



Full wwPDB EM Validation Report ⓘ

Sep 11, 2026 – 07:34 am BST

PDB ID : 8C29 / pdb_00008c29
EMDB ID : EMD-16389
Title : Cryo-EM structure of photosystem II C2S2 supercomplex from Norway spruce (Picea abies) at 2.8 Angstrom resolution
Authors : Kopecny, D.; Semchonok, D.A.; Kouril, R.
Deposited on : 2022-12-21
Resolution : 2.79 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

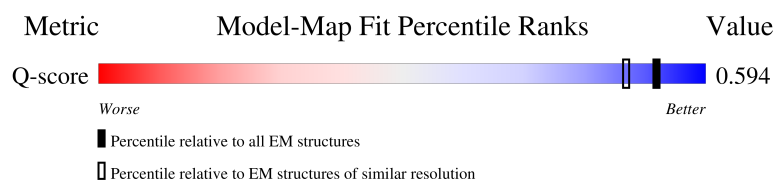
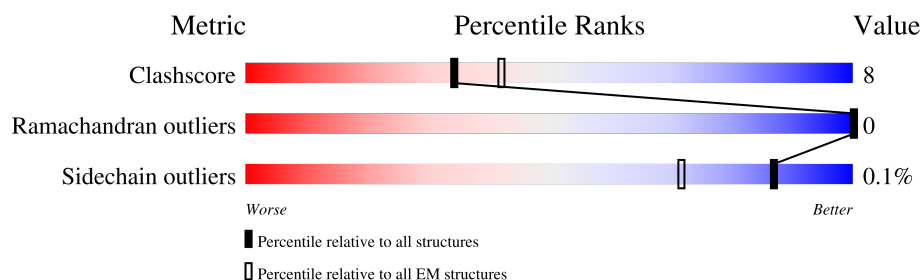
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.79 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	10740 (2.29 - 3.28)

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	353	77% 14% 9%
1	a	353	76% 14% 9%
2	B	508	81% 15% 5%
2	b	508	80% 15% 5%

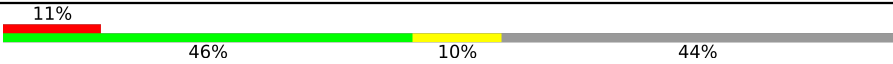
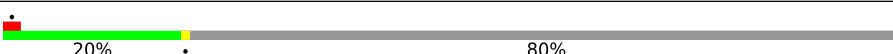
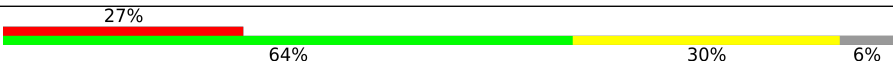
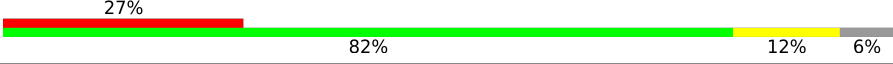
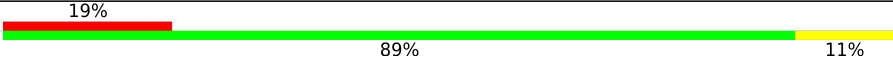
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Mol	Chain	Length	Quality of chain
3	C	473	
3	c	473	
4	D	353	
4	d	353	
5	E	83	
5	e	83	
6	F	39	
6	f	39	
7	G	275	
7	N	275	
7	Y	275	
7	g	275	
7	n	275	
7	y	275	
8	H	75	
8	h	75	
9	I	36	
9	i	36	
10	K	59	
10	k	59	
11	L	38	
11	l	38	
12	M	37	
12	m	37	
13	O	341	

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Mol	Chain	Length	Quality of chain
13	o	341	
14	R	300	
14	r	300	
15	S	303	
15	s	303	
16	T	35	
16	t	35	
17	U	133	
17	u	133	
18	V	33	
18	v	33	
19	W	146	
19	w	146	
20	X	129	
20	x	129	
21	Z	62	
21	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
36	BCT	D	401	-	-	X	-
36	BCT	d	401	-	-	X	-

2 Entry composition [i](#)

There are 43 unique types of molecules in this entry. The entry contains 71174 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	321	Total	C	N	O	S	0	0
			2502	1637	412	440	13		
1	a	321	Total	C	N	O	S	0	0
			2502	1637	412	440	13		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	295	PHE	LEU	conflict	UNP P50155
a	295	PHE	LEU	conflict	UNP P50155

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	485	Total	C	N	O	S	0	0
			3812	2503	638	657	14		
2	b	485	Total	C	N	O	S	0	0
			3812	2503	638	657	14		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	464	PHE	SER	conflict	UNP R4ZGX1
b	464	PHE	SER	conflict	UNP R4ZGX1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	433	Total	C	N	O	S	0	0
			3377	2224	565	578	10		
3	c	433	Total	C	N	O	S	0	0
			3377	2224	565	578	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	175	LEU	PRO	conflict	UNP R4ZGZ0
C	433	LEU	PRO	conflict	UNP R4ZGZ0
c	175	LEU	PRO	conflict	UNP R4ZGZ0
c	433	LEU	PRO	conflict	UNP R4ZGZ0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	337	Total	C	N	O	S	0	0
			2686	1781	439	455	11		
4	d	337	Total	C	N	O	S	0	0
			2685	1781	439	454	11		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	280	LEU	SER	conflict	UNP R4ZGX6
D	312	PHE	SER	conflict	UNP R4ZGX6
d	280	LEU	SER	conflict	UNP R4ZGX6
d	312	PHE	SER	conflict	UNP R4ZGX6

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	65	Total	C	N	O	0	0
			537	353	84	100		
5	e	65	Total	C	N	O	0	0
			537	353	84	100		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	30	Total	C	N	O	S	0	0
			240	160	41	38	1		
6	f	30	Total	C	N	O	S	0	0
			240	160	41	38	1		

- Molecule 7 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	218	Total	C	N	O	S	0	0
			1659	1080	268	305	6		
7	N	218	Total	C	N	O	S	0	0
			1659	1080	268	305	6		
7	Y	218	Total	C	N	O	S	0	0
			1659	1080	268	305	6		
7	g	218	Total	C	N	O	S	0	0
			1659	1080	268	305	6		
7	n	218	Total	C	N	O	S	0	0
			1659	1080	268	305	6		
7	y	218	Total	C	N	O	S	0	0
			1659	1080	268	305	6		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	224	ILE	LEU	conflict	UNP Q40771
G	249	LEU	ILE	conflict	UNP Q40771
G	261	ASN	THR	conflict	UNP Q40771
N	224	ILE	LEU	conflict	UNP Q40771
N	249	LEU	ILE	conflict	UNP Q40771
N	261	ASN	THR	conflict	UNP Q40771
Y	224	ILE	LEU	conflict	UNP Q40771
Y	249	LEU	ILE	conflict	UNP Q40771
Y	261	ASN	THR	conflict	UNP Q40771
g	224	ILE	LEU	conflict	UNP Q40771
g	249	LEU	ILE	conflict	UNP Q40771
g	261	ASN	THR	conflict	UNP Q40771
n	224	ILE	LEU	conflict	UNP Q40771
n	249	LEU	ILE	conflict	UNP Q40771
n	261	ASN	THR	conflict	UNP Q40771
y	224	ILE	LEU	conflict	UNP Q40771
y	249	LEU	ILE	conflict	UNP Q40771
y	261	ASN	THR	conflict	UNP Q40771

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	62	Total	C	N	O	S	0	0
			462	305	71	84	2		
8	h	62	Total	C	N	O	S	0	0
			462	305	71	84	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	36	Total	C	N	O	S	0	0
			297	202	46	48	1		
9	i	36	Total	C	N	O	S	0	0
			297	202	46	48	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	37	Total	C	N	O	S	0	0
			302	211	43	47	1		
10	k	37	Total	C	N	O	S	0	0
			302	211	43	47	1		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	31	PHE	SER	conflict	UNP R4ZGX8
K	45	PHE	SER	conflict	UNP R4ZGX8
k	31	PHE	SER	conflict	UNP R4ZGX8
k	45	PHE	SER	conflict	UNP R4ZGX8

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	36	Total	C	N	O		0	0
			302	200	49	53			
11	l	36	Total	C	N	O		0	0
			302	200	49	53			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	31	Total	C	N	O		0	0
			238	165	33	40			
12	m	31	Total	C	N	O		0	0
			238	165	33	40			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	25	LEU	PRO	conflict	UNP A2CHR7

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Chain	Residue	Modelled	Actual	Comment	Reference
m	25	LEU	PRO	conflict	UNP A2CHR7

- Molecule 13 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	190	Total	C	N	O	S	0	0
			1470	936	236	293	5		
13	o	190	Total	C	N	O	S	0	0
			1470	936	236	293	5		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	219	Total	C	N	O	S	0	0
			1722	1132	272	314	4		
14	r	219	Total	C	N	O	S	0	0
			1722	1132	272	314	4		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	54	THR	PRO	conflict	UNP A9NKKX0
R	56	ALA	-	insertion	UNP A9NKKX0
R	57	VAL	-	insertion	UNP A9NKKX0
R	58	ALA	-	insertion	UNP A9NKKX0
R	59	LYS	-	insertion	UNP A9NKKX0
R	60	PRO	-	insertion	UNP A9NKKX0
R	61	LYS	-	insertion	UNP A9NKKX0
R	62	THR	-	insertion	UNP A9NKKX0
R	63	LYS	-	insertion	UNP A9NKKX0
R	64	ALA	-	insertion	UNP A9NKKX0
R	65	VAL	-	insertion	UNP A9NKKX0
R	66	ALA	-	insertion	UNP A9NKKX0
R	67	LYS	-	insertion	UNP A9NKKX0
r	54	THR	PRO	conflict	UNP A9NKKX0
r	56	ALA	-	insertion	UNP A9NKKX0
r	57	VAL	-	insertion	UNP A9NKKX0
r	58	ALA	-	insertion	UNP A9NKKX0
r	59	LYS	-	insertion	UNP A9NKKX0
r	60	PRO	-	insertion	UNP A9NKKX0
r	61	LYS	-	insertion	UNP A9NKKX0
r	62	THR	-	insertion	UNP A9NKKX0

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Chain	Residue	Modelled	Actual	Comment	Reference
r	63	LYS	-	insertion	UNP A9NKKX0
r	64	ALA	-	insertion	UNP A9NKKX0
r	65	VAL	-	insertion	UNP A9NKKX0
r	66	ALA	-	insertion	UNP A9NKKX0
r	67	LYS	-	insertion	UNP A9NKKX0

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	211	Total	C	N	O	S	0	0
			1626	1067	261	294	4		
15	s	211	Total	C	N	O	S	0	0
			1626	1067	261	294	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	213	LEU	ALA	conflict	UNP A9NKM0
s	213	LEU	ALA	conflict	UNP A9NKM0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	31	Total	C	N	O	S	0	0
			254	177	36	40	1		
16	t	31	Total	C	N	O	S	0	0
			254	177	36	40	1		

- Molecule 17 is a protein called Photosystem II 5 kDa protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	27	Total	C	N	O	S	0	0
			205	127	39	36	3		
17	u	27	Total	C	N	O	S	0	0
			205	127	39	36	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
18	V	31	Total	C	N	O	0	0
			228	151	37	40		

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Mol	Chain	Residues	Atoms				AltConf	Trace
18	v	31	Total	C	N	O	0	0
			228	151	37	40		

- Molecule 19 is a protein called PSII 6.1 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	54	Total	C	N	O	S	0	0
			415	271	61	82	1		
19	w	54	Total	C	N	O	S	0	0
			415	271	61	82	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	98	MET	LEU	conflict	UNP A9NLC2
w	98	MET	LEU	conflict	UNP A9NLC2

- Molecule 20 is a protein called Photosystem II PsbX.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	X	34	Total	C	N	O	0	0
			226	146	37	43		
20	x	34	Total	C	N	O	0	0
			226	146	37	43		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	80	ALA	VAL	conflict	UNP A9NTS2
x	80	ALA	VAL	conflict	UNP A9NTS2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	62	Total	C	N	O	S	0	0
			453	305	68	79	1		
21	z	62	Total	C	N	O	S	0	0
			453	305	68	79	1		

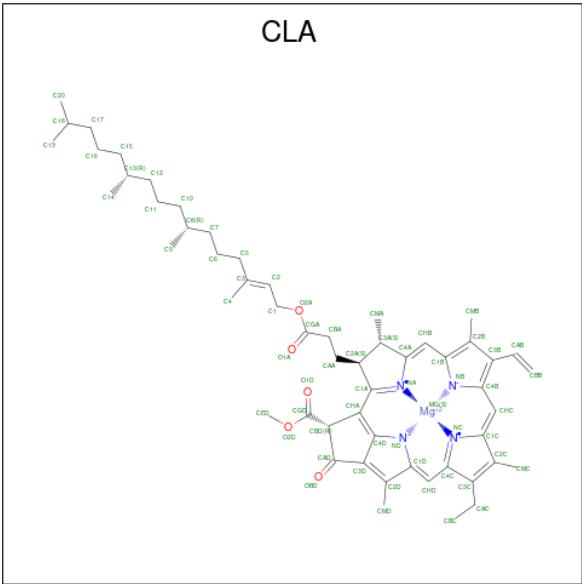
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	17	LEU	PHE	conflict	UNP R4ZGT1
z	17	LEU	PHE	conflict	UNP R4ZGT1

- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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

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Mol	Chain	Residues	Atoms					AltConf
23	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	S	1	Total 57	C 47	Mg 1	N 4	O 5	0
23	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	S	1	Total 56	C 46	Mg 1	N 4	O 5	0
23	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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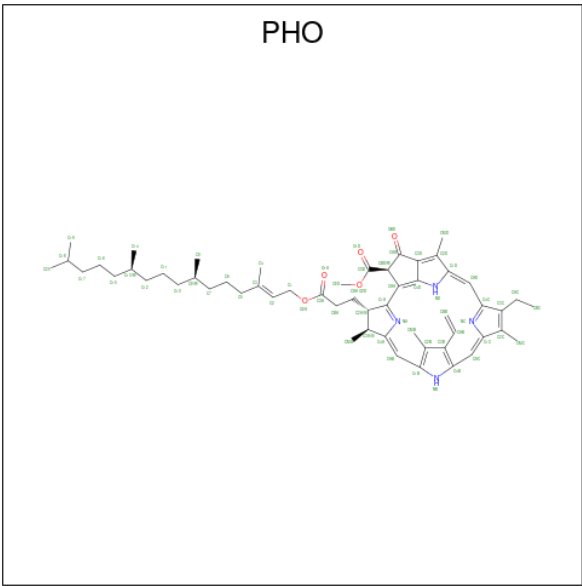
Mol	Chain	Residues	Atoms					AltConf
23	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	r	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	r	1	Total 65	C 55	Mg 1	N 4	O 5	0

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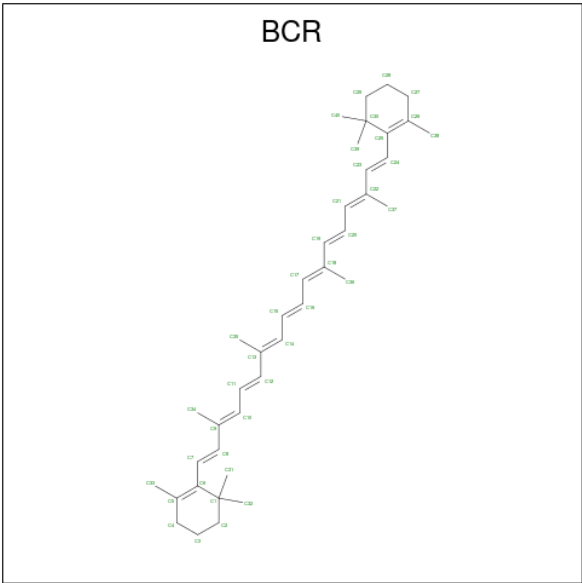
Mol	Chain	Residues	Atoms					AltConf
23	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	s	1	Total 57	C 47	Mg 1	N 4	O 5	0
23	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	s	1	Total 56	C 46	Mg 1	N 4	O 5	0
23	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	y	1	Total 65	C 55	Mg 1	N 4	O 5	0

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



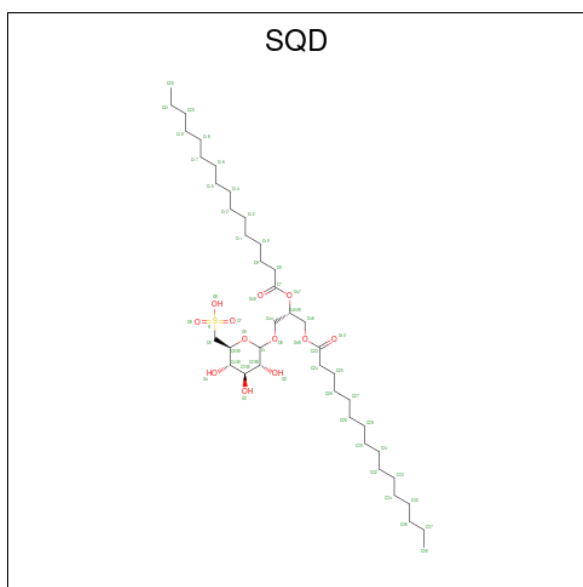
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	N	O	0
			64	55	4	5	
24	D	1	Total	C	N	O	0
			64	55	4	5	
24	a	1	Total	C	N	O	0
			64	55	4	5	
24	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



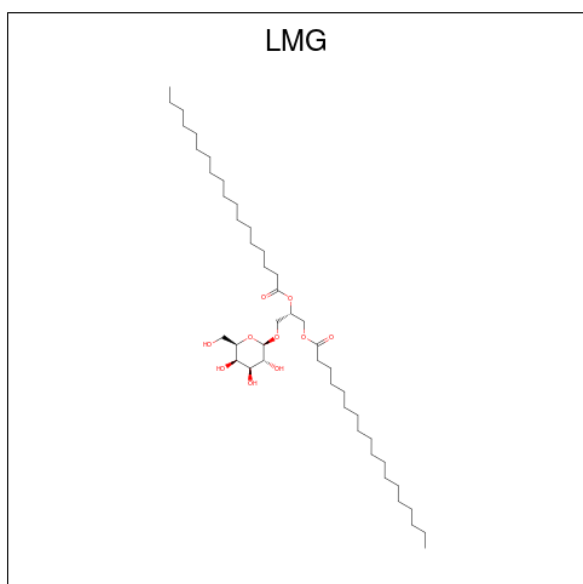
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 39 39	0
25	B	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	D	1	Total C 40 40	0
25	H	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	V	1	Total C 40 40	0
25	Z	1	Total C 40 40	0
25	a	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	c	1	Total C 40 40	0
25	d	1	Total C 40 40	0
25	h	1	Total C 40 40	0
25	k	1	Total C 40 40	0
25	v	1	Total C 40 40	0
25	z	1	Total C 40 40	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



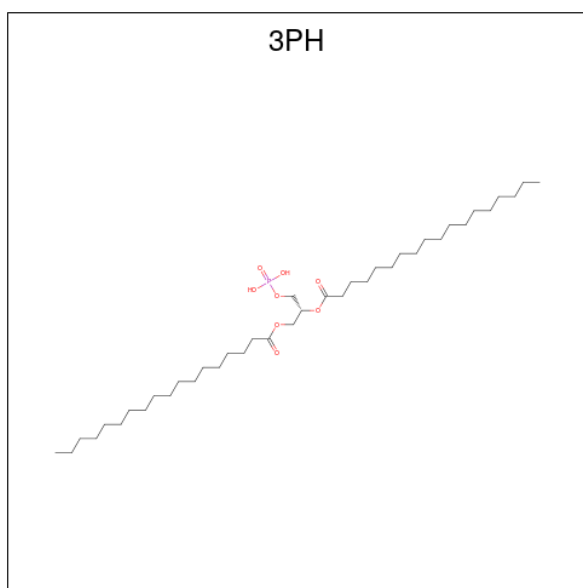
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	S	0
			50	37	12	1	
26	L	1	Total	C	O	S	0
			54	41	12	1	
26	M	1	Total	C	O	S	0
			50	37	12	1	
26	a	1	Total	C	O	S	0
			48	35	12	1	

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



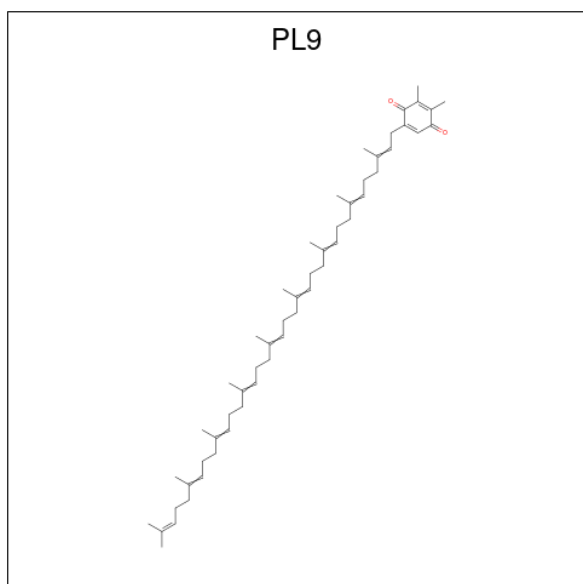
Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			53	43	10	
27	B	1	Total	C	O	0
			48	38	10	
27	B	1	Total	C	O	0
			49	39	10	
27	C	1	Total	C	O	0
			45	35	10	
27	D	1	Total	C	O	0
			36	26	10	
27	R	1	Total	C	O	0
			51	41	10	
27	b	1	Total	C	O	0
			51	41	10	
27	b	1	Total	C	O	0
			50	40	10	
27	c	1	Total	C	O	0
			46	36	10	
27	d	1	Total	C	O	0
			46	36	10	
27	r	1	Total	C	O	0
			51	41	10	
27	w	1	Total	C	O	0
			48	38	10	

- Molecule 28 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



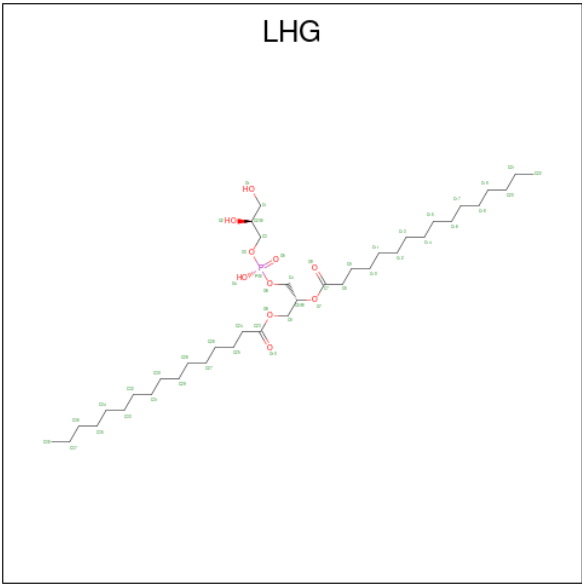
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	O	P	0
			48	39	8	1	
28	C	1	Total	C	O	P	0
			48	39	8	1	
28	D	1	Total	C	O	P	0
			38	29	8	1	
28	L	1	Total	C	O	P	0
			41	32	8	1	
28	T	1	Total	C	O	P	0
			48	39	8	1	
28	W	1	Total	C	O	P	0
			46	37	8	1	
28	X	1	Total	C	O	P	0
			46	37	8	1	
28	a	1	Total	C	O	P	0
			48	39	8	1	
28	d	1	Total	C	O	P	0
			38	29	8	1	
28	s	1	Total	C	O	P	0
			38	29	8	1	
28	w	1	Total	C	O	P	0
			48	39	8	1	
28	x	1	Total	C	O	P	0
			46	37	8	1	

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			55	53	2	
29	D	1	Total	C	O	0
			55	53	2	
29	a	1	Total	C	O	0
			55	53	2	
29	d	1	Total	C	O	0
			55	53	2	

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



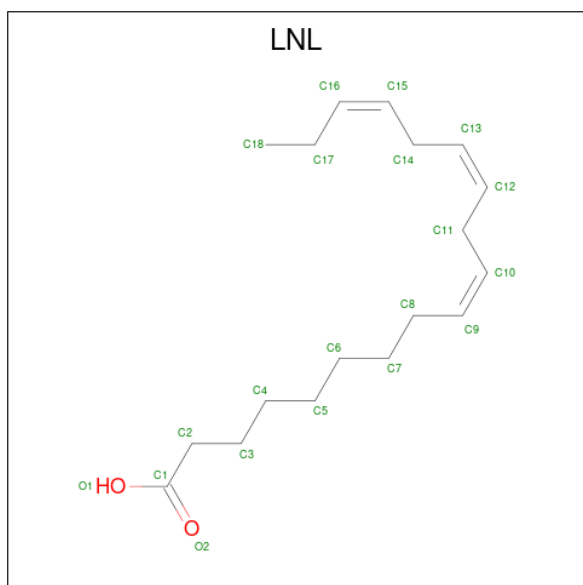
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	P	0
			37	26	10	1	
30	D	1	Total	C	O	P	0
			43	32	10	1	
30	D	1	Total	C	O	P	0
			49	38	10	1	
30	G	1	Total	C	O	P	0
			49	38	10	1	
30	L	1	Total	C	O	P	0
			49	38	10	1	
30	N	1	Total	C	O	P	0
			49	38	10	1	
30	R	1	Total	C	O	P	0
			38	27	10	1	

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Mol	Chain	Residues	Atoms				AltConf
30	S	1	Total	C	O	P	0
			49	38	10	1	
30	Y	1	Total	C	O	P	0
			49	38	10	1	
30	a	1	Total	C	O	P	0
			49	38	10	1	
30	b	1	Total	C	O	P	0
			49	38	10	1	
30	d	1	Total	C	O	P	0
			49	38	10	1	
30	d	1	Total	C	O	P	0
			49	38	10	1	
30	g	1	Total	C	O	P	0
			49	38	10	1	
30	n	1	Total	C	O	P	0
			45	34	10	1	
30	r	1	Total	C	O	P	0
			37	26	10	1	
30	s	1	Total	C	O	P	0
			49	38	10	1	
30	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 31 is ALPHA-LINOLENIC ACID (CCD ID: LNL) (formula: $C_{18}H_{30}O_2$).



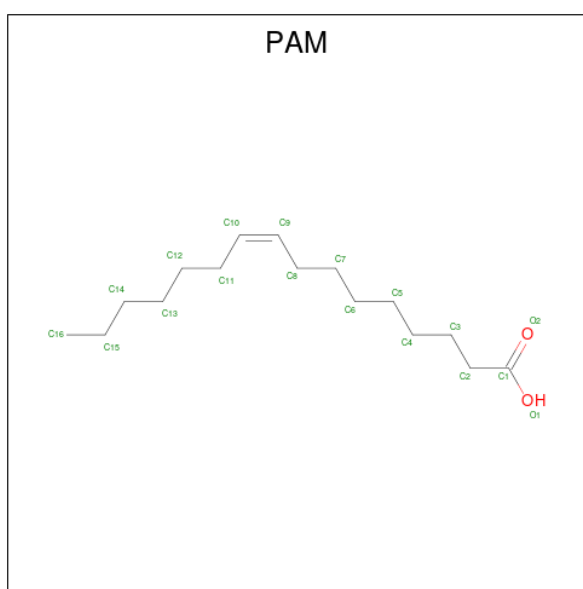
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			20	18	2	
31	A	1	Total	C	O	0
			20	18	2	
31	B	1	Total	C	O	0
			20	18	2	
31	B	1	Total	C	O	0
			20	18	2	
31	B	1	Total	C	O	0
			20	18	2	
31	B	1	Total	C	O	0
			20	18	2	
31	C	1	Total	C	O	0
			20	18	2	
31	C	1	Total	C	O	0
			20	18	2	
31	C	1	Total	C	O	0
			20	18	2	
31	C	1	Total	C	O	0
			20	18	2	
31	C	1	Total	C	O	0
			20	18	2	
31	C	1	Total	C	O	0
			20	18	2	
31	C	1	Total	C	O	0
			20	18	2	
31	I	1	Total	C	O	0
			20	18	2	
31	a	1	Total	C	O	0
			20	18	2	
31	a	1	Total	C	O	0
			20	18	2	
31	b	1	Total	C	O	0
			20	18	2	
31	b	1	Total	C	O	0
			20	18	2	
31	b	1	Total	C	O	0
			20	18	2	
31	b	1	Total	C	O	0
			20	18	2	
31	c	1	Total	C	O	0
			20	18	2	
31	c	1	Total	C	O	0
			20	18	2	
31	c	1	Total	C	O	0
			20	18	2	

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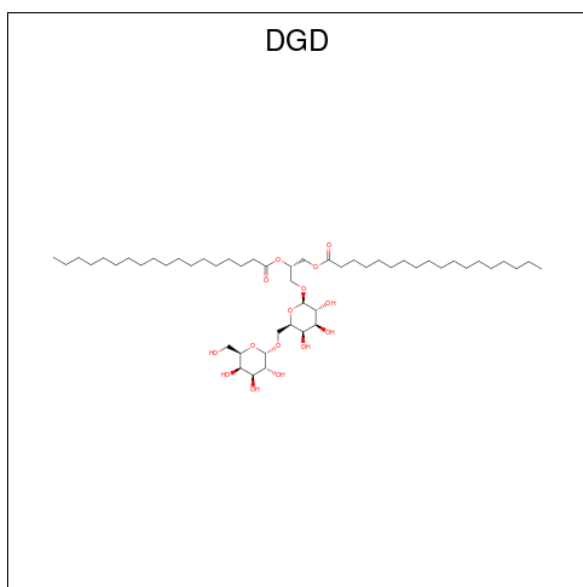
Mol	Chain	Residues	Atoms			AltConf
31	c	1	Total	C	O	0
			20	18	2	
31	c	1	Total	C	O	0
			20	18	2	
31	c	1	Total	C	O	0
			20	18	2	
31	i	1	Total	C	O	0
			20	18	2	

- Molecule 32 is PALMITOLEIC ACID (CCD ID: PAM) (formula: $C_{16}H_{30}O_2$).



Mol	Chain	Residues	Atoms			AltConf
32	B	1	Total	C	O	0
			18	16	2	
32	b	1	Total	C	O	0
			18	16	2	

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).

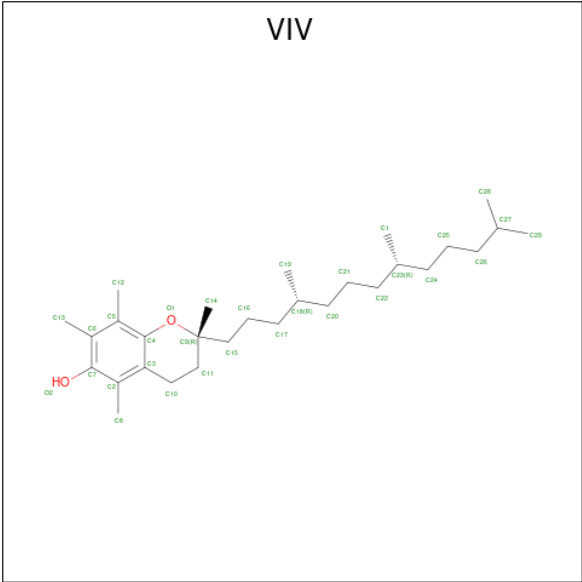


Mol	Chain	Residues	Atoms			AltConf
33	C	1	Total	C	O	0
			66	51	15	
33	H	1	Total	C	O	0
			62	47	15	
33	c	1	Total	C	O	0
			55	40	15	
33	d	1	Total	C	O	0
			62	47	15	

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

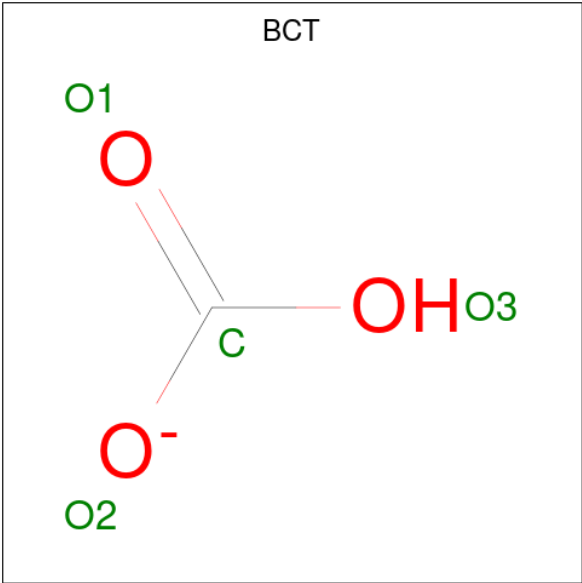
Mol	Chain	Residues	Atoms		AltConf
34	C	1	Total	Mg	0
			1	1	
34	c	1	Total	Mg	0
			1	1	

- Molecule 35 is (2R)-2,5,7,8-TETRAMETHYL-2-[(4R,8R)-4,8,12-TRIMETHYLTRIDECYL]CHROMAN-6-OL (CCD ID: VIV) (formula: C₂₉H₅₀O₂).



Mol	Chain	Residues	Atoms			AltConf
35	C	1	Total	C	O	0
			31	29	2	
35	y	1	Total	C	O	0
			31	29	2	

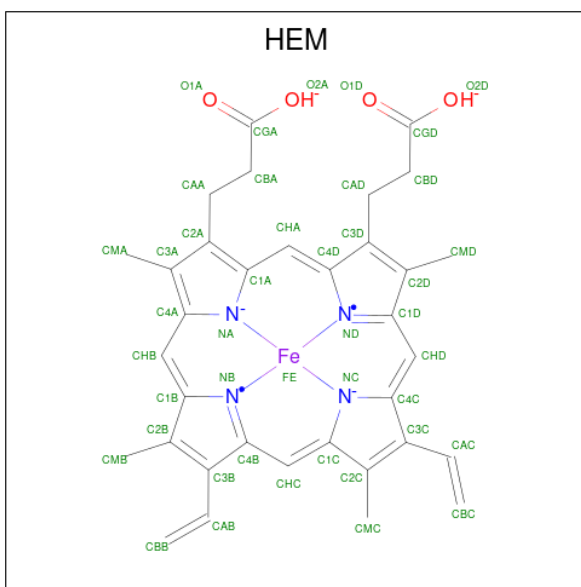
- Molecule 36 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

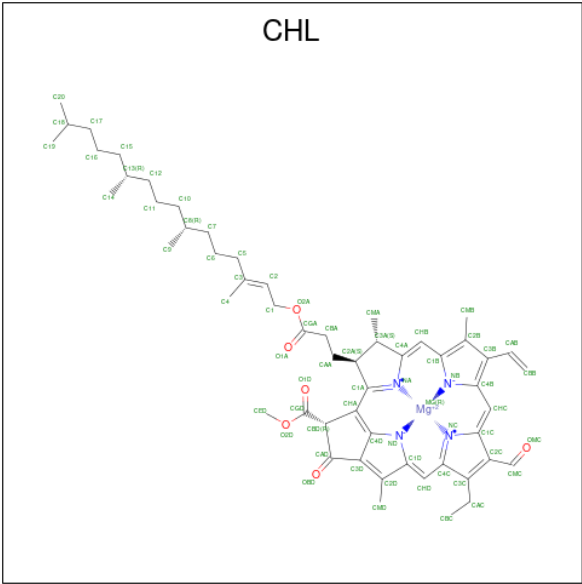
- # DGA
-
- The chemical structure of 1,3-bis(sn-3'-phosphatidyl)sn-glycerol (DGA) is shown. It consists of a central glycerol backbone where the first and third carbons are linked to phosphate groups, which are in turn linked to a second glycerol unit. The second glycerol unit has a phosphate group at the first carbon and a hydroxyl group at the second carbon. The third carbon of the second glycerol unit is linked to a third glycerol unit, which has a phosphate group at the first carbon and a hydroxyl group at the second carbon. The structure is drawn in a zig-zag pattern, with the phosphate groups highlighted in red.

