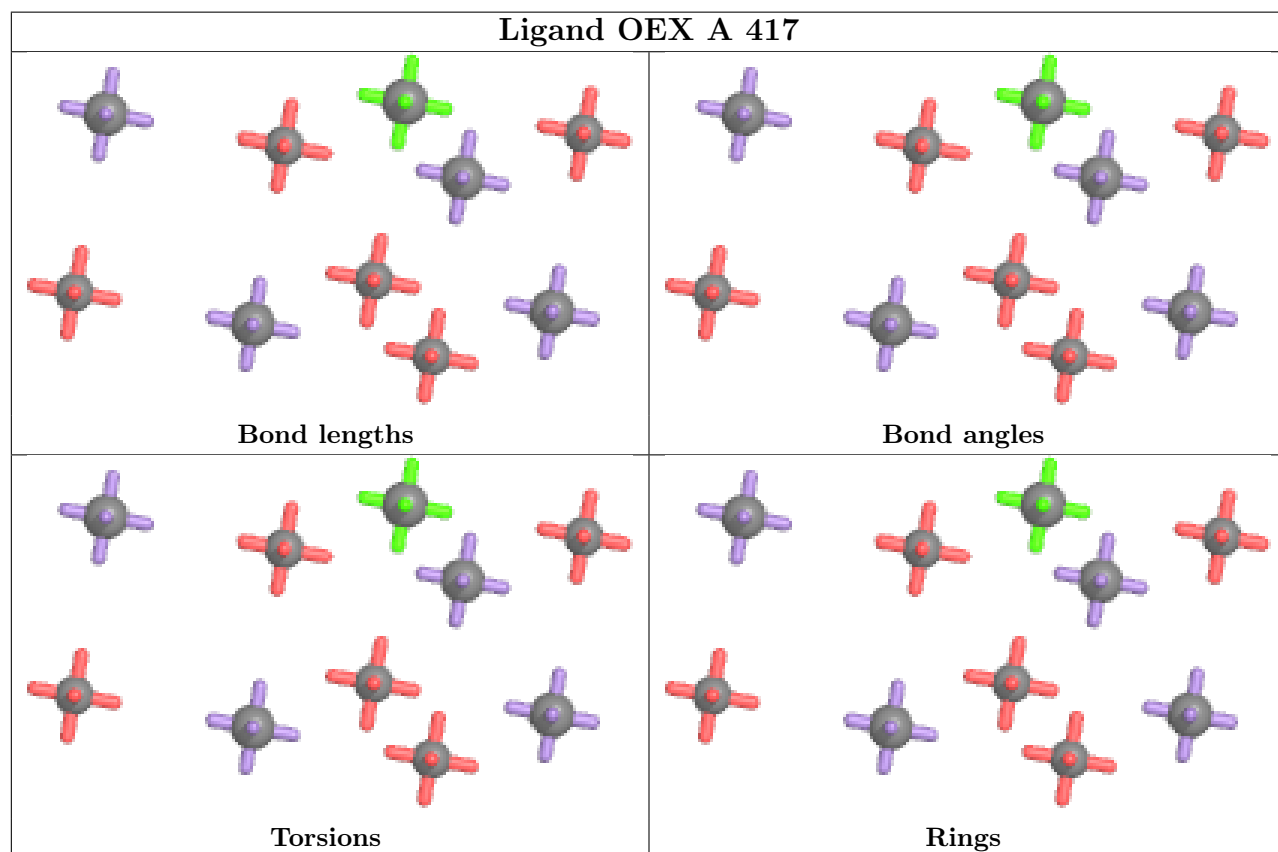
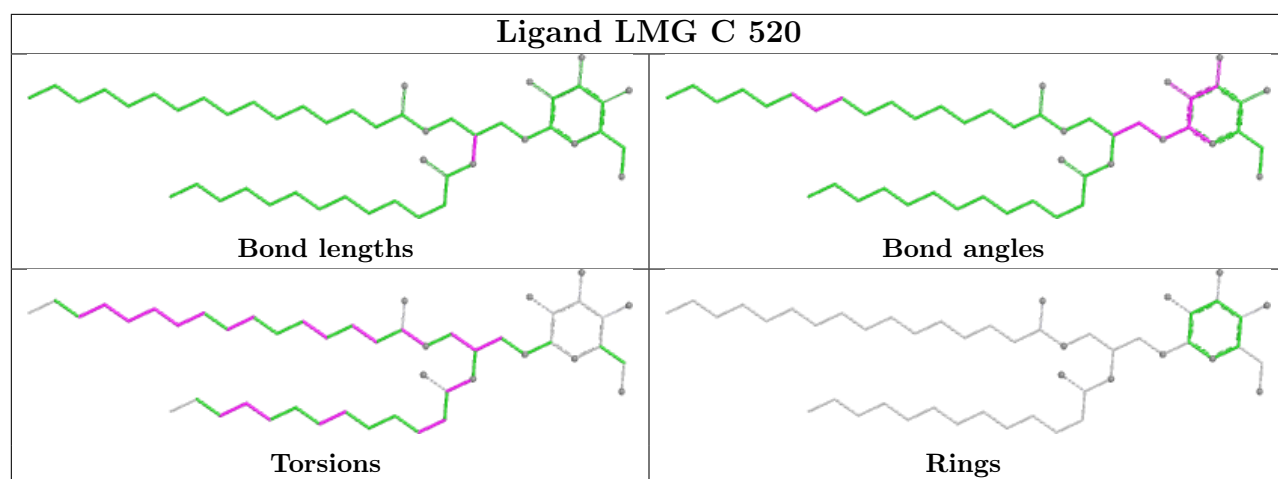


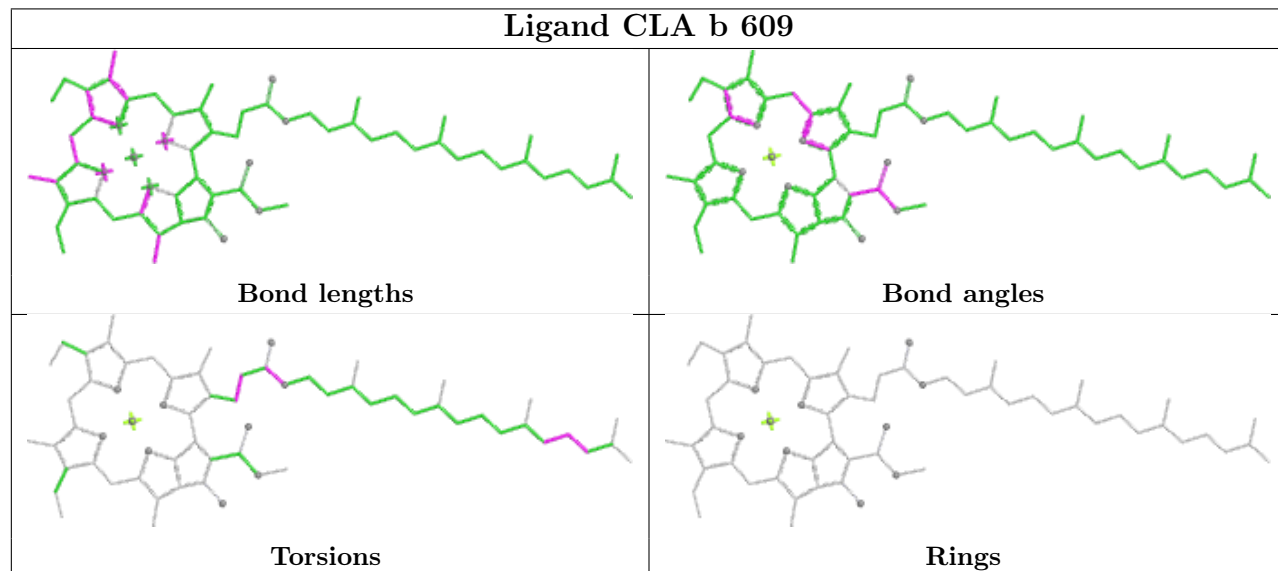
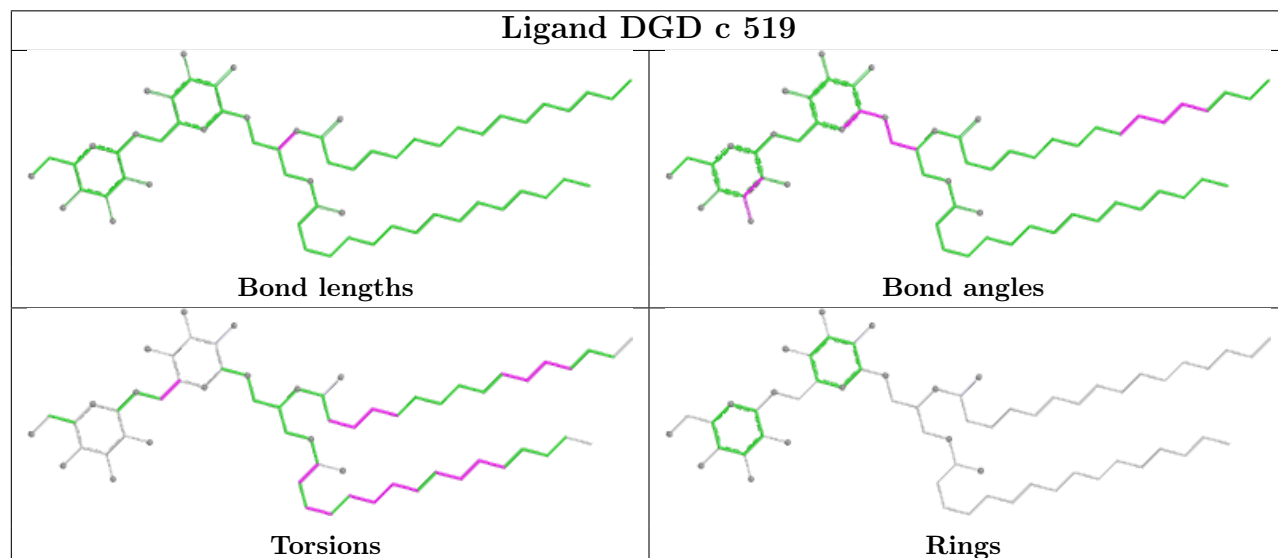
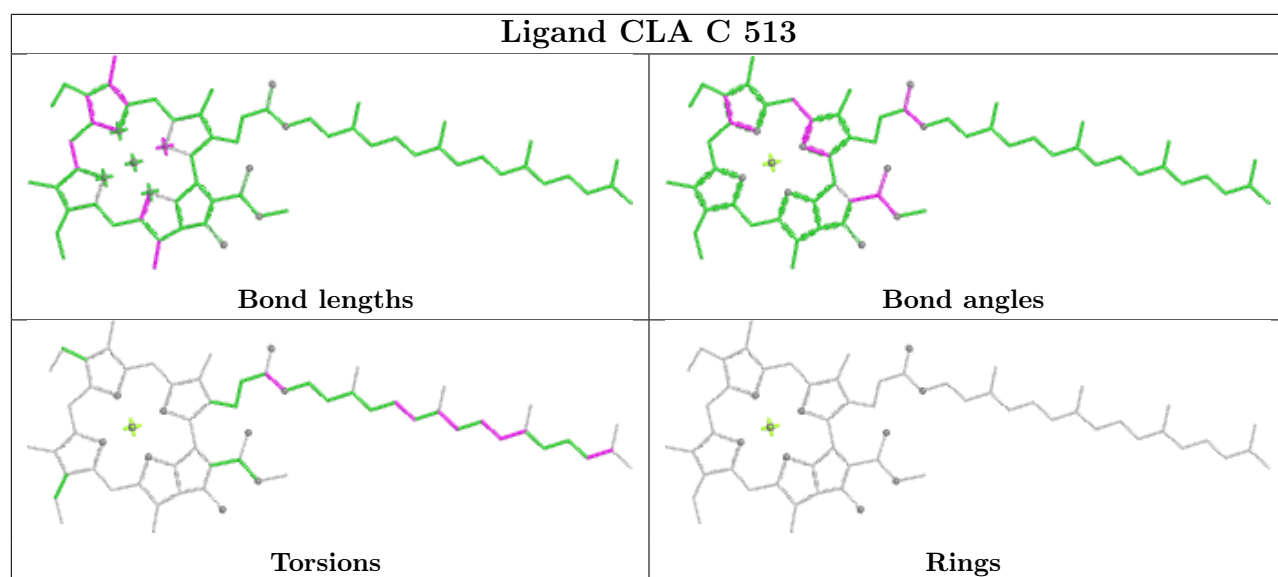