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 39 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
39	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	G	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
39	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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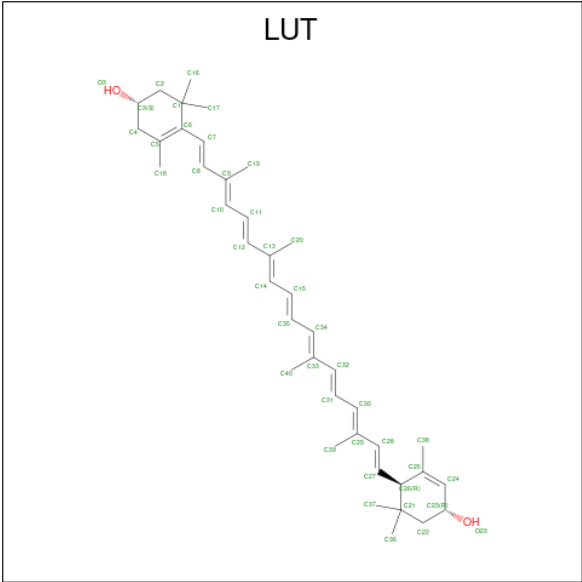
Mol	Chain	Residues	Atoms					AltConf
39	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
39	N	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
39	R	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
39	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
39	S	1	Total 52	C 41	Mg 1	N 4	O 6	0
39	S	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	S	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	S	1	Total 49	C 38	Mg 1	N 4	O 6	0
39	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
39	Y	1	Total 48	C 37	Mg 1	N 4	O 6	0
39	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
39	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
39	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
39	g	1	Total 48	C 37	Mg 1	N 4	O 6	0
39	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
39	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	g	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
39	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	n	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
39	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	r	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	r	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	r	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	s	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
39	s	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	s	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	s	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 40 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



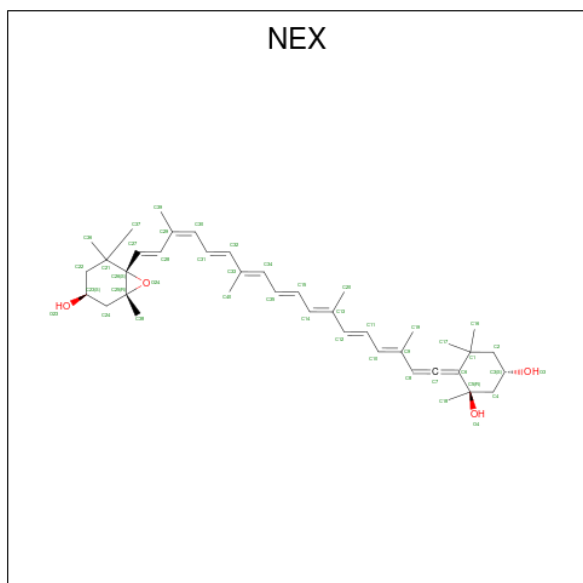
Mol	Chain	Residues	Atoms			AltConf
40	G	1	Total	C	O	0
			42	40	2	
40	G	1	Total	C	O	0
			42	40	2	
40	N	1	Total	C	O	0
			42	40	2	
40	N	1	Total	C	O	0
			42	40	2	
40	R	1	Total	C	O	0
			42	40	2	
40	S	1	Total	C	O	0
			42	40	2	
40	S	1	Total	C	O	0
			42	40	2	
40	Y	1	Total	C	O	0
			42	40	2	
40	Y	1	Total	C	O	0
			42	40	2	
40	g	1	Total	C	O	0
			42	40	2	
40	g	1	Total	C	O	0
			42	40	2	
40	n	1	Total	C	O	0
			42	40	2	
40	n	1	Total	C	O	0
			42	40	2	
40	r	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
40	s	1	Total	C	O	0
			42	40	2	
40	s	1	Total	C	O	0
			42	40	2	
40	y	1	Total	C	O	0
			42	40	2	
40	y	1	Total	C	O	0
			42	40	2	

- Molecule 41 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



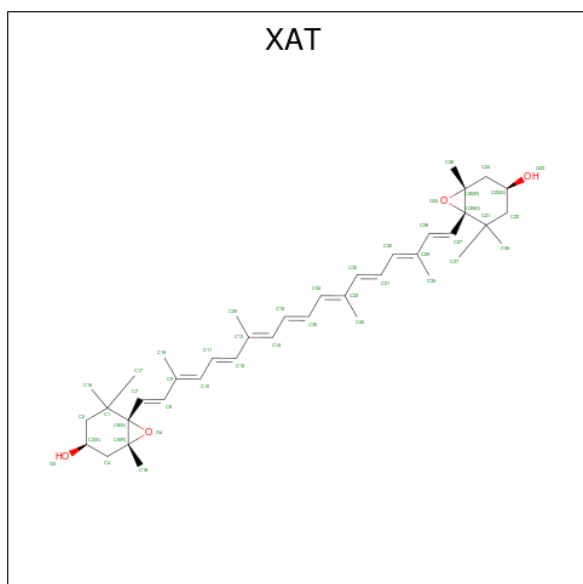
Mol	Chain	Residues	Atoms			AltConf
41	G	1	Total	C	O	0
			24	22	2	
41	N	1	Total	C	O	0
			44	40	4	
41	R	1	Total	C	O	0
			44	40	4	
41	R	1	Total	C	O	0
			44	40	4	
41	S	1	Total	C	O	0
			23	21	2	
41	Y	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
41	g	1	Total	C	O	0
			44	40	4	
41	n	1	Total	C	O	0
			44	40	4	
41	r	1	Total	C	O	0
			44	40	4	
41	s	1	Total	C	O	0
			27	25	2	

- Molecule 42 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'-TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
42	G	1	Total	C	O	0
			44	40	4	
42	N	1	Total	C	O	0
			44	40	4	
42	R	1	Total	C	O	0
			44	40	4	
42	Y	1	Total	C	O	0
			44	40	4	
42	n	1	Total	C	O	0
			44	40	4	
42	n	1	Total	C	O	0
			44	40	4	
42	r	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
42	y	1	Total	C	O	0
			44	40	4	

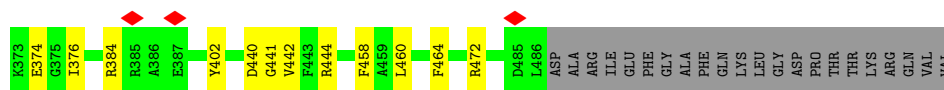
- Molecule 43 is water.

Mol	Chain	Residues	Atoms			AltConf
43	A	28	Total	O		0
			28	28		
43	B	31	Total	O		0
			31	31		
43	C	10	Total	O		0
			10	10		
43	D	18	Total	O		0
			18	18		
43	E	4	Total	O		0
			4	4		
43	H	10	Total	O		0
			10	10		
43	I	1	Total	O		0
			1	1		
43	L	2	Total	O		0
			2	2		
43	N	4	Total	O		0
			4	4		
43	O	4	Total	O		0
			4	4		
43	R	8	Total	O		0
			8	8		
43	S	1	Total	O		0
			1	1		
43	T	5	Total	O		0
			5	5		
43	U	1	Total	O		0
			1	1		
43	V	1	Total	O		0
			1	1		
43	Y	8	Total	O		0
			8	8		
43	Z	1	Total	O		0
			1	1		
43	a	20	Total	O		0
			20	20		

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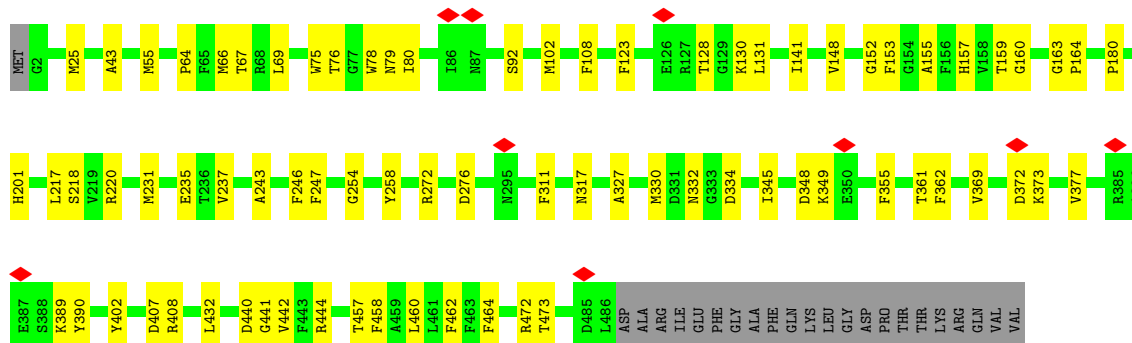
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
43	b	31	Total 31	O 31	0
43	c	14	Total 14	O 14	0
43	d	25	Total 25	O 25	0
43	e	4	Total 4	O 4	0
43	f	1	Total 1	O 1	0
43	g	1	Total 1	O 1	0
43	h	11	Total 11	O 11	0
43	i	2	Total 2	O 2	0
43	l	4	Total 4	O 4	0
43	n	1	Total 1	O 1	0
43	o	2	Total 2	O 2	0
43	r	7	Total 7	O 7	0
43	t	4	Total 4	O 4	0
43	v	2	Total 2	O 2	0
43	x	1	Total 1	O 1	0
43	y	13	Total 13	O 13	0



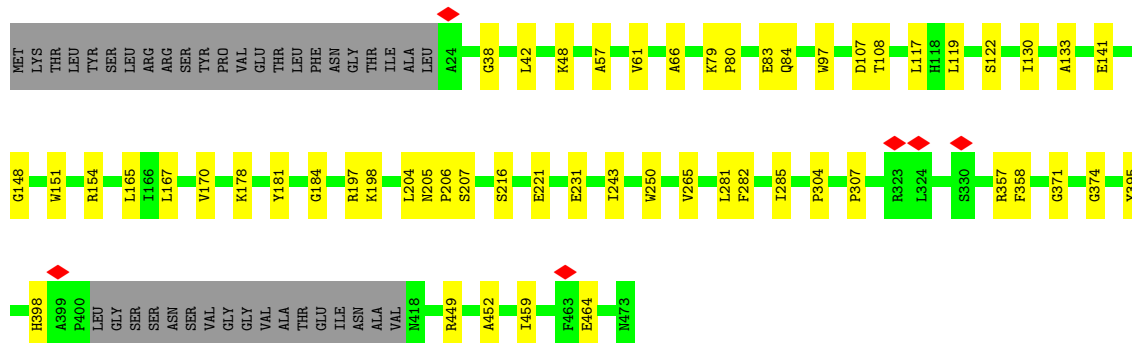
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b: 80% 15% 5%



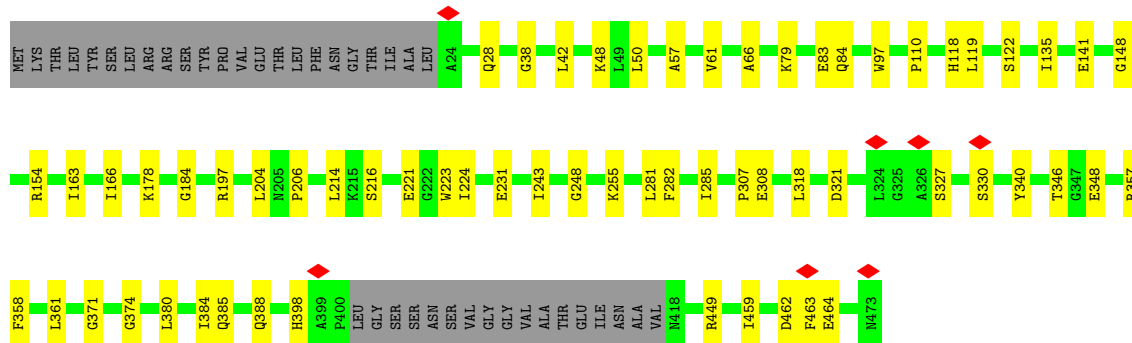
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 80% 12% 8%



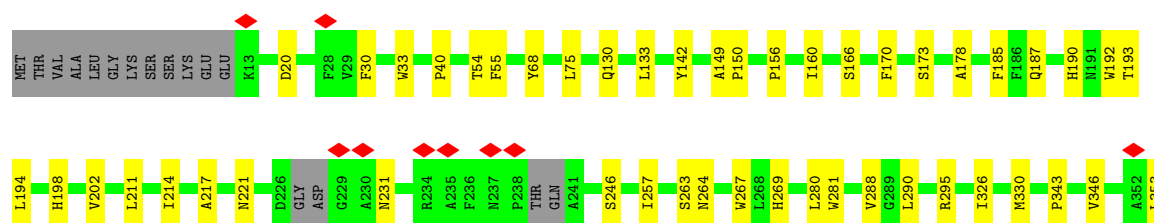
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 78% 13% 8%



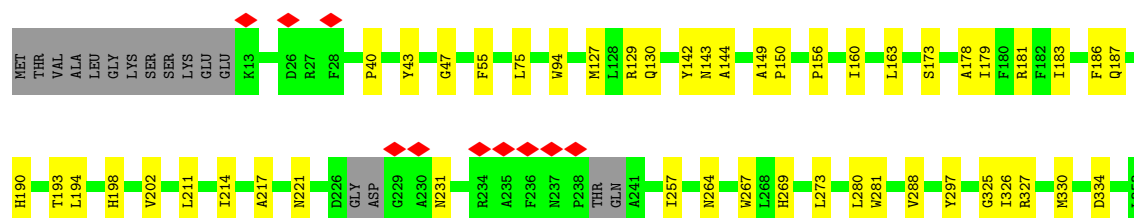
• Molecule 4: Photosystem II D2 protein

Chain D: 



• Molecule 4: Photosystem II D2 protein

Chain d: 



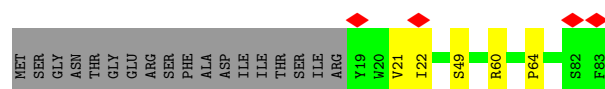
• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 



• Molecule 5: Cytochrome b559 subunit alpha

Chain e: 



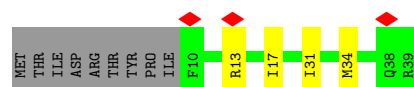
• Molecule 6: Cytochrome b559 subunit beta

Chain F: 

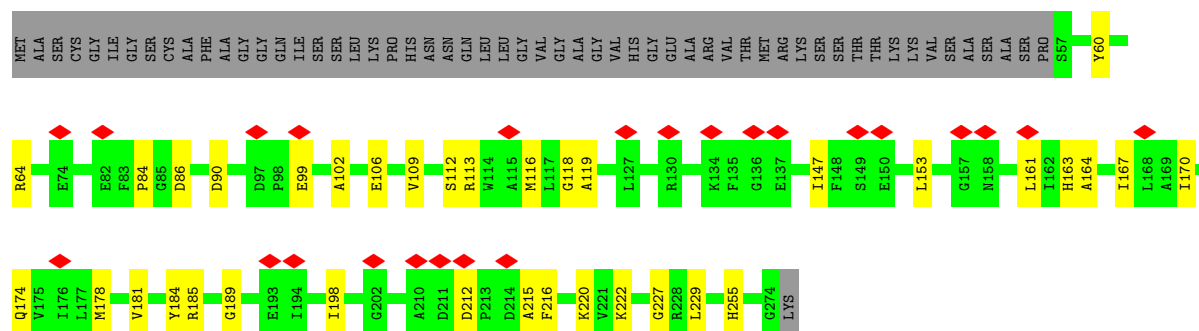


• Molecule 6: Cytochrome b559 subunit beta

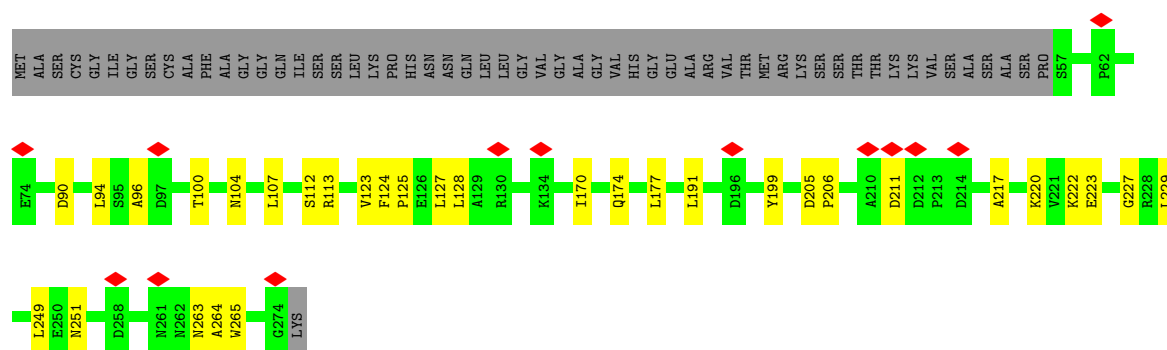
Chain f: 



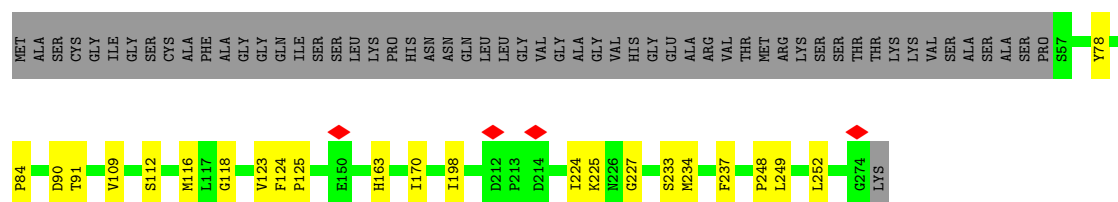
• Molecule 7: Chlorophyll a-b binding protein, chloroplastic



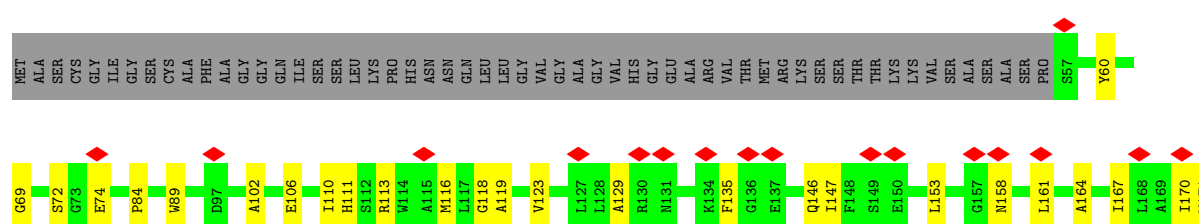
• Molecule 7: Chlorophyll a-b binding protein, chloroplastic

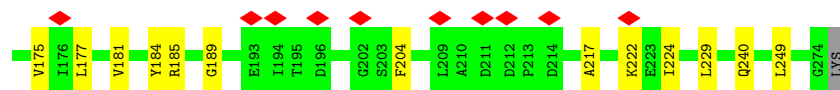


• Molecule 7: Chlorophyll a-b binding protein, chloroplastic

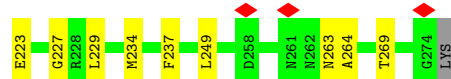
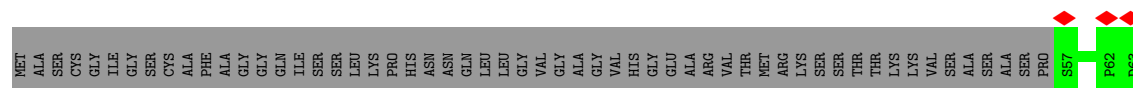


• Molecule 7: Chlorophyll a-b binding protein, chloroplastic

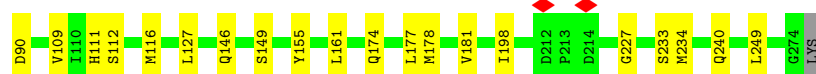
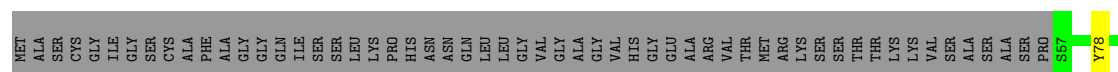




- Molecule 7: Chlorophyll a-b binding protein, chloroplastic



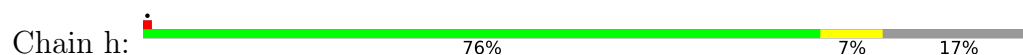
- Molecule 7: Chlorophyll a-b binding protein, chloroplastic



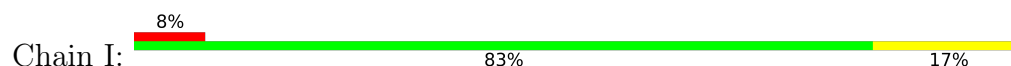
- Molecule 8: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein H

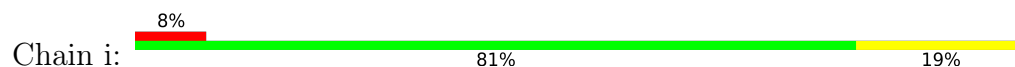


- Molecule 9: Photosystem II reaction center protein I

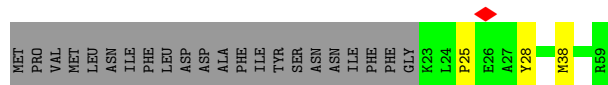




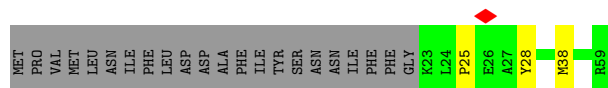
- Molecule 9: Photosystem II reaction center protein I



- Molecule 10: Photosystem II reaction center protein K



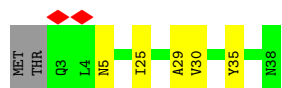
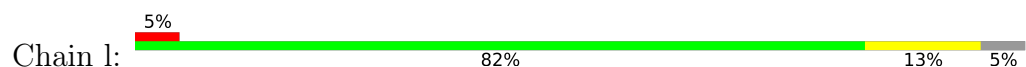
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L

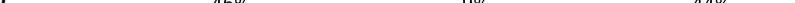


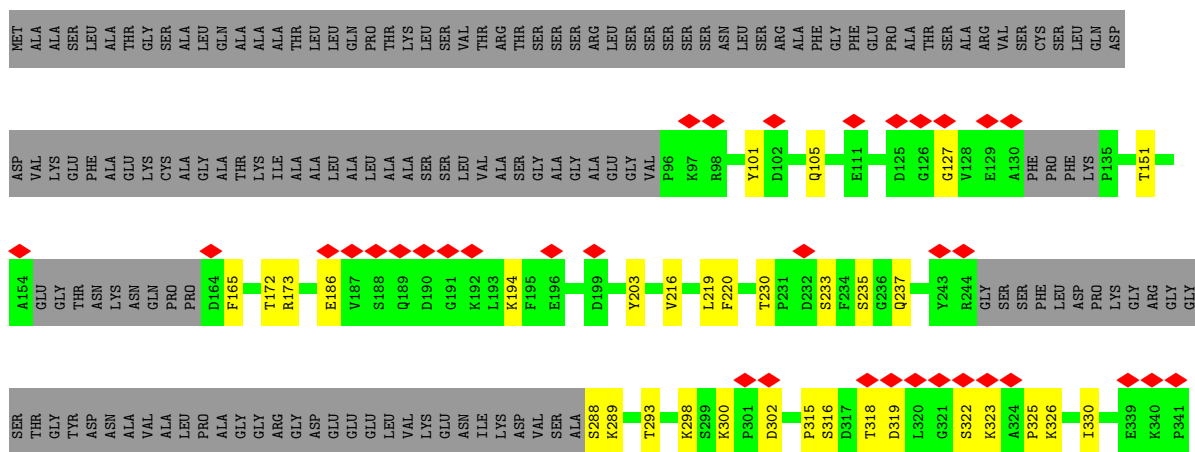
- Molecule 12: Photosystem II reaction center protein M

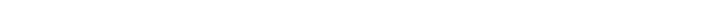


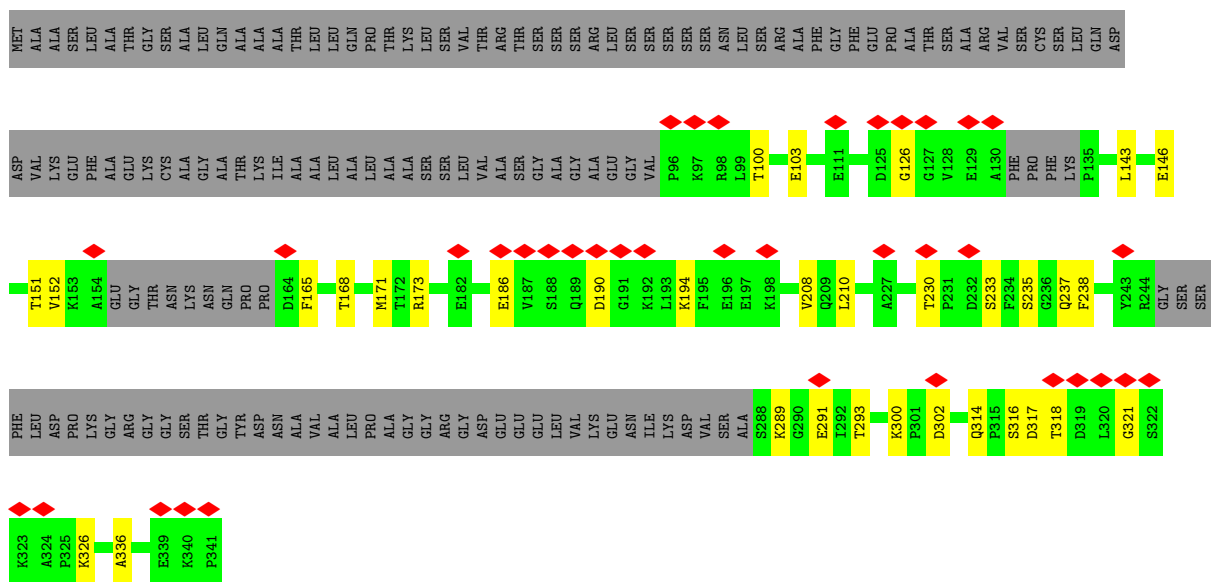
- Molecule 12: Photosystem II reaction center protein M

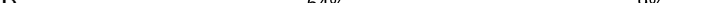


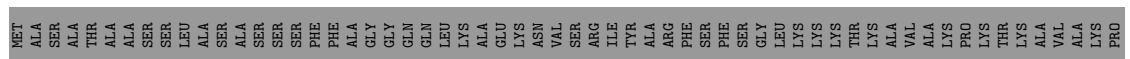
- Chain O: 

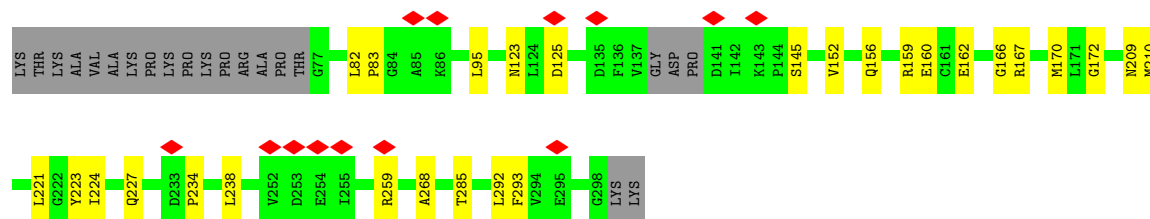


- Chain o: 

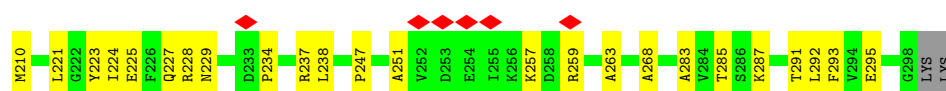
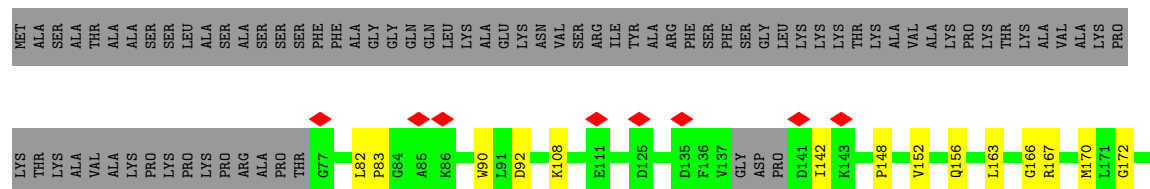


- Chain R: 

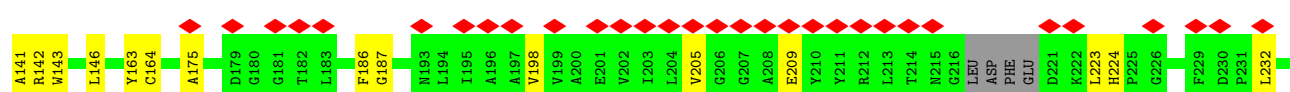
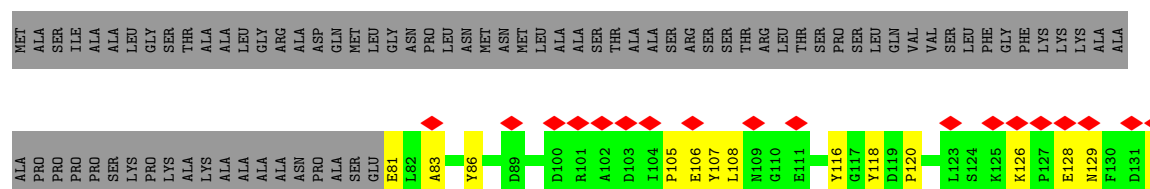




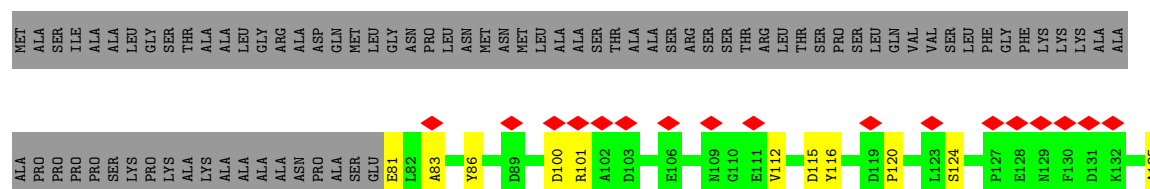
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

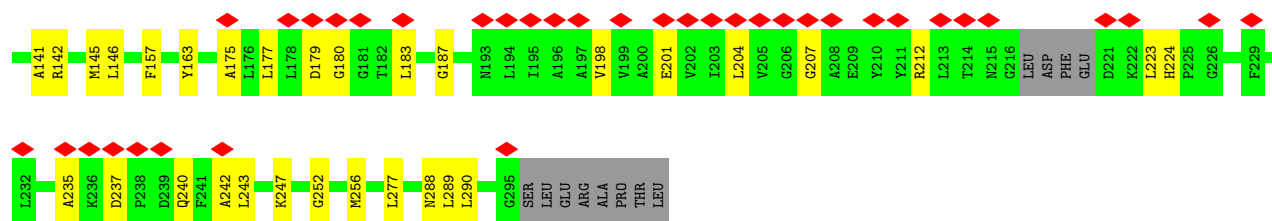


- Molecule 15: Chlorophyll a-b binding protein, chloroplastic

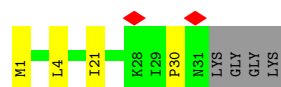
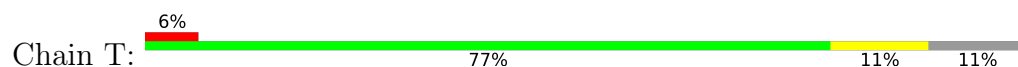


- Molecule 15: Chlorophyll a-b binding protein, chloroplastic

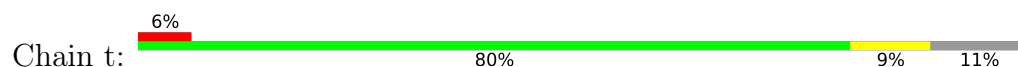




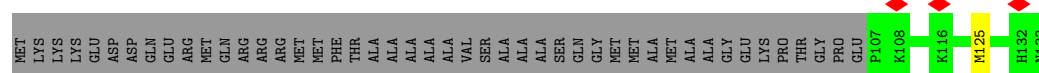
- Molecule 16: Photosystem II reaction center protein T



- Molecule 16: Photosystem II reaction center protein T



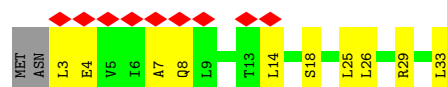
- Molecule 17: Photosystem II 5 kDa protein, chloroplastic

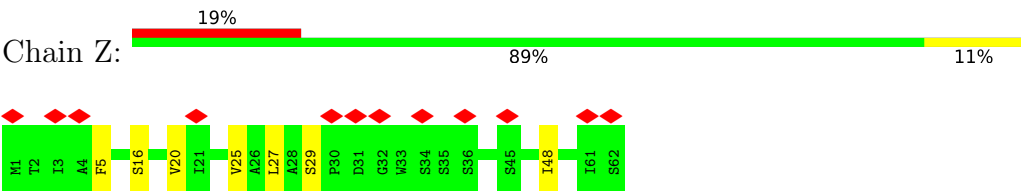


- Molecule 17: Photosystem II 5 kDa protein, chloroplastic

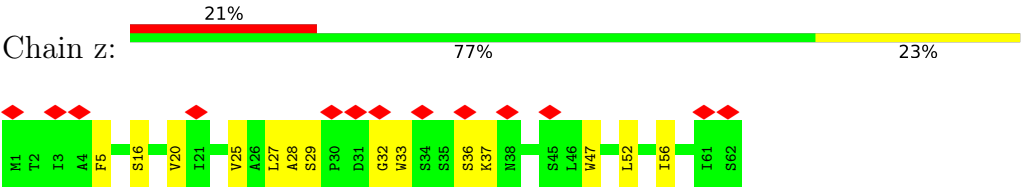


- Molecule 18: Photosystem II reaction center protein Ycf12





• Molecule 21: 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	60956	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	120	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	7.081	Depositor
Minimum map value	-3.771	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.210	Depositor
Recommended contour level	0.886	Depositor
Map size ($\text{\AA}$)	430.64896, 430.64896, 430.64896	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.96127, 0.96127, 0.96127	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, DGD, XAT, FE2, DGA, SQD, PHO, MG, 3PH, PAM, LMG, LUT, VIV, LNL, NEX, HEM, BCT, LHG, PL9, BCR, CHL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.14	0/2578	0.29	0/3513
1	a	0.13	0/2578	0.33	0/3513
2	B	0.13	0/3940	0.29	0/5363
2	b	0.14	0/3940	0.31	0/5363
3	C	0.21	2/3493 (0.1%)	0.28	0/4757
3	c	0.19	1/3493 (0.0%)	0.30	0/4757
4	D	0.12	0/2778	0.28	0/3786
4	d	0.16	0/2777	0.30	0/3786
5	E	0.12	0/555	0.25	0/756
5	e	0.12	0/555	0.27	0/756
6	F	0.11	0/247	0.22	0/333
6	f	0.12	0/247	0.26	0/333
7	G	0.15	0/1712	0.36	0/2335
7	N	0.13	0/1712	0.28	0/2335
7	Y	0.24	2/1712 (0.1%)	0.31	0/2335
7	g	0.15	0/1712	0.34	0/2335
7	n	0.13	0/1712	0.29	0/2335
7	y	0.13	0/1712	0.28	0/2335
8	H	0.18	0/475	0.35	0/647
8	h	0.23	0/475	0.36	0/647
9	I	0.12	0/305	0.29	0/409
9	i	0.12	0/305	0.29	0/409
10	K	0.16	0/313	0.34	0/428
10	k	0.15	0/313	0.34	0/428
11	L	0.09	0/309	0.22	0/421
11	l	0.10	0/309	0.23	0/421
12	M	0.10	0/242	0.23	0/330
12	m	0.12	0/242	0.27	0/330
13	O	0.09	0/1497	0.26	0/2017
13	o	0.10	0/1497	0.27	0/2017
14	R	0.10	0/1767	0.23	0/2397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
14	r	0.11	0/1767	0.26	0/2397
15	S	0.18	0/1673	0.28	0/2272
15	s	0.16	0/1673	0.27	0/2272
16	T	0.09	0/262	0.23	0/356
16	t	0.09	0/262	0.21	0/356
17	U	0.07	0/209	0.20	0/280
17	u	0.08	0/209	0.19	0/280
18	V	0.09	0/228	0.21	0/311
18	v	0.07	0/228	0.20	0/311
19	W	0.11	0/423	0.28	0/574
19	w	0.09	0/423	0.24	0/574
20	X	0.09	0/228	0.21	0/310
20	x	0.09	0/228	0.20	0/310
21	Z	0.10	0/463	0.24	0/633
21	z	0.10	0/463	0.23	0/633
All	All	0.15	5/54241 (0.0%)	0.29	0/73796