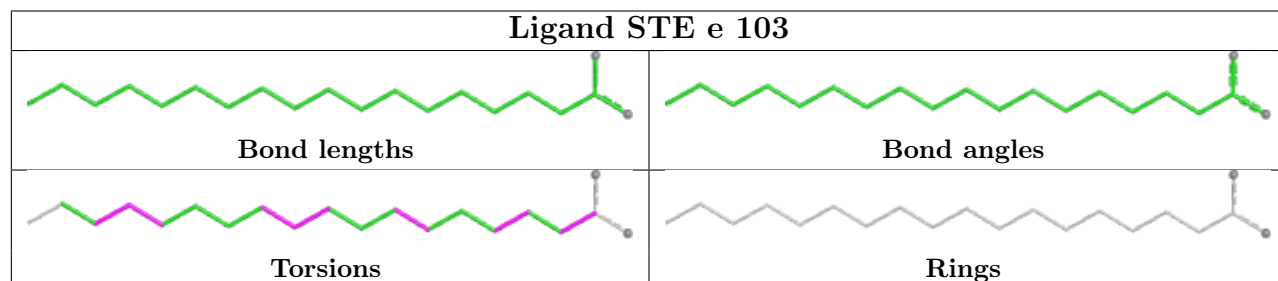
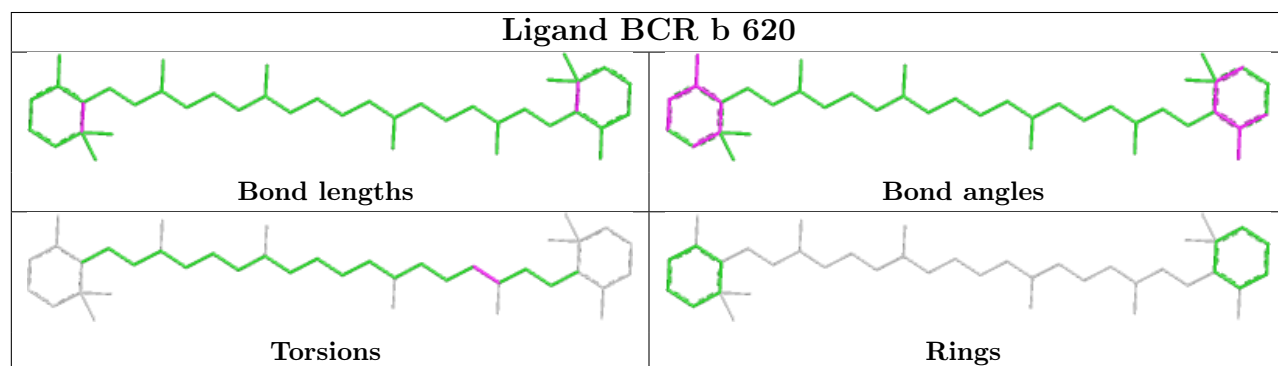
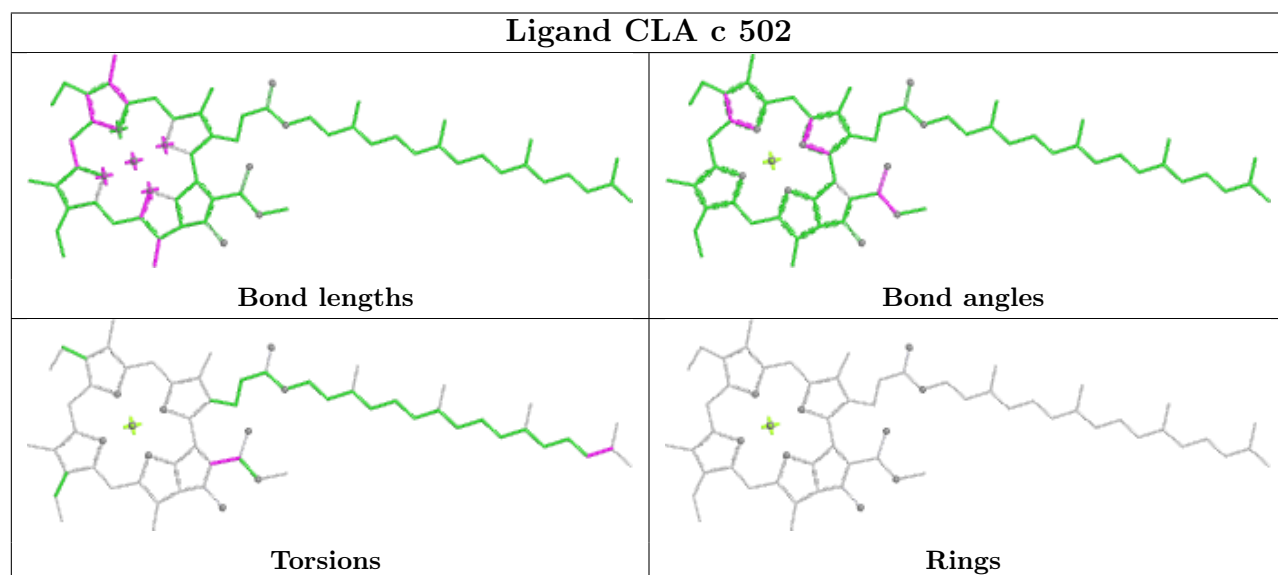
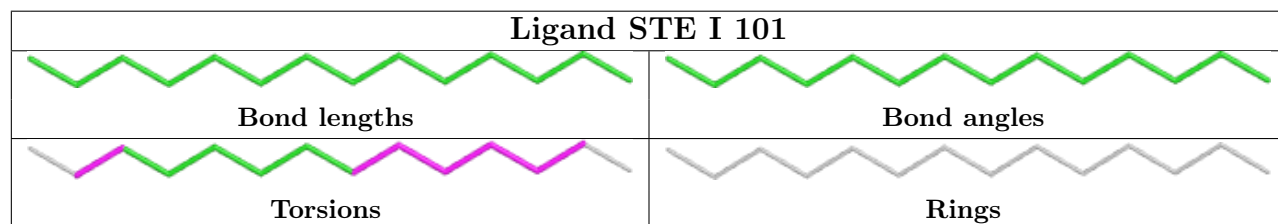
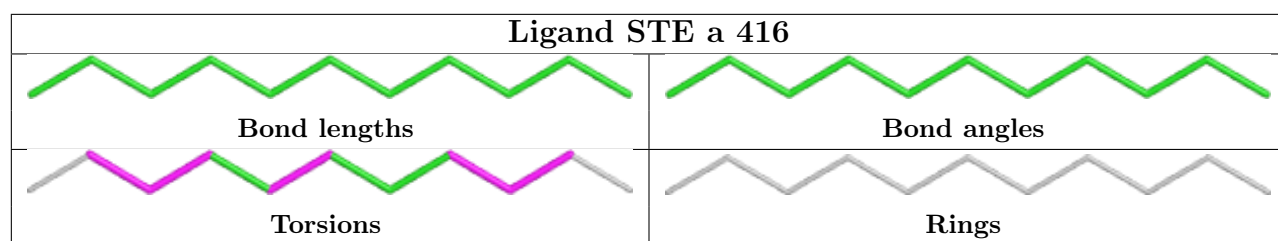


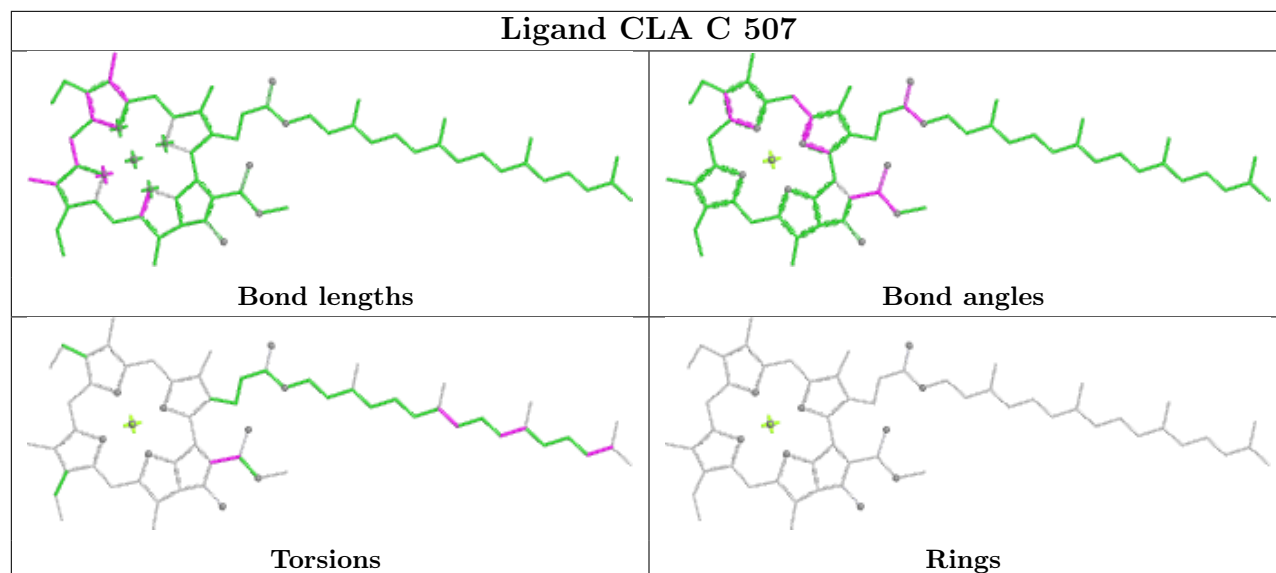
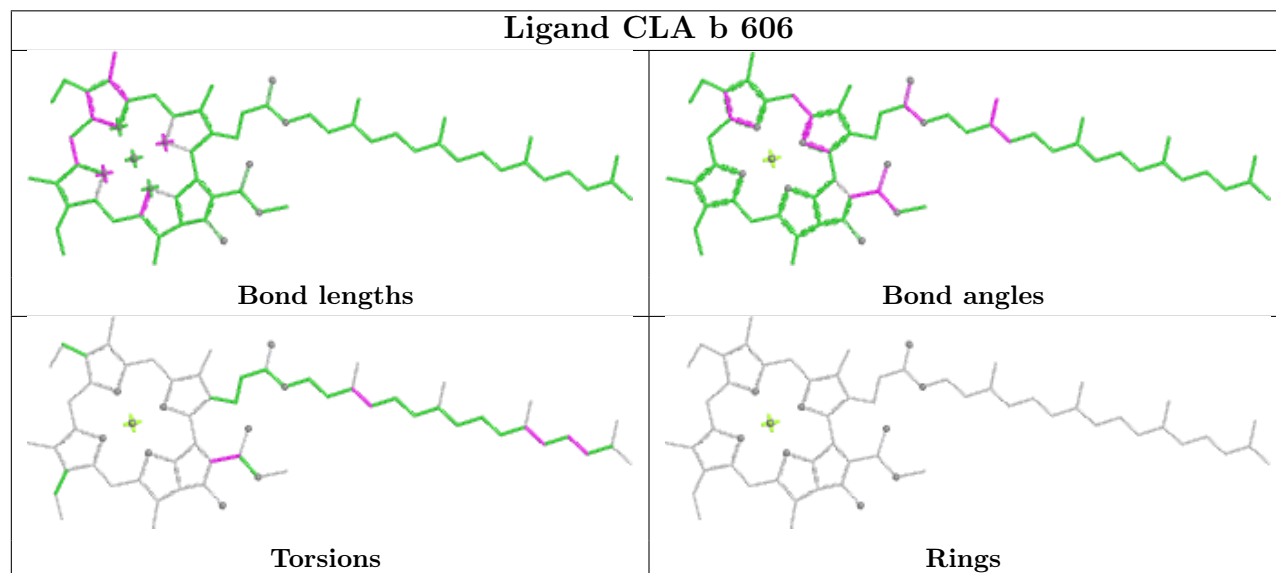
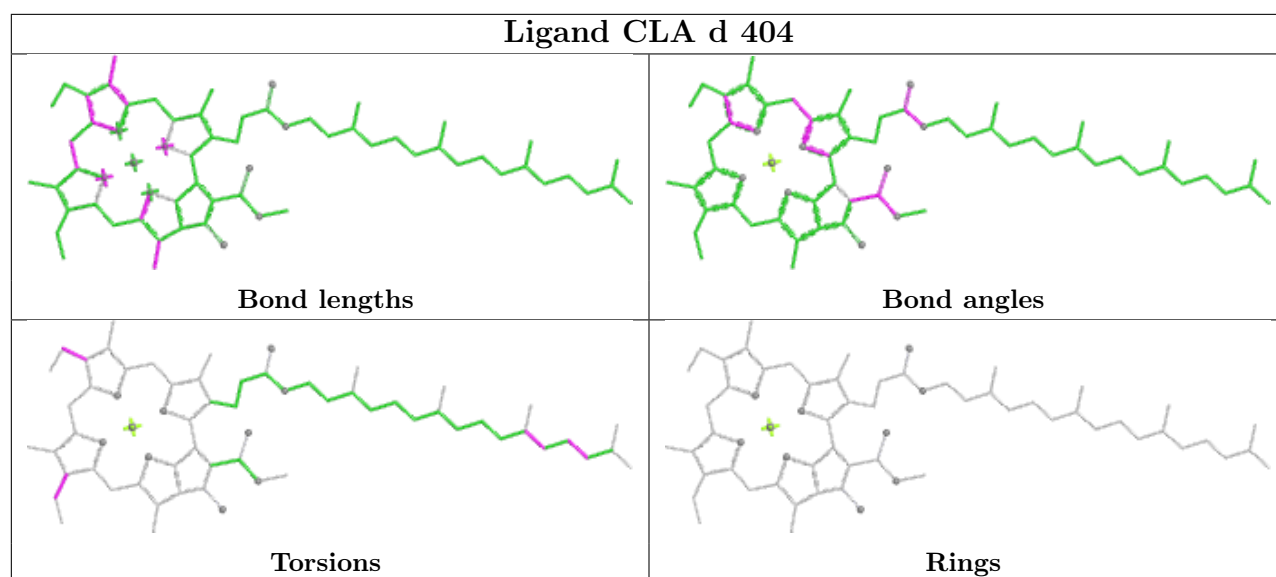


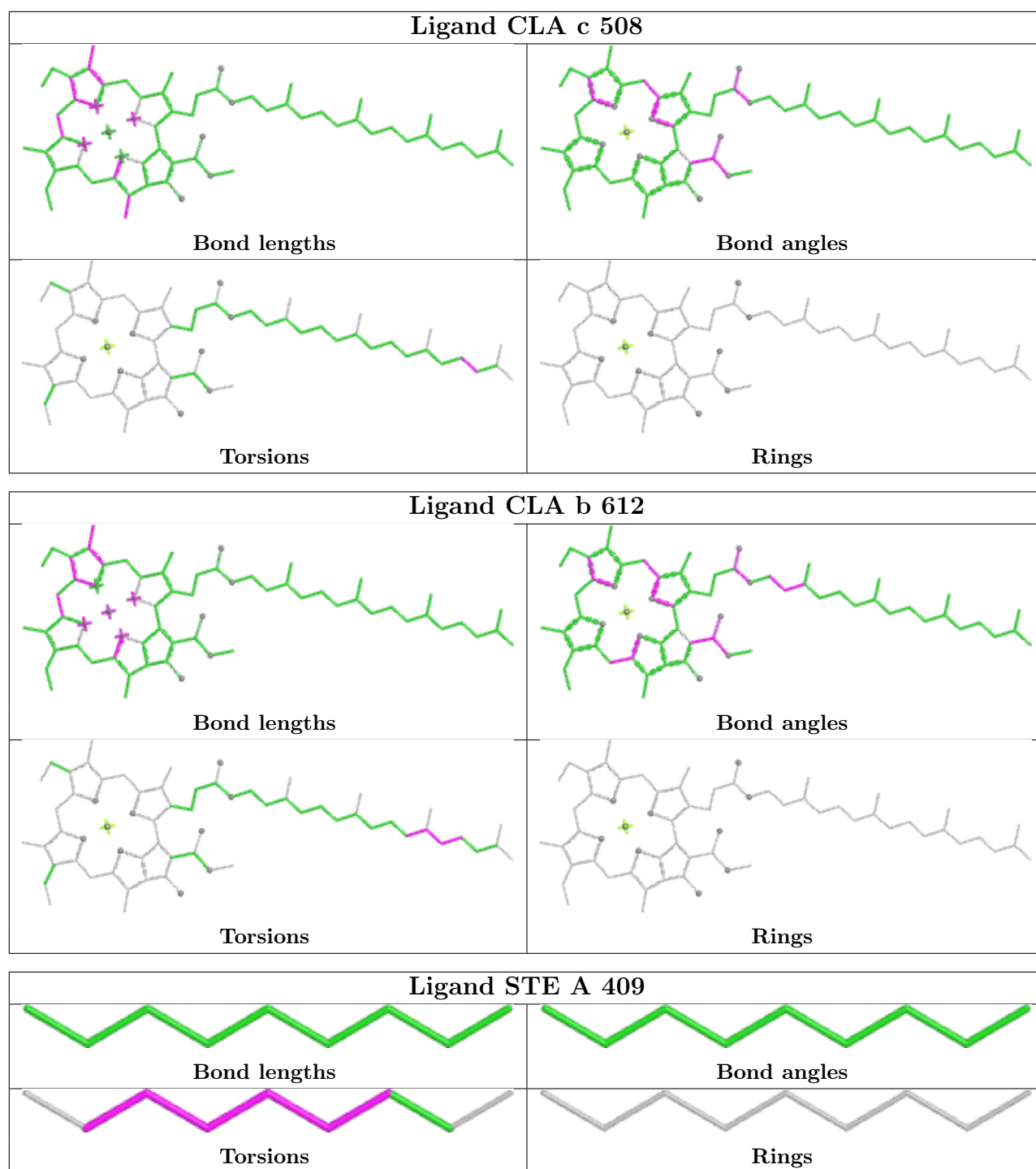


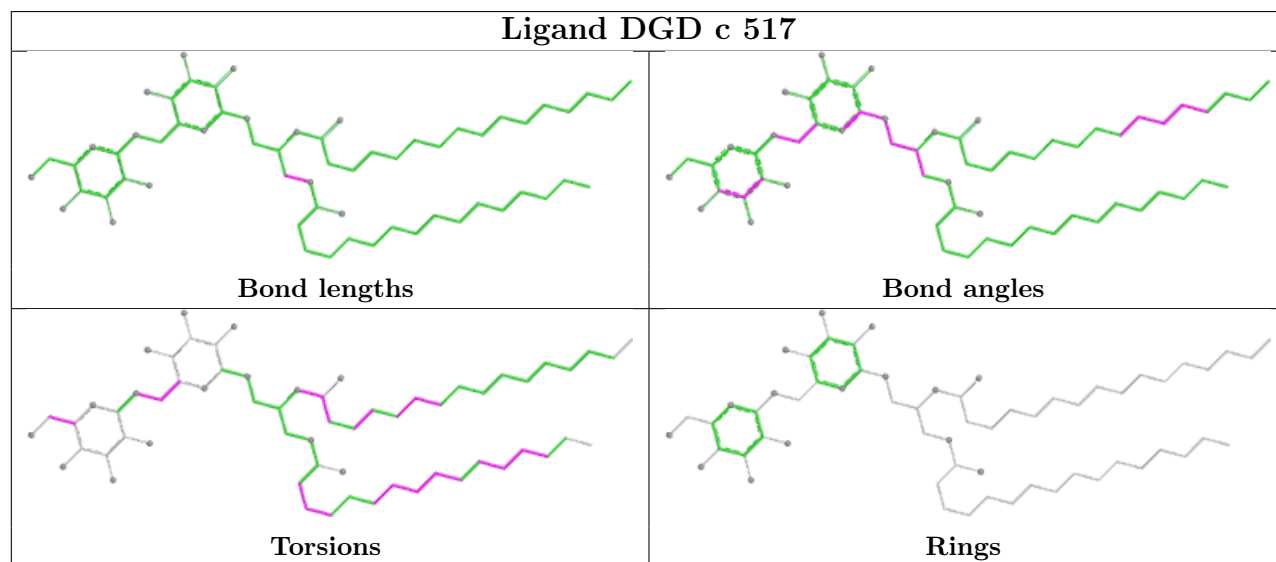
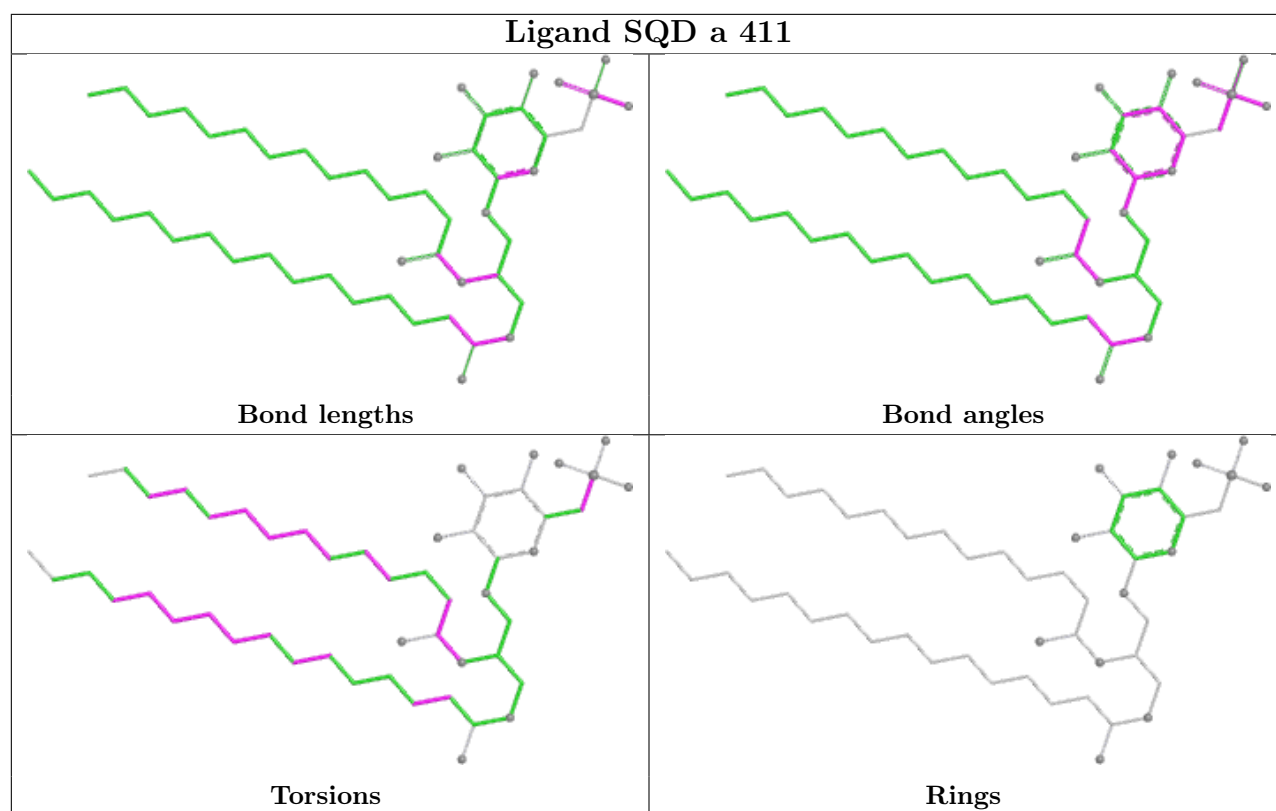