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	97	TRP	C-O	-5.82	1.17	1.24
3	c	97	TRP	C-O	-5.75	1.17	1.24
7	Y	163	HIS	CA-C	-5.53	1.46	1.53
3	C	151	TRP	C-N	5.46	1.42	1.33
7	Y	163	HIS	C-O	-5.09	1.17	1.23

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	2502	0	2425	45	0
1	a	2502	0	2425	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3812	0	3712	54	0
2	b	3812	0	3712	59	0
3	C	3377	0	3299	46	0
3	c	3377	0	3299	45	0
4	D	2686	0	2588	38	0
4	d	2685	0	2588	42	0
5	E	537	0	507	5	0
5	e	537	0	507	3	0
6	F	240	0	242	5	0
6	f	240	0	242	2	0
7	G	1659	0	1591	28	0
7	N	1659	0	1591	32	0
7	Y	1659	0	1591	17	0
7	g	1659	0	1591	32	0
7	n	1659	0	1591	29	0
7	y	1659	0	1591	15	0
8	H	462	0	471	7	0
8	h	462	0	471	5	0
9	I	297	0	310	5	0
9	i	297	0	310	8	0
10	K	302	0	311	3	0
10	k	302	0	311	3	0
11	L	302	0	300	8	0
11	l	302	0	300	5	0
12	M	238	0	256	4	0
12	m	238	0	256	5	0
13	O	1470	0	1468	21	0
13	o	1470	0	1468	21	0
14	R	1722	0	1708	21	0
14	r	1722	0	1708	24	0
15	S	1626	0	1593	29	0
15	s	1626	0	1593	34	0
16	T	254	0	268	4	0
16	t	254	0	268	3	0
17	U	205	0	213	1	0
17	u	205	0	213	1	0
18	V	228	0	267	7	0
18	v	228	0	267	3	0
19	W	415	0	413	9	0
19	w	415	0	413	13	0
20	X	226	0	236	0	0
20	x	226	0	236	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	Z	453	0	480	8	0
21	z	453	0	480	12	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	239	0	242	7	0
23	B	1024	0	1119	48	0
23	C	835	0	913	20	0
23	D	130	0	144	6	0
23	G	451	0	431	20	0
23	N	472	0	477	24	0
23	R	522	0	513	7	0
23	S	494	0	453	21	0
23	Y	520	0	576	23	0
23	a	239	0	242	6	0
23	b	1025	0	1119	39	0
23	c	840	0	923	23	0
23	d	130	0	144	4	0
23	g	472	0	477	19	0
23	n	456	0	444	21	0
23	r	522	0	513	11	0
23	s	494	0	453	26	0
23	y	520	0	576	23	0
24	A	64	0	74	3	0
24	D	64	0	74	4	0
24	a	64	0	74	3	0
24	d	64	0	74	2	0
25	A	40	0	56	4	0
25	B	119	0	165	14	0
25	C	40	0	56	6	0
25	D	40	0	56	2	0
25	H	40	0	56	2	0
25	K	40	0	56	0	0
25	V	40	0	56	0	0
25	Z	40	0	56	3	0
25	a	40	0	56	4	0
25	b	120	0	168	6	0
25	c	40	0	56	3	0
25	d	40	0	56	3	0
25	h	40	0	56	0	0
25	k	40	0	56	1	0
25	v	40	0	56	1	0
25	z	40	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	A	50	0	67	2	0
26	L	54	0	78	4	0
26	M	50	0	67	2	0
26	a	48	0	63	3	0
27	A	53	0	79	5	0
27	B	97	0	137	7	0
27	C	45	0	63	3	0
27	D	36	0	42	1	0
27	R	51	0	75	3	0
27	b	101	0	145	9	0
27	c	46	0	65	2	0
27	d	46	0	62	2	0
27	r	51	0	75	3	0
27	w	48	0	66	1	0
28	A	48	0	75	4	0
28	C	48	0	75	4	0
28	D	38	0	49	2	0
28	L	41	0	58	2	0
28	T	48	0	75	0	0
28	W	46	0	68	2	0
28	X	46	0	68	0	0
28	a	48	0	75	9	0
28	d	38	0	49	3	0
28	s	38	0	52	1	0
28	w	48	0	75	4	0
28	x	46	0	68	3	0
29	A	55	0	80	9	0
29	D	55	0	80	2	0
29	a	55	0	80	7	0
29	d	55	0	80	3	0
30	A	37	0	44	1	0
30	D	92	0	133	6	0
30	G	49	0	74	3	0
30	L	49	0	74	2	0
30	N	49	0	74	3	0
30	R	38	0	49	0	0
30	S	49	0	74	3	0
30	Y	49	0	74	5	0
30	a	49	0	74	4	0
30	b	49	0	74	1	0
30	d	98	0	148	5	0
30	g	49	0	74	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	n	45	0	63	2	0
30	r	37	0	44	0	0
30	s	49	0	74	2	0
30	y	49	0	74	3	0
31	A	40	0	58	3	0
31	B	80	0	116	9	0
31	C	120	0	174	8	0
31	I	20	0	29	0	0
31	a	40	0	58	2	0
31	b	80	0	116	6	0
31	c	120	0	174	7	0
31	i	20	0	29	2	0
32	B	18	0	29	1	0
32	b	18	0	29	0	0
33	C	66	0	96	3	0
33	H	62	0	82	1	0
33	c	55	0	68	1	0
33	d	62	0	82	3	0
34	C	1	0	0	0	0
34	c	1	0	0	0	0
35	C	31	0	49	5	0
35	y	31	0	49	4	0
36	D	4	0	0	5	0
36	d	4	0	0	5	0
37	D	40	0	65	3	0
37	b	44	0	76	4	0
38	F	43	0	30	3	0
38	f	43	0	30	2	0
39	G	412	0	387	19	0
39	N	364	0	354	18	0
39	R	182	0	177	8	0
39	S	201	0	147	9	0
39	Y	296	0	280	11	0
39	g	412	0	387	7	0
39	n	362	0	350	17	0
39	r	182	0	177	9	0
39	s	201	0	147	4	0
39	y	280	0	247	5	0
40	G	84	0	112	12	0
40	N	84	0	112	10	0
40	R	42	0	56	2	0
40	S	84	0	112	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	Y	84	0	112	9	0
40	g	84	0	112	14	0
40	n	84	0	112	11	0
40	r	42	0	56	3	0
40	s	84	0	112	3	0
40	y	84	0	112	5	0
41	G	24	0	29	2	0
41	N	44	0	56	2	0
41	R	88	0	112	2	0
41	S	23	0	28	2	0
41	Y	44	0	56	1	0
41	g	44	0	56	4	0
41	n	44	0	56	4	0
41	r	44	0	56	2	0
41	s	27	0	33	2	0
42	G	44	0	56	4	0
42	N	44	0	56	6	0
42	R	44	0	56	2	0
42	Y	44	0	56	4	0
42	n	88	0	112	8	0
42	r	44	0	56	3	0
42	y	44	0	56	2	0
43	A	28	0	0	0	0
43	B	31	0	0	0	0
43	C	10	0	0	0	0
43	D	18	0	0	0	0
43	E	4	0	0	0	0
43	H	10	0	0	0	0
43	I	1	0	0	1	0
43	L	2	0	0	0	0
43	N	4	0	0	0	0
43	O	4	0	0	0	0
43	R	8	0	0	0	0
43	S	1	0	0	0	0
43	T	5	0	0	0	0
43	U	1	0	0	0	0
43	V	1	0	0	0	0
43	Y	8	0	0	0	0
43	Z	1	0	0	0	0
43	a	20	0	0	0	0
43	b	31	0	0	0	0
43	c	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	d	25	0	0	1	0
43	e	4	0	0	0	0
43	f	1	0	0	0	0
43	g	1	0	0	0	0
43	h	11	0	0	0	0
43	i	2	0	0	0	0
43	l	4	0	0	1	0
43	n	1	0	0	0	0
43	o	2	0	0	0	0
43	r	7	0	0	0	0
43	t	4	0	0	0	0
43	v	2	0	0	1	0
43	x	1	0	0	0	0
43	y	13	0	0	1	0
All	All	71174	0	72294	1166	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1166) 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)
23:b:609:CLA:H2	23:b:610:CLA:HBB2	1.49	0.93
30:D:408:LHG:H262	11:L:23:LEU:HD22	1.60	0.83
3:c:216:SER:OG	3:c:221:GLU:OE2	1.96	0.83
2:b:372:ASP:OD1	2:b:373:LYS:N	2.16	0.79
30:G:618:LHG:H192	42:Y:301:XAT:H12	1.64	0.79
15:s:142:ARG:HB3	23:s:609:CLA:HBC3	1.67	0.77
29:a:411:PL9:H512	4:d:40:PRO:HB3	1.67	0.76
14:r:229:ASN:OD1	14:r:237:ARG:NH2	2.18	0.75
23:g:610:CLA:H52	40:g:615:LUT:H30	1.69	0.75
4:D:187:GLN:HB2	23:D:405:CLA:HBC1	1.69	0.74
39:G:607:CHL:H162	39:G:609:CHL:H92	1.68	0.74
4:d:297:TYR:OH	4:d:327:ARG:NH1	2.20	0.74
3:c:66:ALA:HA	10:k:38:MET:HE3	1.69	0.74
13:O:318:THR:HG22	13:O:325:PRO:HG3	1.69	0.74
1:a:272:HIS:CE1	36:d:401:BCT:O2	2.41	0.74
30:D:408:LHG:H322	16:T:21:ILE:HD11	1.69	0.73
23:b:603:CLA:HAB	23:b:605:CLA:H152	1.70	0.73
7:g:222:LYS:HD3	23:g:612:CLA:HAA2	1.71	0.72
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:HIS:CE1	36:D:401:BCT:O2	2.42	0.72
23:B:607:CLA:H52	27:B:620:LMG:H312	1.72	0.71
13:O:173:ARG:NH2	19:W:101:GLU:OE2	2.22	0.71
3:C:66:ALA:HA	10:K:38:MET:HE3	1.73	0.71
29:a:411:PL9:H402	4:d:43:TYR:HB2	1.72	0.71
4:d:187:GLN:HB2	23:d:405:CLA:HBC1	1.74	0.70
4:d:269:HIS:CE1	36:d:401:BCT:O3	2.45	0.70
27:C:525:LMG:H341	23:Y:314:CLA:H162	1.74	0.70
4:d:193:THR:HG23	23:d:405:CLA:HBC2	1.74	0.70
13:O:316:SER:HB3	13:O:326:LYS:H	1.58	0.69
1:a:140:ARG:NH2	30:a:412:LHG:O5	2.25	0.69
18:v:26:LEU:HB3	18:v:33:LEU:HD11	1.72	0.69
4:D:193:THR:HG23	23:D:405:CLA:HBC2	1.75	0.69
4:D:269:HIS:CE1	36:D:401:BCT:O3	2.45	0.69
2:b:218:SER:HB3	14:r:152:VAL:HG21	1.74	0.68
3:C:178:LYS:NZ	3:C:184:GLY:O	2.27	0.68
4:D:280:LEU:HD22	24:D:402:PHO:HBC3	1.76	0.68
14:R:166:GLY:HA3	14:R:268:ALA:HB1	1.74	0.68
4:d:156:PRO:HA	4:d:160:ILE:HB	1.74	0.68
1:A:184:ILE:HG23	1:A:328:MET:HE2	1.74	0.68
2:B:218:SER:HB3	14:R:152:VAL:HG21	1.74	0.68
1:a:184:ILE:HG23	1:a:328:MET:HE2	1.76	0.68
14:r:166:GLY:HA3	14:r:268:ALA:HB1	1.76	0.68
1:A:104:GLU:OE2	1:A:108:ASN:ND2	2.27	0.68
4:d:280:LEU:HD22	24:d:402:PHO:HBC3	1.76	0.68
13:o:316:SER:HB3	13:o:326:LYS:H	1.58	0.68
27:A:409:LMG:H381	3:C:281:LEU:HD21	1.76	0.67
1:A:120:LEU:HB3	33:C:515:DGD:HAV2	1.75	0.67
2:B:460:LEU:HD11	4:D:288:VAL:HG21	1.75	0.67
2:b:332:ASN:OD1	27:b:620:LMG:O4	2.12	0.67
23:G:610:CLA:H52	40:G:615:LUT:H30	1.77	0.67
7:g:110:ILE:HG13	39:g:609:CHL:HED1	1.76	0.67
23:s:609:CLA:H43	23:s:611:CLA:HBA1	1.76	0.67
31:c:517:LNL:H71	31:c:519:LNL:H52	1.76	0.67
23:n:610:CLA:HBB1	23:n:612:CLA:H3A	1.77	0.67
1:a:43:THR:HG23	25:a:408:BCR:H362	1.76	0.67
3:c:255:LYS:NZ	19:w:140:GLU:OE2	2.28	0.67
14:r:293:PHE:HB2	40:r:613:LUT:H22	1.75	0.67
3:c:178:LYS:NZ	3:c:184:GLY:O	2.28	0.67
23:N:613:CLA:HBA1	23:N:613:CLA:HBD	1.76	0.66
1:A:43:THR:HG23	25:A:407:BCR:H362	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:n:222:LYS:HE2	23:n:612:CLA:HBD	1.77	0.66
1:A:215:HIS:HA	29:A:411:PL9:HC2	1.76	0.66
7:N:222:LYS:NZ	23:N:612:CLA:O1D	2.29	0.66
13:O:101:TYR:O	13:O:105:GLN:NE2	2.29	0.66
2:B:440:ASP:OD1	2:B:441:GLY:N	2.28	0.66
23:B:614:CLA:H121	28:L:102:3PH:H391	1.78	0.66
7:n:206:PRO:HD2	40:n:615:LUT:H23	1.78	0.66
4:D:173:SER:HB2	4:D:178:ALA:HB1	1.79	0.66
7:N:206:PRO:HD2	40:N:615:LUT:H23	1.78	0.65
7:y:234:MET:HE2	40:y:317:LUT:H10	1.78	0.65
1:a:259:ILE:HA	29:a:411:PL9:H303	1.78	0.65
1:A:133:LEU:HD23	4:D:257:ILE:HG12	1.79	0.65
1:A:271:LEU:HD11	29:A:411:PL9:HC8	1.78	0.65
4:d:173:SER:HB2	4:d:178:ALA:HB1	1.79	0.65
23:b:607:CLA:H193	11:l:29:ALA:HA	1.79	0.65
7:g:147:ILE:HG21	7:g:167:ILE:HD12	1.78	0.64
2:b:55:MET:HE1	2:b:67:THR:HG21	1.80	0.64
1:a:100:ALA:N	1:a:104:GLU:OE2	2.31	0.64
2:b:311:PHE:O	2:b:317:ASN:ND2	2.31	0.64
23:G:602:CLA:H162	23:Y:304:CLA:H193	1.78	0.64
3:c:204:LEU:HB3	35:y:301:VIV:H151	1.80	0.64
39:g:607:CHL:H191	39:n:601:CHL:H52	1.80	0.64
23:g:610:CLA:HBA1	40:g:615:LUT:H382	1.80	0.63
31:A:414:LNL:H10	25:b:619:BCR:H382	1.81	0.63
3:c:243:ILE:HG12	35:y:301:VIV:H27	1.80	0.63
15:S:132:LYS:HG3	23:S:608:CLA:H41	1.81	0.63
2:b:276:ASP:OD1	2:b:361:THR:OG1	2.17	0.63
23:s:602:CLA:HAB	40:s:615:LUT:H32	1.79	0.63
3:C:80:PRO:HG2	3:C:83:GLU:HG3	1.81	0.62
39:R:606:CHL:HBB2	23:R:608:CLA:HBC1	1.81	0.62
7:n:191:LEU:HG	39:n:608:CHL:HAB	1.80	0.62
1:a:133:LEU:HD23	4:d:257:ILE:HG12	1.81	0.62
4:d:181:ARG:NH2	4:d:334:ASP:OD1	2.29	0.62
2:B:311:PHE:O	2:B:317:ASN:ND2	2.31	0.62
23:B:603:CLA:HAB	23:B:605:CLA:H162	1.81	0.62
23:B:613:CLA:HED3	23:B:613:CLA:H2	1.81	0.62
23:b:615:CLA:H172	23:b:615:CLA:H91	1.80	0.62
2:B:77:GLY:O	2:B:84:THR:OG1	2.16	0.62
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.81	0.61
2:B:458:PHE:HB3	23:B:604:CLA:HBC2	1.82	0.61
7:N:191:LEU:HD21	39:N:606:CHL:H162	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:128:THR:OG1	2:b:130:LYS:NZ	2.20	0.61
1:A:234:ASN:ND2	30:L:103:LHG:O4	2.33	0.61
2:B:332:ASN:OD1	27:B:620:LMG:O4	2.16	0.61
2:B:157:HIS:HA	2:B:163:GLY:HA3	1.83	0.61
16:T:1:MET:HG2	31:b:622:LNL:H62	1.81	0.61
19:w:109:LEU:HA	19:w:114:LEU:HD23	1.83	0.61
30:N:618:LHG:H121	30:N:618:LHG:H302	1.82	0.61
38:F:501:HEM:HMC2	38:F:501:HEM:HBC2	1.83	0.61
1:a:98:GLU:OE2	19:w:100:THR:OG1	2.19	0.61
27:b:620:LMG:H382	12:m:14:PHE:HB2	1.82	0.61
30:g:618:LHG:H192	42:y:302:XAT:H12	1.83	0.61
2:B:148:VAL:HG13	27:R:617:LMG:H402	1.83	0.61
14:R:159:ARG:NH1	14:R:162:GLU:OE1	2.34	0.61
15:S:120:PRO:HD2	40:S:615:LUT:H23	1.83	0.61
2:b:460:LEU:HD11	4:d:288:VAL:HG21	1.82	0.60
27:B:620:LMG:H381	12:M:14:PHE:HB2	1.82	0.60
4:D:156:PRO:HA	4:D:160:ILE:HB	1.83	0.60
23:B:602:CLA:H41	8:H:58:LEU:HA	1.83	0.60
3:C:181:TYR:O	3:C:198:LYS:NZ	2.32	0.60
38:f:501:HEM:HBC2	38:f:501:HEM:HMC2	1.83	0.60
2:b:458:PHE:HB3	23:b:604:CLA:HBC2	1.84	0.60
23:B:607:CLA:H202	27:B:620:LMG:H361	1.84	0.60
23:G:604:CLA:HBB1	40:G:616:LUT:H192	1.83	0.60
27:c:523:LMG:H112	23:y:312:CLA:H12	1.84	0.60
7:G:112:SER:OG	7:G:227:GLY:HA3	2.02	0.60
7:n:64:ARG:NH1	7:n:80:THR:O	2.35	0.60
2:B:327:ALA:HB1	27:B:620:LMG:HC8	1.84	0.59
31:B:622:LNL:H82	16:t:4:LEU:HG	1.84	0.59
23:N:610:CLA:HBB1	23:N:612:CLA:H3A	1.85	0.59
18:V:26:LEU:HB3	18:V:33:LEU:HD11	1.84	0.59
13:O:216:VAL:HG11	13:O:326:LYS:HD2	1.83	0.59
2:b:157:HIS:HA	2:b:163:GLY:HA3	1.85	0.59
2:B:235:GLU:OE1	2:B:472:ARG:NH1	2.35	0.59
7:G:222:LYS:HD3	23:G:612:CLA:HAA2	1.84	0.59
25:a:408:BCR:H401	28:a:410:3PH:H32	1.83	0.59
3:c:282:PHE:HE1	23:c:501:CLA:H111	1.66	0.59
14:r:221:LEU:HD13	14:r:224:ILE:HD11	1.83	0.59
1:A:188:ALA:HB2	1:A:328:MET:HB3	1.85	0.59
23:S:609:CLA:H92	40:S:614:LUT:H371	1.84	0.59
7:n:170:ILE:HG12	39:n:605:CHL:HAC1	1.83	0.59
7:y:78:TYR:OH	7:y:90:ASP:OD2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.38	0.59
23:g:603:CLA:H51	23:n:603:CLA:H41	1.84	0.59
23:g:604:CLA:HBB1	40:g:616:LUT:H192	1.84	0.59
5:E:21:VAL:HG23	5:E:22:ILE:HD12	1.84	0.58
7:N:100:THR:O	7:N:104:ASN:ND2	2.36	0.58
14:R:221:LEU:HA	14:R:224:ILE:HG12	1.85	0.58
5:e:60:ARG:NE	5:e:64:PRO:HG3	2.18	0.58
7:n:229:LEU:HD22	40:n:615:LUT:H202	1.84	0.58
1:a:93:PHE:HZ	23:a:407:CLA:HAA1	1.69	0.58
15:S:116:TYR:OH	30:S:616:LHG:O5	2.21	0.58
19:W:109:LEU:HA	19:W:114:LEU:HD11	1.84	0.58
1:a:188:ALA:HB2	1:a:328:MET:HB3	1.85	0.58
1:a:77:ILE:HD13	11:l:30:VAL:HG13	1.86	0.58
13:O:319:ASP:HB2	13:O:323:LYS:HE3	1.84	0.58
9:i:35:LYS:HE2	19:w:144:LEU:HD23	1.84	0.58
23:b:607:CLA:H52	27:b:620:LMG:H312	1.85	0.58
29:d:407:PL9:H401	30:d:408:LHG:H202	1.84	0.58
1:a:259:ILE:HG13	1:a:260:PHE:H	1.68	0.58
23:B:606:CLA:HHC	23:B:606:CLA:HBB1	1.85	0.58
7:G:109:VAL:HG11	7:G:198:ILE:HG23	1.86	0.58
7:N:177:LEU:HD22	41:N:617:NEX:H15	1.86	0.58
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.39	0.58
37:b:626:DGA:HB72	28:d:403:3PH:H12	1.85	0.58
27:b:628:LMG:H171	39:r:606:CHL:HBB1	1.86	0.58
3:C:170:VAL:HG13	28:C:524:3PH:H3I3	1.86	0.57
13:o:151:THR:HB	13:o:165:PHE:HB3	1.85	0.57
28:D:403:3PH:H262	37:D:410:DGA:HB92	1.84	0.57
7:y:240:GLN:HE22	40:y:316:LUT:H42	1.69	0.57
13:o:152:VAL:HB	13:o:210:LEU:HD21	1.86	0.57
2:B:348:ASP:OD1	2:B:349:LYS:N	2.36	0.57
3:C:282:PHE:HE1	23:C:501:CLA:H111	1.69	0.57
26:M:101:SQD:H122	23:b:614:CLA:H43	1.87	0.57
42:N:619:XAT:H361	30:Y:318:LHG:HC91	1.86	0.57
7:g:158:ASN:HB2	7:g:161:LEU:HD13	1.86	0.57
7:G:60:TYR:HE1	7:G:84:PRO:HA	1.68	0.57
13:o:146:GLU:OE2	19:w:93:LEU:N	2.38	0.57
1:A:93:PHE:HZ	23:A:406:CLA:HAA1	1.69	0.57
27:C:525:LMG:H112	23:Y:311:CLA:H12	1.87	0.57
38:f:501:HEM:HMB1	38:f:501:HEM:HBB2	1.86	0.57
3:C:42:LEU:HD21	23:C:511:CLA:H2A	1.87	0.57
23:G:610:CLA:HBA1	40:G:615:LUT:H382	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:5:THR:HG21	12:m:5:THR:HG21	1.87	0.57
41:R:618:NEX:H15	7:y:177:LEU:HD22	1.87	0.57
23:N:602:CLA:H72	40:N:616:LUT:H30	1.85	0.56
39:N:609:CHL:H43	39:Y:302:CHL:H12	1.86	0.56
1:a:234:ASN:ND2	30:b:627:LHG:O4	2.33	0.56
2:B:153:PHE:HB2	23:B:606:CLA:HBB1	1.87	0.56
3:C:452:ALA:HB1	19:W:144:LEU:HB3	1.87	0.56
7:N:123:VAL:HG23	7:N:249:LEU:HD11	1.86	0.56
7:N:205:ASP:OD1	40:N:615:LUT:O23	2.20	0.56
30:a:412:LHG:H271	30:a:412:LHG:H321	1.87	0.56
7:g:84:PRO:HB2	7:g:224:ILE:HD12	1.87	0.56
7:g:129:ALA:HB2	7:g:135:PHE:HD1	1.70	0.56
7:g:229:LEU:HD23	40:g:615:LUT:H203	1.86	0.56
14:R:156:GLN:HE21	14:R:234:PRO:HB3	1.69	0.56
23:b:606:CLA:HHC	23:b:606:CLA:HBB1	1.87	0.56
28:w:202:3PH:H3D2	23:y:313:CLA:H141	1.86	0.56
3:C:204:LEU:HB3	35:C:523:VIV:H151	1.86	0.56
3:c:206:PRO:HD3	35:y:301:VIV:H111	1.87	0.56
30:n:619:LHG:H302	30:n:619:LHG:HC82	1.88	0.56
2:b:327:ALA:HB1	27:b:620:LMG:HC8	1.88	0.56
39:n:605:CHL:HBA2	15:s:157:PHE:HE1	1.71	0.56
15:s:179:ASP:OD1	15:s:180:GLY:N	2.36	0.56
26:L:101:SQD:H372	16:t:15:GLY:HA3	1.87	0.56
1:A:98:GLU:OE2	19:W:100:THR:OG1	2.24	0.56
23:G:603:CLA:H51	23:N:603:CLA:H41	1.88	0.56
7:g:129:ALA:HB2	7:g:135:PHE:CD1	2.40	0.56
7:n:191:LEU:HD21	39:n:606:CHL:H171	1.87	0.56
21:z:16:SER:OG	21:z:47:TRP:NE1	2.37	0.56
28:A:410:3PH:H261	31:b:625:LNL:H31	1.87	0.55
3:C:83:GLU:OE2	3:C:398:HIS:NE2	2.39	0.55
31:c:521:LNL:H12	23:y:315:CLA:H112	1.87	0.55
15:s:146:LEU:HG	23:s:604:CLA:HAB	1.88	0.55
2:B:74:SER:HA	2:B:92:SER:HB2	1.86	0.55
38:F:501:HEM:HMB2	38:F:501:HEM:HBB2	1.88	0.55
7:G:106:GLU:HG2	7:G:198:ILE:HD11	1.87	0.55
30:G:618:LHG:HC91	42:Y:301:XAT:H361	1.88	0.55
2:b:440:ASP:OD1	2:b:441:GLY:N	2.40	0.55
27:d:409:LMG:H171	25:d:410:BCR:H332	1.88	0.55
15:s:235:ALA:HB2	23:s:609:CLA:HAA2	1.88	0.55
3:C:464:GLU:OE2	4:D:246:SER:OG	2.25	0.55
3:c:163:ILE:HG23	31:c:517:LNL:H15	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:327:ALA:O	2:b:444:ARG:NH1	2.40	0.55
1:A:64:ARG:HH21	13:O:172:THR:HB	1.71	0.55
2:b:348:ASP:OD1	2:b:349:LYS:N	2.37	0.55
3:C:205:ASN:OD1	3:C:207:SER:OG	2.22	0.55
7:G:212:ASP:HB3	7:G:215:ALA:HB3	1.89	0.55
15:S:235:ALA:HB2	23:S:609:CLA:HAA2	1.89	0.55
3:c:28:GLN:HE22	4:d:231:ASN:HD22	1.54	0.55
3:c:42:LEU:HD21	23:c:511:CLA:H2A	1.88	0.55
23:g:602:CLA:H162	23:y:305:CLA:H193	1.88	0.55
7:G:161:LEU:O	7:G:163:HIS:N	2.39	0.55
7:N:170:ILE:HG12	39:N:605:CHL:HAC1	1.87	0.55
39:G:609:CHL:HBB1	39:N:601:CHL:H52	1.89	0.55
4:D:40:PRO:HB2	23:D:406:CLA:HBB1	1.88	0.54
4:D:192:TRP:CE3	4:D:290:LEU:HD11	2.42	0.54
26:a:409:SQD:O9	4:d:231:ASN:ND2	2.40	0.54
23:n:603:CLA:HBB1	39:n:609:CHL:H161	1.89	0.54
1:A:45:THR:HG23	23:A:403:CLA:H201	1.89	0.54
1:a:45:THR:HG23	23:a:404:CLA:H201	1.89	0.54
23:b:601:CLA:H42	31:b:624:LNL:H61	1.88	0.54
39:n:607:CHL:H8	39:n:609:CHL:H172	1.90	0.54
1:a:259:ILE:HG13	1:a:260:PHE:N	2.21	0.54
1:a:252:HIS:ND1	1:a:265:PHE:O	2.36	0.54
2:b:153:PHE:HB2	23:b:606:CLA:HBB1	1.89	0.54
7:n:263:ASN:OD1	7:n:264:ALA:N	2.41	0.54
39:n:601:CHL:HH1	30:n:619:LHG:HC41	1.90	0.54
1:A:252:HIS:ND1	1:A:265:PHE:O	2.37	0.54
23:G:603:CLA:H122	39:G:609:CHL:H121	1.89	0.54
7:g:102:ALA:O	7:g:106:GLU:HG3	2.08	0.54
14:r:156:GLN:HE21	14:r:234:PRO:HB3	1.72	0.54
30:s:616:LHG:H311	28:s:618:3PH:H3A2	1.90	0.54
21:z:32:GLY:O	21:z:36:SER:CB	2.56	0.54
16:T:4:LEU:HD11	31:b:623:LNL:H81	1.90	0.54
7:n:94:LEU:HD13	23:n:602:CLA:H42	1.89	0.54
3:C:206:PRO:HD3	35:C:523:VIV:H112	1.90	0.54
15:S:146:LEU:HG	23:S:604:CLA:HAB	1.89	0.54
4:D:190:HIS:CE1	4:D:295:ARG:HH21	2.25	0.53
1:a:60:ILE:HD12	1:a:84:PRO:HD2	1.88	0.53
1:a:217:SER:HA	4:d:273:LEU:HD12	1.88	0.53
15:s:116:TYR:OH	30:s:616:LHG:O5	2.25	0.53
15:s:175:ALA:HB2	39:s:606:CHL:HED2	1.90	0.53
15:s:288:ASN:HD21	23:s:613:CLA:H101	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:GLY:HA3	23:C:511:CLA:HMD2	1.90	0.53
4:D:185:PHE:HA	4:D:330:MET:HE1	1.89	0.53
7:n:90:ASP:OD2	7:n:95:SER:OG	2.25	0.53
39:g:606:CHL:HMC	40:g:616:LUT:H162	1.91	0.53
14:r:209:ASN:OD1	14:r:210:MET:N	2.41	0.53
39:G:609:CHL:C4B	39:N:601:CHL:H2	2.39	0.53
23:b:615:CLA:H172	23:b:615:CLA:H112	1.90	0.53
27:r:617:LMG:H341	27:r:617:LMG:H271	1.91	0.53
23:c:511:CLA:H143	21:z:20:VAL:HG13	1.91	0.53
1:A:131:TRP:HZ2	3:C:449:ARG:HG2	1.73	0.53
4:D:194:LEU:O	11:L:35:TYR:OH	2.25	0.53
4:D:202:VAL:HG22	23:D:405:CLA:C1B	2.39	0.53
7:G:118:GLY:HA3	40:G:616:LUT:H10	1.90	0.53
2:b:217:LEU:HB3	23:r:612:CLA:HBA2	1.91	0.53
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.90	0.53
1:A:77:ILE:HD13	11:L:30:VAL:HG13	1.91	0.53
4:d:47:GLY:HA3	25:d:410:BCR:H372	1.90	0.53
4:d:142:TYR:OH	30:d:404:LHG:O4	2.16	0.53
7:G:181:VAL:HA	7:G:184:TYR:HD2	1.74	0.53
15:s:138:LEU:HD23	15:s:223:LEU:HB3	1.91	0.53
7:G:102:ALA:O	7:G:106:GLU:HG3	2.08	0.52
9:I:6:LEU:HD23	19:W:114:LEU:HB3	1.90	0.52
7:Y:112:SER:HB3	7:Y:227:GLY:HA3	1.90	0.52
4:d:202:VAL:HG22	23:d:405:CLA:C1B	2.39	0.52
7:N:113:ARG:NH1	39:N:608:CHL:OBD	2.42	0.52
2:B:345:ILE:HD12	2:B:402:TYR:CE2	2.45	0.52
7:n:123:VAL:HG23	7:n:249:LEU:HD11	1.91	0.52
23:s:602:CLA:H2A	23:s:602:CLA:HED2	1.91	0.52
1:A:110:GLY:N	1:A:111:PRO:HD2	2.25	0.52
4:D:264:ASN:HB3	4:D:267:TRP:HB3	1.91	0.52
23:G:602:CLA:H91	23:Y:304:CLA:H61	1.90	0.52
7:n:146:GLN:HE21	7:n:153:LEU:HG	1.74	0.52
15:s:145:MET:HG3	15:s:252:GLY:HA2	1.91	0.52
2:b:457:THR:HG21	27:b:620:LMG:H241	1.92	0.52
23:c:505:CLA:CMD	23:c:507:CLA:HAB	2.39	0.52
8:H:72:VAL:HG12	8:H:72:VAL:O	2.09	0.52
26:M:101:SQD:H151	23:b:614:CLA:H151	1.91	0.52
27:b:620:LMG:O10	12:m:4:ASN:ND2	2.43	0.52
4:d:264:ASN:HB3	4:d:267:TRP:HB3	1.90	0.52
15:s:204:LEU:HD12	39:s:605:CHL:HMA2	1.91	0.52
26:L:101:SQD:H242	26:L:101:SQD:H81	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ASN:HD21	1:A:322:ASN:HD22	1.58	0.52
26:A:408:SQD:H292	23:C:508:CLA:H71	1.91	0.52
28:A:410:3PH:H3D1	2:b:102:MET:HE2	1.92	0.52
23:C:505:CLA:CMD	23:C:507:CLA:HAB	2.40	0.52
4:D:55:PHE:O	5:E:49:SER:OG	2.28	0.52
6:F:20:LEU:O	6:F:24:THR:OG1	2.25	0.52
15:S:232:LEU:HD22	40:S:614:LUT:H363	1.91	0.52
23:S:609:CLA:H43	23:S:611:CLA:HBA1	1.90	0.52
7:g:177:LEU:HD22	41:g:617:NEX:H15	1.91	0.52
13:o:237:GLN:HB3	13:o:289:LYS:HE2	1.92	0.52
14:r:167:ARG:NH1	39:r:607:CHL:OBD	2.43	0.52
14:r:285:THR:HG22	14:r:287:LYS:HG2	1.92	0.52
23:B:614:CLA:H122	26:L:101:SQD:H152	1.92	0.52
15:S:141:ALA:HB1	15:S:252:GLY:HA3	1.92	0.52
18:V:26:LEU:HD21	21:Z:25:VAL:HA	1.92	0.52
3:c:38:GLY:HA3	23:c:511:CLA:HMD2	1.90	0.52
23:R:609:CLA:H52	40:R:613:LUT:H30	1.92	0.51
2:b:464:PHE:HD2	23:b:611:CLA:HAC2	1.74	0.51
21:z:32:GLY:O	21:z:36:SER:HB2	2.11	0.51
14:r:163:LEU:HD12	14:r:238:LEU:HD21	1.93	0.51
23:s:603:CLA:HBC1	23:s:608:CLA:HAC1	1.92	0.51
23:y:314:CLA:HBB1	30:y:318:LHG:H321	1.91	0.51
1:A:84:PRO:HA	1:A:112:TYR:CG	2.46	0.51
23:C:513:CLA:H101	25:Z:101:BCR:H23C	1.91	0.51
7:N:127:LEU:HD11	23:N:611:CLA:H201	1.92	0.51
15:S:175:ALA:HB2	39:S:606:CHL:HED2	1.93	0.51
7:g:113:ARG:NH1	39:g:608:CHL:OBD	2.41	0.51
39:y:303:CHL:HMA3	30:y:318:LHG:H112	1.92	0.51
2:B:76:THR:HG1	2:B:78:TRP:CD1	2.28	0.51
3:C:250:TRP:HB2	23:Y:314:CLA:H141	1.92	0.51
9:I:28:PRO:HB3	19:W:144:LEU:HD12	1.93	0.51
13:O:319:ASP:HB3	13:O:322:SER:HB2	1.91	0.51
39:S:607:CHL:HMA1	41:S:617:NEX:H203	1.93	0.51
23:R:604:CLA:H92	39:R:605:CHL:HBA2	1.93	0.51
15:S:118:TYR:OH	39:S:601:CHL:O1A	2.28	0.51
2:b:25:MET:HE1	2:b:108:PHE:HD1	1.76	0.51
27:A:409:LMG:H141	33:C:515:DGD:HAT1	1.93	0.51
2:b:76:THR:HG1	2:b:78:TRP:CD1	2.28	0.51
3:c:385:GLN:HB2	3:c:388:GLN:HG3	1.93	0.51
1:A:280:VAL:HG11	30:A:412:LHG:H282	1.92	0.51
2:B:297:SER:OG	2:B:300:GLU:OE1	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:50:LEU:HD11	23:c:513:CLA:HMB2	1.92	0.51
4:d:269:HIS:HE1	36:d:401:BCT:O3	1.92	0.51
39:n:606:CHL:HBA1	41:n:618:NEX:H403	1.92	0.51
26:A:408:SQD:O7	4:D:231:ASN:ND2	2.43	0.51