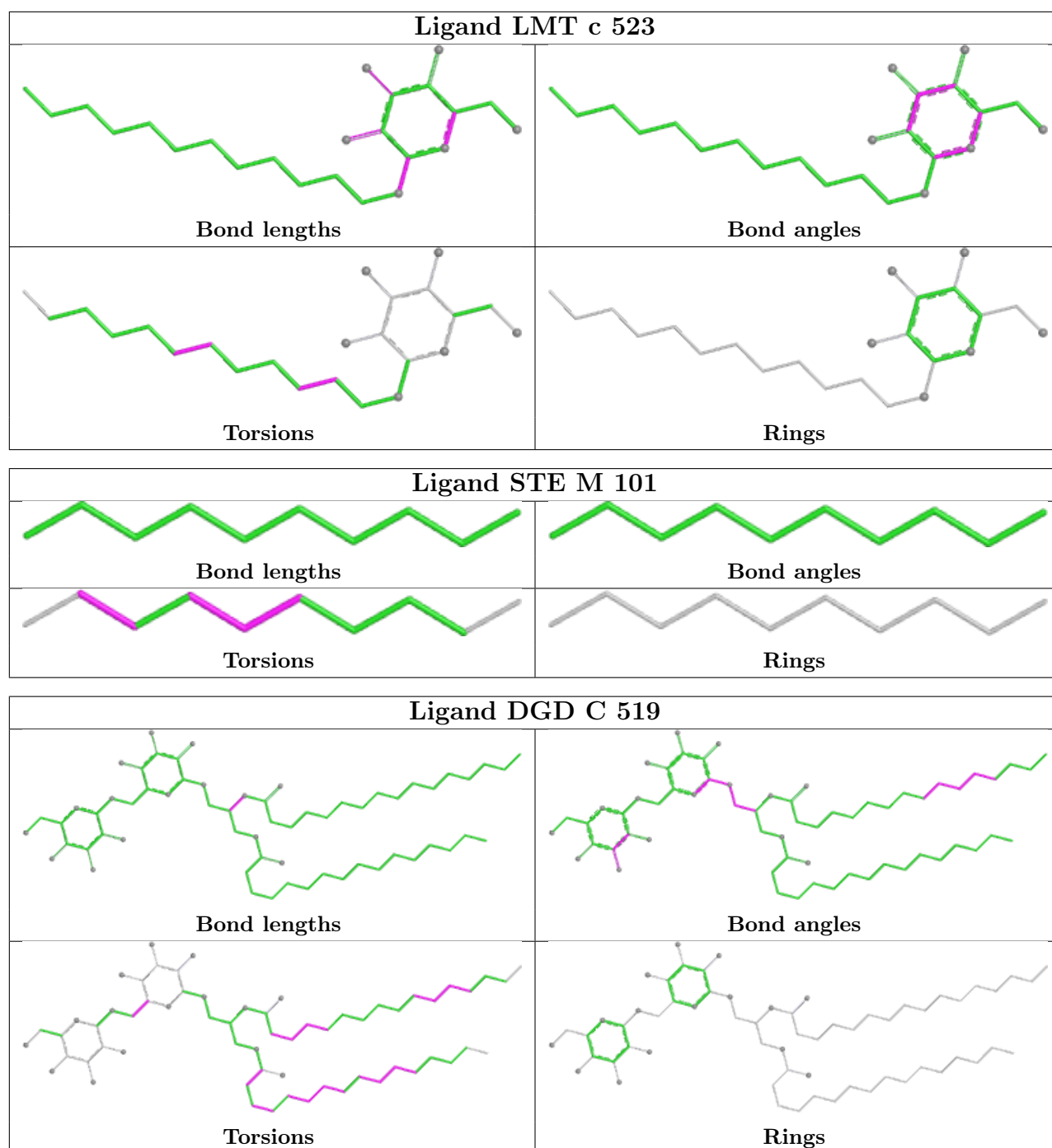


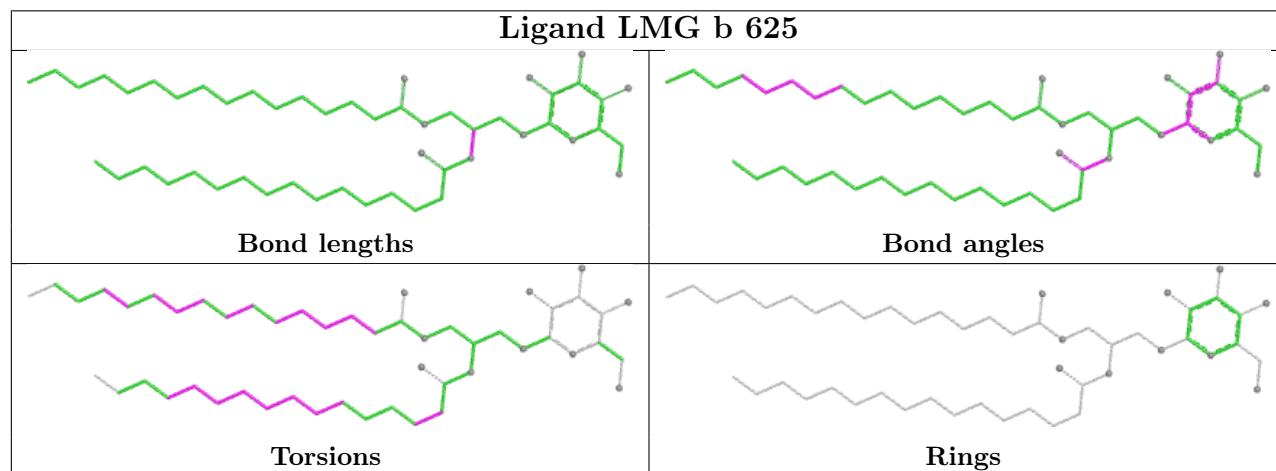
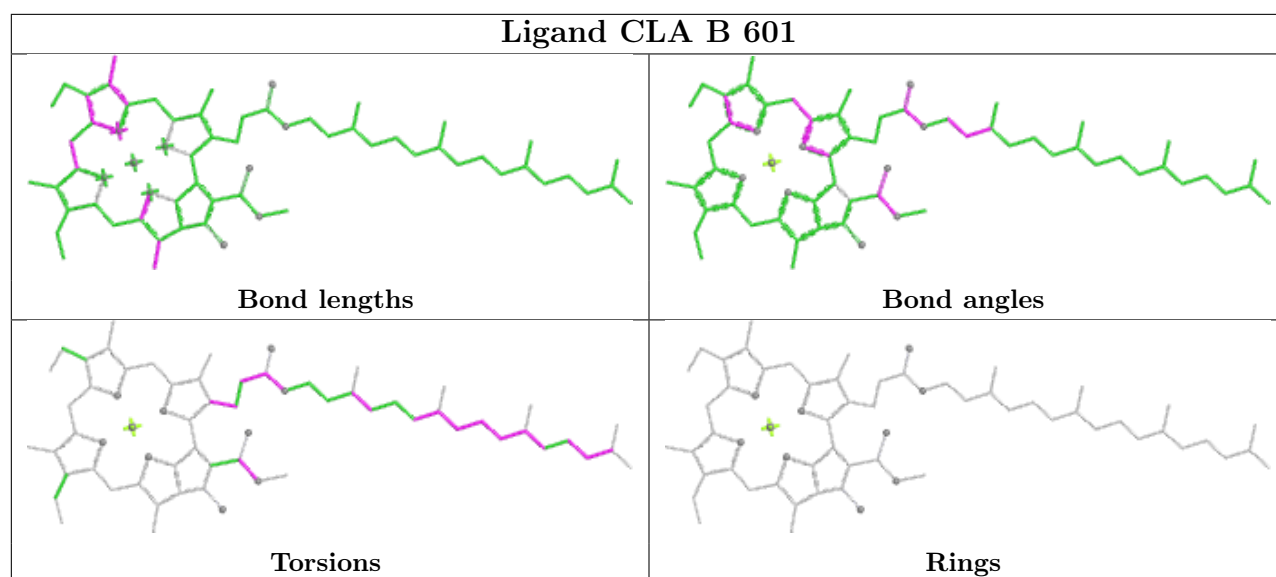