27:A:409:LMG:H242	25:C:514:BCR:H331	1.92	0.51
35:C:523:VIV:H143	23:Y:314:CLA:HMB1	1.93	0.51
2:b:123:PHE:HB2	2:b:131:LEU:HD22	1.93	0.51
23:g:604:CLA:H12	41:g:617:NEX:H241	1.93	0.51
2:B:25:MET:HE1	2:B:108:PHE:HD1	1.76	0.51
3:C:48:LYS:NZ	3:C:133:ALA:O	2.43	0.51
42:N:619:XAT:H193	23:Y:313:CLA:H43	1.92	0.51
23:b:609:CLA:H42	8:h:47:MET:HE1	1.93	0.51
2:B:464:PHE:HD2	23:B:611:CLA:HAC2	1.75	0.51
15:S:142:ARG:HB3	23:S:609:CLA:HBC3	1.93	0.51
13:o:316:SER:OG	13:o:317:ASP:N	2.44	0.51
7:N:112:SER:HB2	7:N:227:GLY:HA3	1.93	0.50
13:O:186:GLU:HG2	13:O:194:LYS:HB3	1.92	0.50
1:a:103:ASP:HB3	13:o:171:MET:HE1	1.91	0.50
23:g:602:CLA:HBA1	40:g:616:LUT:H382	1.93	0.50
21:z:25:VAL:O	21:z:29:SER:OG	2.23	0.50
15:s:142:ARG:HH22	15:s:224:HIS:CD2	2.28	0.50
2:B:374:GLU:HG3	2:B:376:ILE:HG12	1.93	0.50
4:D:142:TYR:OH	30:D:404:LHG:O4	2.13	0.50
3:c:135:ILE:HD13	21:z:27:LEU:HD22	1.92	0.50
7:G:64:ARG:HD2	7:G:86:ASP:O	2.10	0.50
14:R:209:ASN:OD1	14:R:210:MET:N	2.42	0.50
1:a:131:TRP:CZ2	3:c:449:ARG:HD2	2.45	0.50
1:a:131:TRP:CH2	23:c:505:CLA:HAA2	2.46	0.50
3:c:110:PRO:HB3	31:c:520:LNL:H51	1.93	0.50
7:n:234:MET:HG3	40:n:616:LUT:H12	1.93	0.50
25:B:617:BCR:H323	31:B:623:LNL:H9	1.94	0.50
25:B:617:BCR:H383	26:L:101:SQD:H102	1.92	0.50
25:B:619:BCR:H382	31:a:401:LNL:H111	1.94	0.50
15:S:105:PRO:HG2	15:S:108:LEU:HD12	1.93	0.50
2:B:141:ILE:HG21	23:B:615:CLA:HBB1	1.93	0.50
14:R:167:ARG:NH1	39:R:607:CHL:OBD	2.44	0.50
23:c:510:CLA:H2	23:c:510:CLA:HED2	1.93	0.50
7:g:222:LYS:HD3	23:g:612:CLA:HBD	1.93	0.50
3:C:216:SER:OG	3:C:221:GLU:OE1	2.22	0.50
13:O:151:THR:HB	13:O:165:PHE:HB3	1.94	0.50
39:S:605:CHL:HMC	39:S:606:CHL:C4C	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:166:SER:HB2	4:D:170:PHE:HE2	1.77	0.50
19:W:123:THR:HG21	28:W:201:3PH:H3H1	1.93	0.50
7:Y:78:TYR:OH	7:Y:90:ASP:OD2	2.23	0.50
7:Y:116:MET:SD	23:Y:310:CLA:HAB	2.52	0.50
7:g:118:GLY:HA3	40:g:616:LUT:H10	1.94	0.50
7:g:185:ARG:HG3	39:g:608:CHL:C1D	2.41	0.50
1:A:286:THR:HG22	23:A:402:CLA:O1D	2.12	0.49
1:a:34:GLY:HA2	1:a:37:MET:HB3	1.94	0.49
1:a:286:THR:HG22	23:a:403:CLA:O1D	2.12	0.49
1:A:131:TRP:CH2	23:C:505:CLA:HAA2	2.48	0.49
25:C:514:BCR:HC41	9:I:24:LEU:HG	1.94	0.49
5:E:55:TYR:O	5:E:60:ARG:NH2	2.45	0.49
23:N:602:CLA:HBA1	40:N:616:LUT:H382	1.94	0.49
4:d:130:GLN:NE2	24:d:402:PHO:OBD	2.45	0.49
1:A:27:ARG:H	31:A:414:LNL:H32	1.76	0.49
23:G:602:CLA:HBA1	40:G:616:LUT:H382	1.93	0.49
15:S:232:LEU:HB2	40:S:614:LUT:H222	1.94	0.49
14:r:251:ALA:HB1	14:r:257:LYS:HG2	1.93	0.49
15:s:141:ALA:HB2	15:s:256:MET:HE2	1.93	0.49
14:R:293:PHE:HB2	40:R:613:LUT:H22	1.93	0.49
7:Y:123:VAL:HG13	7:Y:249:LEU:HD11	1.95	0.49
1:a:110:GLY:N	1:a:111:PRO:HD2	2.28	0.49
13:o:237:GLN:NE2	13:o:291:GLU:OE1	2.45	0.49
14:R:285:THR:HG21	14:R:292:LEU:HD21	1.94	0.49
3:c:281:LEU:O	3:c:285:ILE:HG13	2.13	0.49
7:y:116:MET:SD	23:y:311:CLA:HAB	2.52	0.49
7:y:178:MET:HA	7:y:181:VAL:HG22	1.94	0.49
7:G:189:GLY:N	39:G:608:CHL:OMC	2.45	0.49
13:O:230:THR:HG23	13:O:233:SER:H	1.78	0.49
27:R:617:LMG:H321	27:R:617:LMG:O8	2.12	0.49
1:a:84:PRO:HA	1:a:112:TYR:CG	2.47	0.49
4:d:55:PHE:O	5:e:49:SER:OG	2.29	0.49
15:s:141:ALA:HB1	15:s:252:GLY:HA3	1.94	0.49
23:y:304:CLA:HHC	40:y:317:LUT:H32	1.95	0.49
23:B:607:CLA:H193	11:L:29:ALA:HA	1.94	0.49
7:N:191:LEU:HG	39:N:608:CHL:HAB	1.95	0.49
29:A:411:PL9:H471	29:A:411:PL9:H451	1.47	0.49
2:B:220:ARG:HG3	8:H:32:LYS:HE3	1.95	0.49
39:N:609:CHL:HAA2	7:Y:91:THR:HG21	1.94	0.49
39:G:606:CHL:HMC	40:G:616:LUT:H162	1.94	0.49
15:S:86:TYR:CE2	15:S:242:ALA:HB1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:V:26:LEU:HG	21:Z:25:VAL:HG12	1.95	0.49
23:B:607:CLA:H2	27:B:620:LMG:H152	1.95	0.48
7:N:229:LEU:HD13	23:N:611:CLA:HBC1	1.94	0.48
2:b:231:MET:HE2	23:b:610:CLA:HMC2	1.94	0.48
30:d:408:LHG:H122	30:d:408:LHG:H271	1.94	0.48
39:G:601:CHL:H41	30:G:618:LHG:H172	1.95	0.48
7:N:100:THR:HG22	7:N:104:ASN:HD21	1.78	0.48
7:N:217:ALA:HA	7:N:220:LYS:HD3	1.95	0.48
3:C:57:ALA:O	3:C:61:VAL:HG23	2.13	0.48
11:L:9:GLN:NE2	14:R:123:ASN:OD1	2.42	0.48
23:Y:313:CLA:HMA2	40:Y:315:LUT:H3	1.95	0.48
3:c:380:LEU:HA	3:c:384:ILE:HD11	1.95	0.48
23:r:604:CLA:H92	39:r:605:CHL:HBA2	1.95	0.48
31:B:625:LNL:H31	28:a:410:3PH:H251	1.96	0.48
3:C:79:LYS:HB3	3:C:84:GLN:NE2	2.29	0.48
1:a:201:GLY:HA3	1:a:286:THR:OG1	2.14	0.48
3:c:57:ALA:O	3:c:61:VAL:HG23	2.13	0.48
23:r:604:CLA:HBA1	39:r:605:CHL:C1D	2.43	0.48
2:B:102:MET:HE2	28:a:410:3PH:H3E2	1.96	0.48
7:G:90:ASP:OD1	40:G:616:LUT:O23	2.30	0.48
7:G:222:LYS:HD3	23:G:612:CLA:HBD	1.96	0.48
7:N:107:LEU:HD13	23:N:603:CLA:HBA1	1.95	0.48
1:a:272:HIS:NE2	36:d:401:BCT:O2	2.47	0.48
23:b:602:CLA:H121	23:b:602:CLA:H161	1.58	0.48
23:n:613:CLA:H122	23:n:613:CLA:H161	1.71	0.48
42:n:620:XAT:H193	23:y:314:CLA:H43	1.95	0.48
23:S:604:CLA:HBB1	40:S:615:LUT:H192	1.94	0.48
2:b:389:LYS:HG3	2:b:390:TYR:CD1	2.48	0.48
23:b:616:CLA:H91	23:b:616:CLA:H112	1.63	0.48
23:c:506:CLA:H41	28:w:202:3PH:H262	1.96	0.48
7:n:64:ARG:NH2	7:n:86:ASP:OD1	2.47	0.48
15:s:124:SER:OG	23:s:602:CLA:HBA1	2.14	0.48
1:A:272:HIS:NE2	36:D:401:BCT:O2	2.46	0.48
3:C:307:PRO:HB3	3:C:358:PHE:HB3	1.95	0.48
3:c:141:GLU:HG3	3:c:148:GLY:HA3	1.96	0.48
4:d:194:LEU:O	11:l:35:TYR:OH	2.25	0.48
7:n:90:ASP:HA	40:n:616:LUT:H24	1.96	0.48
15:s:81:GLU:HG3	15:s:83:ALA:H	1.79	0.48
39:G:620:CHL:H161	39:Y:309:CHL:H72	1.95	0.47
15:S:265:GLN:O	15:S:269:THR:OG1	2.25	0.47
1:a:102:VAL:HB	28:a:410:3PH:H222	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:69:GLY:O	7:g:72:SER:OG	2.28	0.47
23:s:602:CLA:H3A	23:s:602:CLA:HBA2	1.36	0.47
39:y:303:CHL:H92	39:y:303:CHL:H62	1.78	0.47
23:Y:312:CLA:H112	23:Y:312:CLA:H72	1.65	0.47
23:b:607:CLA:H2	27:b:620:LMG:H152	1.96	0.47
27:b:620:LMG:H381	12:m:13:LEU:HD22	1.95	0.47
13:O:235:SER:HB2	13:O:293:THR:HG23	1.96	0.47
23:R:604:CLA:HBA1	39:R:605:CHL:C1D	2.44	0.47
3:c:281:LEU:HD21	27:w:201:LMG:H201	1.96	0.47
4:d:94:TRP:HB3	28:x:201:3PH:H221	1.94	0.47
33:d:411:DGD:O5D	33:d:411:DGD:O4D	2.31	0.47
23:g:613:CLA:H11	23:g:613:CLA:H52	1.71	0.47
9:I:35:LYS:NZ	43:I:201:HOH:O	2.47	0.47
15:S:205:VAL:O	15:S:209:GLU:HG2	2.13	0.47
3:c:166:ILE:HG13	3:c:248:GLY:HA3	1.96	0.47
3:C:117:LEU:HD13	31:C:519:LNL:H12	1.97	0.47
7:N:223:GLU:HB2	23:N:610:CLA:C1B	2.44	0.47
18:V:4:GLU:O	18:V:8:GLN:HG2	2.15	0.47
7:G:185:ARG:NH2	39:G:609:CHL:O1D	2.47	0.47
42:G:619:XAT:H11	42:G:619:XAT:H191	1.71	0.47
29:a:411:PL9:H18	29:a:411:PL9:H221	1.56	0.47
9:i:4:LEU:HD22	31:i:101:LNL:H51	1.96	0.47
14:r:225:GLU:OE1	14:r:228:ARG:NH2	2.38	0.47
23:s:609:CLA:H3A	23:s:609:CLA:HBA2	1.65	0.47
23:B:616:CLA:H11	25:B:619:BCR:H361	1.97	0.47
3:C:197:ARG:NH2	3:C:231:GLU:OE2	2.48	0.47
4:D:269:HIS:HE1	36:D:401:BCT:O3	1.92	0.47
23:G:613:CLA:H2	23:G:613:CLA:H61	1.59	0.47
7:N:174:GLN:OE1	39:N:607:CHL:HMC	2.15	0.47
23:N:603:CLA:CBB	40:N:616:LUT:H35	2.45	0.47
15:S:163:TYR:CD2	15:S:187:GLY:HA2	2.50	0.47
2:b:334:ASP:OD1	2:b:334:ASP:N	2.46	0.47
3:c:214:LEU:HB3	19:w:107:LEU:H	1.79	0.47
11:l:5:ASN:ND2	43:l:102:HOH:O	2.48	0.47
13:o:316:SER:N	13:o:326:LYS:O	2.45	0.47
39:s:606:CHL:HBA2	39:s:606:CHL:H3A	1.74	0.47
7:y:109:VAL:HG21	7:y:198:ILE:HD12	1.97	0.47
35:y:301:VIV:H143	23:y:315:CLA:HMB2	1.97	0.47
23:B:614:CLA:H8	25:B:617:BCR:H362	1.96	0.47
26:a:409:SQD:H142	26:a:409:SQD:H171	1.48	0.47
2:B:55:MET:HE1	2:B:67:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:V:25:LEU:O	18:V:29:ARG:HG3	2.14	0.47
7:Y:84:PRO:HB2	7:Y:224:ILE:HD12	1.95	0.47
3:c:459:ILE:HG21	3:c:464:GLU:HG3	1.96	0.47
31:c:521:LNL:H13	31:c:521:LNL:H10	1.62	0.47
7:g:146:GLN:HB2	7:g:153:LEU:HD12	1.97	0.47
42:n:617:XAT:H391	42:n:617:XAT:H31	1.68	0.47
1:A:34:GLY:HA2	1:A:37:MET:HB3	1.97	0.47
1:A:201:GLY:HA3	1:A:286:THR:OG1	2.14	0.47
10:K:25:PRO:HG2	10:K:28:TYR:HD1	1.80	0.47
7:N:263:ASN:OD1	7:N:264:ALA:N	2.47	0.47
31:C:522:LNL:H9	31:C:522:LNL:H62	1.75	0.46
13:O:288:SER:HB2	13:O:315:PRO:HG2	1.97	0.46
23:Y:303:CLA:HHC	40:Y:316:LUT:H32	1.96	0.46
3:c:197:ARG:NH2	3:c:231:GLU:OE2	2.46	0.46
7:G:164:ALA:HB1	7:G:170:ILE:HD11	1.97	0.46
7:N:124:PHE:HB3	7:N:125:PRO:HD3	1.97	0.46
39:S:606:CHL:HBA2	39:S:606:CHL:H3A	1.71	0.46
23:Y:305:CLA:H2	23:Y:305:CLA:H61	1.53	0.46
2:b:272:ARG:NH2	2:b:276:ASP:OD2	2.34	0.46
7:n:112:SER:HB2	7:n:227:GLY:HA3	1.97	0.46
2:b:201:HIS:HB2	23:b:602:CLA:CHB	2.45	0.46
2:b:462:PHE:HA	23:b:611:CLA:HMC2	1.97	0.46
7:n:107:LEU:HD13	23:n:603:CLA:HBA1	1.96	0.46
7:n:177:LEU:HD22	41:n:618:NEX:H15	1.98	0.46
30:D:408:LHG:H272	30:D:408:LHG:H242	1.57	0.46
7:G:147:ILE:HG21	7:G:167:ILE:HB	1.97	0.46
23:Y:305:CLA:H62	23:Y:305:CLA:H101	1.65	0.46
1:a:127:MET:HG3	1:a:144:ALA:HB1	1.96	0.46
39:G:609:CHL:H61	39:G:609:CHL:H41	1.62	0.46
7:n:153:LEU:HB3	7:n:164:ALA:HB3	1.97	0.46
42:n:617:XAT:H401	42:n:617:XAT:H35	1.79	0.46
13:o:238:PHE:HZ	13:o:314:GLN:HG2	1.80	0.46
14:r:170:MET:HE3	23:r:609:CLA:HMC2	1.97	0.46
7:y:127:LEU:HG	7:y:249:LEU:HD21	1.97	0.46
7:y:155:TYR:HB3	7:y:161:LEU:HB3	1.97	0.46
24:A:405:PHO:H61	24:A:405:PHO:H2	1.68	0.46
23:G:610:CLA:HHC	40:G:615:LUT:H32	1.97	0.46
14:R:95:LEU:HB3	14:R:159:ARG:HH21	1.81	0.46
1:a:272:HIS:HE1	36:d:401:BCT:O2	1.95	0.46
23:b:616:CLA:H141	23:b:616:CLA:H161	1.79	0.46
7:n:223:GLU:HB2	23:n:610:CLA:C1B	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:r:607:CHL:HBA2	39:r:607:CHL:H3A	1.63	0.46
21:z:32:GLY:O	21:z:36:SER:OG	2.33	0.46
2:B:128:THR:HG23	2:B:130:LYS:HG2	1.96	0.46
2:B:201:HIS:HB2	23:B:602:CLA:C1B	2.46	0.46
23:N:604:CLA:HMA1	40:N:616:LUT:H3	1.98	0.46
14:R:82:LEU:HD12	14:R:83:PRO:HD2	1.96	0.46
2:B:273:TYR:HA	2:B:276:ASP:HB2	1.97	0.46
3:C:42:LEU:HD22	3:C:48:LYS:HB3	1.97	0.46
7:G:216:PHE:CE2	7:G:220:LYS:HE3	2.51	0.46
11:L:17:SER:HG	30:L:103:LHG:H02	1.61	0.46
23:g:613:CLA:H12	23:g:613:CLA:NA	2.31	0.46
14:r:247:PRO:HD2	40:r:613:LUT:H23	1.98	0.46
23:s:604:CLA:C1C	41:s:617:NEX:H22	2.45	0.46
18:v:29:ARG:NH2	43:v:201:HOH:O	2.48	0.46
23:A:403:CLA:H141	23:A:403:CLA:H161	1.67	0.46
37:D:410:DGA:HAF2	8:H:47:MET:HE2	1.98	0.46
41:N:617:NEX:H191	41:N:617:NEX:H12	1.98	0.46
1:a:153:ALA:HB1	23:a:403:CLA:HED1	1.98	0.46
2:b:69:LEU:HD23	23:b:606:CLA:HMA1	1.97	0.46
2:b:247:PHE:HB2	23:b:608:CLA:HBC1	1.98	0.46
3:c:307:PRO:HB3	3:c:358:PHE:HB3	1.97	0.46
4:d:330:MET:O	4:d:334:ASP:HB3	2.16	0.46
39:n:605:CHL:HBA2	15:s:157:PHE:CE1	2.51	0.46
1:A:135:PHE:CE1	3:C:449:ARG:HG3	2.51	0.46
3:C:119:LEU:O	3:C:122:SER:OG	2.33	0.46
42:G:619:XAT:H15	42:G:619:XAT:H201	1.69	0.46
23:N:610:CLA:H141	23:N:610:CLA:H162	1.82	0.46
3:c:83:GLU:OE2	3:c:398:HIS:NE2	2.49	0.46
13:o:300:LYS:HG2	13:o:302:ASP:OD1	2.16	0.46
23:r:612:CLA:HBA2	23:r:612:CLA:H3A	1.48	0.46
2:B:231:MET:HE2	23:B:610:CLA:HMC2	1.99	0.45
23:B:615:CLA:H91	23:B:615:CLA:H112	1.74	0.45
39:N:601:CHL:H3A	39:N:601:CHL:HBA1	1.68	0.45
40:N:615:LUT:H12	40:N:615:LUT:H191	1.98	0.45
7:Y:234:MET:HG3	40:Y:316:LUT:H12	1.98	0.45
7:Y:248:PRO:O	40:Y:315:LUT:O3	2.24	0.45
39:Y:302:CHL:H62	39:Y:302:CHL:H41	1.48	0.45
1:a:211:PHE:HB3	29:a:411:PL9:H101	1.97	0.45
23:a:404:CLA:HBB1	24:a:406:PHO:H141	1.98	0.45
25:a:408:BCR:H15C	25:a:408:BCR:H351	1.85	0.45
7:g:123:VAL:HG13	7:g:249:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:k:25:PRO:HG2	10:k:28:TYR:HD1	1.80	0.45
23:n:610:CLA:H52	40:n:615:LUT:H30	1.97	0.45
42:n:620:XAT:H31	42:n:620:XAT:H391	1.63	0.45
14:r:223:TYR:O	14:r:227:GLN:HG2	2.16	0.45
20:x:102:SER:HA	28:x:201:3PH:H241	1.98	0.45
1:A:153:ALA:HB1	23:A:402:CLA:HED1	1.98	0.45
23:B:615:CLA:H2	23:B:616:CLA:HBB2	1.98	0.45
14:R:259:ARG:HG2	23:R:610:CLA:HED1	1.98	0.45
39:R:606:CHL:H93	39:R:606:CHL:H62	1.81	0.45
23:Y:313:CLA:H2	23:Y:313:CLA:H61	1.68	0.45
23:c:503:CLA:HMB1	23:c:512:CLA:H192	1.98	0.45
1:A:240:GLY:HA3	16:T:30:PRO:HG3	1.97	0.45
3:C:371:GLY:N	3:C:374:GLY:O	2.47	0.45
4:D:130:GLN:NE2	24:D:402:PHO:OBD	2.50	0.45
29:D:407:PL9:H401	30:D:408:LHG:H211	1.99	0.45
1:A:55:ALA:O	1:A:70:SER:OG	2.29	0.45
25:B:619:BCR:H361	25:B:619:BCR:H20C	1.85	0.45
14:R:223:TYR:O	14:R:227:GLN:HG2	2.16	0.45
2:b:407:ASP:OD2	2:b:408:ARG:NH2	2.50	0.45
3:c:154:ARG:HH12	19:w:141:ASP:HA	1.81	0.45
40:n:615:LUT:H35	40:n:615:LUT:H401	1.77	0.45
13:o:186:GLU:HB2	13:o:194:LYS:HB3	1.98	0.45
23:y:306:CLA:H41	23:y:306:CLA:H121	1.98	0.45
2:B:358:ARG:HB2	17:U:125:MET:SD	2.57	0.45
23:C:511:CLA:H143	21:Z:20:VAL:HG13	1.98	0.45
23:G:604:CLA:H12	41:G:617:NEX:H241	1.97	0.45
14:R:160:GLU:HG2	23:R:608:CLA:HED2	1.98	0.45
39:Y:302:CHL:H161	30:Y:318:LHG:H211	1.98	0.45
39:r:606:CHL:HBB2	23:r:608:CLA:HBC3	1.98	0.45
1:A:186:PHE:CE2	1:A:192:ILE:HD12	2.52	0.45
2:B:247:PHE:HB2	23:B:608:CLA:HBC1	1.98	0.45
31:C:521:LNL:H41	27:C:525:LMG:HC61	1.97	0.45
3:c:79:LYS:HB3	3:c:84:GLN:NE2	2.31	0.45
9:i:5:LYS:HD2	19:w:98:MET:HE1	1.97	0.45
39:n:606:CHL:H161	41:n:618:NEX:H10	1.99	0.45
13:o:173:ARG:HA	19:w:97:ARG:NH2	2.32	0.45
29:A:411:PL9:H162	24:D:402:PHO:HED1	1.99	0.45
23:B:616:CLA:H91	25:a:408:BCR:H312	1.99	0.45
23:S:609:CLA:CBB	23:S:611:CLA:H3A	2.47	0.45
1:a:170:ASP:OD2	3:c:357:ARG:NH1	2.48	0.45
2:b:345:ILE:HD12	2:b:402:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:g:611:CLA:HBC3	30:g:618:LHG:HC62	1.97	0.45
1:A:102:VAL:HB	28:A:410:3PH:H222	1.99	0.45
2:B:164:PRO:HG3	23:B:606:CLA:O1D	2.16	0.45
2:B:201:HIS:HB2	23:B:602:CLA:CHB	2.47	0.45
3:C:141:GLU:HG3	3:C:148:GLY:HA3	1.98	0.45
3:C:459:ILE:HG21	3:C:464:GLU:HG3	1.98	0.45
23:C:507:CLA:H91	23:C:507:CLA:H112	1.67	0.45
25:C:514:BCR:H15C	25:C:514:BCR:H351	1.86	0.45
39:G:606:CHL:HHC	39:G:606:CHL:HBB1	1.99	0.45
7:N:211:ASP:OD1	7:N:211:ASP:N	2.49	0.45
23:S:604:CLA:C1C	41:S:617:NEX:H22	2.47	0.45
42:Y:301:XAT:H31	42:Y:301:XAT:H391	1.80	0.45
3:c:118:HIS:CE1	23:c:503:CLA:NA	2.85	0.45
23:c:505:CLA:H202	23:c:505:CLA:H162	1.82	0.45
23:y:304:CLA:H141	23:y:304:CLA:H161	1.71	0.45
23:y:315:CLA:H93	23:y:315:CLA:H62	1.71	0.45
2:B:38:THR:HG23	2:B:66:MET:HE1	1.99	0.45
15:S:138:LEU:HD23	15:S:223:LEU:HB3	1.99	0.45
23:Y:314:CLA:H161	23:Y:314:CLA:H122	1.63	0.45
23:y:314:CLA:H2	23:y:314:CLA:H61	1.68	0.45
1:A:170:ASP:OD2	3:C:357:ARG:NH1	2.49	0.45
7:N:222:LYS:HD3	23:N:612:CLA:HAA2	1.98	0.45
7:N:263:ASN:HD21	7:N:265:TRP:HD1	1.65	0.45
3:c:119:LEU:O	3:c:122:SER:OG	2.33	0.45
25:k:101:BCR:H24C	25:k:101:BCR:H371	1.81	0.45
13:o:100:THR:HB	13:o:103:GLU:OE1	2.17	0.45
15:s:290:LEU:HD22	23:s:613:CLA:H72	1.99	0.45
3:C:130:ILE:HG22	21:Z:27:LEU:HD12	1.99	0.44
3:C:165:LEU:HG	23:C:507:CLA:HED1	1.99	0.44
13:O:316:SER:N	13:O:326:LYS:O	2.46	0.44
39:R:607:CHL:H3A	39:R:607:CHL:HBA2	1.71	0.44
1:a:131:TRP:HZ2	3:c:449:ARG:HD2	1.81	0.44
2:b:330:MET:HA	2:b:444:ARG:HB2	1.99	0.44
37:b:626:DGA:HAW2	8:h:47:MET:HE2	1.99	0.44
14:r:285:THR:HG21	14:r:292:LEU:HD21	1.98	0.44
19:w:122:PHE:CZ	28:w:202:3PH:H291	2.52	0.44
7:y:111:HIS:NE2	23:y:305:CLA:ND	2.65	0.44
2:B:7:ARG:O	2:B:10:THR:OG1	2.35	0.44
2:B:36:SER:HB3	31:B:623:LNL:H15	1.99	0.44
3:C:304:PRO:HG3	3:C:395:TYR:CG	2.52	0.44
39:G:607:CHL:H201	39:N:601:CHL:H62	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:618:BCR:H15C	25:b:618:BCR:H351	1.84	0.44
23:c:504:CLA:H91	23:c:504:CLA:H112	1.74	0.44
30:g:618:LHG:HC62	30:g:618:LHG:H242	1.62	0.44
15:s:163:TYR:CD2	15:s:187:GLY:HA2	2.53	0.44
15:s:277:LEU:HD13	23:s:613:CLA:HBC2	1.99	0.44
23:s:602:CLA:H61	23:s:602:CLA:H41	1.70	0.44
23:s:613:CLA:H141	23:s:613:CLA:H161	1.69	0.44
3:C:107:ASP:OD1	3:C:108:THR:N	2.50	0.44
7:N:251:ASN:HB3	23:N:613:CLA:O1D	2.18	0.44
30:S:616:LHG:H271	30:S:616:LHG:HC82	1.99	0.44
4:d:130:GLN:NE2	4:d:143:ASN:OD1	2.50	0.44
30:d:408:LHG:H321	16:t:21:ILE:HD11	1.98	0.44
42:n:617:XAT:H15	42:n:617:XAT:H201	1.68	0.44
23:B:613:CLA:H143	23:B:613:CLA:H161	1.80	0.44
3:C:281:LEU:O	3:C:285:ILE:HG13	2.18	0.44
10:K:28:TYR:CZ	21:Z:5:PHE:HZ	2.35	0.44
15:S:141:ALA:HB2	15:S:256:MET:HE2	1.98	0.44
2:b:237:VAL:HG22	23:b:610:CLA:HBC2	2.00	0.44
37:b:626:DGA:HBT2	28:d:403:3PH:H262	1.99	0.44
37:b:626:DGA:HBW1	28:d:403:3PH:H282	1.99	0.44
23:c:512:CLA:H111	23:c:512:CLA:H152	1.41	0.44
7:g:240:GLN:HE22	40:g:615:LUT:H42	1.82	0.44
1:A:303:ASN:ND2	1:A:322:ASN:HD22	2.14	0.44
7:N:191:LEU:HD21	39:N:606:CHL:H141	1.99	0.44
7:Y:225:LYS:NZ	30:Y:318:LHG:O4	2.49	0.44
7:g:189:GLY:N	39:g:608:CHL:OMC	2.50	0.44
14:r:259:ARG:NH1	14:r:263:ALA:HB2	2.32	0.44
4:D:211:LEU:HA	4:D:214:ILE:HG22	2.00	0.44
7:N:199:TYR:HB3	23:N:610:CLA:HED2	2.00	0.44
39:N:601:CHL:HED3	30:N:618:LHG:H132	2.00	0.44
42:N:619:XAT:H391	42:N:619:XAT:H31	1.70	0.44
23:R:610:CLA:H172	23:R:611:CLA:HMC3	1.99	0.44
24:a:406:PHO:H141	24:a:406:PHO:H161	1.66	0.44
23:c:512:CLA:H92	23:c:512:CLA:H61	1.70	0.44
2:B:297:SER:HG	2:B:300:GLU:CD	2.23	0.44
23:B:614:CLA:H41	23:B:614:CLA:H61	1.51	0.44
23:B:615:CLA:H2	23:B:616:CLA:CBB	2.48	0.44
23:G:610:CLA:HMB1	23:G:610:CLA:HBB1	2.00	0.44
42:G:619:XAT:H10	39:N:601:CHL:H13	1.99	0.44
39:G:620:CHL:H152	39:Y:309:CHL:H102	1.99	0.44
21:Z:25:VAL:O	21:Z:29:SER:OG	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:303:ASN:HD21	1:a:322:ASN:HD22	1.66	0.44
2:b:235:GLU:HB3	2:b:473:THR:HB	2.00	0.44
7:n:237:PHE:HE1	40:n:615:LUT:H41	1.83	0.44
14:r:283:ALA:HB2	39:r:606:CHL:H143	1.99	0.44
23:r:610:CLA:H172	23:r:611:CLA:HMC3	1.98	0.44
23:s:609:CLA:H92	23:s:609:CLA:H61	1.72	0.44
19:w:122:PHE:HZ	28:w:202:3PH:H272	1.83	0.44
7:y:116:MET:HE2	7:y:227:GLY:CA	2.48	0.44
23:A:403:CLA:H172	29:D:407:PL9:H512	2.00	0.44
23:B:616:CLA:H171	30:d:408:LHG:H382	1.99	0.44
28:C:524:3PH:H3G1	28:C:524:3PH:H3D1	1.71	0.44
31:c:519:LNL:H9	31:c:519:LNL:H62	1.68	0.44
42:r:615:XAT:H11	42:r:615:XAT:H191	1.66	0.44
23:s:613:CLA:H2	23:s:613:CLA:H61	1.70	0.44
29:A:411:PL9:H311	29:A:411:PL9:H262	1.98	0.44
23:B:610:CLA:H202	23:B:610:CLA:H161	1.73	0.44
25:H:501:BCR:H20C	25:H:501:BCR:H361	1.82	0.44
23:b:603:CLA:H141	23:b:603:CLA:H161	1.81	0.44
3:c:327:SER:OG	3:c:330:SER:O	2.35	0.44
23:n:604:CLA:HMA1	40:n:616:LUT:H3	2.00	0.44
23:A:403:CLA:HBB1	24:A:405:PHO:H141	1.99	0.43
29:A:411:PL9:H422	29:A:411:PL9:H401	1.73	0.43
7:G:113:ARG:HA	7:G:116:MET:HE3	2.00	0.43
23:G:602:CLA:H142	23:G:602:CLA:H112	1.79	0.43
8:H:25:PRO:HG2	14:R:145:SER:HB2	1.99	0.43
3:c:371:GLY:N	3:c:374:GLY:O	2.49	0.43
14:r:82:LEU:HD12	14:r:83:PRO:HD2	2.00	0.43
14:r:142:ILE:HG23	14:r:148:PRO:HB2	2.00	0.43
7:y:233:SER:HB3	40:y:316:LUT:H8	2.00	0.43
13:O:173:ARG:HA	19:W:97:ARG:NH2	2.33	0.43
7:Y:116:MET:HE2	7:Y:227:GLY:CA	2.48	0.43
2:b:152:GLY:HA3	27:r:617:LMG:H221	2.01	0.43
23:b:604:CLA:H152	23:b:604:CLA:H112	1.77	0.43
9:i:7:PHE:O	9:i:11:VAL:HG23	2.19	0.43
7:Y:170:ILE:HG12	39:Y:306:CHL:HAC1	1.99	0.43
4:d:186:PHE:CD1	4:d:190:HIS:HD2	2.37	0.43
7:n:174:GLN:OE1	39:n:607:CHL:HMC	2.17	0.43
23:n:610:CLA:H92	23:n:610:CLA:H61	1.86	0.43
7:y:112:SER:HB3	7:y:227:GLY:HA3	2.00	0.43
23:B:608:CLA:H8	23:B:609:CLA:H13	2.00	0.43
3:C:243:ILE:HG12	35:C:523:VIV:H261	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:R:607:CHL:HMC	39:R:607:CHL:H171	2.00	0.43
23:S:609:CLA:HBA2	23:S:609:CLA:H3A	1.46	0.43
7:Y:252:LEU:HD11	23:Y:314:CLA:HMC2	2.00	0.43
1:a:331:MET:HG3	4:d:325:GLY:HA3	2.01	0.43
2:b:43:ALA:HB1	31:b:622:LNL:H52	2.00	0.43
27:d:409:LMG:H321	27:d:409:LMG:H352	1.82	0.43
23:g:610:CLA:H92	23:g:610:CLA:H61	1.86	0.43
23:n:602:CLA:HBA1	40:n:616:LUT:H382	2.01	0.43
41:r:614:NEX:H35	41:r:614:NEX:H401	1.77	0.43
15:s:100:ASP:OD1	15:s:101:ARG:N	2.51	0.43
23:y:314:CLA:HMA1	40:y:316:LUT:H3	2.01	0.43
1:A:196:PRO:HG3	1:A:300:PHE:CE2	2.53	0.43
23:C:512:CLA:H162	23:C:512:CLA:H122	1.62	0.43
7:g:164:ALA:HB1	7:g:170:ILE:HD11	2.00	0.43
10:k:28:TYR:CZ	21:z:5:PHE:HZ	2.36	0.43
42:n:620:XAT:H11	42:n:620:XAT:H191	1.90	0.43
13:o:168:THR:HB	13:o:208:VAL:HB	2.01	0.43
23:r:609:CLA:H52	40:r:613:LUT:H30	2.00	0.43
23:B:602:CLA:H2	23:B:602:CLA:H62	1.75	0.43
28:C:524:3PH:H2G1	28:C:524:3PH:H2D2	1.82	0.43
7:N:94:LEU:HD12	40:N:616:LUT:H221	2.01	0.43
23:S:602:CLA:H111	40:S:615:LUT:H30	2.00	0.43
28:W:201:3PH:H341	28:W:201:3PH:H391	2.00	0.43
7:Y:109:VAL:HG21	7:Y:198:ILE:HD12	2.00	0.43
23:g:613:CLA:H102	42:y:302:XAT:H15	2.01	0.43
13:o:230:THR:HG23	13:o:233:SER:H	1.84	0.43
21:z:33:TRP:NE1	21:z:37:LYS:HE2	2.33	0.43
2:B:141:ILE:HG13	2:B:217:LEU:HD21	2.00	0.43
23:B:609:CLA:H92	23:B:609:CLA:H62	1.84	0.43
23:B:614:CLA:H61	23:B:614:CLA:H102	1.91	0.43
25:B:617:BCR:H15C	25:B:617:BCR:H351	1.82	0.43
31:B:625:LNL:H52	28:a:410:3PH:H271	2.00	0.43
33:C:515:DGD:HGB2	33:C:515:DGD:HBN2	1.85	0.43
31:C:521:LNL:H61	31:C:521:LNL:H32	1.37	0.43
4:D:198:HIS:CE1	23:D:405:CLA:NC	2.87	0.43
7:G:229:LEU:HD23	40:G:615:LUT:H203	2.01	0.43
7:N:100:THR:HG22	7:N:104:ASN:ND2	2.33	0.43
15:S:126:LYS:HB3	15:S:129:ASN:HB2	2.01	0.43
15:S:198:VAL:HG22	39:S:606:CHL:HBC1	2.00	0.43
7:Y:233:SER:HB3	40:Y:315:LUT:H8	2.01	0.43
25:Z:101:BCR:H15C	25:Z:101:BCR:H351	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:302:PHE:HE2	4:d:75:LEU:HD12	1.83	0.43
2:b:160:GLY:HA3	2:b:180:PRO:HB3	2.00	0.43
2:b:334:ASP:HB2	2:b:432:LEU:HD13	2.00	0.43
25:c:514:BCR:H15C	25:c:514:BCR:H351	1.87	0.43
23:n:610:CLA:H62	23:n:610:CLA:H41	1.89	0.43
13:o:126:GLY:H	13:o:300:LYS:HE2	1.84	0.43
23:s:610:CLA:H93	23:s:610:CLA:H62	1.80	0.43
3:C:117:LEU:HD21	23:S:613:CLA:H2	2.00	0.43
23:C:506:CLA:H62	23:C:506:CLA:H2	1.77	0.43