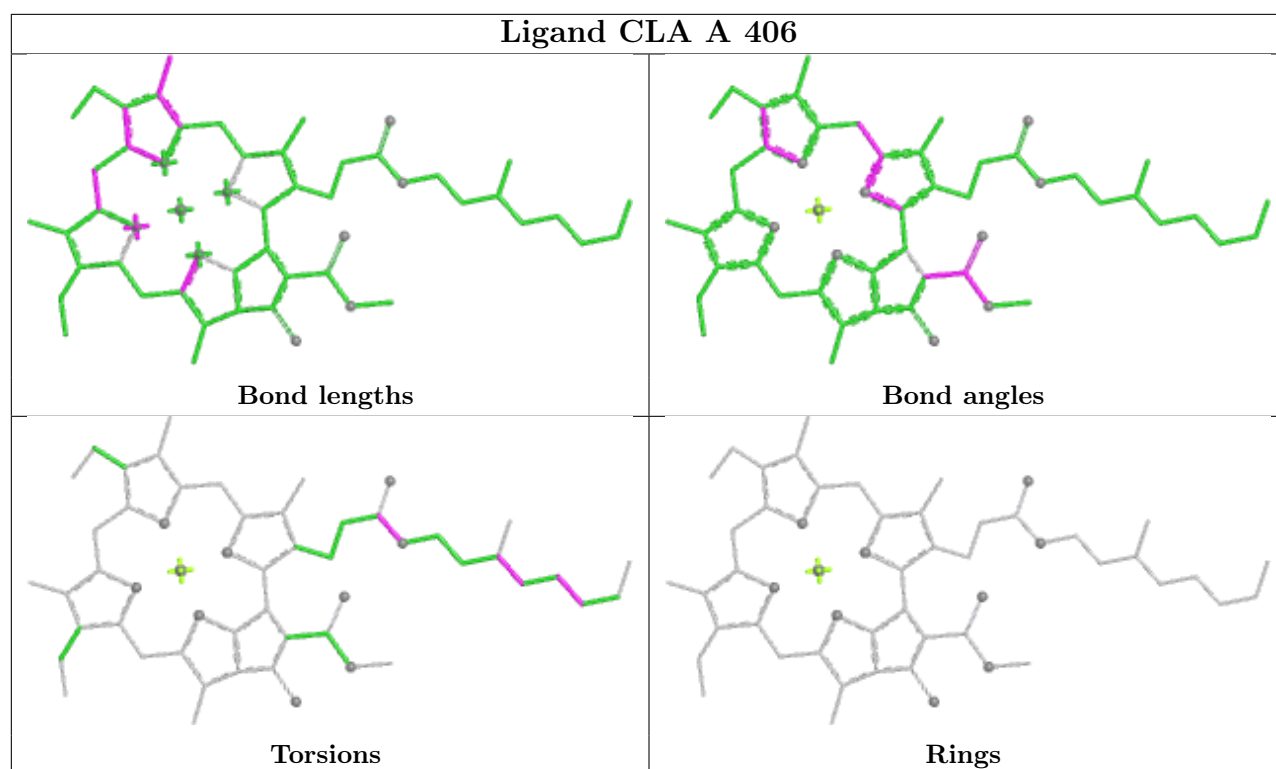












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

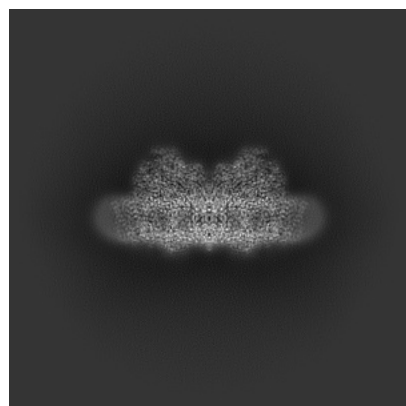
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50019. These allow visual inspection of the internal detail of the map and identification of artifacts.

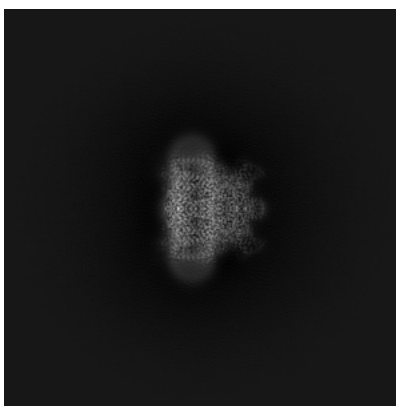
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

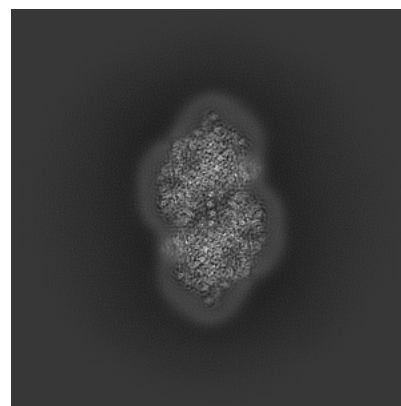
6.1.1 Primary map



X

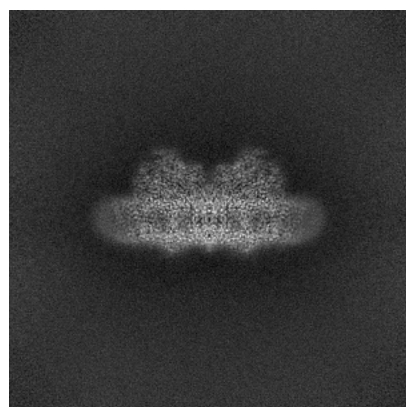


Y

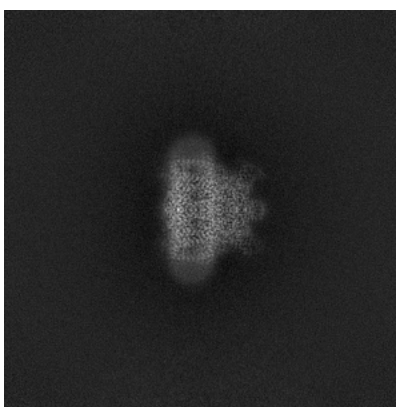


Z

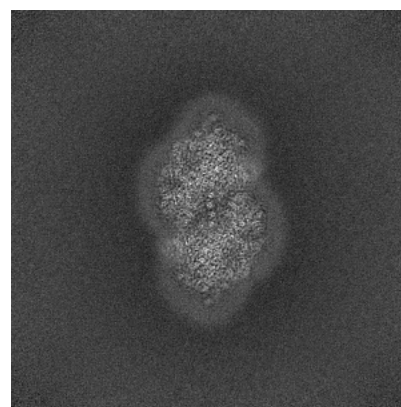
6.1.2 Raw map



X



Y

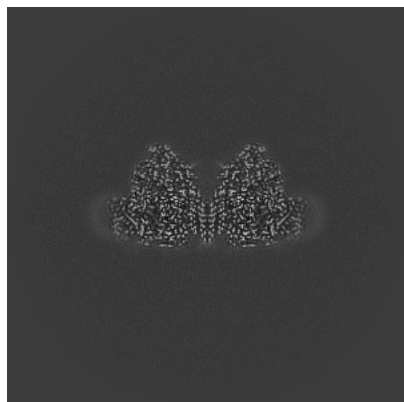


Z

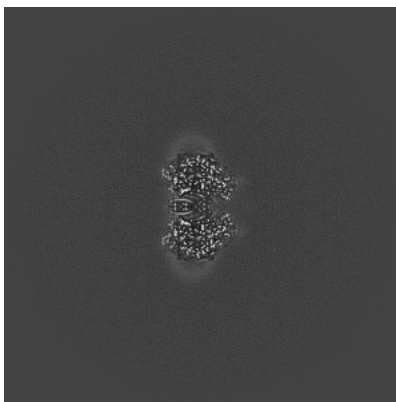
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

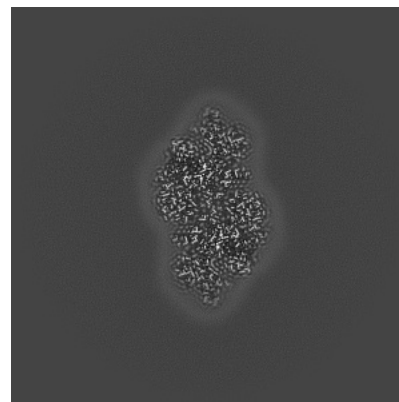
6.2.1 Primary map



X Index: 360

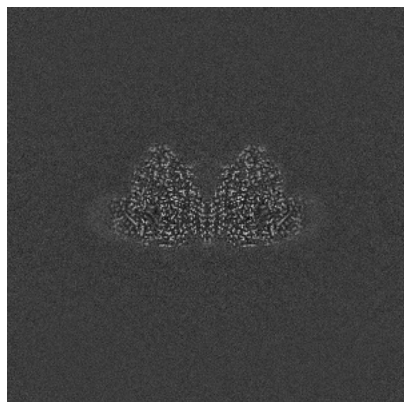


Y Index: 360

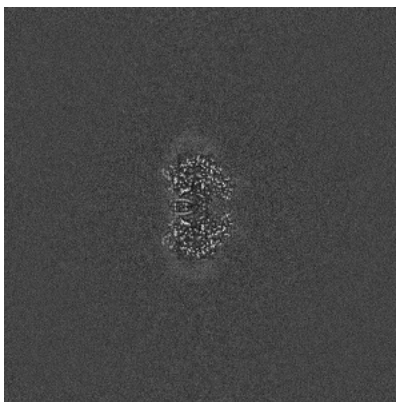


Z Index: 360

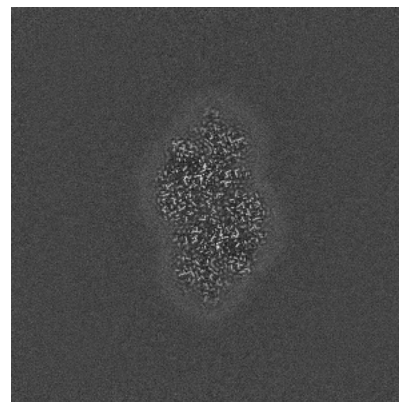
6.2.2 Raw map



X Index: 360



Y Index: 360

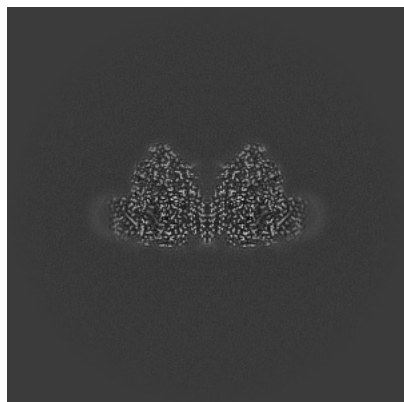


Z Index: 360

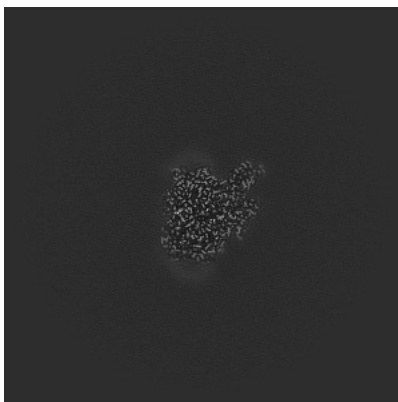
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

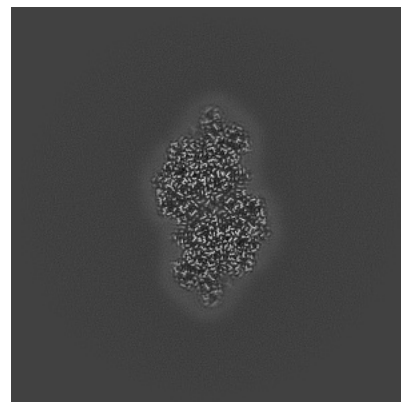
6.3.1 Primary map



X Index: 360

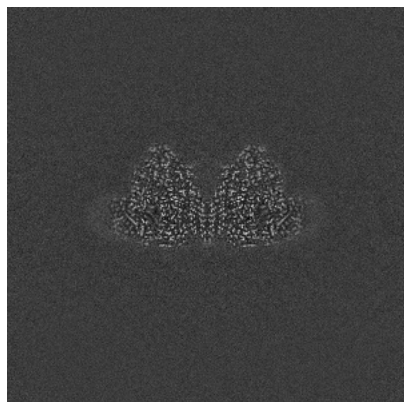


Y Index: 420

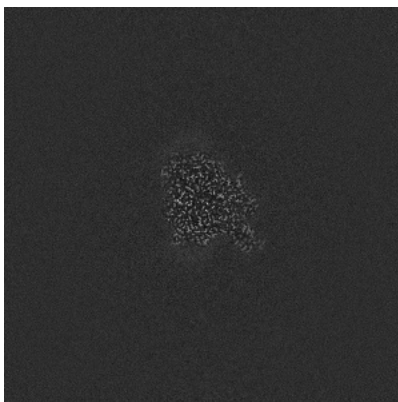


Z Index: 369

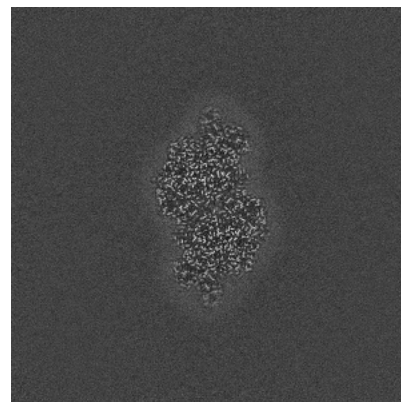
6.3.2 Raw map



X Index: 360



Y Index: 300

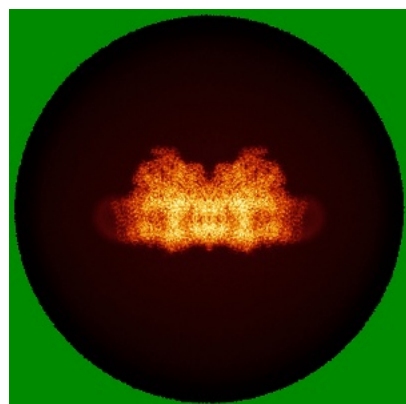


Z Index: 369

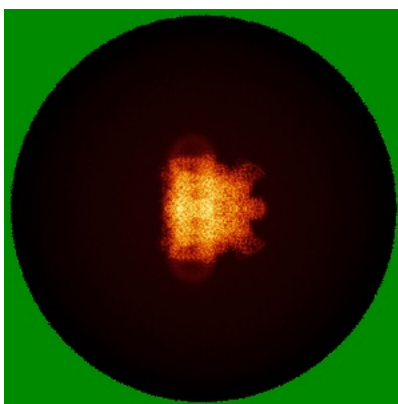
The images above show the largest variance slices of the map in three orthogonal directions.

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

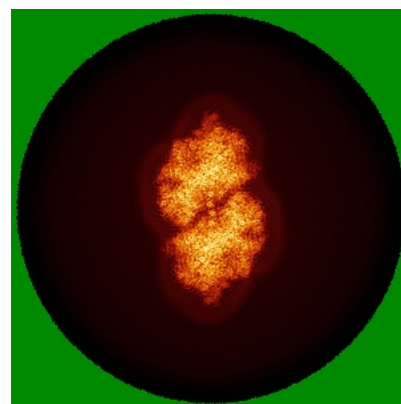
6.4.1 Primary map



X

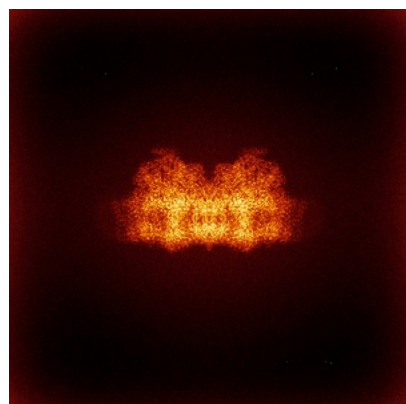


Y

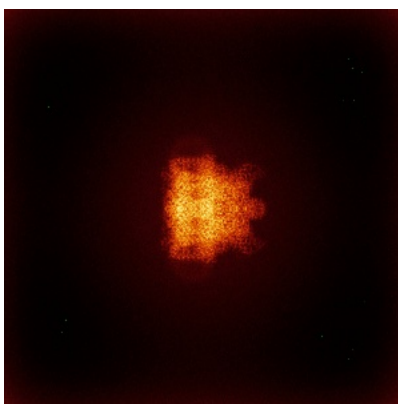


Z

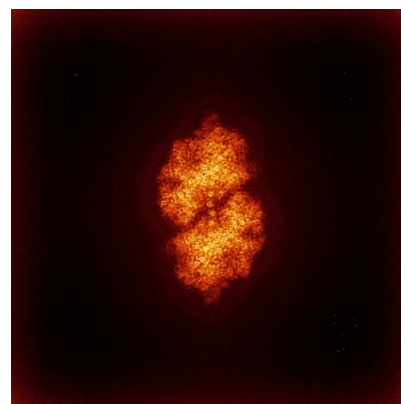
6.4.2 Raw map



X



Y

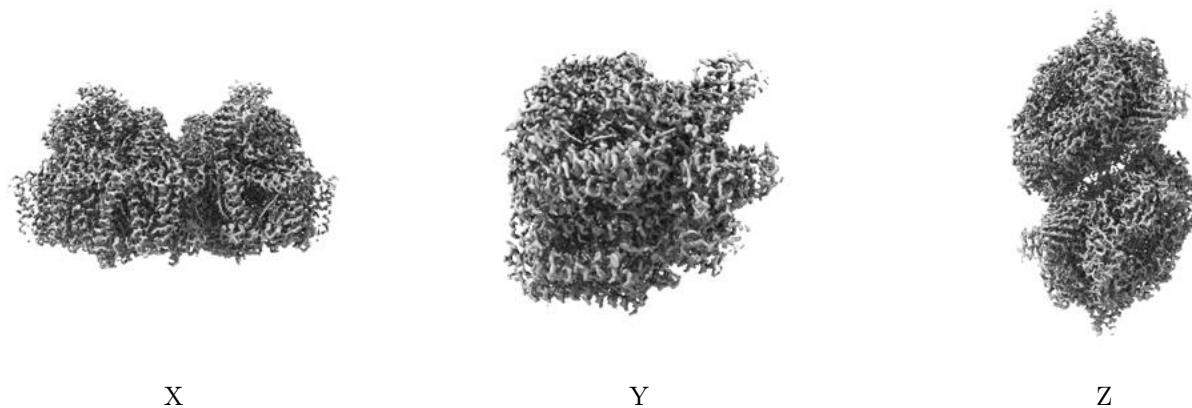


Z

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.

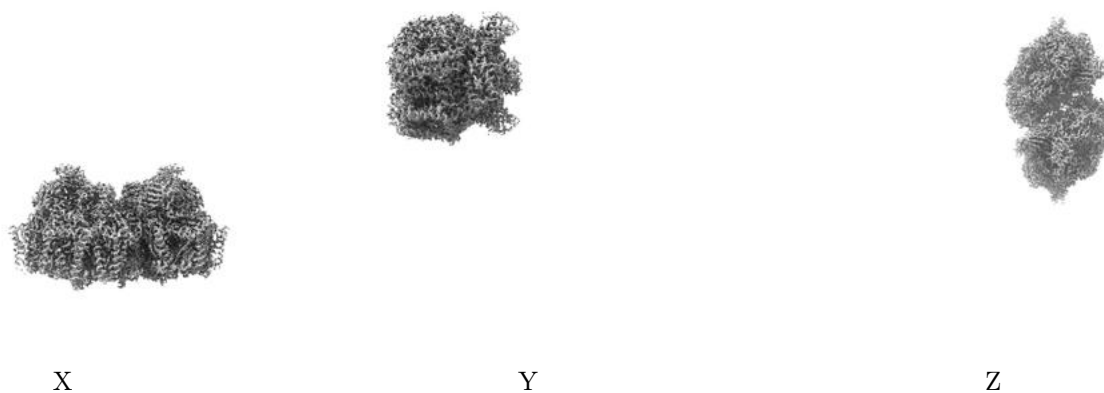
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. 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.

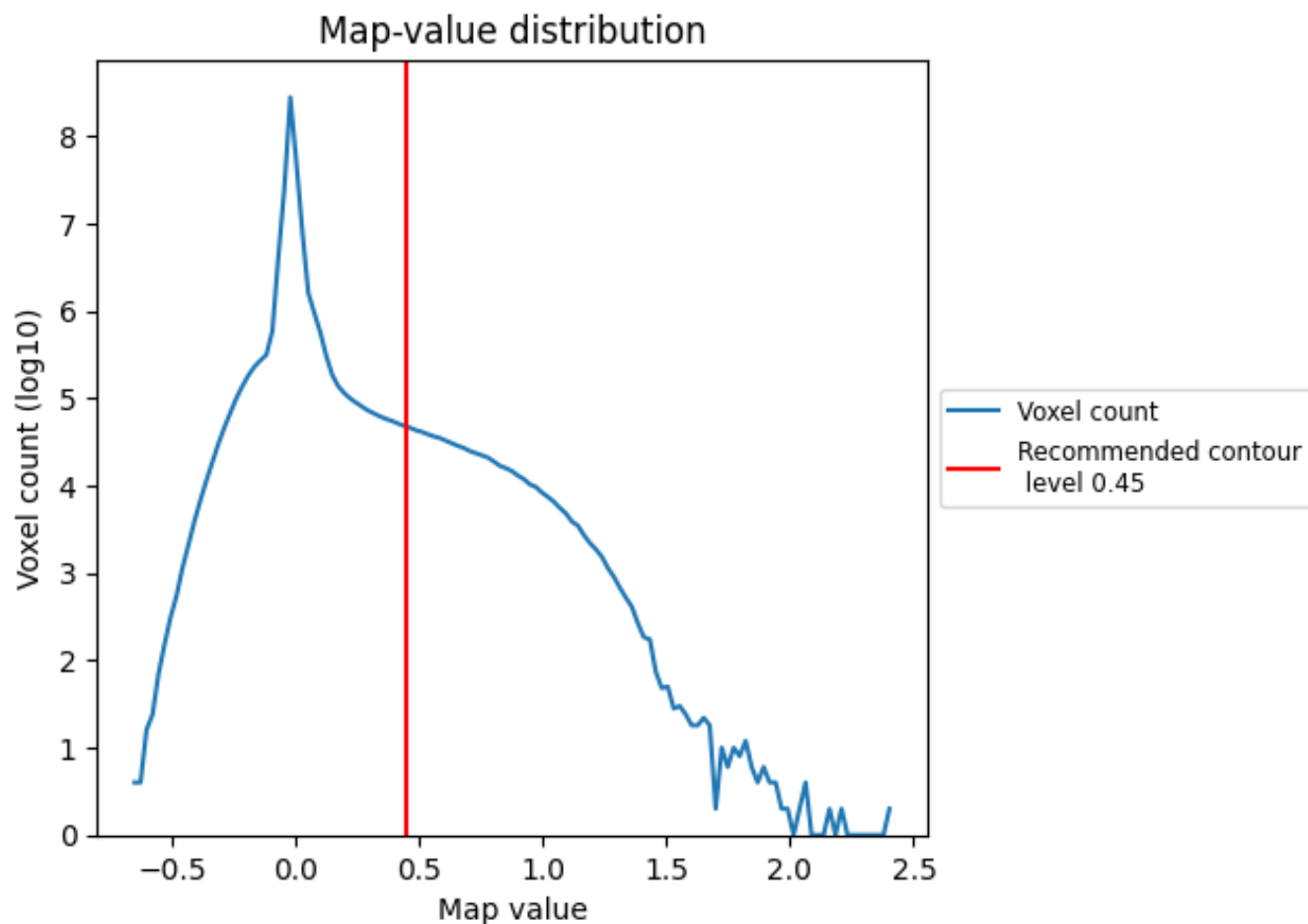
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