23:C:508:CLA:H41	23:C:508:CLA:H62	1.77	0.43
25:C:514:BCR:H24C	25:C:514:BCR:H371	1.81	0.43
7:G:178:MET:HG3	39:G:609:CHL:HMC	2.00	0.43
23:G:603:CLA:H93	23:N:603:CLA:H93	2.01	0.43
15:S:107:TYR:CD2	15:S:108:LEU:HG	2.53	0.43
23:Y:303:CLA:H111	23:Y:303:CLA:H93	1.75	0.43
4:d:198:HIS:CE1	23:d:405:CLA:NC	2.87	0.43
23:g:603:CLA:H93	23:n:603:CLA:H93	2.00	0.43
23:B:608:CLA:H2	28:D:403:3PH:H291	2.01	0.43
3:C:265:VAL:HG21	3:C:449:ARG:HD3	2.01	0.43
7:G:99:GLU:OE2	7:N:96:ALA:HB1	2.18	0.43
40:G:615:LUT:H171	40:G:615:LUT:H8	2.00	0.43
42:G:619:XAT:H35	42:G:619:XAT:H401	1.82	0.43
42:R:615:XAT:H191	42:R:615:XAT:H11	1.66	0.43
23:Y:310:CLA:H62	23:Y:310:CLA:H41	1.90	0.43
29:a:411:PL9:HC8	29:a:411:PL9:H121	1.61	0.43
2:b:164:PRO:HG3	23:b:606:CLA:O1D	2.18	0.43
23:c:506:CLA:H122	23:c:506:CLA:H162	1.50	0.43
4:d:211:LEU:HA	4:d:214:ILE:HG22	2.00	0.43
7:n:155:TYR:OH	41:n:618:NEX:O23	2.26	0.43
1:A:257:ARG:HB3	4:D:133:LEU:HD11	1.99	0.43
27:A:409:LMG:O5	3:C:221:GLU:OE2	2.18	0.43
2:B:372:ASP:OD1	2:B:376:ILE:N	2.48	0.43
23:C:505:CLA:H141	23:C:505:CLA:H161	1.84	0.43
23:C:512:CLA:H202	23:S:613:CLA:HMB1	2.01	0.43
28:C:524:3PH:H2D2	28:C:524:3PH:H2A2	1.79	0.43
13:O:186:GLU:CG	13:O:194:LYS:HB3	2.48	0.43
14:R:160:GLU:HG3	14:R:238:LEU:HD13	2.00	0.43
23:S:609:CLA:H92	23:S:609:CLA:H61	1.79	0.43
1:a:303:ASN:ND2	1:a:322:ASN:HD22	2.17	0.43
25:c:514:BCR:HC41	9:i:24:LEU:HG	2.00	0.43
7:g:181:VAL:HA	7:g:184:TYR:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:405:PHO:H141	24:A:405:PHO:H161	1.66	0.42
35:C:523:VIV:HC12	35:C:523:VIV:H211	1.69	0.42
42:N:619:XAT:H363	30:Y:318:LHG:HC41	2.01	0.42
15:S:81:GLU:HG3	15:S:83:ALA:H	1.83	0.42
21:Z:16:SER:O	21:Z:20:VAL:HG23	2.18	0.42
31:b:622:LNL:H51	31:b:622:LNL:H22	1.72	0.42
3:c:223:TRP:CG	3:c:224:ILE:H	2.37	0.42
2:B:79:ASN:OD1	2:B:80:ILE:N	2.52	0.42
2:B:460:LEU:CD1	4:D:288:VAL:HG21	2.48	0.42
4:D:263:SER:OG	30:D:408:LHG:O4	2.34	0.42
25:D:411:BCR:H20C	25:D:411:BCR:H361	1.84	0.42
11:L:25:ILE:HG13	12:M:18:SER:HB3	2.01	0.42
23:b:607:CLA:H162	23:b:607:CLA:H141	1.65	0.42
23:c:513:CLA:H93	23:c:513:CLA:H61	1.78	0.42
4:d:217:ALA:O	4:d:221:ASN:ND2	2.44	0.42
7:g:119:ALA:HB1	40:g:615:LUT:H12	2.00	0.42
7:n:113:ARG:NH1	39:n:608:CHL:OBD	2.47	0.42
7:n:218:GLU:O	7:n:222:LYS:HG3	2.19	0.42
13:o:143:LEU:HD13	13:o:336:ALA:HB2	2.01	0.42
15:s:135:ALA:HA	15:s:223:LEU:HD11	2.01	0.42
15:s:207:GLY:HA3	41:s:617:NEX:H403	2.00	0.42
23:B:602:CLA:H152	23:B:602:CLA:H18	1.86	0.42
1:a:280:VAL:HG11	30:a:412:LHG:H132	2.01	0.42
2:b:155:ALA:O	2:b:159:THR:OG1	2.37	0.42
31:c:517:LNL:H142	31:c:517:LNL:H112	1.85	0.42
11:l:25:ILE:HG13	12:m:18:SER:HB3	2.01	0.42
42:n:620:XAT:H15	42:n:620:XAT:H201	1.68	0.42
42:r:615:XAT:H31	42:r:615:XAT:H391	1.84	0.42
15:s:112:VAL:HG22	15:s:115:ASP:HB2	2.01	0.42
39:y:303:CHL:H61	39:y:303:CHL:H41	1.48	0.42
2:B:160:GLY:HA3	2:B:180:PRO:HB3	2.01	0.42
7:G:60:TYR:CE1	7:G:84:PRO:HA	2.53	0.42
15:S:106:GLU:CD	15:S:106:GLU:H	2.28	0.42
23:a:404:CLA:H172	29:d:407:PL9:H512	2.01	0.42
3:c:281:LEU:HG	3:c:285:ILE:HD11	2.01	0.42
23:n:613:CLA:H61	23:n:613:CLA:H2	1.74	0.42
2:B:283:GLU:OE1	2:B:286:ARG:NH1	2.53	0.42
25:B:618:BCR:H15C	25:B:618:BCR:H351	1.82	0.42
25:B:618:BCR:H371	25:B:618:BCR:H24C	1.83	0.42
4:D:217:ALA:O	4:D:221:ASN:ND2	2.38	0.42
6:F:13:ARG:NH2	38:F:501:HEM:O1D	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:G:610:CLA:H8	40:G:615:LUT:C30	2.49	0.42
23:N:611:CLA:H52	23:N:612:CLA:HMD2	2.02	0.42
42:N:619:XAT:H15	42:N:619:XAT:H201	1.68	0.42
13:O:220:PHE:CD1	13:O:330:ILE:HD13	2.55	0.42
39:R:606:CHL:H11	39:R:606:CHL:H51	1.77	0.42
23:Y:313:CLA:HBB1	30:Y:318:LHG:H331	2.00	0.42
25:b:617:BCR:H15C	25:b:617:BCR:H351	1.80	0.42
3:c:361:LEU:HD12	33:c:515:DGD:O3E	2.20	0.42
23:c:510:CLA:H3A	23:c:510:CLA:HBA1	1.84	0.42
4:d:149:ALA:HB3	4:d:150:PRO:HD3	2.02	0.42
7:n:211:ASP:OD1	7:n:211:ASP:N	2.50	0.42
15:s:212:ARG:HG2	39:s:607:CHL:C4C	2.50	0.42
23:B:614:CLA:H42	28:L:102:3PH:H351	2.02	0.42
3:C:79:LYS:HB3	3:C:84:GLN:HE21	1.85	0.42
4:D:68:TYR:O	27:D:409:LMG:O5	2.31	0.42
7:G:153:LEU:HB3	7:G:164:ALA:HB3	2.02	0.42
7:G:255:HIS:CG	23:G:613:CLA:HAA2	2.55	0.42
9:I:7:PHE:O	9:I:11:VAL:HG23	2.19	0.42
23:N:610:CLA:H61	23:N:610:CLA:H92	1.79	0.42
42:N:619:XAT:H35	42:N:619:XAT:H401	1.88	0.42
29:d:407:PL9:H122	29:d:407:PL9:H101	1.84	0.42
7:g:111:HIS:NE2	23:g:603:CLA:ND	2.67	0.42
23:n:603:CLA:H91	39:n:609:CHL:H142	2.01	0.42
23:C:504:CLA:H91	23:C:504:CLA:H112	1.72	0.42
4:D:343:PRO:O	4:D:346:VAL:HG22	2.20	0.42
13:O:127:GLY:HA3	13:O:298:LYS:HB3	2.02	0.42
14:R:125:ASP:OD1	14:R:125:ASP:N	2.52	0.42
1:a:328:MET:HG3	4:d:326:ILE:HG12	2.01	0.42
23:b:609:CLA:H161	23:b:609:CLA:H141	1.79	0.42
7:g:113:ARG:HA	7:g:116:MET:HE3	2.02	0.42
13:o:235:SER:HB3	13:o:293:THR:HG23	2.01	0.42
1:A:131:TRP:CZ2	3:C:449:ARG:HG2	2.54	0.42
13:O:237:GLN:HG3	13:O:289:LYS:HE2	2.01	0.42
1:a:196:PRO:HG3	1:a:300:PHE:CE2	2.55	0.42
26:a:409:SQD:H441	26:a:409:SQD:H2	1.79	0.42
28:a:410:3PH:H3C2	28:a:410:3PH:H371	2.01	0.42
30:a:412:LHG:H332	30:a:412:LHG:H361	1.76	0.42
41:g:617:NEX:H12	41:g:617:NEX:H191	2.01	0.42
9:i:28:PRO:HB3	19:w:144:LEU:HD12	2.01	0.42
23:n:613:CLA:H2	23:n:614:CLA:HMD1	2.01	0.42
23:r:602:CLA:H171	23:r:603:CLA:HBB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:y:311:CLA:HBB1	23:y:313:CLA:H3A	2.02	0.42
2:B:75:TRP:HB3	28:a:410:3PH:H31	2.02	0.42
2:B:237:VAL:HG22	23:B:610:CLA:HBC2	2.01	0.42
31:B:623:LNL:H31	12:M:6:LEU:HD11	2.01	0.42
25:C:514:BCR:H20C	25:C:514:BCR:H361	1.88	0.42
31:C:517:LNL:H9	31:C:517:LNL:H61	1.82	0.42
25:D:411:BCR:H363	6:F:27:PHE:HB3	2.02	0.42
1:a:218:LEU:HD12	29:a:411:PL9:C3	2.50	0.42
2:b:464:PHE:HB2	4:d:281:TRP:CH2	2.55	0.42
3:c:42:LEU:HD22	3:c:48:LYS:HB3	2.01	0.42
23:c:510:CLA:H193	23:c:510:CLA:H162	1.76	0.42
39:n:601:CHL:HBA1	39:n:601:CHL:H3A	1.93	0.42
13:o:318:THR:HG22	13:o:321:GLY:HA2	2.02	0.42
14:r:172:GLY:HA2	42:r:615:XAT:H181	2.01	0.42
23:r:603:CLA:H92	23:r:603:CLA:H62	1.84	0.42
31:C:521:LNL:H52	31:C:521:LNL:H81	1.53	0.42
33:H:502:DGD:HB32	33:H:502:DGD:HB62	1.71	0.42
15:S:142:ARG:HD3	39:S:607:CHL:OBD	2.20	0.42
18:V:3:LEU:O	18:V:7:ALA:N	2.49	0.42
2:b:201:HIS:HB2	23:b:602:CLA:C1B	2.50	0.42
23:c:505:CLA:H161	23:c:505:CLA:H141	1.85	0.42
23:c:506:CLA:HAC2	23:y:315:CLA:H143	2.02	0.42
7:g:74:GLU:N	7:g:74:GLU:OE1	2.53	0.42
39:r:605:CHL:HMC	39:r:606:CHL:C1C	2.49	0.42
23:s:613:CLA:H11	25:z:101:BCR:H352	2.02	0.42
1:A:303:ASN:OD1	1:A:322:ASN:ND2	2.53	0.41
31:B:622:LNL:H142	31:B:622:LNL:H111	1.86	0.41
3:C:167:LEU:HD23	3:C:167:LEU:HA	1.91	0.41
5:E:23:HIS:HA	5:E:26:THR:OG1	2.19	0.41
39:N:606:CHL:H18	23:S:611:CLA:H42	2.01	0.41
15:S:289:LEU:N	23:S:612:CLA:O1A	2.52	0.41
2:b:79:ASN:OD1	2:b:80:ILE:N	2.53	0.41
23:b:614:CLA:H172	23:b:614:CLA:H13	1.93	0.41
25:b:619:BCR:H20C	25:b:619:BCR:H361	1.85	0.41
25:c:514:BCR:H371	25:c:514:BCR:H24C	1.81	0.41
7:g:60:TYR:CE1	7:g:217:ALA:HB1	2.55	0.41
7:g:89:TRP:O	40:g:616:LUT:H24	2.20	0.41
7:g:240:GLN:NE2	40:g:615:LUT:H42	2.35	0.41
23:y:305:CLA:HED1	39:y:310:CHL:H92	2.02	0.41
27:A:409:LMG:H331	27:A:409:LMG:H362	1.78	0.41
28:A:410:3PH:H222	28:A:410:3PH:H251	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:R:172:GLY:HA2	42:R:615:XAT:H181	2.01	0.41
31:a:413:LNL:H72	4:d:75:LEU:HD21	2.01	0.41
23:n:612:CLA:H12	23:n:612:CLA:HED2	2.03	0.41
14:r:92:ASP:OD1	14:r:92:ASP:N	2.50	0.41
39:r:607:CHL:H92	39:r:607:CHL:H62	1.91	0.41
15:s:243:LEU:O	15:s:247:LYS:HG3	2.20	0.41
23:y:304:CLA:H93	23:y:304:CLA:H111	1.75	0.41
21:z:16:SER:O	21:z:20:VAL:HG23	2.19	0.41
25:B:619:BCR:H11C	25:B:619:BCR:H341	1.94	0.41
23:C:508:CLA:H92	23:C:508:CLA:H61	1.87	0.41
23:G:603:CLA:H142	23:G:603:CLA:H112	1.91	0.41
23:N:602:CLA:H141	23:N:602:CLA:H161	1.87	0.41
23:N:611:CLA:H101	23:N:611:CLA:H62	1.74	0.41
13:O:203:TYR:HB2	13:O:219:LEU:HD21	2.00	0.41
7:Y:118:GLY:HA2	40:Y:316:LUT:H8	2.03	0.41
2:b:355:PHE:CE2	2:b:373:LYS:HD3	2.54	0.41
23:b:613:CLA:H72	23:b:613:CLA:H112	1.71	0.41
3:c:321:ASP:OD2	3:c:340:TYR:OH	2.33	0.41
4:d:129:ARG:NH1	43:d:502:HOH:O	2.42	0.41
23:s:612:CLA:H51	23:s:612:CLA:H11	1.87	0.41
29:A:411:PL9:H101	29:A:411:PL9:H122	1.85	0.41
31:A:413:LNL:H72	4:D:75:LEU:HD21	2.02	0.41
2:B:235:GLU:CD	2:B:472:ARG:HH11	2.27	0.41
3:C:154:ARG:HH12	19:W:141:ASP:HA	1.85	0.41
23:C:509:CLA:H141	23:C:509:CLA:H161	1.78	0.41
4:D:149:ALA:HB3	4:D:150:PRO:HD3	2.02	0.41
7:G:119:ALA:HB1	40:G:615:LUT:H12	2.03	0.41
39:G:601:CHL:H142	42:Y:301:XAT:H10	2.02	0.41
7:N:124:PHE:CZ	7:N:128:LEU:HD11	2.55	0.41
23:N:613:CLA:H151	23:N:614:CLA:H11	2.02	0.41
23:S:603:CLA:HBC1	23:S:608:CLA:HAC1	2.02	0.41
1:a:161:TYR:HB3	1:a:162:PRO:HD3	2.03	0.41
2:b:66:MET:HE3	2:b:66:MET:HB2	1.94	0.41
2:b:141:ILE:HG13	2:b:217:LEU:HD21	2.02	0.41
23:b:612:CLA:H61	23:b:612:CLA:H102	1.84	0.41
25:b:618:BCR:H11C	25:b:618:BCR:H341	1.92	0.41
27:c:523:LMG:H453	30:y:318:LHG:H301	2.02	0.41
15:s:120:PRO:HD2	40:s:615:LUT:H24	2.02	0.41
15:s:177:LEU:HD11	15:s:183:LEU:CD1	2.51	0.41
39:y:303:CHL:HBA1	39:y:303:CHL:H3A	1.78	0.41
23:y:306:CLA:H162	23:y:306:CLA:H193	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:ALA:O	2:B:159:THR:OG1	2.35	0.41
2:B:464:PHE:HB2	4:D:281:TRP:CH2	2.55	0.41
23:B:607:CLA:H203	11:L:36:LEU:HD11	2.02	0.41
23:C:507:CLA:H142	25:C:514:BCR:H362	2.01	0.41
23:N:603:CLA:HED1	39:N:609:CHL:H92	2.02	0.41
23:S:609:CLA:H41	23:S:609:CLA:H62	1.67	0.41
39:Y:307:CHL:HBB2	40:Y:316:LUT:H193	2.02	0.41
2:b:64:PRO:HA	2:b:67:THR:HG22	2.02	0.41
3:c:308:GLU:HA	3:c:361:LEU:CD2	2.50	0.41
7:n:199:TYR:HB3	23:n:610:CLA:HED2	2.02	0.41
7:n:269:THR:O	7:n:269:THR:HG22	2.20	0.41
23:r:604:CLA:C1B	41:r:614:NEX:H383	2.50	0.41
1:A:328:MET:HG3	4:D:326:ILE:HG12	2.01	0.41
25:A:407:BCR:H15C	25:A:407:BCR:H351	1.85	0.41
25:A:407:BCR:H371	25:A:407:BCR:H24C	1.83	0.41
23:C:509:CLA:H3A	23:C:509:CLA:HBA1	1.86	0.41
15:S:224:HIS:ND1	23:S:609:CLA:O1D	2.53	0.41
18:V:14:LEU:O	18:V:18:SER:OG	2.33	0.41
23:Y:303:CLA:H141	23:Y:303:CLA:H161	1.72	0.41
28:a:410:3PH:H382	28:a:410:3PH:H351	1.88	0.41
2:b:440:ASP:OD2	2:b:444:ARG:NH2	2.53	0.41
2:b:460:LEU:CD1	4:d:288:VAL:HG21	2.49	0.41
23:c:506:CLA:H62	23:c:506:CLA:H92	1.87	0.41
15:s:289:LEU:HD13	23:s:612:CLA:HMD2	2.03	0.41
2:B:91:TRP:HE1	32:B:621:PAM:H82	1.85	0.41
2:B:324:LEU:HD11	23:B:607:CLA:H92	2.03	0.41
23:B:615:CLA:H92	23:B:615:CLA:H61	1.79	0.41
4:D:54:THR:HG22	6:F:34:MET:HE1	2.03	0.41
39:N:601:CHL:ND	30:N:618:LHG:HC92	2.35	0.41
2:b:258:TYR:OH	4:d:163:LEU:O	2.37	0.41
2:b:440:ASP:OD1	2:b:442:VAL:HG22	2.21	0.41
3:c:346:THR:OG1	3:c:348:GLU:OE1	2.25	0.41
4:d:127:MET:HE3	4:d:144:ALA:O	2.21	0.41
33:d:411:DGD:HBW1	33:d:411:DGD:HBN2	1.82	0.41
23:g:602:CLA:H142	23:g:602:CLA:H112	1.81	0.41
23:n:610:CLA:H152	40:n:615:LUT:H391	2.02	0.41
17:u:117:LEU:HD23	17:u:117:LEU:HA	1.89	0.41
7:y:174:GLN:HB2	43:y:408:HOH:O	2.21	0.41
23:B:610:CLA:H2	23:B:610:CLA:HED1	2.03	0.41
25:B:617:BCR:C32	31:B:623:LNL:H9	2.50	0.41
4:D:30:PHE:CD2	4:D:133:LEU:HD12	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:D:405:CLA:H91	23:D:405:CLA:H112	1.88	0.41
25:H:501:BCR:H24C	25:H:501:BCR:H371	1.81	0.41
15:S:143:TRP:CE2	39:S:607:CHL:HED2	2.56	0.41
15:S:164:CYS:HA	15:S:186:PHE:H	1.85	0.41
2:b:148:VAL:HG13	27:r:617:LMG:H232	2.02	0.41
2:b:369:VAL:HG13	2:b:377:VAL:HG13	2.01	0.41
25:d:410:BCR:H15C	25:d:410:BCR:H351	1.88	0.41
6:f:31:ILE:HA	6:f:34:MET:HE3	2.02	0.41
8:h:53:PHE:O	8:h:56:ILE:HG22	2.21	0.41
7:n:171:TRP:O	7:n:175:VAL:HG23	2.20	0.41
42:n:620:XAT:H35	42:n:620:XAT:H401	1.89	0.41
14:r:291:THR:O	14:r:295:GLU:OE1	2.38	0.41
23:s:613:CLA:H61	23:s:613:CLA:H92	1.70	0.41
1:A:272:HIS:HE1	36:D:401:BCT:O2	1.97	0.41
1:A:303:ASN:HB3	1:A:304:GLN:NE2	2.36	0.41
2:B:94:GLU:HG2	28:a:410:3PH:H321	2.02	0.41
25:B:617:BCR:H312	27:B:620:LMG:H342	2.02	0.41
4:D:20:ASP:OD1	4:D:33:TRP:NE1	2.50	0.41
39:G:606:CHL:CGA	41:G:617:NEX:H403	2.51	0.41
7:N:90:ASP:HA	40:N:616:LUT:H24	2.03	0.41
40:N:615:LUT:H15	40:N:615:LUT:H201	1.91	0.41
23:S:610:CLA:H93	23:S:610:CLA:H62	1.80	0.41
30:S:616:LHG:H223	21:Z:48:ILE:HG12	2.01	0.41
1:a:82:ILE:HB	1:a:174:LEU:HB2	2.02	0.41
23:b:602:CLA:H12	8:h:61:TYR:HD2	1.86	0.41
23:b:610:CLA:H202	23:b:610:CLA:H161	1.73	0.41
3:c:462:ASP:OD1	3:c:463:PHE:N	2.54	0.41
4:d:179:ILE:O	4:d:183:ILE:HG13	2.21	0.41
9:i:5:LYS:HE2	19:w:114:LEU:HD21	2.02	0.41
39:n:607:CHL:H92	39:n:607:CHL:H62	1.85	0.41
39:n:607:CHL:H152	39:n:609:CHL:H93	2.03	0.41
14:r:90:TRP:CE3	14:r:108:LYS:HG3	2.56	0.41
25:v:101:BCR:H15C	25:v:101:BCR:H351	1.94	0.41
23:y:312:CLA:H102	23:y:313:CLA:H143	2.03	0.41
25:A:407:BCR:H11C	25:A:407:BCR:H341	1.93	0.41
2:B:123:PHE:HB2	2:B:131:LEU:HD22	2.02	0.41
2:B:442:VAL:HG23	2:B:444:ARG:NH1	2.36	0.41
23:B:612:CLA:H162	23:B:612:CLA:H122	1.67	0.41
23:B:615:CLA:HBA1	23:B:615:CLA:H3A	1.87	0.41
23:B:616:CLA:H141	23:B:616:CLA:H161	1.90	0.41
25:B:617:BCR:H24C	25:B:617:BCR:H371	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:D:402:PHO:H72	24:D:402:PHO:H112	1.85	0.41
5:E:35:TRP:HA	6:F:33:ALA:HB2	2.03	0.41
23:G:610:CLA:H62	23:G:610:CLA:H41	1.84	0.41
14:R:210:MET:HE2	27:R:617:LMG:H111	2.02	0.41
15:S:128:GLU:HG2	15:S:129:ASN:N	2.36	0.41
23:b:610:CLA:H102	23:b:615:CLA:HAA1	2.02	0.41
23:b:616:CLA:H61	23:b:616:CLA:H92	1.81	0.41
9:i:35:LYS:HD3	9:i:35:LYS:HA	1.79	0.41
18:v:32:ASN:HB3	21:z:28:ALA:HB1	2.03	0.41
2:B:384:ARG:HD2	4:D:353:LEU:HD23	2.02	0.40
23:B:604:CLA:H92	23:B:604:CLA:H41	2.03	0.40
25:B:619:BCR:H15C	25:B:619:BCR:H351	1.90	0.40
3:C:304:PRO:HG3	3:C:395:TYR:CD1	2.56	0.40
23:S:610:CLA:H2	23:S:610:CLA:H61	1.77	0.40
7:Y:124:PHE:HB3	7:Y:125:PRO:HD3	2.03	0.40
7:Y:237:PHE:HE1	40:Y:315:LUT:H41	1.86	0.40
2:b:235:GLU:OE1	2:b:472:ARG:NH1	2.54	0.40
23:b:609:CLA:HBA1	23:b:609:CLA:H3A	1.92	0.40
7:g:153:LEU:HB3	7:g:164:ALA:HB3	2.03	0.40
7:g:204:PHE:O	40:g:615:LUT:H24	2.20	0.40
23:g:610:CLA:HMB3	23:g:612:CLA:HAA1	2.02	0.40
40:g:616:LUT:H35	40:g:616:LUT:H401	1.94	0.40
41:g:617:NEX:H35	41:g:617:NEX:H401	1.83	0.40
15:s:86:TYR:CE2	15:s:242:ALA:HB1	2.56	0.40
23:s:609:CLA:CBB	23:s:611:CLA:H3A	2.51	0.40
23:y:305:CLA:H102	23:y:305:CLA:H13	1.90	0.40
23:B:602:CLA:H72	23:B:602:CLA:H111	1.95	0.40
31:C:522:LNL:H16	31:C:522:LNL:H13	1.69	0.40
37:D:410:DGA:HAW1	8:H:44:GLY:HA2	2.03	0.40
39:G:609:CHL:CMB	39:N:601:CHL:HHB	2.51	0.40
8:H:53:PHE:O	8:H:56:ILE:HG22	2.20	0.40
2:b:254:GLY:HA2	33:d:411:DGD:HBH1	2.04	0.40
25:b:619:BCR:H371	25:b:619:BCR:H24C	1.79	0.40
6:f:13:ARG:O	6:f:17:ILE:HG12	2.20	0.40
7:g:171:TRP:O	7:g:175:VAL:HG23	2.22	0.40
39:g:606:CHL:HHC	39:g:606:CHL:HBB1	2.03	0.40
40:g:615:LUT:H35	40:g:615:LUT:H401	1.95	0.40
28:x:201:3PH:H342	28:x:201:3PH:H271	2.01	0.40
7:y:146:GLN:O	7:y:149:SER:OG	2.32	0.40
7:N:263:ASN:ND2	7:N:265:TRP:HD1	2.19	0.40
41:R:618:NEX:H383	23:y:306:CLA:C1B	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:305:CLA:H141	23:Y:305:CLA:H162	1.77	0.40
39:Y:307:CHL:H51	39:Y:307:CHL:H11	1.79	0.40
2:b:75:TRP:CD1	2:b:92:SER:HG	2.40	0.40
4:d:181:ARG:C	4:d:181:ARG:HD3	2.46	0.40
5:e:21:VAL:HG13	5:e:22:ILE:HG13	2.03	0.40
15:s:237:ASP:HB3	15:s:240:GLN:HB2	2.03	0.40
23:s:610:CLA:HBD	23:s:611:CLA:OBD	2.21	0.40
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.02	0.40
23:B:607:CLA:H141	23:B:607:CLA:H162	1.84	0.40
23:B:610:CLA:H102	23:B:615:CLA:HAA1	2.03	0.40
31:B:625:LNL:H111	31:i:101:LNL:H111	2.03	0.40
3:C:250:TRP:HE3	31:C:521:LNL:H12	1.85	0.40
23:N:614:CLA:H2A	23:N:614:CLA:HED2	2.03	0.40
23:c:513:CLA:H112	23:c:513:CLA:H91	1.89	0.40
7:g:60:TYR:CZ	7:g:217:ALA:HB1	2.57	0.40
15:s:120:PRO:HD2	40:s:615:LUT:C24	2.52	0.40
15:s:198:VAL:O	15:s:201:GLU:HG3	2.20	0.40
15:s:289:LEU:N	23:s:612:CLA:O1A	2.53	0.40
29:A:411:PL9:H172	29:A:411:PL9:H151	1.94	0.40
29:A:411:PL9:H322	29:A:411:PL9:H361	1.92	0.40
7:G:174:GLN:HA	39:G:606:CHL:HMA3	2.04	0.40
7:G:185:ARG:HG3	39:G:608:CHL:C1D	2.51	0.40
13:O:300:LYS:HG2	13:O:302:ASP:OD1	2.21	0.40
14:R:167:ARG:HA	14:R:170:MET:HE3	2.04	0.40
39:S:607:CHL:HBA1	39:S:607:CHL:H3A	1.89	0.40
23:Y:303:CLA:H92	23:Y:304:CLA:HMA3	2.04	0.40
23:Y:303:CLA:H112	40:Y:316:LUT:H30	2.03	0.40
39:Y:307:CHL:H41	39:Y:307:CHL:H62	1.88	0.40
39:Y:307:CHL:HMB2	39:Y:309:CHL:HMC	2.04	0.40
39:Y:308:CHL:CBB	41:Y:317:NEX:H11	2.52	0.40
25:Z:101:BCR:H20C	25:Z:101:BCR:H361	1.86	0.40
24:a:406:PHO:H2	24:a:406:PHO:H61	1.63	0.40
2:b:220:ARG:HG3	8:h:32:LYS:HE3	2.03	0.40
23:b:605:CLA:H92	23:b:605:CLA:H61	1.86	0.40
3:c:318:LEU:HD13	3:c:340:TYR:HB3	2.04	0.40
23:g:612:CLA:H2A	23:g:612:CLA:O2A	2.22	0.40
23:n:613:CLA:H61	23:n:613:CLA:H102	1.92	0.40
40:n:616:LUT:H35	40:n:616:LUT:H401	1.95	0.40
13:o:190:ASP:OD1	13:o:190:ASP:N	2.49	0.40
21:z:52:LEU:O	21:z:56:ILE:HG12	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	317/353 (90%)	312 (98%)	5 (2%)	0	100	100
1	a	317/353 (90%)	313 (99%)	4 (1%)	0	100	100
2	B	483/508 (95%)	473 (98%)	10 (2%)	0	100	100
2	b	483/508 (95%)	473 (98%)	10 (2%)	0	100	100
3	C	429/473 (91%)	420 (98%)	9 (2%)	0	100	100
3	c	429/473 (91%)	419 (98%)	10 (2%)	0	100	100
4	D	331/353 (94%)	319 (96%)	12 (4%)	0	100	100
4	d	331/353 (94%)	322 (97%)	9 (3%)	0	100	100
5	E	63/83 (76%)	61 (97%)	2 (3%)	0	100	100
5	e	63/83 (76%)	62 (98%)	1 (2%)	0	100	100
6	F	28/39 (72%)	28 (100%)	0	0	100	100
6	f	28/39 (72%)	28 (100%)	0	0	100	100
7	G	216/275 (78%)	206 (95%)	10 (5%)	0	100	100
7	N	216/275 (78%)	209 (97%)	7 (3%)	0	100	100
7	Y	216/275 (78%)	211 (98%)	5 (2%)	0	100	100
7	g	216/275 (78%)	207 (96%)	9 (4%)	0	100	100
7	n	216/275 (78%)	209 (97%)	7 (3%)	0	100	100
7	y	216/275 (78%)	212 (98%)	4 (2%)	0	100	100
8	H	60/75 (80%)	58 (97%)	2 (3%)	0	100	100
8	h	60/75 (80%)	59 (98%)	1 (2%)	0	100	100
9	I	34/36 (94%)	34 (100%)	0	0	100	100
9	i	34/36 (94%)	34 (100%)	0	0	100	100
10	K	35/59 (59%)	33 (94%)	2 (6%)	0	100	100
10	k	35/59 (59%)	32 (91%)	3 (9%)	0	100	100
11	L	34/38 (90%)	34 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	l	34/38 (90%)	34 (100%)	0	0	100	100
12	M	29/37 (78%)	29 (100%)	0	0	100	100
12	m	29/37 (78%)	29 (100%)	0	0	100	100
13	O	182/341 (53%)	175 (96%)	7 (4%)	0	100	100
13	o	182/341 (53%)	173 (95%)	9 (5%)	0	100	100
14	R	215/300 (72%)	213 (99%)	2 (1%)	0	100	100
14	r	215/300 (72%)	211 (98%)	4 (2%)	0	100	100
15	S	207/303 (68%)	196 (95%)	11 (5%)	0	100	100
15	s	207/303 (68%)	196 (95%)	11 (5%)	0	100	100
16	T	29/35 (83%)	29 (100%)	0	0	100	100
16	t	29/35 (83%)	29 (100%)	0	0	100	100
17	U	25/133 (19%)	25 (100%)	0	0	100	100
17	u	25/133 (19%)	25 (100%)	0	0	100	100
18	V	29/33 (88%)	26 (90%)	3 (10%)	0	100	100
18	v	29/33 (88%)	29 (100%)	0	0	100	100
19	W	52/146 (36%)	51 (98%)	1 (2%)	0	100	100
19	w	52/146 (36%)	51 (98%)	1 (2%)	0	100	100
20	X	32/129 (25%)	31 (97%)	1 (3%)	0	100	100
20	x	32/129 (25%)	32 (100%)	0	0	100	100
21	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
21	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	6644/8722 (76%)	6469 (97%)	175 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	257/282 (91%)	256 (100%)	1 (0%)	84	93
1	a	257/282 (91%)	256 (100%)	1 (0%)	84	93
2	B	387/406 (95%)	386 (100%)	1 (0%)	86	94
2	b	387/406 (95%)	386 (100%)	1 (0%)	86	94
3	C	338/371 (91%)	338 (100%)	0	100	100
3	c	338/371 (91%)	338 (100%)	0	100	100
4	D	271/284 (95%)	271 (100%)	0	100	100
4	d	271/284 (95%)	271 (100%)	0	100	100
5	E	59/74 (80%)	59 (100%)	0	100	100
5	e	59/74 (80%)	59 (100%)	0	100	100
6	F	25/34 (74%)	25 (100%)	0	100	100
6	f	25/34 (74%)	25 (100%)	0	100	100
7	G	166/208 (80%)	166 (100%)	0	100	100
7	N	166/208 (80%)	166 (100%)	0	100	100
7	Y	166/208 (80%)	166 (100%)	0	100	100
7	g	166/208 (80%)	166 (100%)	0	100	100
7	n	166/208 (80%)	166 (100%)	0	100	100
7	y	166/208 (80%)	166 (100%)	0	100	100
8	H	50/62 (81%)	50 (100%)	0	100	100
8	h	50/62 (81%)	50 (100%)	0	100	100
9	I	33/33 (100%)	33 (100%)	0	100	100
9	i	33/33 (100%)	33 (100%)	0	100	100
10	K	32/52 (62%)	32 (100%)	0	100	100
10	k	32/52 (62%)	32 (100%)	0	100	100
11	L	34/36 (94%)	34 (100%)	0	100	100
11	l	34/36 (94%)	34 (100%)	0	100	100
12	M	25/30 (83%)	25 (100%)	0	100	100
12	m	25/30 (83%)	25 (100%)	0	100	100
13	O	164/275 (60%)	164 (100%)	0	100	100
13	o	164/275 (60%)	164 (100%)	0	100	100
14	R	180/241 (75%)	180 (100%)	0	100	100
14	r	180/241 (75%)	180 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	S	162/230 (70%)	162 (100%)	0	100	100
15	s	162/230 (70%)	162 (100%)	0	100	100
16	T	28/30 (93%)	28 (100%)	0	100	100
16	t	28/30 (93%)	28 (100%)	0	100	100
17	U	23/103 (22%)	23 (100%)	0	100	100
17	u	23/103 (22%)	23 (100%)	0	100	100
18	V	27/29 (93%)	27 (100%)	0	100	100
18	v	27/29 (93%)	27 (100%)	0	100	100
19	W	46/116 (40%)	46 (100%)	0	100	100
19	w	46/116 (40%)	46 (100%)	0	100	100
20	X	23/94 (24%)	23 (100%)	0	100	100
20	x	23/94 (24%)	23 (100%)	0	100	100
21	Z	51/51 (100%)	51 (100%)	0	100	100
21	z	51/51 (100%)	51 (100%)	0	100	100
All	All	5426/6914 (78%)	5422 (100%)	4 (0%)	87	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	332	HIS
2	B	362	PHE
1	a	332	HIS
2	b	362	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	303	ASN
1	A	304	GLN
1	A	322	ASN
2	B	202	HIS
2	B	216	HIS
2	B	223	GLN
2	B	317	ASN
3	C	118	HIS
3	C	201	ASN