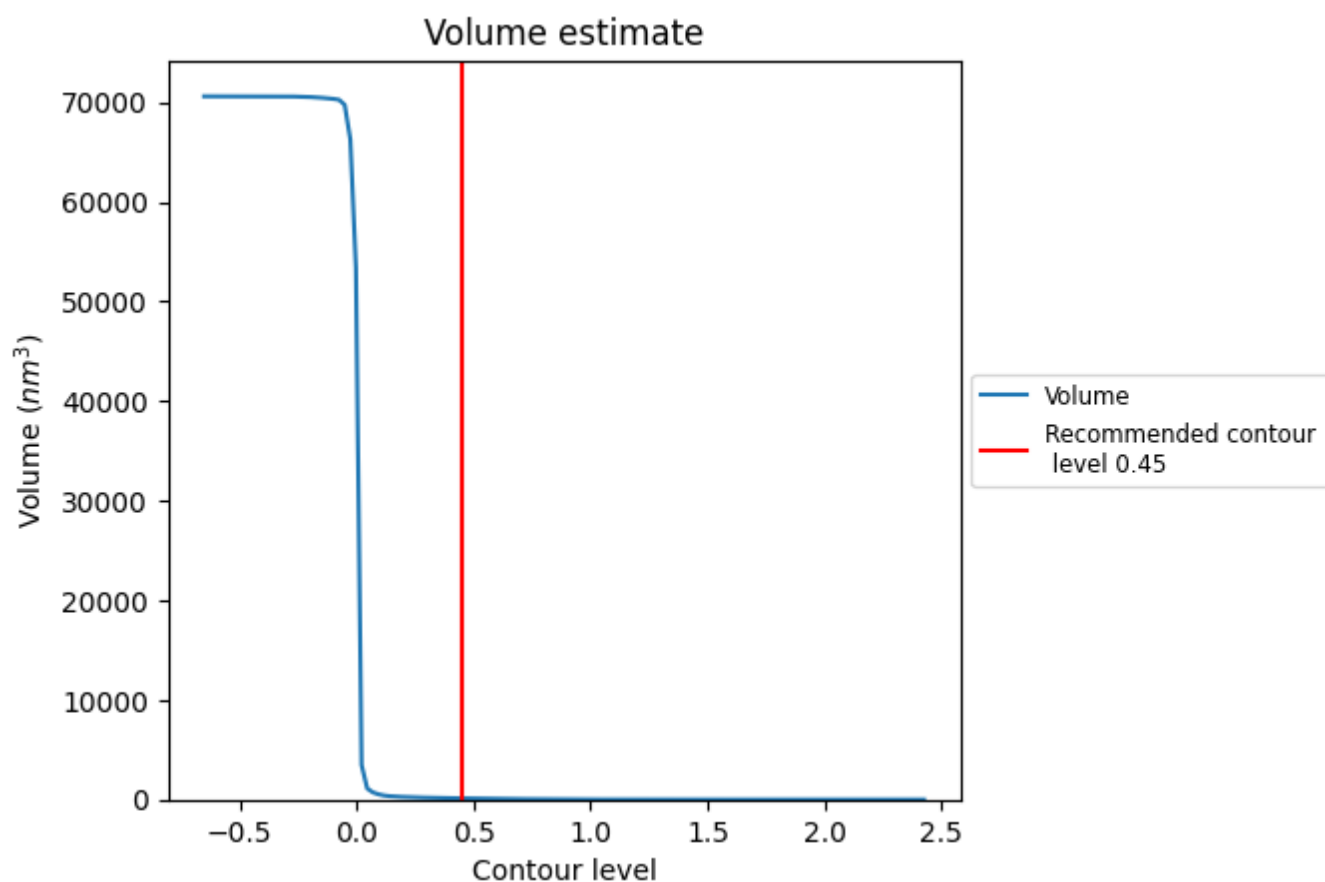
This section contains the results of statistical analysis of the map.

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.

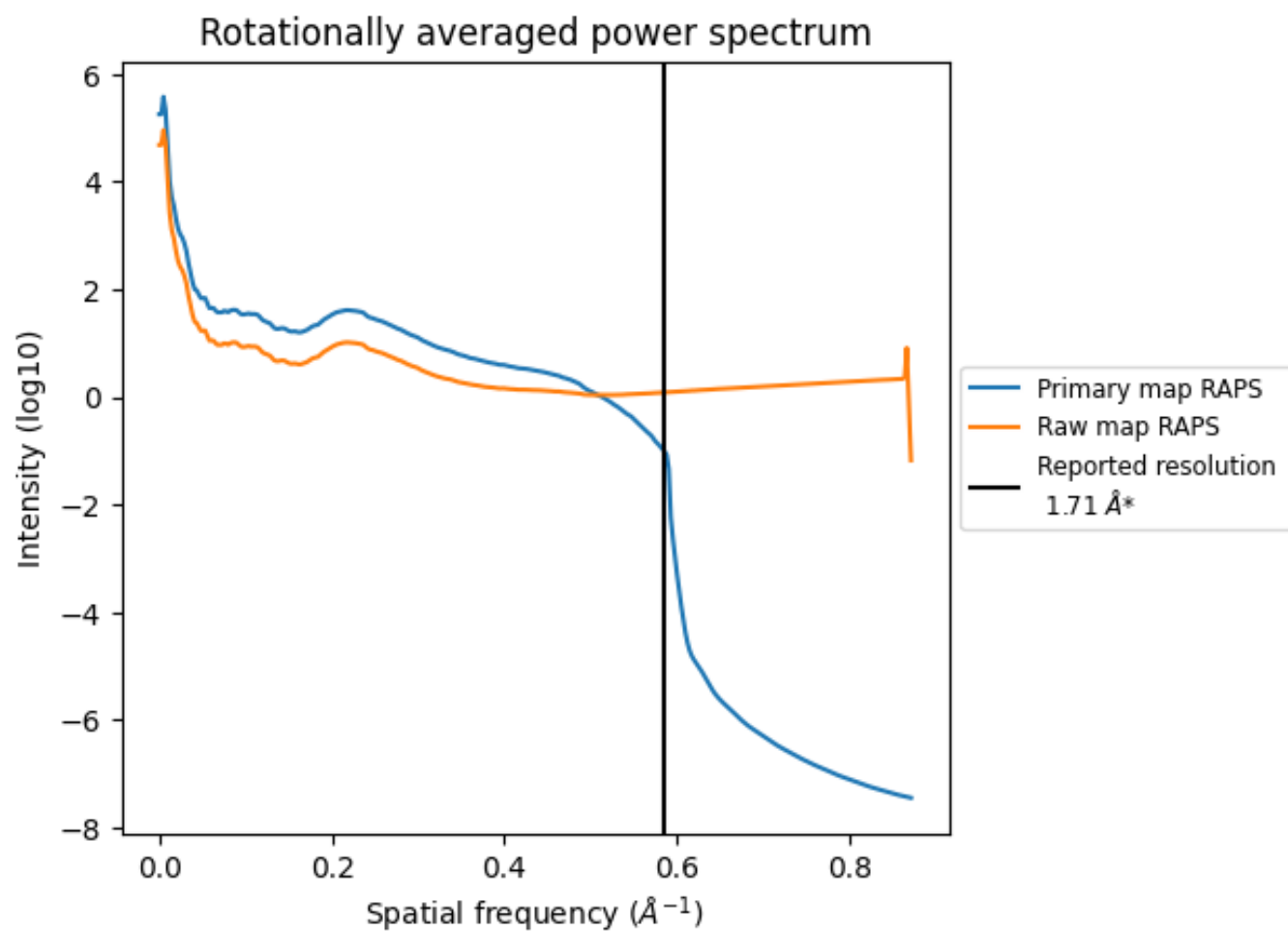
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 121 nm³; this corresponds to an approximate mass of 109 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 ⓘ

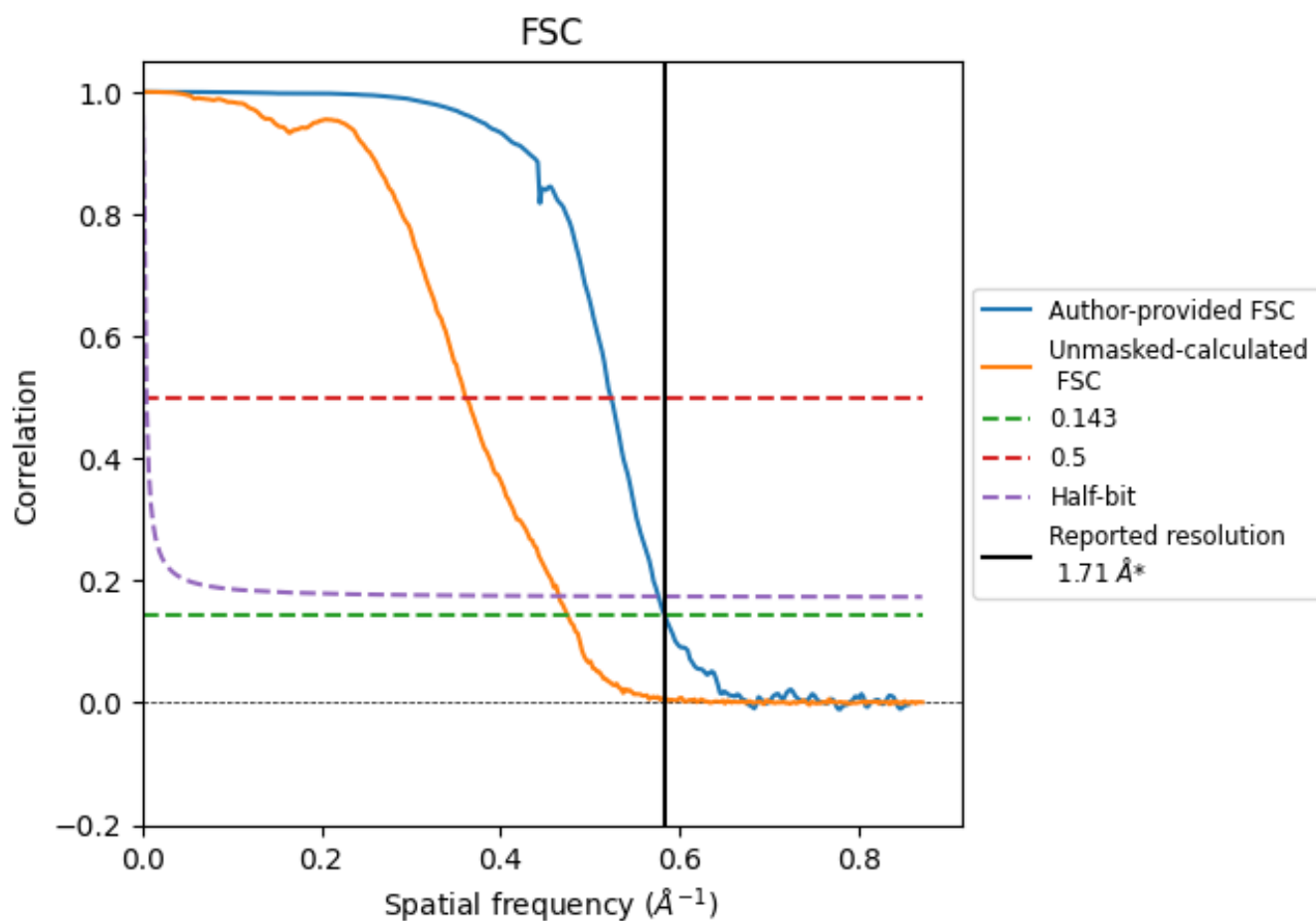


*Reported resolution corresponds to spatial frequency of $0.585 \text{ \AA}^{-1}$