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Mol	Chain	Res	Type
3	C	313	GLN
4	D	231	ASN
4	D	335	GLN
7	G	240	GLN
7	G	251	ASN
7	N	104	ASN
13	O	337	GLN
14	R	156	GLN
15	S	129	ASN
15	S	251	ASN
16	T	31	ASN
7	Y	240	GLN
21	Z	6	GLN
1	a	303	ASN
1	a	322	ASN
2	b	202	HIS
2	b	317	ASN
3	c	118	HIS
3	c	313	GLN
4	d	231	ASN
4	d	335	GLN
7	n	146	GLN
13	o	120	GLN
13	o	189	GLN
13	o	224	GLN
13	o	237	GLN
14	r	147	GLN
14	r	156	GLN
15	s	224	HIS
15	s	251	ASN
7	y	226	ASN
7	y	240	GLN
7	y	251	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 358 ligands modelled in this entry, 4 are monoatomic - leaving 354 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	$\# Z > 2$
23	CLA	n	610	7	69,73,73	1.25	8 (11%)	83,113,113	1.26	6 (7%)
31	LNL	C	521	-	19,19,19	0.45	0	18,19,19	0.93	1 (5%)
30	LHG	a	412	-	48,48,48	1.40	8 (16%)	51,54,54	0.73	2 (3%)
30	LHG	A	412	-	36,36,48	1.52	8 (22%)	39,42,54	0.89	2 (5%)
40	LUT	s	615	-	42,43,43	2.55	21 (50%)	51,60,60	3.15	24 (47%)
27	LMG	d	409	-	46,46,55	0.19	0	54,54,63	0.15	0
23	CLA	C	509	3	69,73,73	1.25	7 (10%)	83,113,113	1.27	6 (7%)
39	CHL	R	607	-	70,74,74	1.04	5 (7%)	80,114,114	1.68	13 (16%)
39	CHL	g	601	7	70,74,74	1.02	4 (5%)	80,114,114	1.65	10 (12%)
25	BCR	B	618	-	40,40,41	1.09	2 (5%)	52,54,56	1.25	6 (11%)
39	CHL	G	601	7	70,74,74	1.02	4 (5%)	80,114,114	1.66	10 (12%)
33	DGD	C	515	-	67,67,67	0.88	2 (2%)	81,81,81	1.46	10 (12%)
23	CLA	s	613	15	69,73,73	1.25	7 (10%)	83,113,113	1.27	7 (8%)
23	CLA	B	602	2	69,73,73	1.26	7 (10%)	83,113,113	1.29	9 (10%)
23	CLA	N	604	-	53,57,73	1.43	9 (16%)	62,93,113	1.42	8 (12%)
25	BCR	z	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	5 (8%)
31	LNL	C	519	-	19,19,19	0.43	0	18,19,19	0.95	1 (5%)
23	CLA	a	404	43	69,73,73	1.25	9 (13%)	83,113,113	1.32	7 (8%)
25	BCR	Z	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	5 (8%)
28	3PH	L	102	-	40,40,47	0.68	1 (2%)	44,45,52	0.64	1 (2%)
23	CLA	D	406	4	69,73,73	1.26	8 (11%)	83,113,113	1.30	6 (7%)
41	NEX	s	617	-	23,27,46	4.08	19 (82%)	28,38,70	3.76	14 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	507	43	69,73,73	1.26	8 (11%)	83,113,113	1.31	5 (6%)
31	LNL	A	413	-	19,19,19	0.44	0	18,19,19	0.89	1 (5%)
23	CLA	r	611	14	53,57,73	1.43	7 (13%)	62,93,113	1.42	5 (8%)
40	LUT	n	616	-	42,43,43	2.36	19 (45%)	51,60,60	3.07	21 (41%)
33	DGD	d	411	-	63,63,67	0.85	1 (1%)	77,77,81	1.35	7 (9%)
23	CLA	G	610	7	69,73,73	1.25	6 (8%)	83,113,113	1.30	8 (9%)
23	CLA	g	602	7	69,73,73	1.26	7 (10%)	83,113,113	1.29	6 (7%)
40	LUT	G	616	-	42,43,43	2.41	20 (47%)	51,60,60	3.11	21 (41%)
42	XAT	n	617	-	39,47,47	3.04	21 (53%)	54,74,74	4.50	30 (55%)
23	CLA	s	610	30	69,73,73	1.26	7 (10%)	83,113,113	1.27	6 (7%)
23	CLA	N	612	7	53,57,73	1.43	8 (15%)	62,93,113	1.41	5 (8%)
30	LHG	Y	318	23	48,48,48	1.39	8 (16%)	51,54,54	0.69	2 (3%)
23	CLA	R	612	14	53,57,73	1.44	7 (13%)	62,93,113	1.40	5 (8%)
23	CLA	r	602	14	69,73,73	1.26	7 (10%)	83,113,113	1.29	6 (7%)
39	CHL	s	601	-	56,60,74	1.15	3 (5%)	63,97,114	1.86	10 (15%)
23	CLA	c	504	43	69,73,73	1.26	7 (10%)	83,113,113	1.28	4 (4%)
23	CLA	y	314	7	69,73,73	1.26	8 (11%)	83,113,113	1.29	6 (7%)
27	LMG	D	409	-	36,36,55	0.20	0	44,44,63	0.14	0
23	CLA	n	613	7	69,73,73	1.26	7 (10%)	83,113,113	1.30	5 (6%)
28	3PH	W	201	-	45,45,47	0.64	1 (2%)	49,50,52	0.60	1 (2%)
23	CLA	c	501	3	69,73,73	1.25	8 (11%)	83,113,113	1.26	6 (7%)
23	CLA	y	305	7	69,73,73	1.25	6 (8%)	83,113,113	1.31	6 (7%)
23	CLA	Y	303	7	69,73,73	1.25	7 (10%)	83,113,113	1.29	7 (8%)
41	NEX	S	617	-	19,23,46	4.24	16 (84%)	23,33,70	4.24	11 (47%)
31	LNL	b	625	-	19,19,19	0.44	0	18,19,19	0.92	1 (5%)
39	CHL	g	608	-	54,58,74	1.19	4 (7%)	59,94,114	1.84	10 (16%)
31	LNL	C	522	-	19,19,19	0.44	0	18,19,19	0.91	1 (5%)
31	LNL	I	101	-	19,19,19	0.43	0	18,19,19	0.91	1 (5%)
23	CLA	c	505	3	69,73,73	1.25	8 (11%)	83,113,113	1.26	6 (7%)
26	SQD	a	409	-	47,48,54	1.61	7 (14%)	56,59,65	1.45	6 (10%)
28	3PH	C	524	-	47,47,47	0.63	1 (2%)	51,52,52	0.60	1 (1%)
28	3PH	X	201	-	45,45,47	0.65	1 (2%)	49,50,52	0.60	1 (2%)
31	LNL	A	414	-	19,19,19	0.43	0	18,19,19	0.92	1 (5%)
30	LHG	L	103	-	48,48,48	1.36	8 (16%)	51,54,54	0.71	2 (3%)
23	CLA	Y	313	-	69,73,73	1.26	7 (10%)	83,113,113	1.28	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CHL	G	606	-	54,58,74	1.21	3 (5%)	59,94,114	1.94	9 (15%)
23	CLA	Y	311	30	69,73,73	1.25	7 (10%)	83,113,113	1.27	6 (7%)
23	CLA	r	610	30	69,73,73	1.26	7 (10%)	83,113,113	1.33	7 (8%)
39	CHL	r	605	-	54,58,74	1.16	5 (9%)	59,94,114	1.91	11 (18%)
25	BCR	h	501	-	41,41,41	1.15	2 (4%)	56,56,56	1.20	4 (7%)
23	CLA	a	405	43	53,57,73	1.42	6 (11%)	62,93,113	1.44	7 (11%)
23	CLA	d	406	4	69,73,73	1.25	7 (10%)	83,113,113	1.31	6 (7%)
39	CHL	S	606	-	54,58,74	1.18	4 (7%)	59,94,114	1.93	11 (18%)
23	CLA	b	608	2	69,73,73	1.25	7 (10%)	83,113,113	1.28	7 (8%)
39	CHL	s	606	-	54,58,74	1.17	4 (7%)	59,94,114	1.87	10 (16%)
39	CHL	n	608	-	54,58,74	1.18	4 (7%)	59,94,114	1.92	10 (16%)
23	CLA	a	407	1	64,68,73	1.30	7 (10%)	77,107,113	1.34	7 (9%)
23	CLA	Y	312	7	69,73,73	1.27	6 (8%)	83,113,113	1.26	6 (7%)
23	CLA	s	608	-	53,57,73	1.44	6 (11%)	62,93,113	1.36	5 (8%)
23	CLA	c	512	3	69,73,73	1.25	7 (10%)	83,113,113	1.28	8 (9%)
25	BCR	k	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.23	6 (10%)
23	CLA	g	603	7	69,73,73	1.26	7 (10%)	83,113,113	1.29	6 (7%)
23	CLA	c	513	3	64,68,73	1.29	8 (12%)	77,107,113	1.31	6 (7%)
23	CLA	g	611	-	69,73,73	1.25	7 (10%)	83,113,113	1.27	5 (6%)
41	NEX	g	617	-	38,46,46	4.18	33 (86%)	50,70,70	4.94	24 (48%)
35	VIV	C	523	-	32,32,32	0.93	2 (6%)	41,45,45	1.14	4 (9%)
41	NEX	n	618	-	38,46,46	4.08	32 (84%)	50,70,70	4.99	22 (44%)
23	CLA	R	603	14	64,68,73	1.30	8 (12%)	77,107,113	1.33	7 (9%)
23	CLA	G	604	-	53,57,73	1.43	8 (15%)	62,93,113	1.41	7 (11%)
23	CLA	A	404	43	53,57,73	1.42	7 (13%)	62,93,113	1.44	6 (9%)
23	CLA	B	601	-	53,57,73	1.42	6 (11%)	62,93,113	1.45	6 (9%)
23	CLA	a	403	1	69,73,73	1.25	8 (11%)	83,113,113	1.30	6 (7%)
23	CLA	B	616	2	69,73,73	1.25	7 (10%)	83,113,113	1.30	7 (8%)
23	CLA	n	604	-	53,57,73	1.43	9 (16%)	62,93,113	1.42	8 (12%)
39	CHL	g	619	43	70,74,74	1.03	4 (5%)	80,114,114	1.70	11 (13%)
39	CHL	G	609	7	70,74,74	1.08	4 (5%)	80,114,114	1.76	9 (11%)
23	CLA	s	604	-	53,57,73	1.42	9 (16%)	62,93,113	1.44	7 (11%)
40	LUT	R	613	-	42,43,43	2.53	21 (50%)	51,60,60	3.16	25 (49%)
23	CLA	N	613	7	69,73,73	1.26	6 (8%)	83,113,113	1.39	7 (8%)
30	LHG	N	618	23	48,48,48	1.45	8 (16%)	51,54,54	0.69	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LNL	b	624	-	19,19,19	0.43	0	18,19,19	0.88	1 (5%)
23	CLA	c	508	3	69,73,73	1.25	7 (10%)	83,113,113	1.30	8 (9%)
23	CLA	c	503	3	69,73,73	1.25	7 (10%)	83,113,113	1.29	5 (6%)
23	CLA	R	610	30	69,73,73	1.27	7 (10%)	83,113,113	1.27	6 (7%)
23	CLA	C	502	3	69,73,73	1.25	8 (11%)	83,113,113	1.30	6 (7%)
23	CLA	B	615	2	69,73,73	1.26	7 (10%)	83,113,113	1.28	5 (6%)
23	CLA	b	615	2	69,73,73	1.25	7 (10%)	83,113,113	1.31	5 (6%)
23	CLA	Y	304	7	69,73,73	1.25	7 (10%)	83,113,113	1.31	5 (6%)
39	CHL	R	605	-	54,58,74	1.17	4 (7%)	59,94,114	1.90	11 (18%)
32	PAM	B	621	-	17,17,17	0.61	0	17,17,17	0.78	0
23	CLA	y	311	7	69,73,73	1.25	8 (11%)	83,113,113	1.28	8 (9%)
39	CHL	R	606	-	70,74,74	1.03	4 (5%)	80,114,114	1.66	12 (15%)
36	BCT	D	401	22	2,3,3	1.16	0	2,3,3	4.53	2 (100%)
40	LUT	Y	315	-	42,43,43	1.78	10 (23%)	51,60,60	2.77	20 (39%)
30	LHG	d	408	-	48,48,48	1.36	8 (16%)	51,54,54	0.74	2 (3%)
23	CLA	C	513	3	69,73,73	1.24	7 (10%)	83,113,113	1.33	8 (9%)
23	CLA	G	613	7	69,73,73	1.26	7 (10%)	83,113,113	1.30	6 (7%)
27	LMG	b	628	-	50,50,55	0.19	0	58,58,63	0.18	0
23	CLA	r	603	14	64,68,73	1.30	8 (12%)	77,107,113	1.32	7 (9%)
23	CLA	B	610	43	69,73,73	1.26	7 (10%)	83,113,113	1.27	7 (8%)
23	CLA	b	610	43	69,73,73	1.27	7 (10%)	83,113,113	1.28	7 (8%)
24	PHO	A	405	-	58,69,69	2.04	10 (17%)	56,99,99	1.48	8 (14%)
25	BCR	C	514	-	41,41,41	1.14	2 (4%)	56,56,56	1.20	7 (12%)
23	CLA	c	506	3	69,73,73	1.26	9 (13%)	83,113,113	1.27	6 (7%)
30	LHG	r	616	23	36,36,48	1.60	8 (22%)	39,42,54	0.82	2 (5%)
23	CLA	y	312	30	69,73,73	1.25	7 (10%)	83,113,113	1.27	8 (9%)
23	CLA	C	508	3	69,73,73	1.25	7 (10%)	83,113,113	1.31	7 (8%)
40	LUT	y	317	-	42,43,43	2.38	20 (47%)	51,60,60	3.16	23 (45%)
26	SQD	L	101	-	53,54,54	1.53	8 (15%)	62,65,65	1.40	6 (9%)
32	PAM	b	621	-	17,17,17	0.63	0	17,17,17	0.78	0
39	CHL	N	608	-	54,58,74	1.17	4 (7%)	59,94,114	1.92	11 (18%)
40	LUT	g	616	-	42,43,43	2.40	19 (45%)	51,60,60	3.11	21 (41%)
27	LMG	A	409	-	53,53,55	0.19	0	61,61,63	0.19	0
42	XAT	R	615	-	39,47,47	3.21	20 (51%)	54,74,74	4.68	31 (57%)
25	BCR	b	618	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	n	603	7	69,73,73	1.25	8 (11%)	83,113,113	1.30	6 (7%)
27	LMG	b	620	-	51,51,55	0.19	0	59,59,63	0.22	0
23	CLA	R	604	43	59,63,73	1.35	9 (15%)	71,101,113	1.36	7 (9%)
24	PHO	d	402	-	58,69,69	2.06	10 (17%)	56,99,99	1.52	7 (12%)
23	CLA	A	402	1	69,73,73	1.26	8 (11%)	83,113,113	1.30	6 (7%)
25	BCR	A	407	-	41,41,41	1.12	2 (4%)	56,56,56	1.19	5 (8%)
23	CLA	s	602	15	61,65,73	1.34	7 (11%)	73,103,113	1.33	5 (6%)
23	CLA	C	506	3	59,63,73	1.35	9 (15%)	71,101,113	1.33	7 (9%)
23	CLA	B	609	2	69,73,73	1.25	7 (10%)	83,113,113	1.26	7 (8%)
25	BCR	b	617	-	41,41,41	1.13	2 (4%)	56,56,56	1.33	8 (14%)
39	CHL	y	309	-	54,58,74	1.18	4 (7%)	59,94,114	1.88	9 (15%)
25	BCR	D	411	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	6 (10%)
23	CLA	G	614	7	53,57,73	1.44	6 (11%)	62,93,113	1.36	6 (9%)
42	XAT	N	619	-	39,47,47	3.16	23 (58%)	54,74,74	4.58	32 (59%)
26	SQD	M	101	-	49,50,54	1.59	8 (16%)	58,61,65	1.38	6 (10%)
39	CHL	S	607	-	53,57,74	1.20	5 (9%)	59,93,114	1.87	11 (18%)
41	NEX	R	614	-	38,46,46	4.09	32 (84%)	50,70,70	4.87	22 (44%)
31	LNL	C	517	-	19,19,19	0.43	0	18,19,19	0.92	1 (5%)
39	CHL	g	605	7	52,56,74	1.20	4 (7%)	58,92,114	2.09	11 (18%)
40	LUT	S	614	-	42,43,43	2.60	21 (50%)	51,60,60	3.23	25 (49%)
39	CHL	g	606	-	54,58,74	1.21	4 (7%)	59,94,114	1.95	11 (18%)
23	CLA	c	511	3	69,73,73	1.26	8 (11%)	83,113,113	1.31	7 (8%)
28	3PH	T	101	-	47,47,47	0.63	1 (2%)	51,52,52	0.61	1 (1%)
23	CLA	c	509	3	69,73,73	1.25	8 (11%)	83,113,113	1.27	5 (6%)
42	XAT	Y	301	-	39,47,47	3.30	24 (61%)	54,74,74	4.45	32 (59%)
35	VIV	y	301	-	32,32,32	0.88	1 (3%)	41,45,45	1.13	5 (12%)
25	BCR	B	617	-	41,41,41	1.10	2 (4%)	56,56,56	1.29	8 (14%)
23	CLA	n	614	7	53,57,73	1.43	7 (13%)	62,93,113	1.40	6 (9%)
31	LNL	c	522	-	19,19,19	0.43	0	18,19,19	0.94	1 (5%)
28	3PH	w	202	-	47,47,47	0.63	1 (2%)	51,52,52	0.59	1 (1%)
40	LUT	g	615	-	42,43,43	1.88	10 (23%)	51,60,60	2.93	21 (41%)
40	LUT	G	615	-	42,43,43	1.97	12 (28%)	51,60,60	2.89	22 (43%)
23	CLA	S	608	-	53,57,73	1.43	6 (11%)	62,93,113	1.34	5 (8%)
23	CLA	A	403	43	69,73,73	1.25	8 (11%)	83,113,113	1.31	7 (8%)
23	CLA	G	612	7	53,57,73	1.43	7 (13%)	62,93,113	1.42	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	S	609	15	60,64,73	1.35	8 (13%)	72,102,113	1.30	8 (11%)
23	CLA	B	612	2	69,73,73	1.24	8 (11%)	83,113,113	1.32	6 (7%)
28	3PH	x	201	-	45,45,47	0.65	1 (2%)	49,50,52	0.60	1 (2%)
23	CLA	B	604	2	69,73,73	1.25	8 (11%)	83,113,113	1.36	6 (7%)
27	LMG	R	617	-	51,51,55	0.18	0	59,59,63	0.26	0
25	BCR	d	410	-	41,41,41	1.14	2 (4%)	56,56,56	1.21	6 (10%)
36	BCT	d	401	22	2,3,3	1.15	0	2,3,3	4.51	2 (100%)
30	LHG	D	408	-	48,48,48	1.13	4 (8%)	51,54,54	0.93	3 (5%)
29	PL9	a	411	-	55,55,55	0.11	0	68,69,69	0.28	0
23	CLA	b	609	-	69,73,73	1.25	6 (8%)	83,113,113	1.28	7 (8%)
23	CLA	A	406	1	64,68,73	1.29	6 (9%)	77,107,113	1.33	7 (9%)
30	LHG	n	619	23	44,44,48	1.45	8 (18%)	47,50,54	0.75	2 (4%)
28	3PH	a	410	-	47,47,47	0.63	1 (2%)	51,52,52	0.56	1 (1%)
23	CLA	b	616	2	69,73,73	1.25	8 (11%)	83,113,113	1.30	7 (8%)
40	LUT	S	615	-	42,43,43	2.65	22 (52%)	51,60,60	3.22	24 (47%)
23	CLA	B	605	2	69,73,73	1.25	8 (11%)	83,113,113	1.26	6 (7%)
40	LUT	n	615	-	42,43,43	1.89	11 (26%)	51,60,60	2.97	19 (37%)
23	CLA	S	610	30	69,73,73	1.27	6 (8%)	83,113,113	1.28	6 (7%)
31	LNL	a	401	-	19,19,19	0.43	0	18,19,19	0.93	1 (5%)
30	LHG	b	627	-	48,48,48	1.36	8 (16%)	51,54,54	0.73	2 (3%)
23	CLA	C	511	3	69,73,73	1.26	7 (10%)	83,113,113	1.31	6 (7%)
39	CHL	Y	302	7	70,74,74	1.04	4 (5%)	80,114,114	1.64	11 (13%)
25	BCR	B	619	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	5 (8%)
30	LHG	g	618	-	48,48,48	1.40	8 (16%)	51,54,54	0.77	2 (3%)
23	CLA	B	607	-	69,73,73	1.25	7 (10%)	83,113,113	1.30	6 (7%)
40	LUT	N	616	-	42,43,43	2.59	22 (52%)	51,60,60	3.21	22 (43%)
23	CLA	B	611	2	69,73,73	1.25	7 (10%)	83,113,113	1.28	7 (8%)
23	CLA	N	603	7	69,73,73	1.24	8 (11%)	83,113,113	1.31	6 (7%)
23	CLA	C	503	3	69,73,73	1.25	6 (8%)	83,113,113	1.29	5 (6%)
23	CLA	S	612	15	59,63,73	1.36	7 (11%)	71,101,113	1.37	5 (7%)
23	CLA	b	605	2	69,73,73	1.25	8 (11%)	83,113,113	1.25	5 (6%)
23	CLA	s	612	15	59,63,73	1.36	7 (11%)	71,101,113	1.36	5 (7%)
28	3PH	A	410	-	47,47,47	0.62	1 (2%)	51,52,52	0.60	1 (1%)
31	LNL	c	520	-	19,19,19	0.43	0	18,19,19	0.95	1 (5%)
23	CLA	b	604	2	69,73,73	1.25	8 (11%)	83,113,113	1.36	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	SQD	A	408	-	49,50,54	1.57	7 (14%)	58,61,65	1.45	7 (12%)
25	BCR	c	514	-	41,41,41	1.14	2 (4%)	56,56,56	1.20	7 (12%)
37	DGA	b	626	-	43,43,43	0.19	0	45,45,45	0.15	0
23	CLA	y	313	7	69,73,73	1.26	6 (8%)	83,113,113	1.26	6 (7%)
39	CHL	r	606	-	70,74,74	1.03	4 (5%)	80,114,114	1.65	11 (13%)
40	LUT	r	613	-	42,43,43	2.49	20 (47%)	51,60,60	3.11	24 (47%)
39	CHL	Y	306	7	52,56,74	1.19	4 (7%)	58,92,114	2.12	9 (15%)
23	CLA	G	602	7	69,73,73	1.26	8 (11%)	83,113,113	1.30	7 (8%)
23	CLA	N	614	7	53,57,73	1.42	6 (11%)	62,93,113	1.39	6 (9%)
42	XAT	r	615	-	39,47,47	3.22	20 (51%)	54,74,74	4.70	31 (57%)
23	CLA	r	601	14	53,57,73	1.44	6 (11%)	62,93,113	1.38	5 (8%)
23	CLA	C	504	43	69,73,73	1.25	7 (10%)	83,113,113	1.29	4 (4%)
23	CLA	S	602	15	61,65,73	1.35	7 (11%)	73,103,113	1.34	6 (8%)
24	PHO	D	402	-	58,69,69	2.05	10 (17%)	56,99,99	1.50	6 (10%)
39	CHL	G	620	-	70,74,74	1.04	4 (5%)	80,114,114	1.70	11 (13%)
23	CLA	C	512	3	69,73,73	1.26	7 (10%)	83,113,113	1.29	6 (7%)
40	LUT	Y	316	-	42,43,43	2.36	20 (47%)	51,60,60	3.15	23 (45%)
39	CHL	N	605	7	54,58,74	1.18	3 (5%)	59,94,114	2.15	9 (15%)
25	BCR	V	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.19	4 (7%)
31	LNL	c	517	-	19,19,19	0.44	0	18,19,19	0.93	1 (5%)
23	CLA	d	405	4	69,73,73	1.25	8 (11%)	83,113,113	1.28	4 (4%)
41	NEX	N	617	-	38,46,46	4.10	32 (84%)	50,70,70	4.96	22 (44%)
23	CLA	B	614	2	69,73,73	1.25	8 (11%)	83,113,113	1.29	5 (6%)
33	DGD	H	502	-	63,63,67	0.87	1 (1%)	77,77,81	1.33	7 (9%)
23	CLA	b	613	2	69,73,73	1.26	7 (10%)	83,113,113	1.27	5 (6%)
23	CLA	c	510	3	69,73,73	1.25	7 (10%)	83,113,113	1.29	5 (6%)
39	CHL	n	606	-	70,74,74	1.03	4 (5%)	80,114,114	1.59	10 (12%)
39	CHL	g	607	-	70,74,74	1.03	5 (7%)	80,114,114	1.71	10 (12%)
23	CLA	n	612	7	53,57,73	1.43	7 (13%)	62,93,113	1.39	4 (6%)
23	CLA	b	607	-	69,73,73	1.26	8 (11%)	83,113,113	1.30	6 (7%)
30	LHG	s	616	23	48,48,48	1.39	8 (16%)	51,54,54	0.74	2 (3%)
40	LUT	N	615	-	42,43,43	2.58	21 (50%)	51,60,60	3.25	24 (47%)
41	NEX	R	618	-	38,46,46	3.93	31 (81%)	50,70,70	4.85	20 (40%)
23	CLA	n	611	30	53,57,73	1.43	7 (13%)	62,93,113	1.39	6 (9%)
42	XAT	y	302	-	39,47,47	3.39	24 (61%)	54,74,74	4.46	31 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	611	2	69,73,73	1.25	8 (11%)	83,113,113	1.30	9 (10%)
31	LNL	a	413	-	19,19,19	0.44	0	18,19,19	0.93	1 (5%)
23	CLA	B	606	2	69,73,73	1.27	9 (13%)	83,113,113	1.30	7 (8%)
23	CLA	C	501	3	69,73,73	1.25	7 (10%)	83,113,113	1.27	6 (7%)
39	CHL	s	607	-	53,57,74	1.19	4 (7%)	59,93,114	1.86	11 (18%)
23	CLA	y	306	-	69,73,73	1.26	8 (11%)	83,113,113	1.29	9 (10%)
31	LNL	i	101	-	19,19,19	0.45	0	18,19,19	0.89	1 (5%)
23	CLA	B	603	2	69,73,73	1.25	8 (11%)	83,113,113	1.26	6 (7%)
23	CLA	G	611	30	53,57,73	1.43	8 (15%)	62,93,113	1.40	6 (9%)
39	CHL	Y	309	7	70,74,74	1.05	4 (5%)	80,114,114	1.61	10 (12%)
23	CLA	g	610	7	69,73,73	1.24	6 (8%)	83,113,113	1.30	8 (9%)
39	CHL	n	609	7	70,74,74	1.02	5 (7%)	80,114,114	1.61	11 (13%)
23	CLA	b	601	-	54,58,73	1.41	7 (12%)	65,95,113	1.42	7 (10%)
39	CHL	N	609	7	70,74,74	1.03	5 (7%)	80,114,114	1.62	11 (13%)
42	XAT	G	619	-	39,47,47	3.01	22 (56%)	54,74,74	4.57	30 (55%)
28	3PH	s	618	-	37,37,47	0.70	1 (2%)	41,42,52	0.64	1 (2%)
23	CLA	C	507	43	69,73,73	1.26	7 (10%)	83,113,113	1.30	5 (6%)
23	CLA	B	613	2	69,73,73	1.26	6 (8%)	83,113,113	1.27	5 (6%)
23	CLA	R	602	14	69,73,73	1.26	7 (10%)	83,113,113	1.28	4 (4%)
23	CLA	Y	314	7	69,73,73	1.26	9 (13%)	83,113,113	1.28	8 (9%)
23	CLA	g	612	7	53,57,73	1.43	7 (13%)	62,93,113	1.46	5 (8%)
39	CHL	Y	307	-	70,74,74	1.03	4 (5%)	80,114,114	1.64	9 (11%)
23	CLA	g	614	7	53,57,73	1.42	7 (13%)	62,93,113	1.38	6 (9%)
27	LMG	r	617	-	51,51,55	0.19	0	59,59,63	0.16	0
39	CHL	r	607	-	70,74,74	1.05	5 (7%)	80,114,114	1.68	12 (15%)
25	BCR	H	501	-	41,41,41	1.15	2 (4%)	56,56,56	1.20	4 (7%)
23	CLA	S	611	15	53,57,73	1.43	7 (13%)	62,93,113	1.40	5 (8%)
31	LNL	B	623	-	19,19,19	0.45	0	18,19,19	0.86	1 (5%)
23	CLA	s	611	15	53,57,73	1.43	7 (13%)	62,93,113	1.40	4 (6%)
39	CHL	N	601	7	70,74,74	1.04	5 (7%)	80,114,114	1.69	11 (13%)
23	CLA	R	601	14	53,57,73	1.44	7 (13%)	62,93,113	1.40	6 (9%)
23	CLA	b	606	2	69,73,73	1.27	8 (11%)	83,113,113	1.29	8 (9%)
23	CLA	C	510	3	69,73,73	1.25	8 (11%)	83,113,113	1.28	5 (6%)
31	LNL	B	622	-	19,19,19	0.45	0	18,19,19	0.93	1 (5%)
23	CLA	D	405	4	69,73,73	1.24	8 (11%)	83,113,113	1.27	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMG	C	525	-	45,45,55	0.20	0	53,53,63	0.14	0
37	DGA	D	410	-	39,39,43	0.20	0	41,41,45	0.15	0
42	XAT	n	620	-	39,47,47	3.15	23 (58%)	54,74,74	4.56	31 (57%)
23	CLA	r	608	-	69,73,73	1.25	8 (11%)	83,113,113	1.29	6 (7%)
23	CLA	N	611	30	69,73,73	1.26	7 (10%)	83,113,113	1.25	6 (7%)
39	CHL	G	605	7	52,56,74	1.21	3 (5%)	58,92,114	2.07	12 (20%)
23	CLA	r	609	14	69,73,73	1.25	7 (10%)	83,113,113	1.26	7 (8%)
31	LNL	b	623	-	19,19,19	0.45	0	18,19,19	0.89	1 (5%)
30	LHG	d	404	-	48,48,48	1.36	8 (16%)	51,54,54	0.78	2 (3%)
39	CHL	G	607	-	70,74,74	1.04	4 (5%)	80,114,114	1.71	10 (12%)
23	CLA	b	612	2	69,73,73	1.25	7 (10%)	83,113,113	1.31	6 (7%)
31	LNL	c	518	-	19,19,19	0.44	0	18,19,19	0.92	1 (5%)
30	LHG	S	616	23	48,48,48	1.43	8 (16%)	51,54,54	0.73	2 (3%)
41	NEX	r	614	-	38,46,46	3.97	31 (81%)	50,70,70	4.87	22 (44%)
23	CLA	b	614	2	69,73,73	1.24	8 (11%)	83,113,113	1.28	6 (7%)
38	HEM	f	501	6,5	50,50,50	1.52	7 (14%)	66,82,82	1.21	7 (10%)
31	LNL	C	520	-	19,19,19	0.44	0	18,19,19	0.90	1 (5%)
41	NEX	Y	317	-	38,46,46	4.00	31 (81%)	50,70,70	4.95	22 (44%)
23	CLA	c	502	3	69,73,73	1.25	8 (11%)	83,113,113	1.29	6 (7%)
39	CHL	y	310	7	70,74,74	1.03	4 (5%)	80,114,114	1.59	11 (13%)
23	CLA	R	609	14	69,73,73	1.26	7 (10%)	83,113,113	1.26	5 (6%)
40	LUT	y	316	-	42,43,43	1.80	10 (23%)	51,60,60	2.77	19 (37%)
39	CHL	N	606	-	70,74,74	1.03	4 (5%)	80,114,114	1.60	10 (12%)
23	CLA	n	602	7	69,73,73	1.26	8 (11%)	83,113,113	1.29	7 (8%)
39	CHL	g	609	7	70,74,74	1.04	4 (5%)	80,114,114	1.68	11 (13%)
25	BCR	a	408	-	41,41,41	1.13	2 (4%)	56,56,56	1.19	6 (10%)
39	CHL	n	605	7	52,56,74	1.19	4 (7%)	58,92,114	2.07	10 (17%)
24	PHO	a	406	-	58,69,69	2.03	10 (17%)	56,99,99	1.47	6 (10%)
23	CLA	g	604	-	53,57,73	1.43	8 (15%)	62,93,113	1.41	7 (11%)
39	CHL	n	607	-	70,74,74	1.04	4 (5%)	80,114,114	1.70	9 (11%)
31	LNL	B	625	-	19,19,19	0.45	0	18,19,19	0.91	1 (5%)
30	LHG	G	618	23	48,48,48	1.39	8 (16%)	51,54,54	0.75	2 (3%)
39	CHL	s	605	-	54,58,74	1.17	3 (5%)	59,94,114	1.91	11 (18%)
39	CHL	Y	308	-	54,58,74	1.17	4 (7%)	59,94,114	1.91	9 (15%)
27	LMG	c	523	-	46,46,55	0.19	0	54,54,63	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LHG	y	318	23	48,48,48	1.39	8 (16%)	51,54,54	0.71	2 (3%)
23	CLA	g	613	7	69,73,73	1.26	6 (8%)	83,113,113	1.31	7 (8%)
23	CLA	r	612	14	53,57,73	1.43	7 (13%)	62,93,113	1.37	5 (8%)
23	CLA	y	315	7	69,73,73	1.27	8 (11%)	83,113,113	1.27	7 (8%)
23	CLA	Y	310	7	69,73,73	1.25	7 (10%)	83,113,113	1.28	8 (9%)
39	CHL	S	601	-	56,60,74	1.14	3 (5%)	63,97,114	1.86	10 (15%)
23	CLA	C	505	3	69,73,73	1.25	8 (11%)	83,113,113	1.26	6 (7%)
23	CLA	R	608	-	69,73,73	1.25	7 (10%)	83,113,113	1.30	7 (8%)
23	CLA	N	610	7	69,73,73	1.25	8 (11%)	83,113,113	1.26	8 (9%)
23	CLA	B	608	2	69,73,73	1.25	9 (13%)	83,113,113	1.27	7 (8%)
27	LMG	B	626	-	49,49,55	0.19	0	57,57,63	0.14	0
23	CLA	S	604	-	53,57,73	1.42	8 (15%)	62,93,113	1.44	6 (9%)
23	CLA	Y	305	-	69,73,73	1.26	8 (11%)	83,113,113	1.29	8 (9%)
23	CLA	y	304	7	69,73,73	1.26	7 (10%)	83,113,113	1.29	7 (8%)
29	PL9	A	411	-	55,55,55	0.11	0	68,69,69	0.42	0
31	LNL	c	519	-	19,19,19	0.43	0	18,19,19	0.93	1 (5%)
23	CLA	G	603	7	64,68,73	1.30	8 (12%)	77,107,113	1.31	5 (6%)
23	CLA	s	609	15	60,64,73	1.36	8 (13%)	72,102,113	1.34	8 (11%)
23	CLA	R	611	14	53,57,73	1.43	7 (13%)	62,93,113	1.40	5 (8%)
29	PL9	D	407	-	55,55,55	0.08	0	68,69,69	0.21	0
39	CHL	G	608	-	54,58,74	1.19	5 (9%)	59,94,114	1.86	10 (16%)
23	CLA	S	613	15	69,73,73	1.26	6 (8%)	83,113,113	1.28	7 (8%)
31	LNL	C	518	-	19,19,19	0.44	0	18,19,19	0.97	1 (5%)
25	BCR	K	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	6 (10%)
39	CHL	S	605	-	54,58,74	1.17	4 (7%)	59,94,114	1.94	10 (16%)
39	CHL	y	307	7	52,56,74	1.19	4 (7%)	58,92,114	2.09	9 (15%)
28	3PH	D	403	-	37,37,47	0.70	1 (2%)	41,42,52	0.65	1 (2%)
39	CHL	y	308	43	54,58,74	1.17	4 (7%)	59,94,114	1.90	9 (15%)
31	LNL	c	521	-	19,19,19	0.43	0	18,19,19	0.94	1 (5%)
30	LHG	D	404	-	42,42,48	1.43	8 (19%)	45,48,54	0.80	2 (4%)
40	LUT	s	614	-	42,43,43	2.74	23 (54%)	51,60,60	3.28	24 (47%)
25	BCR	v	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.20	4 (7%)
23	CLA	N	602	7	69,73,73	1.26	7 (10%)	83,113,113	1.29	6 (7%)
31	LNL	B	624	-	19,19,19	0.44	0	18,19,19	0.90	1 (5%)
30	LHG	R	616	23	37,37,48	1.56	8 (21%)	40,43,54	0.86	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CHL	n	601	7	70,74,74	1.03	4 (5%)	80,114,114	1.68	9 (11%)
27	LMG	w	201	-	48,48,55	0.19	0	56,56,63	0.18	0
39	CHL	y	303	7	70,74,74	1.03	5 (7%)	80,114,114	1.67	11 (13%)
23	CLA	b	602	2	69,73,73	1.25	6 (8%)	83,113,113	1.29	6 (7%)
39	CHL	N	607	-	70,74,74	1.04	4 (5%)	80,114,114	1.68	9 (11%)
25	BCR	b	619	-	41,41,41	1.10	2 (4%)	56,56,56	1.17	5 (8%)
29	PL9	d	407	-	55,55,55	0.08	0	68,69,69	0.22	0
33	DGD	c	515	-	56,56,67	0.95	2 (3%)	70,70,81	1.45	9 (12%)
23	CLA	b	603	2	69,73,73	1.25	8 (11%)	83,113,113	1.27	6 (7%)
41	NEX	G	617	-	21,25,46	4.26	19 (90%)	28,38,70	5.44	11 (39%)
38	HEM	F	501	-	50,50,50	1.41	6 (12%)	66,82,82	1.22	6 (9%)
23	CLA	S	603	15	53,57,73	1.43	7 (13%)	62,93,113	1.42	5 (8%)
23	CLA	r	604	43	59,63,73	1.35	8 (13%)	71,101,113	1.37	8 (11%)
23	CLA	s	603	15	53,57,73	1.43	8 (15%)	62,93,113	1.41	6 (9%)
28	3PH	d	403	-	37,37,47	0.71	1 (2%)	41,42,52	0.66	1 (2%)
31	LNL	b	622	-	19,19,19	0.44	0	18,19,19	0.93	1 (5%)
27	LMG	B	620	-	48,48,55	0.19	0	56,56,63	0.19	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
23	CLA	n	610	7	-	11/39/115/115	-
31	LNL	C	521	-	-	11/17/17/17	-
30	LHG	a	412	-	-	26/53/53/53	-
30	LHG	A	412	-	-	21/41/41/53	-
40	LUT	s	615	-	-	11/29/67/67	0/2/2/2
27	LMG	d	409	-	-	6/41/61/70	0/1/1/1
23	CLA	C	509	3	-	10/39/115/115	-
39	CHL	R	607	-	-	11/41/117/117	-
39	CHL	g	601	7	-	8/41/117/117	-
25	BCR	B	618	-	-	3/29/60/63	0/2/2/2
39	CHL	G	601	7	-	11/41/117/117	-
33	DGD	C	515	-	-	20/55/95/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	s	613	15	-	16/39/115/115	-
23	CLA	B	602	2	-	14/39/115/115	-
23	CLA	N	604	-	-	7/20/96/115	-
25	BCR	z	101	-	-	5/29/63/63	0/2/2/2
31	LNL	C	519	-	-	5/17/17/17	-
23	CLA	a	404	43	-	11/39/115/115	-
25	BCR	Z	101	-	-	5/29/63/63	0/2/2/2
28	3PH	L	102	-	-	14/42/42/49	-
23	CLA	D	406	4	-	17/39/115/115	-
41	NEX	s	617	-	-	8/15/40/83	0/1/1/3
23	CLA	c	507	43	-	8/39/115/115	-
31	LNL	A	413	-	-	10/17/17/17	-
23	CLA	r	611	14	-	6/20/96/115	-
40	LUT	n	616	-	-	14/29/67/67	0/2/2/2
33	DGD	d	411	-	-	18/51/91/95	0/2/2/2
23	CLA	G	610	7	-	10/39/115/115	-
23	CLA	g	602	7	-	5/39/115/115	-
40	LUT	G	616	-	-	9/29/67/67	0/2/2/2
42	XAT	n	617	-	-	6/31/93/93	0/4/4/4
23	CLA	s	610	30	-	16/39/115/115	-
23	CLA	N	612	7	-	9/20/96/115	-
30	LHG	Y	318	23	-	21/53/53/53	-
23	CLA	R	612	14	-	10/20/96/115	-
23	CLA	r	602	14	-	13/39/115/115	-
39	CHL	s	601	-	-	8/25/101/117	-
23	CLA	c	504	43	-	8/39/115/115	-
23	CLA	y	314	7	-	14/39/115/115	-
27	LMG	D	409	-	-	1/31/51/70	0/1/1/1
23	CLA	n	613	7	-	6/39/115/115	-
28	3PH	W	201	-	-	23/47/47/49	-
23	CLA	c	501	3	-	15/39/115/115	-
23	CLA	y	305	7	-	12/39/115/115	-
23	CLA	Y	303	7	-	13/39/115/115	-
41	NEX	S	617	-	-	6/11/36/83	0/1/1/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LNL	b	625	-	-	9/17/17/17	-
39	CHL	g	608	-	-	10/22/98/117	-
31	LNL	C	522	-	-	11/17/17/17	-
31	LNL	I	101	-	-	11/17/17/17	-
23	CLA	c	505	3	-	8/39/115/115	-
26	SQD	a	409	-	-	18/43/63/69	0/1/1/1
28	3PH	C	524	-	-	19/49/49/49	-
28	3PH	X	201	-	-	13/47/47/49	-
31	LNL	A	414	-	-	8/17/17/17	-
30	LHG	L	103	-	-	25/53/53/53	-
23	CLA	Y	313	-	-	10/39/115/115	-
39	CHL	G	606	-	-	4/22/98/117	-
23	CLA	Y	311	30	-	9/39/115/115	-
23	CLA	r	610	30	-	12/39/115/115	-
39	CHL	r	605	-	-	6/22/98/117	-
25	BCR	h	501	-	-	7/29/63/63	0/2/2/2
23	CLA	a	405	43	-	1/20/96/115	-
23	CLA	d	406	4	-	7/39/115/115	-
39	CHL	S	606	-	-	8/22/98/117	-
23	CLA	b	608	2	-	10/39/115/115	-
39	CHL	s	606	-	-	6/22/98/117	-
39	CHL	n	608	-	-	6/22/98/117	-
23	CLA	a	407	1	-	5/33/109/115	-
23	CLA	Y	312	7	-	9/39/115/115	-
23	CLA	s	608	-	-	9/20/96/115	-
23	CLA	c	512	3	-	21/39/115/115	-
25	BCR	k	101	-	-	4/29/63/63	0/2/2/2
23	CLA	g	603	7	-	10/39/115/115	-
23	CLA	c	513	3	-	8/33/109/115	-
23	CLA	g	611	-	-	11/39/115/115	-
41	NEX	g	617	-	-	14/27/83/83	0/3/3/3
35	VIV	C	523	-	-	12/19/30/30	0/2/2/2
41	NEX	n	618	-	-	14/27/83/83	0/3/3/3
23	CLA	R	603	14	-	5/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	G	604	-	-	6/20/96/115	-
23	CLA	A	404	43	-	5/20/96/115	-
23	CLA	B	601	-	-	12/20/96/115	-
23	CLA	a	403	1	-	10/39/115/115	-
23	CLA	B	616	2	-	11/39/115/115	-
23	CLA	n	604	-	-	7/20/96/115	-
39	CHL	g	619	43	-	10/41/117/117	-
39	CHL	G	609	7	-	12/41/117/117	-
23	CLA	s	604	-	-	8/20/96/115	-
40	LUT	R	613	-	-	16/29/67/67	0/2/2/2
23	CLA	N	613	7	-	12/39/115/115	-
30	LHG	N	618	23	-	25/53/53/53	-
31	LNL	b	624	-	-	9/17/17/17	-
23	CLA	c	508	3	-	3/39/115/115	-
23	CLA	c	503	3	-	7/39/115/115	-
23	CLA	R	610	30	-	11/39/115/115	-
23	CLA	C	502	3	-	12/39/115/115	-
23	CLA	B	615	2	-	9/39/115/115	-
23	CLA	b	615	2	-	6/39/115/115	-
23	CLA	Y	304	7	-	12/39/115/115	-
39	CHL	R	605	-	-	4/22/98/117	-
32	PAM	B	621	-	-	5/15/15/15	-
23	CLA	y	311	7	-	10/39/115/115	-
39	CHL	R	606	-	-	11/41/117/117	-
40	LUT	Y	315	-	-	17/29/67/67	0/2/2/2
30	LHG	d	408	-	-	15/53/53/53	-
23	CLA	C	513	3	-	12/39/115/115	-
23	CLA	G	613	7	-	12/39/115/115	-
27	LMG	b	628	-	-	11/45/65/70	0/1/1/1
23	CLA	r	603	14	-	5/33/109/115	-
23	CLA	B	610	43	-	8/39/115/115	-
23	CLA	b	610	43	-	10/39/115/115	-
24	PHO	A	405	-	-	10/37/103/103	0/5/6/6
25	BCR	C	514	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	506	3	-	15/39/115/115	-
30	LHG	r	616	23	-	19/41/41/53	-
23	CLA	y	312	30	-	8/39/115/115	-
23	CLA	C	508	3	-	7/39/115/115	-
40	LUT	y	317	-	-	15/29/67/67	0/2/2/2
26	SQD	L	101	-	-	24/49/69/69	0/1/1/1
32	PAM	b	621	-	-	3/15/15/15	-
39	CHL	N	608	-	-	8/22/98/117	-
40	LUT	g	616	-	-	10/29/67/67	0/2/2/2
27	LMG	A	409	-	-	11/48/68/70	0/1/1/1
42	XAT	R	615	-	-	14/31/93/93	0/4/4/4
25	BCR	b	618	-	-	5/29/63/63	0/2/2/2
23	CLA	n	603	7	-	11/39/115/115	-
27	LMG	b	620	-	-	8/46/66/70	0/1/1/1
23	CLA	R	604	43	-	9/27/103/115	-
24	PHO	d	402	-	-	5/37/103/103	0/5/6/6
23	CLA	A	402	1	-	10/39/115/115	-
25	BCR	A	407	-	-	4/29/63/63	0/2/2/2
23	CLA	s	602	15	-	9/30/106/115	-
23	CLA	C	506	3	-	9/27/103/115	-
23	CLA	B	609	2	-	8/39/115/115	-
25	BCR	b	617	-	-	11/29/63/63	0/2/2/2
39	CHL	y	309	-	-	5/22/98/117	-
25	BCR	D	411	-	-	5/29/63/63	0/2/2/2
23	CLA	G	614	7	-	8/20/96/115	-
42	XAT	N	619	-	-	13/31/93/93	0/4/4/4
26	SQD	M	101	-	-	24/45/65/69	0/1/1/1
39	CHL	S	607	-	-	7/21/97/117	-
41	NEX	R	614	-	-	13/27/83/83	0/3/3/3
31	LNL	C	517	-	-	12/17/17/17	-
39	CHL	g	605	7	-	7/20/96/117	-
40	LUT	S	614	-	-	15/29/67/67	0/2/2/2
39	CHL	g	606	-	-	4/22/98/117	-
23	CLA	c	511	3	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	3PH	T	101	-	-	22/49/49/49	-
23	CLA	c	509	3	-	10/39/115/115	-
42	XAT	Y	301	-	-	17/31/93/93	0/4/4/4
35	VIV	y	301	-	-	15/19/30/30	0/2/2/2
25	BCR	B	617	-	-	10/29/63/63	0/2/2/2
23	CLA	n	614	7	-	10/20/96/115	-
31	LNL	c	522	-	-	7/17/17/17	-
28	3PH	w	202	-	-	17/49/49/49	-
40	LUT	g	615	-	-	19/29/67/67	0/2/2/2
40	LUT	G	615	-	-	22/29/67/67	0/2/2/2
23	CLA	S	608	-	-	3/20/96/115	-
23	CLA	A	403	43	-	10/39/115/115	-
23	CLA	G	612	7	-	8/20/96/115	-
23	CLA	S	609	15	-	12/29/105/115	-
23	CLA	B	612	2	-	11/39/115/115	-
28	3PH	x	201	-	-	13/47/47/49	-
23	CLA	B	604	2	-	9/39/115/115	-
27	LMG	R	617	-	-	14/46/66/70	0/1/1/1
25	BCR	d	410	-	-	9/29/63/63	0/2/2/2
30	LHG	D	408	-	-	29/53/53/53	-
29	PL9	a	411	-	-	12/53/73/73	0/1/1/1
23	CLA	b	609	-	-	10/39/115/115	-
23	CLA	A	406	1	-	1/33/109/115	-
30	LHG	n	619	23	-	23/49/49/53	-
28	3PH	a	410	-	-	21/49/49/49	-
23	CLA	b	616	2	-	12/39/115/115	-
40	LUT	S	615	-	-	16/29/67/67	0/2/2/2
23	CLA	B	605	2	-	13/39/115/115	-
40	LUT	n	615	-	-	14/29/67/67	0/2/2/2
23	CLA	S	610	30	-	16/39/115/115	-
31	LNL	a	401	-	-	11/17/17/17	-
30	LHG	b	627	-	-	22/53/53/53	-
23	CLA	C	511	3	-	11/39/115/115	-
39	CHL	Y	302	7	-	13/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	B	619	-	-	4/29/63/63	0/2/2/2
30	LHG	g	618	-	-	15/53/53/53	-
23	CLA	B	607	-	-	21/39/115/115	-
40	LUT	N	616	-	-	20/29/67/67	0/2/2/2
23	CLA	B	611	2	-	10/39/115/115	-
23	CLA	N	603	7	-	10/39/115/115	-
23	CLA	C	503	3	-	8/39/115/115	-
23	CLA	S	612	15	-	9/27/103/115	-
23	CLA	b	605	2	-	15/39/115/115	-
23	CLA	s	612	15	-	7/27/103/115	-
28	3PH	A	410	-	-	18/49/49/49	-
31	LNL	c	520	-	-	6/17/17/17	-
23	CLA	b	604	2	-	6/39/115/115	-
26	SQD	A	408	-	-	29/45/65/69	0/1/1/1
25	BCR	c	514	-	-	7/29/63/63	0/2/2/2
37	DGA	b	626	-	-	14/45/45/45	-
23	CLA	y	313	7	-	9/39/115/115	-
39	CHL	r	606	-	-	12/41/117/117	-
40	LUT	r	613	-	-	11/29/67/67	0/2/2/2
39	CHL	Y	306	7	-	4/20/96/117	-
23	CLA	G	602	7	-	5/39/115/115	-
23	CLA	N	614	7	-	7/20/96/115	-
42	XAT	r	615	-	-	14/31/93/93	0/4/4/4
23	CLA	r	601	14	-	12/20/96/115	-
23	CLA	C	504	43	-	8/39/115/115	-
23	CLA	S	602	15	-	10/30/106/115	-
24	PHO	D	402	-	-	9/37/103/103	0/5/6/6
39	CHL	G	620	-	-	14/41/117/117	-
23	CLA	C	512	3	-	17/39/115/115	-
40	LUT	Y	316	-	-	15/29/67/67	0/2/2/2
39	CHL	N	605	7	-	7/22/98/117	-
25	BCR	V	101	-	-	11/29/63/63	0/2/2/2
31	LNL	c	517	-	-	5/17/17/17	-
23	CLA	d	405	4	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	NEX	N	617	-	-	12/27/83/83	0/3/3/3
23	CLA	B	614	2	-	13/39/115/115	-
33	DGD	H	502	-	-	24/51/91/95	0/2/2/2
23	CLA	b	613	2	-	13/39/115/115	-
23	CLA	c	510	3	-	14/39/115/115	-
39	CHL	n	606	-	-	8/41/117/117	-
39	CHL	g	607	-	-	15/41/117/117	-
23	CLA	n	612	7	-	5/20/96/115	-
23	CLA	b	607	-	-	16/39/115/115	-
30	LHG	s	616	23	-	19/53/53/53	-
40	LUT	N	615	-	-	13/29/67/67	0/2/2/2
41	NEX	R	618	-	-	12/27/83/83	0/3/3/3
23	CLA	n	611	30	-	7/20/96/115	-
42	XAT	y	302	-	-	18/31/93/93	0/4/4/4
23	CLA	b	611	2	-	6/39/115/115	-
31	LNL	a	413	-	-	9/17/17/17	-
23	CLA	B	606	2	-	9/39/115/115	-
23	CLA	C	501	3	-	13/39/115/115	-
39	CHL	s	607	-	-	8/21/97/117	-
23	CLA	y	306	-	-	20/39/115/115	-
31	LNL	i	101	-	-	9/17/17/17	-
23	CLA	B	603	2	-	10/39/115/115	-
23	CLA	G	611	30	-	10/20/96/115	-
39	CHL	Y	309	7	-	6/41/117/117	-
23	CLA	g	610	7	-	10/39/115/115	-
39	CHL	n	609	7	-	10/41/117/117	-
23	CLA	b	601	-	-	7/21/97/115	-
39	CHL	N	609	7	-	8/41/117/117	-
42	XAT	G	619	-	-	11/31/93/93	0/4/4/4
28	3PH	s	618	-	-	14/39/39/49	-
23	CLA	C	507	43	-	11/39/115/115	-
23	CLA	B	613	2	-	8/39/115/115	-
23	CLA	R	602	14	-	6/39/115/115	-
23	CLA	Y	314	7	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	g	612	7	-	6/20/96/115	-
39	CHL	Y	307	-	-	3/41/117/117	-
23	CLA	g	614	7	-	8/20/96/115	-
27	LMG	r	617	-	-	11/46/66/70	0/1/1/1
39	CHL	r	607	-	-	11/41/117/117	-
25	BCR	H	501	-	-	7/29/63/63	0/2/2/2
23	CLA	S	611	15	-	9/20/96/115	-
31	LNL	B	623	-	-	10/17/17/17	-
23	CLA	s	611	15	-	8/20/96/115	-
39	CHL	N	601	7	-	9/41/117/117	-
23	CLA	R	601	14	-	12/20/96/115	-
23	CLA	b	606	2	-	10/39/115/115	-
23	CLA	C	510	3	-	12/39/115/115	-
31	LNL	B	622	-	-	7/17/17/17	-
23	CLA	D	405	4	-	9/39/115/115	-
27	LMG	C	525	-	-	10/40/60/70	0/1/1/1
37	DGA	D	410	-	-	12/41/41/45	-
42	XAT	n	620	-	-	9/31/93/93	0/4/4/4
23	CLA	r	608	-	-	9/39/115/115	-
23	CLA	N	611	30	-	11/39/115/115	-
39	CHL	G	605	7	-	8/20/96/117	-
23	CLA	r	609	14	-	7/39/115/115	-
31	LNL	b	623	-	-	10/17/17/17	-
30	LHG	d	404	-	-	20/53/53/53	-
39	CHL	G	607	-	-	11/41/117/117	-
23	CLA	b	612	2	-	12/39/115/115	-
31	LNL	c	518	-	-	12/17/17/17	-
30	LHG	S	616	23	-	14/53/53/53	-
41	NEX	r	614	-	-	9/27/83/83	0/3/3/3
23	CLA	b	614	2	-	12/39/115/115	-
38	HEM	f	501	6,5	-	1/14/54/54	-
31	LNL	C	520	-	-	11/17/17/17	-
41	NEX	Y	317	-	-	14/27/83/83	0/3/3/3
23	CLA	c	502	3	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	y	310	7	-	10/41/117/117	-
23	CLA	R	609	14	-	6/39/115/115	-
40	LUT	y	316	-	-	17/29/67/67	0/2/2/2
39	CHL	N	606	-	-	9/41/117/117	-
23	CLA	n	602	7	-	11/39/115/115	-
39	CHL	g	609	7	-	13/41/117/117	-
25	BCR	a	408	-	-	4/29/63/63	0/2/2/2
39	CHL	n	605	7	-	6/20/96/117	-
24	PHO	a	406	-	-	10/37/103/103	0/5/6/6
23	CLA	g	604	-	-	8/20/96/115	-
39	CHL	n	607	-	-	10/41/117/117	-
31	LNL	B	625	-	-	7/17/17/17	-
30	LHG	G	618	23	-	19/53/53/53	-
39	CHL	s	605	-	-	5/22/98/117	-
39	CHL	Y	308	-	-	8/22/98/117	-
27	LMG	c	523	-	-	9/41/61/70	0/1/1/1
30	LHG	y	318	23	-	22/53/53/53	-
23	CLA	g	613	7	-	10/39/115/115	-
23	CLA	r	612	14	-	7/20/96/115	-
23	CLA	y	315	7	-	20/39/115/115	-
23	CLA	Y	310	7	-	13/39/115/115	-
39	CHL	S	601	-	-	6/25/101/117	-
23	CLA	C	505	3	-	6/39/115/115	-
23	CLA	R	608	-	-	7/39/115/115	-
23	CLA	N	610	7	-	10/39/115/115	-
23	CLA	B	608	2	-	10/39/115/115	-
27	LMG	B	626	-	-	8/44/64/70	0/1/1/1
23	CLA	S	604	-	-	7/20/96/115	-
23	CLA	Y	305	-	-	12/39/115/115	-
23	CLA	y	304	7	-	13/39/115/115	-
29	PL9	A	411	-	-	7/53/73/73	0/1/1/1
31	LNL	c	519	-	-	11/17/17/17	-
23	CLA	G	603	7	-	3/33/109/115	-
23	CLA	s	609	15	-	11/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	R	611	14	-	8/20/96/115	-
29	PL9	D	407	-	-	10/53/73/73	0/1/1/1
39	CHL	G	608	-	-	10/22/98/117	-
23	CLA	S	613	15	-	14/39/115/115	-
31	LNL	C	518	-	-	8/17/17/17	-
25	BCR	K	101	-	-	4/29/63/63	0/2/2/2
39	CHL	S	605	-	-	6/22/98/117	-
39	CHL	y	307	7	-	4/20/96/117	-
28	3PH	D	403	-	-	13/39/39/49	-
39	CHL	y	308	43	-	5/22/98/117	-
31	LNL	c	521	-	-	7/17/17/17	-
30	LHG	D	404	-	-	10/47/47/53	-
40	LUT	s	614	-	-	18/29/67/67	0/2/2/2
25	BCR	v	101	-	-	10/29/63/63	0/2/2/2
23	CLA	N	602	7	-	4/39/115/115	-
31	LNL	B	624	-	-	8/17/17/17	-
30	LHG	R	616	23	-	17/42/42/53	-
39	CHL	n	601	7	-	10/41/117/117	-
27	LMG	w	201	-	-	5/43/63/70	0/1/1/1
39	CHL	y	303	7	-	15/41/117/117	-
23	CLA	b	602	2	-	12/39/115/115	-
39	CHL	N	607	-	-	9/41/117/117	-
25	BCR	b	619	-	-	6/29/63/63	0/2/2/2
29	PL9	d	407	-	-	10/53/73/73	0/1/1/1
33	DGD	c	515	-	-	13/44/84/95	0/2/2/2
23	CLA	b	603	2	-	11/39/115/115	-
41	NEX	G	617	-	-	7/16/47/83	0/2/2/3
38	HEM	F	501	-	-	3/14/54/54	-
23	CLA	S	603	15	-	12/20/96/115	-
23	CLA	r	604	43	-	8/27/103/115	-
23	CLA	s	603	15	-	12/20/96/115	-
28	3PH	d	403	-	-	10/39/39/49	-
31	LNL	b	622	-	-	8/17/17/17	-
27	LMG	B	620	-	-	7/43/63/70	0/1/1/1