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 0.585 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

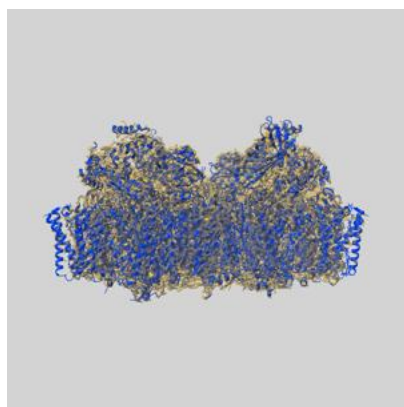
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.71	-	-
Author-provided FSC curve	1.71	1.91	1.73
Unmasked-calculated*	2.10	2.77	2.15

*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 2.10 differs from the reported value 1.71 by more than 10 %

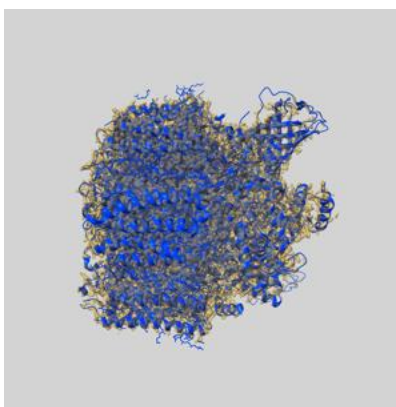
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50019 and PDB model 9EVX. Per-residue inclusion information can be found in section 3 on page 29.

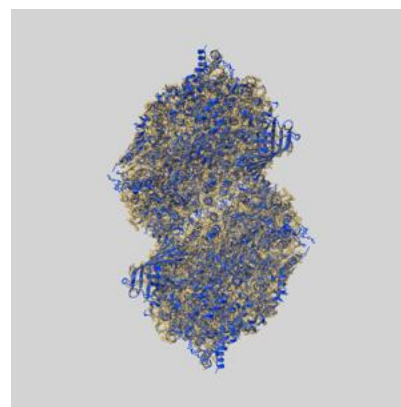
9.1 Map-model overlay [i](#)



X



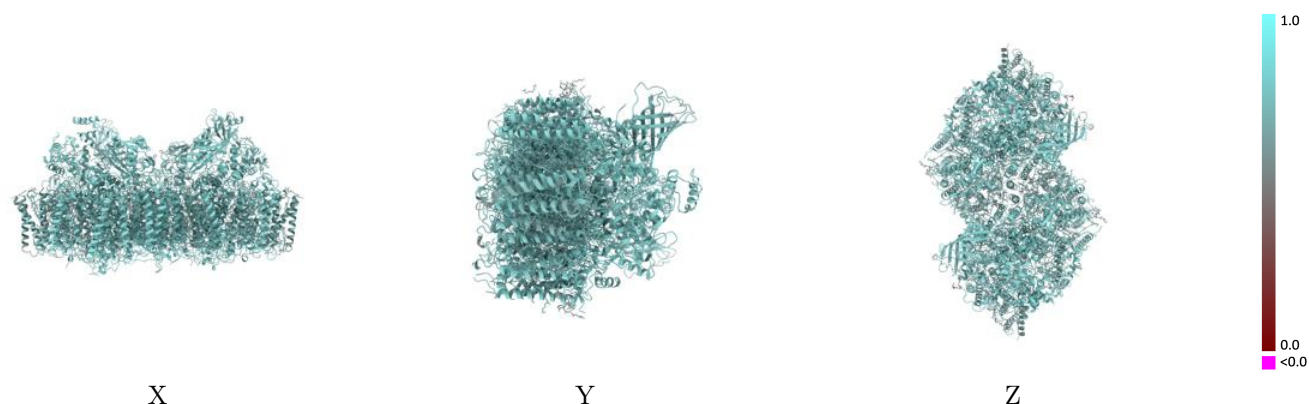
Y



Z

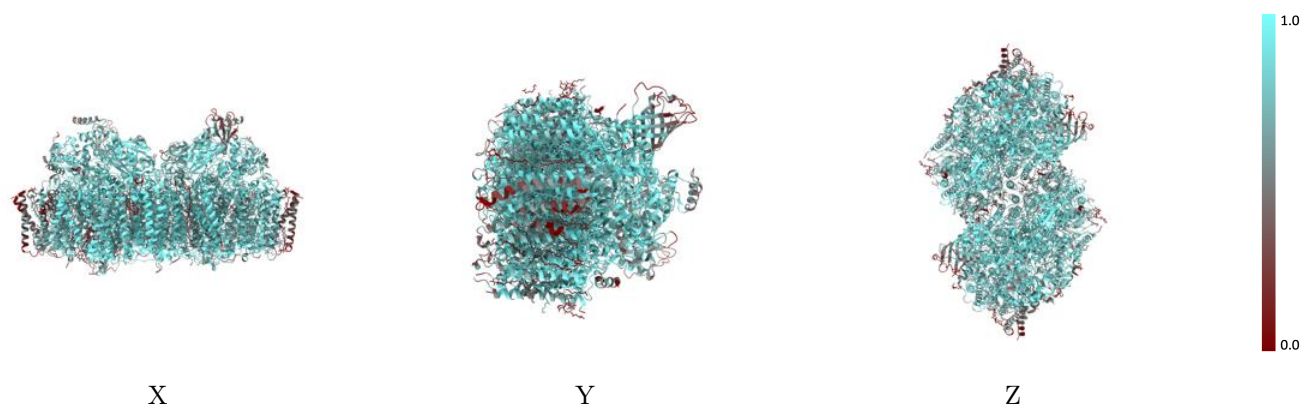
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



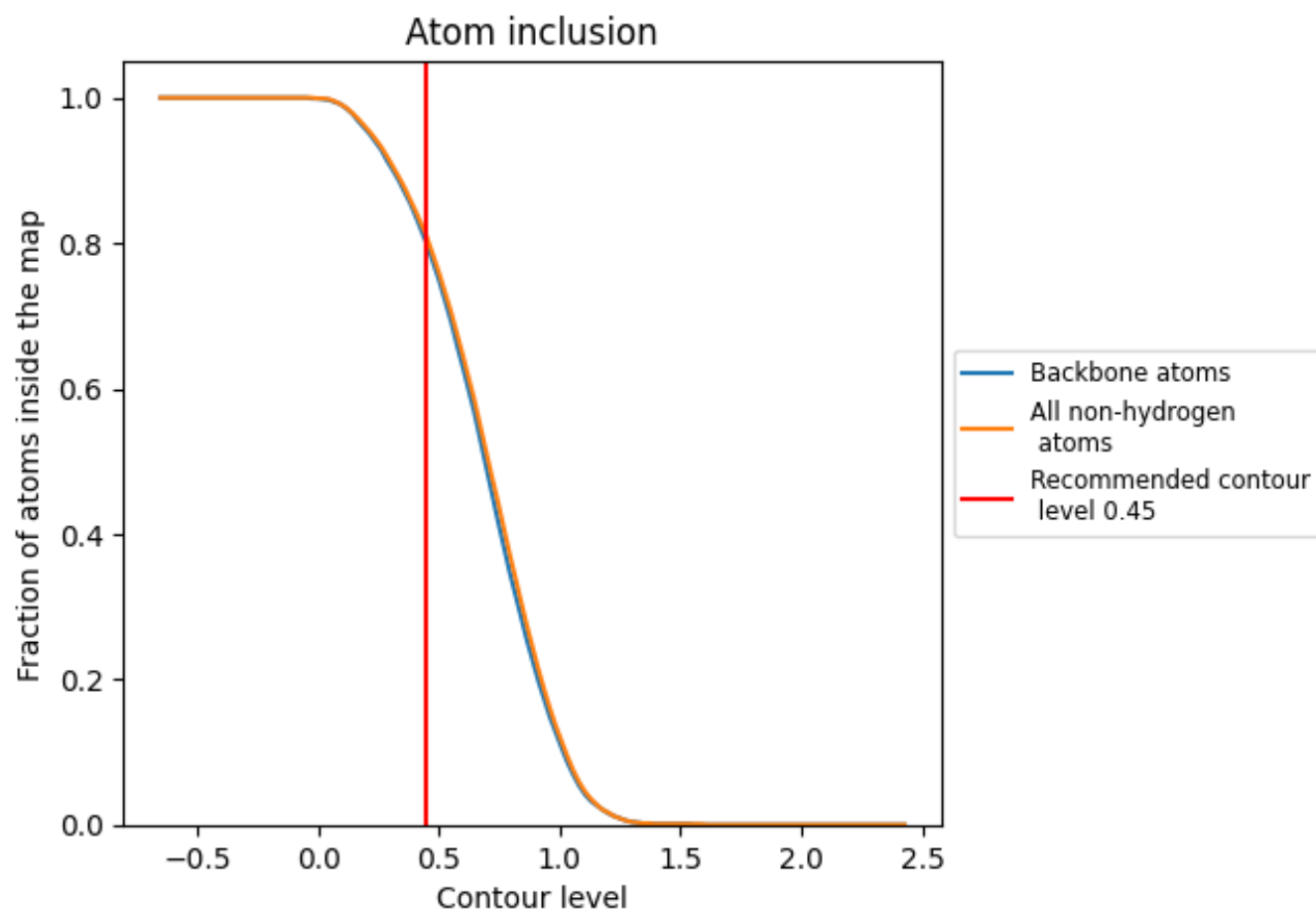
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).

9.4 Atom inclusion ⓘ



At the recommended contour level, 80% of all backbone atoms, 81% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8090	 0.7490
A	 0.8620	 0.7700
B	 0.8650	 0.7580
C	 0.8280	 0.7430
D	 0.9200	 0.7740
E	 0.6740	 0.7180
F	 0.8070	 0.7480
H	 0.7480	 0.7330
I	 0.7760	 0.7400
J	 0.6490	 0.7220
K	 0.7580	 0.7240
L	 0.8560	 0.7730
M	 0.8230	 0.7650
O	 0.6540	 0.7220
T	 0.8380	 0.7700
U	 0.7510	 0.7380
V	 0.7740	 0.7400
X	 0.6100	 0.7120
Y	 0.3950	 0.6670
Z	 0.3280	 0.6400
a	 0.8630	 0.7680
b	 0.8670	 0.7610
c	 0.8290	 0.7420
d	 0.9230	 0.7760
e	 0.6780	 0.7250
f	 0.8550	 0.7490
h	 0.7570	 0.7350
i	 0.7830	 0.7380
j	 0.6700	 0.7280
k	 0.7470	 0.7310
l	 0.8730	 0.7740
m	 0.8230	 0.7690
o	 0.6590	 0.7240
t	 0.8230	 0.7690
u	 0.7500	 0.7460



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Chain	Atom inclusion	Q-score
v	 0.7880	 0.7410
x	 0.6160	 0.7190
y	 0.4200	 0.6760
z	 0.3520	 0.6440