All (2393) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	405	PHO	C1B-C2B	9.46	1.50	1.39
24	d	402	PHO	C1B-C2B	9.39	1.50	1.39
24	D	402	PHO	C1B-C2B	9.37	1.50	1.39
24	a	406	PHO	C1B-C2B	9.33	1.49	1.39
42	y	302	XAT	C10-C9	8.32	1.46	1.35
40	s	614	LUT	C34-C33	8.21	1.46	1.35
42	n	620	XAT	C10-C9	8.08	1.46	1.35
40	N	616	LUT	C34-C33	8.05	1.46	1.35
40	S	615	LUT	C34-C33	8.04	1.46	1.35
42	N	619	XAT	C10-C9	7.97	1.46	1.35
42	Y	301	XAT	C10-C9	7.94	1.46	1.35
40	S	614	LUT	C34-C33	7.89	1.46	1.35
41	G	617	NEX	C34-C33	7.84	1.46	1.35
40	R	613	LUT	C34-C33	7.84	1.46	1.35
40	s	615	LUT	C34-C33	7.74	1.46	1.35
40	N	615	LUT	C34-C33	7.73	1.46	1.35
40	r	613	LUT	C34-C33	7.72	1.46	1.35
24	D	402	PHO	C3B-C4B	7.71	1.50	1.41
24	d	402	PHO	C3B-C4B	7.69	1.50	1.41
24	a	406	PHO	C3B-C4B	7.64	1.50	1.41
24	A	405	PHO	C3B-C4B	7.55	1.50	1.41
41	g	617	NEX	C34-C33	7.53	1.45	1.35
40	G	616	LUT	C34-C33	7.37	1.45	1.35
40	y	317	LUT	C34-C33	7.36	1.45	1.35
40	n	616	LUT	C34-C33	7.34	1.45	1.35
40	g	616	LUT	C34-C33	7.30	1.45	1.35
40	Y	316	LUT	C34-C33	7.28	1.45	1.35
41	n	618	NEX	C34-C33	7.16	1.45	1.35
41	R	614	NEX	C34-C33	7.12	1.45	1.35
41	N	617	NEX	C34-C33	7.08	1.45	1.35
41	S	617	NEX	C12-C13	7.08	1.61	1.45
41	G	617	NEX	C28-C29	7.07	1.61	1.45
41	g	617	NEX	C28-C29	7.00	1.61	1.45
41	s	617	NEX	C12-C13	6.96	1.60	1.45
42	G	619	XAT	C12-C13	-6.91	1.31	1.45
42	n	617	XAT	C10-C9	6.90	1.44	1.35
41	r	614	NEX	C34-C33	6.86	1.44	1.35
41	Y	317	NEX	C34-C33	6.83	1.44	1.35
41	N	617	NEX	C28-C29	6.80	1.60	1.45
41	n	618	NEX	C28-C29	6.80	1.60	1.45
41	g	617	NEX	C12-C13	6.77	1.60	1.45
41	R	614	NEX	C12-C13	6.75	1.60	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	R	618	NEX	C34-C33	6.74	1.44	1.35
42	r	615	XAT	C14-C13	6.70	1.44	1.35
41	S	617	NEX	C10-C9	6.68	1.44	1.35
42	n	617	XAT	C12-C13	-6.66	1.31	1.45
42	R	615	XAT	C14-C13	6.63	1.44	1.35
39	G	609	CHL	C4B-NB	6.61	1.45	1.37
41	s	617	NEX	C10-C9	6.60	1.44	1.35
41	n	618	NEX	C12-C13	6.60	1.60	1.45
41	R	614	NEX	C10-C9	6.60	1.44	1.35
42	r	615	XAT	C10-C9	6.54	1.44	1.35
42	N	619	XAT	C12-C13	-6.53	1.31	1.45
41	g	617	NEX	C10-C9	6.53	1.44	1.35
41	R	614	NEX	C28-C29	6.50	1.59	1.45
41	N	617	NEX	C10-C9	6.49	1.44	1.35
41	N	617	NEX	C12-C13	6.49	1.59	1.45
42	n	620	XAT	C12-C13	-6.47	1.32	1.45
42	R	615	XAT	C12-C13	-6.45	1.32	1.45
42	R	615	XAT	C10-C9	6.44	1.44	1.35
42	r	615	XAT	C12-C13	-6.43	1.32	1.45
39	G	606	CHL	C4B-NB	6.41	1.45	1.37
41	r	614	NEX	C12-C13	6.41	1.59	1.45
39	g	606	CHL	C4B-NB	6.41	1.45	1.37
40	G	615	LUT	C34-C33	6.40	1.44	1.35
41	r	614	NEX	C28-C29	6.32	1.59	1.45
41	R	618	NEX	C10-C9	6.29	1.44	1.35
41	Y	317	NEX	C12-C13	6.28	1.59	1.45
39	g	608	CHL	C4B-NB	6.27	1.45	1.37
41	S	617	NEX	C14-C13	6.27	1.44	1.35
39	G	608	CHL	C4B-NB	6.26	1.45	1.37
42	y	302	XAT	C34-C33	6.25	1.44	1.35
39	G	605	CHL	C4B-NB	6.25	1.45	1.37
41	Y	317	NEX	C28-C29	6.24	1.59	1.45
42	Y	301	XAT	C12-C13	-6.23	1.32	1.45
40	n	615	LUT	C34-C33	6.23	1.44	1.35
41	R	618	NEX	C28-C29	6.22	1.59	1.45
39	g	609	CHL	C4B-NB	6.21	1.45	1.37
39	Y	309	CHL	C4B-NB	6.21	1.45	1.37
42	y	302	XAT	C14-C13	6.20	1.44	1.35
39	r	607	CHL	C4B-NB	6.20	1.45	1.37
41	Y	317	NEX	C10-C9	6.19	1.44	1.35
39	R	607	CHL	C4B-NB	6.17	1.45	1.37
39	s	607	CHL	C4B-NB	6.17	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	n	601	CHL	C4B-NB	6.17	1.45	1.37
39	N	601	CHL	C4B-NB	6.16	1.45	1.37
39	S	607	CHL	C4B-NB	6.16	1.45	1.37
40	g	615	LUT	C34-C33	6.16	1.43	1.35
39	Y	302	CHL	C4B-NB	6.15	1.45	1.37
39	S	606	CHL	C4B-NB	6.15	1.45	1.37
41	n	618	NEX	C10-C9	6.13	1.43	1.35
39	Y	308	CHL	C4B-NB	6.12	1.45	1.37
42	r	615	XAT	C30-C29	6.12	1.43	1.35
39	n	606	CHL	C4B-NB	6.11	1.45	1.37
41	R	618	NEX	C12-C13	6.10	1.59	1.45
39	y	309	CHL	C4B-NB	6.10	1.45	1.37
39	N	606	CHL	C4B-NB	6.10	1.45	1.37
39	g	619	CHL	C4B-NB	6.09	1.45	1.37
39	n	608	CHL	C4B-NB	6.09	1.45	1.37
39	N	605	CHL	C4B-NB	6.09	1.45	1.37
39	s	605	CHL	C4B-NB	6.08	1.45	1.37
39	R	605	CHL	C4B-NB	6.08	1.45	1.37
39	n	607	CHL	C4B-NB	6.08	1.45	1.37
39	S	605	CHL	C4B-NB	6.07	1.45	1.37
39	n	605	CHL	C4B-NB	6.07	1.45	1.37
39	y	303	CHL	C4B-NB	6.07	1.45	1.37
39	G	607	CHL	C4B-NB	6.07	1.45	1.37
42	y	302	XAT	C12-C13	-6.06	1.32	1.45
39	s	606	CHL	C4B-NB	6.05	1.45	1.37
39	N	608	CHL	C4B-NB	6.05	1.45	1.37
42	R	615	XAT	C30-C29	6.05	1.43	1.35
39	N	607	CHL	C4B-NB	6.04	1.45	1.37
39	s	601	CHL	C4B-NB	6.03	1.45	1.37
39	G	620	CHL	C4B-NB	6.02	1.45	1.37
39	N	609	CHL	C4B-NB	6.02	1.45	1.37
39	g	607	CHL	C4B-NB	6.01	1.45	1.37
39	y	310	CHL	C4B-NB	6.01	1.45	1.37
39	S	601	CHL	C4B-NB	6.01	1.45	1.37
39	Y	306	CHL	C4B-NB	6.01	1.45	1.37
39	G	601	CHL	C4B-NB	6.00	1.45	1.37
39	Y	307	CHL	C4B-NB	6.00	1.45	1.37
39	g	605	CHL	C4B-NB	5.99	1.45	1.37
39	y	308	CHL	C4B-NB	5.98	1.45	1.37
39	y	307	CHL	C4B-NB	5.97	1.45	1.37
39	g	601	CHL	C4B-NB	5.96	1.45	1.37
41	r	614	NEX	C10-C9	5.95	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	R	606	CHL	C4B-NB	5.95	1.45	1.37
39	n	609	CHL	C4B-NB	5.94	1.45	1.37
41	Y	317	NEX	C1-C6	5.94	1.64	1.54
39	r	605	CHL	C4B-NB	5.93	1.45	1.37
39	r	606	CHL	C4B-NB	5.90	1.45	1.37
41	s	617	NEX	C14-C13	5.80	1.43	1.35
42	n	617	XAT	C32-C33	-5.78	1.33	1.45
40	y	316	LUT	C34-C33	5.70	1.43	1.35
42	r	615	XAT	C32-C33	-5.68	1.33	1.45
40	Y	315	LUT	C34-C33	5.67	1.43	1.35
41	n	618	NEX	C1-C6	5.66	1.64	1.54
42	R	615	XAT	C32-C33	-5.65	1.33	1.45
42	y	302	XAT	C32-C33	-5.64	1.33	1.45
42	G	619	XAT	C32-C33	-5.64	1.33	1.45
42	Y	301	XAT	C14-C13	5.58	1.43	1.35
41	N	617	NEX	C1-C6	5.58	1.63	1.54
42	Y	301	XAT	C32-C33	-5.58	1.34	1.45
42	n	620	XAT	C32-C33	-5.57	1.34	1.45
41	g	617	NEX	C14-C13	5.57	1.43	1.35
40	s	614	LUT	C14-C13	5.57	1.43	1.35
42	N	619	XAT	C32-C33	-5.49	1.34	1.45
41	G	617	NEX	C31-C30	5.39	1.60	1.43
40	N	616	LUT	C14-C13	5.36	1.42	1.35
42	Y	301	XAT	C34-C33	5.36	1.42	1.35
40	S	615	LUT	C14-C13	5.34	1.42	1.35
41	R	618	NEX	C1-C6	5.33	1.63	1.54
42	n	620	XAT	C14-C13	5.31	1.42	1.35
40	N	615	LUT	C14-C13	5.28	1.42	1.35
42	Y	301	XAT	C30-C29	5.27	1.42	1.35
41	n	618	NEX	C14-C13	5.26	1.42	1.35
42	N	619	XAT	C14-C13	5.26	1.42	1.35
41	R	614	NEX	C14-C13	5.25	1.42	1.35
41	g	617	NEX	C31-C30	5.24	1.59	1.43
40	R	613	LUT	C14-C13	5.24	1.42	1.35
40	S	614	LUT	C14-C13	5.22	1.42	1.35
42	R	615	XAT	C34-C33	5.21	1.42	1.35
41	S	617	NEX	C1-C6	5.21	1.63	1.54
40	s	615	LUT	C14-C13	5.20	1.42	1.35
41	n	618	NEX	C31-C30	5.18	1.59	1.43
42	r	615	XAT	C34-C33	5.18	1.42	1.35
41	R	614	NEX	C31-C30	5.17	1.59	1.43
41	N	617	NEX	C14-C13	5.16	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	s	617	NEX	C1-C6	5.14	1.63	1.54
41	N	617	NEX	C24-C23	5.14	1.59	1.52
41	N	617	NEX	C31-C30	5.14	1.59	1.43
42	y	302	XAT	C2-C3	5.13	1.59	1.52
42	G	619	XAT	C10-C9	5.13	1.42	1.35
41	R	614	NEX	C1-C6	5.12	1.63	1.54
41	n	618	NEX	C24-C23	5.11	1.59	1.52
40	r	613	LUT	C14-C13	5.09	1.42	1.35
42	Y	301	XAT	C2-C3	5.08	1.59	1.52
41	r	614	NEX	C31-C30	5.08	1.59	1.43
41	g	617	NEX	C1-C6	5.06	1.63	1.54
41	Y	317	NEX	C31-C30	5.05	1.59	1.43
42	N	619	XAT	C34-C33	5.04	1.42	1.35
41	Y	317	NEX	C14-C13	5.03	1.42	1.35
41	G	617	NEX	C24-C23	5.01	1.59	1.52
41	R	618	NEX	C31-C30	5.01	1.59	1.43
41	Y	317	NEX	C24-C23	4.98	1.59	1.52
41	r	614	NEX	C14-C13	4.97	1.42	1.35
41	R	618	NEX	C24-C23	4.96	1.59	1.52
41	r	614	NEX	C24-C23	4.95	1.59	1.52
41	r	614	NEX	C1-C6	4.95	1.62	1.54
41	g	617	NEX	C24-C23	4.93	1.59	1.52
40	g	616	LUT	C14-C13	4.93	1.42	1.35
41	R	614	NEX	C24-C23	4.92	1.59	1.52
41	g	617	NEX	C22-C23	4.92	1.59	1.52
40	G	616	LUT	C14-C13	4.89	1.42	1.35
40	n	616	LUT	C14-C13	4.87	1.42	1.35
41	G	617	NEX	C22-C23	4.85	1.59	1.52
41	R	618	NEX	C14-C13	4.83	1.42	1.35
41	G	617	NEX	C35-C34	4.83	1.58	1.43
41	s	617	NEX	C35-C34	4.83	1.58	1.43
42	G	619	XAT	C30-C29	4.82	1.42	1.35
40	N	615	LUT	C10-C9	4.81	1.42	1.35
41	R	614	NEX	C22-C23	4.77	1.59	1.52
41	n	618	NEX	C22-C23	4.76	1.59	1.52
41	r	614	NEX	C2-C3	4.76	1.59	1.52
40	s	614	LUT	C10-C9	4.73	1.42	1.35
42	n	620	XAT	C34-C33	4.73	1.42	1.35
42	G	619	XAT	C34-C33	4.73	1.42	1.35
41	S	617	NEX	C11-C10	4.73	1.58	1.43
41	G	617	NEX	C24-C25	4.72	1.58	1.52
41	R	618	NEX	C22-C23	4.72	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	N	617	NEX	C22-C23	4.71	1.59	1.52
26	M	101	SQD	O48-C23	4.70	1.47	1.33
41	Y	317	NEX	C2-C3	4.69	1.59	1.52
41	Y	317	NEX	C22-C23	4.69	1.59	1.52
41	G	617	NEX	C32-C33	4.68	1.56	1.45
41	r	614	NEX	C22-C23	4.67	1.59	1.52
40	y	317	LUT	C14-C13	4.67	1.42	1.35
41	s	617	NEX	C11-C10	4.67	1.57	1.43
40	Y	316	LUT	C14-C13	4.66	1.42	1.35
26	L	101	SQD	O48-C23	4.65	1.46	1.33
26	a	409	SQD	O48-C23	4.64	1.46	1.33
41	g	617	NEX	C35-C34	4.63	1.57	1.43
41	s	617	NEX	C2-C3	4.63	1.59	1.52
41	N	617	NEX	C24-C25	4.63	1.58	1.52
41	R	614	NEX	C2-C3	4.61	1.59	1.52
26	A	408	SQD	O48-C23	4.61	1.46	1.33
41	n	618	NEX	C24-C25	4.59	1.58	1.52
41	R	614	NEX	C11-C10	4.59	1.57	1.43
41	g	617	NEX	C24-C25	4.57	1.58	1.52
41	g	617	NEX	C11-C10	4.55	1.57	1.43
41	g	617	NEX	C18-C5	4.53	1.60	1.52
41	S	617	NEX	C7-C8	4.53	1.39	1.32
41	s	617	NEX	C34-C33	4.52	1.46	1.35
41	Y	317	NEX	C18-C5	4.51	1.60	1.52
41	R	618	NEX	C2-C3	4.51	1.58	1.52
41	R	614	NEX	C18-C5	4.51	1.60	1.52
41	g	617	NEX	C32-C33	4.51	1.55	1.45
41	r	614	NEX	C18-C5	4.49	1.60	1.52
42	n	620	XAT	C2-C3	4.48	1.58	1.52
41	S	617	NEX	C2-C3	4.48	1.58	1.52
41	N	617	NEX	C11-C10	4.48	1.57	1.43
42	N	619	XAT	C2-C3	4.48	1.58	1.52
41	s	617	NEX	C7-C8	4.48	1.39	1.32
41	Y	317	NEX	C24-C25	4.47	1.58	1.52
41	N	617	NEX	C2-C3	4.47	1.58	1.52
41	R	614	NEX	C35-C34	4.47	1.57	1.43
42	n	617	XAT	C30-C29	4.47	1.41	1.35
41	n	618	NEX	C18-C5	4.47	1.60	1.52
41	s	617	NEX	C15-C14	4.47	1.57	1.43
41	g	617	NEX	C4-C3	4.45	1.58	1.52
41	n	618	NEX	C32-C33	4.45	1.55	1.45
41	R	618	NEX	C24-C25	4.45	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	G	617	NEX	C28-C27	4.45	1.42	1.32
41	r	614	NEX	C4-C3	4.44	1.58	1.52
41	R	614	NEX	C4-C3	4.44	1.58	1.52
40	r	613	LUT	C10-C9	4.44	1.41	1.35
41	N	617	NEX	C18-C5	4.43	1.60	1.52
40	N	616	LUT	C10-C9	4.43	1.41	1.35
41	n	618	NEX	C35-C34	4.42	1.57	1.43
41	G	617	NEX	C30-C29	4.42	1.41	1.35
40	S	615	LUT	C10-C9	4.41	1.41	1.35
41	g	617	NEX	C7-C8	4.41	1.39	1.32
41	R	618	NEX	C18-C5	4.41	1.59	1.52
40	R	613	LUT	C10-C9	4.40	1.41	1.35
41	N	617	NEX	C35-C34	4.40	1.57	1.43
40	S	614	LUT	C10-C9	4.39	1.41	1.35
42	G	619	XAT	C8-C9	-4.39	1.36	1.45
41	R	618	NEX	C11-C10	4.38	1.57	1.43
40	s	615	LUT	C10-C9	4.37	1.41	1.35
41	N	617	NEX	C32-C33	4.36	1.55	1.45
41	R	614	NEX	C7-C8	4.35	1.39	1.32
41	Y	317	NEX	C11-C10	4.35	1.56	1.43
42	n	617	XAT	C14-C13	4.35	1.41	1.35
42	R	615	XAT	C2-C3	4.35	1.58	1.52
41	Y	317	NEX	C35-C34	4.35	1.56	1.43
41	s	617	NEX	C18-C5	4.34	1.59	1.52
41	n	618	NEX	C11-C10	4.33	1.56	1.43
38	f	501	HEM	FE-ND	4.33	2.08	1.94
42	y	302	XAT	C30-C29	4.32	1.41	1.35
41	N	617	NEX	C7-C8	4.32	1.39	1.32
41	Y	317	NEX	C4-C3	4.32	1.58	1.52
42	r	615	XAT	C2-C3	4.32	1.58	1.52
40	G	616	LUT	C10-C9	4.31	1.41	1.35
41	g	617	NEX	C28-C27	4.29	1.42	1.32
41	r	614	NEX	C11-C10	4.28	1.56	1.43
41	n	618	NEX	C7-C8	4.28	1.39	1.32
40	g	616	LUT	C10-C9	4.28	1.41	1.35
41	S	617	NEX	C18-C5	4.27	1.59	1.52
41	R	614	NEX	C32-C33	4.26	1.55	1.45
41	N	617	NEX	C4-C3	4.26	1.58	1.52
41	g	617	NEX	C15-C14	4.25	1.56	1.43
41	s	617	NEX	C4-C3	4.25	1.58	1.52
41	n	618	NEX	C2-C3	4.25	1.58	1.52
41	r	614	NEX	C35-C34	4.24	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	S	617	NEX	C15-C14	4.23	1.58	1.45
42	G	619	XAT	C22-C23	4.23	1.58	1.52
40	n	615	LUT	C14-C13	4.23	1.41	1.35
42	n	617	XAT	C8-C9	-4.23	1.36	1.45
41	R	618	NEX	C35-C34	4.22	1.56	1.43
41	r	614	NEX	C7-C8	4.21	1.39	1.32
41	S	617	NEX	C4-C3	4.21	1.58	1.52
41	N	617	NEX	C28-C27	4.21	1.41	1.32
24	D	402	PHO	C1D-C2D	4.21	1.44	1.39
41	Y	317	NEX	C7-C8	4.21	1.39	1.32
41	R	614	NEX	C24-C25	4.20	1.58	1.52
41	n	618	NEX	C28-C27	4.19	1.41	1.32
41	r	614	NEX	C24-C25	4.19	1.58	1.52
42	Y	301	XAT	C8-C9	-4.18	1.37	1.45
42	y	302	XAT	C8-C9	-4.18	1.37	1.45
41	R	614	NEX	C15-C14	4.17	1.56	1.43
41	n	618	NEX	C15-C14	4.15	1.56	1.43
40	s	614	LUT	C30-C29	4.15	1.41	1.35
40	n	616	LUT	C10-C9	4.14	1.41	1.35
41	g	617	NEX	C30-C29	4.12	1.41	1.35
41	N	617	NEX	C15-C14	4.12	1.56	1.43
40	Y	316	LUT	C10-C9	4.10	1.41	1.35
40	y	317	LUT	C10-C9	4.10	1.41	1.35
41	Y	317	NEX	C32-C33	4.10	1.54	1.45
42	r	615	XAT	C8-C9	-4.09	1.37	1.45
41	R	614	NEX	C28-C27	4.08	1.41	1.32
41	R	618	NEX	C7-C8	4.08	1.38	1.32
42	n	620	XAT	C22-C23	4.08	1.58	1.52
24	d	402	PHO	C1D-C2D	4.07	1.44	1.39
24	a	406	PHO	C1D-C2D	4.06	1.44	1.39
42	R	615	XAT	C8-C9	-4.06	1.37	1.45
42	G	619	XAT	C11-C10	-4.05	1.30	1.43
41	R	618	NEX	C32-C33	4.04	1.54	1.45
40	S	614	LUT	C30-C29	4.04	1.41	1.35
41	Y	317	NEX	C15-C14	4.04	1.56	1.43
40	s	614	LUT	C12-C13	4.03	1.54	1.45
42	y	302	XAT	C11-C12	4.03	1.45	1.34
41	r	614	NEX	C32-C33	4.01	1.54	1.45
24	A	405	PHO	C1D-C2D	4.00	1.44	1.39
42	y	302	XAT	C22-C23	4.00	1.58	1.52
41	r	614	NEX	C15-C14	4.00	1.55	1.43
41	R	618	NEX	C4-C3	3.99	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	G	613	CLA	C1D-ND	3.99	1.42	1.37
23	n	611	CLA	C1D-ND	3.98	1.42	1.37
40	S	615	LUT	C30-C29	3.95	1.41	1.35
23	s	609	CLA	C1D-ND	3.95	1.42	1.37
23	s	612	CLA	C1D-ND	3.94	1.42	1.37
23	S	608	CLA	C1D-ND	3.94	1.42	1.37
23	s	608	CLA	C1D-ND	3.94	1.42	1.37
23	S	610	CLA	C1D-ND	3.93	1.42	1.37
41	g	617	NEX	C2-C3	3.93	1.58	1.52
23	a	405	CLA	C1D-ND	3.92	1.42	1.37
41	r	614	NEX	C28-C27	3.92	1.41	1.32
23	S	602	CLA	C1D-ND	3.92	1.42	1.37
23	n	610	CLA	C1D-ND	3.92	1.42	1.37
40	N	616	LUT	C30-C29	3.92	1.41	1.35
23	r	610	CLA	C1D-ND	3.92	1.42	1.37
41	R	618	NEX	C15-C14	3.92	1.55	1.43
23	G	612	CLA	C1D-ND	3.91	1.42	1.37
23	n	602	CLA	C1D-ND	3.91	1.42	1.37
23	r	601	CLA	C1D-ND	3.91	1.42	1.37
23	c	504	CLA	C1D-ND	3.91	1.42	1.37
23	D	406	CLA	C1D-ND	3.91	1.42	1.37
23	g	613	CLA	C1D-ND	3.91	1.42	1.37
23	Y	314	CLA	C1D-ND	3.90	1.42	1.37
23	r	602	CLA	C1D-ND	3.90	1.42	1.37
23	N	613	CLA	C1D-ND	3.90	1.42	1.37
23	R	612	CLA	C1D-ND	3.90	1.42	1.37
42	N	619	XAT	C22-C23	3.90	1.57	1.52
23	c	507	CLA	C1D-ND	3.90	1.42	1.37
23	y	311	CLA	C1D-ND	3.90	1.42	1.37
23	y	315	CLA	C1D-ND	3.90	1.42	1.37
23	B	615	CLA	C1D-ND	3.90	1.42	1.37
23	g	612	CLA	C1D-ND	3.90	1.42	1.37
23	r	612	CLA	C1D-ND	3.89	1.42	1.37
23	N	602	CLA	C1D-ND	3.89	1.42	1.37
23	R	610	CLA	C1D-ND	3.89	1.42	1.37
23	c	502	CLA	C1D-ND	3.89	1.42	1.37
42	G	619	XAT	C14-C13	3.89	1.40	1.35
23	G	614	CLA	C1D-ND	3.89	1.42	1.37
23	R	602	CLA	C1D-ND	3.89	1.42	1.37
23	r	611	CLA	C1D-ND	3.89	1.42	1.37
23	R	601	CLA	C1D-ND	3.89	1.42	1.37
23	A	404	CLA	C1D-ND	3.88	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	Y	301	XAT	C11-C12	3.88	1.44	1.34
23	G	610	CLA	C1D-ND	3.88	1.42	1.37
23	n	613	CLA	C1D-ND	3.88	1.42	1.37
23	y	305	CLA	C1D-ND	3.88	1.42	1.37
23	S	611	CLA	C1D-ND	3.88	1.42	1.37
41	Y	317	NEX	C28-C27	3.88	1.41	1.32
23	G	611	CLA	C1D-ND	3.88	1.42	1.37
23	R	609	CLA	C1D-ND	3.88	1.42	1.37
23	S	603	CLA	C1D-ND	3.88	1.42	1.37
23	N	612	CLA	C1D-ND	3.88	1.42	1.37
23	R	611	CLA	C1D-ND	3.87	1.42	1.37
23	d	406	CLA	C1D-ND	3.87	1.42	1.37
23	s	604	CLA	C1D-ND	3.87	1.42	1.37
40	S	615	LUT	C12-C13	3.87	1.54	1.45
23	G	604	CLA	C1D-ND	3.87	1.42	1.37
23	Y	304	CLA	C1D-ND	3.87	1.42	1.37
23	Y	303	CLA	C1D-ND	3.87	1.42	1.37
23	s	610	CLA	C1D-ND	3.87	1.42	1.37
23	S	612	CLA	C1D-ND	3.87	1.42	1.37
42	n	617	XAT	C2-C3	3.87	1.57	1.52
42	G	619	XAT	C2-C3	3.87	1.57	1.52
42	n	617	XAT	C11-C10	-3.87	1.31	1.43
23	s	611	CLA	C1D-ND	3.87	1.42	1.37
23	s	602	CLA	C1D-ND	3.86	1.42	1.37
23	Y	313	CLA	C1D-ND	3.86	1.42	1.37
23	C	511	CLA	C1D-ND	3.86	1.42	1.37
23	Y	310	CLA	C1D-ND	3.86	1.42	1.37
23	y	314	CLA	C1D-ND	3.86	1.42	1.37
41	n	618	NEX	C4-C3	3.86	1.57	1.52
23	g	611	CLA	C1D-ND	3.86	1.42	1.37
23	n	612	CLA	C1D-ND	3.86	1.42	1.37
23	B	616	CLA	C1D-ND	3.85	1.42	1.37
23	S	609	CLA	C1D-ND	3.85	1.42	1.37
23	a	407	CLA	C1D-ND	3.85	1.42	1.37
23	N	614	CLA	C1D-ND	3.85	1.42	1.37
23	c	508	CLA	C1D-ND	3.85	1.42	1.37
23	B	610	CLA	C1D-ND	3.84	1.42	1.37
23	C	501	CLA	C1D-ND	3.84	1.42	1.37
23	b	611	CLA	C1D-ND	3.84	1.42	1.37
23	C	507	CLA	C1D-ND	3.84	1.42	1.37
23	a	404	CLA	C1D-ND	3.84	1.42	1.37
23	N	610	CLA	C1D-ND	3.84	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	504	CLA	C1D-ND	3.84	1.42	1.37
38	f	501	HEM	FE-NC	3.84	2.08	1.95
23	n	614	CLA	C1D-ND	3.84	1.42	1.37
23	b	610	CLA	C1D-ND	3.84	1.42	1.37
23	C	509	CLA	C1D-ND	3.84	1.42	1.37
23	r	609	CLA	C1D-ND	3.84	1.42	1.37
23	g	602	CLA	C1D-ND	3.84	1.42	1.37
23	y	306	CLA	C1D-ND	3.84	1.42	1.37
41	R	618	NEX	C28-C27	3.84	1.41	1.32
23	b	616	CLA	C1D-ND	3.83	1.42	1.37
23	Y	311	CLA	C1D-ND	3.83	1.42	1.37
23	c	509	CLA	C1D-ND	3.83	1.42	1.37
40	S	614	LUT	C12-C13	3.83	1.54	1.45
23	B	611	CLA	C1D-ND	3.83	1.42	1.37
23	B	607	CLA	C1D-ND	3.83	1.42	1.37
23	c	506	CLA	C1D-ND	3.83	1.42	1.37
23	c	505	CLA	C1D-ND	3.83	1.42	1.37
23	S	604	CLA	C1D-ND	3.83	1.42	1.37
23	s	603	CLA	C1D-ND	3.83	1.42	1.37
23	B	601	CLA	C1D-ND	3.83	1.42	1.37
23	C	508	CLA	C1D-ND	3.83	1.42	1.37
23	y	304	CLA	C1D-ND	3.83	1.42	1.37
23	r	603	CLA	C1D-ND	3.82	1.42	1.37
23	B	602	CLA	C1D-ND	3.82	1.42	1.37
23	b	606	CLA	C1D-ND	3.82	1.42	1.37
23	g	610	CLA	C1D-ND	3.82	1.42	1.37
23	C	510	CLA	C1D-ND	3.82	1.42	1.37
23	S	613	CLA	C1D-ND	3.82	1.42	1.37
23	b	601	CLA	C1D-ND	3.82	1.42	1.37
23	b	613	CLA	C1D-ND	3.82	1.42	1.37
40	R	613	LUT	C30-C29	3.82	1.40	1.35
23	G	602	CLA	C1D-ND	3.82	1.42	1.37
23	b	615	CLA	C1D-ND	3.81	1.42	1.37
23	N	611	CLA	C1D-ND	3.81	1.42	1.37
23	Y	305	CLA	C1D-ND	3.81	1.42	1.37
23	c	501	CLA	C1D-ND	3.81	1.42	1.37
23	g	604	CLA	C1D-ND	3.81	1.42	1.37
23	B	613	CLA	C1D-ND	3.81	1.42	1.37
23	A	402	CLA	C1D-ND	3.81	1.42	1.37
23	Y	312	CLA	C1D-ND	3.81	1.42	1.37
41	n	618	NEX	C30-C29	3.81	1.40	1.35
23	B	604	CLA	C1D-ND	3.81	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	604	CLA	C1D-ND	3.81	1.42	1.37
42	N	619	XAT	C30-C29	3.81	1.40	1.35
23	r	608	CLA	C1D-ND	3.80	1.42	1.37
23	y	313	CLA	C1D-ND	3.80	1.42	1.37
23	b	603	CLA	C1D-ND	3.80	1.42	1.37
23	B	614	CLA	C1D-ND	3.80	1.42	1.37
23	A	403	CLA	C1D-ND	3.80	1.42	1.37
23	b	614	CLA	C1D-ND	3.80	1.42	1.37
42	R	615	XAT	C11-C10	-3.80	1.31	1.43
23	c	511	CLA	C1D-ND	3.80	1.42	1.37
23	c	503	CLA	C1D-ND	3.80	1.42	1.37
23	B	609	CLA	C1D-ND	3.79	1.42	1.37
42	n	617	XAT	C31-C30	-3.79	1.31	1.43
40	N	615	LUT	C12-C13	3.79	1.54	1.45
23	R	603	CLA	C1D-ND	3.79	1.42	1.37
42	N	619	XAT	C8-C9	-3.79	1.37	1.45
23	r	604	CLA	C1D-ND	3.79	1.42	1.37
23	G	603	CLA	C1D-ND	3.79	1.42	1.37
41	N	617	NEX	C30-C29	3.78	1.40	1.35
23	b	602	CLA	C1D-ND	3.78	1.42	1.37
23	B	605	CLA	C1D-ND	3.78	1.42	1.37
23	R	608	CLA	C1D-ND	3.78	1.42	1.37
23	C	502	CLA	C1D-ND	3.78	1.42	1.37
23	g	603	CLA	C1D-ND	3.78	1.42	1.37
23	N	604	CLA	C1D-ND	3.78	1.42	1.37
23	A	406	CLA	C1D-ND	3.77	1.42	1.37
23	b	607	CLA	C1D-ND	3.77	1.42	1.37
23	y	312	CLA	C1D-ND	3.77	1.42	1.37
23	b	609	CLA	C1D-ND	3.77	1.42	1.37
40	N	616	LUT	C12-C13	3.77	1.54	1.45
23	C	505	CLA	C1D-ND	3.77	1.42	1.37
42	r	615	XAT	C11-C10	-3.77	1.31	1.43
23	c	512	CLA	C1D-ND	3.77	1.42	1.37
23	C	513	CLA	C1D-ND	3.77	1.42	1.37
23	n	603	CLA	C1D-ND	3.77	1.42	1.37
23	C	503	CLA	C1D-ND	3.77	1.42	1.37
42	n	617	XAT	C22-C23	3.77	1.57	1.52
42	n	620	XAT	C31-C30	-3.76	1.31	1.43
23	C	512	CLA	C1D-ND	3.76	1.42	1.37
40	s	615	LUT	C30-C29	3.76	1.40	1.35
23	C	506	CLA	C1D-ND	3.76	1.42	1.37
23	s	613	CLA	C1D-ND	3.76	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	N	615	LUT	C30-C29	3.76	1.40	1.35
23	a	403	CLA	C1D-ND	3.75	1.42	1.37
23	c	510	CLA	C1D-ND	3.75	1.42	1.37
42	y	302	XAT	C31-C30	-3.75	1.31	1.43
23	B	603	CLA	C1D-ND	3.75	1.42	1.37
23	c	513	CLA	C1D-ND	3.74	1.42	1.37
23	g	614	CLA	C1D-ND	3.74	1.42	1.37
23	n	604	CLA	C1D-ND	3.74	1.42	1.37
42	n	617	XAT	C34-C33	3.74	1.40	1.35
23	b	608	CLA	C1D-ND	3.74	1.42	1.37
23	B	608	CLA	C1D-ND	3.74	1.42	1.37
42	n	620	XAT	C8-C9	-3.73	1.37	1.45
23	B	606	CLA	C1D-ND	3.73	1.42	1.37
40	r	613	LUT	C12-C13	3.73	1.54	1.45
23	b	605	CLA	C1D-ND	3.72	1.42	1.37
40	s	614	LUT	C26-C27	3.72	1.55	1.50
23	N	603	CLA	C1D-ND	3.72	1.42	1.37
40	S	614	LUT	C26-C27	3.72	1.55	1.50
40	s	615	LUT	C12-C13	3.72	1.53	1.45
41	R	614	NEX	C30-C29	3.71	1.40	1.35
23	R	604	CLA	C1D-ND	3.70	1.42	1.37
42	G	619	XAT	C31-C30	-3.69	1.32	1.43
42	N	619	XAT	C31-C30	-3.69	1.32	1.43
41	g	617	NEX	C22-C21	3.67	1.60	1.54
23	B	612	CLA	C1D-ND	3.67	1.42	1.37
42	n	617	XAT	C15-C14	-3.66	1.32	1.43
42	Y	301	XAT	C31-C30	-3.65	1.32	1.43
41	R	614	NEX	C22-C21	3.65	1.60	1.54
42	R	615	XAT	C22-C23	3.65	1.57	1.52
41	R	618	NEX	C36-C21	3.63	1.60	1.53
41	r	614	NEX	C36-C21	3.63	1.60	1.53
41	G	617	NEX	C22-C21	3.63	1.60	1.54
42	G	619	XAT	C15-C14	-3.62	1.32	1.43
41	Y	317	NEX	C36-C21	3.62	1.60	1.53
35	y	301	VIV	C10-C3	-3.62	1.45	1.51
42	R	615	XAT	C31-C30	-3.61	1.32	1.43
41	R	614	NEX	C36-C21	3.61	1.60	1.53
41	n	618	NEX	C36-C21	3.61	1.60	1.53
24	d	402	PHO	C4D-CHA	3.61	1.45	1.39
42	r	615	XAT	C31-C30	-3.60	1.32	1.43
40	r	613	LUT	C30-C29	3.59	1.40	1.35
40	G	615	LUT	C14-C13	3.59	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	r	615	XAT	C22-C23	3.58	1.57	1.52
23	B	606	CLA	C4B-NB	3.58	1.42	1.37
23	Y	312	CLA	C4B-NB	3.58	1.42	1.37
40	R	613	LUT	C12-C13	3.58	1.53	1.45
41	N	617	NEX	C36-C21	3.57	1.60	1.53
42	N	619	XAT	C11-C10	-3.57	1.32	1.43
40	y	316	LUT	C10-C9	3.57	1.40	1.35
42	n	617	XAT	C35-C34	-3.56	1.32	1.43
41	r	614	NEX	C17-C1	3.55	1.60	1.53
23	D	405	CLA	C1D-ND	3.55	1.42	1.37
23	b	612	CLA	C1D-ND	3.55	1.42	1.37
25	h	501	BCR	C1-C6	-3.55	1.48	1.53
41	g	617	NEX	C17-C1	3.55	1.60	1.53
25	d	410	BCR	C1-C6	-3.54	1.48	1.53
25	v	101	BCR	C1-C6	-3.54	1.48	1.53
23	y	313	CLA	C4B-NB	3.54	1.42	1.37
41	g	617	NEX	C36-C21	3.54	1.60	1.53
40	n	615	LUT	C10-C9	3.53	1.40	1.35
41	n	618	NEX	C17-C1	3.53	1.60	1.53
38	f	501	HEM	FE-NB	3.53	2.05	1.94
40	Y	315	LUT	C10-C9	3.52	1.40	1.35
42	Y	301	XAT	C22-C23	3.52	1.57	1.52
40	S	615	LUT	C26-C27	3.52	1.55	1.50
41	r	614	NEX	C22-C21	3.52	1.60	1.54
25	H	501	BCR	C1-C6	-3.52	1.48	1.53
40	Y	316	LUT	C30-C29	3.51	1.40	1.35
42	n	620	XAT	C11-C10	-3.51	1.32	1.43
41	G	617	NEX	C36-C21	3.50	1.60	1.53
23	b	606	CLA	C4B-NB	3.50	1.42	1.37
41	R	614	NEX	C17-C1	3.50	1.60	1.53
25	V	101	BCR	C1-C6	-3.50	1.49	1.53
42	Y	301	XAT	C15-C14	-3.50	1.32	1.43
40	y	317	LUT	C30-C29	3.49	1.40	1.35
41	R	618	NEX	C22-C21	3.49	1.60	1.54
42	N	619	XAT	C15-C14	-3.49	1.32	1.43
25	d	410	BCR	C30-C25	-3.48	1.49	1.53
23	d	405	CLA	C1D-ND	3.48	1.42	1.37
42	Y	301	XAT	C11-C10	-3.48	1.32	1.43
41	g	617	NEX	C39-C29	3.47	1.58	1.50
26	M	101	SQD	O5-C1	3.47	1.50	1.41
23	G	614	CLA	C4B-NB	3.47	1.42	1.37
23	s	608	CLA	C4B-NB	3.47	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	n	620	XAT	C15-C14	-3.47	1.32	1.43
25	B	618	BCR	C1-C6	-3.46	1.49	1.53
42	y	302	XAT	C11-C10	-3.46	1.32	1.43
41	Y	317	NEX	C22-C21	3.46	1.59	1.54
41	G	617	NEX	C39-C29	3.46	1.58	1.50
23	y	315	CLA	C4B-NB	3.45	1.42	1.37
23	R	601	CLA	C4B-NB	3.45	1.42	1.37
23	B	615	CLA	C4B-NB	3.45	1.42	1.37
42	n	620	XAT	C35-C34	-3.45	1.32	1.43
26	M	101	SQD	O47-C7	3.45	1.44	1.34
25	C	514	BCR	C1-C6	-3.44	1.49	1.53
41	N	617	NEX	C17-C1	3.44	1.60	1.53
26	A	408	SQD	O47-C45	-3.44	1.38	1.46
41	s	617	NEX	C17-C1	3.44	1.60	1.53
25	c	514	BCR	C1-C6	-3.44	1.49	1.53
26	a	409	SQD	O47-C45	-3.44	1.38	1.46
42	G	619	XAT	C35-C34	-3.44	1.32	1.43
40	G	616	LUT	C30-C29	3.44	1.40	1.35
42	N	619	XAT	C35-C34	-3.44	1.32	1.43
41	r	614	NEX	C30-C29	3.43	1.40	1.35
23	N	611	CLA	C4B-NB	3.43	1.42	1.37
40	s	614	LUT	C11-C10	3.43	1.54	1.43
25	K	101	BCR	C1-C6	-3.43	1.49	1.53
40	g	616	LUT	C30-C29	3.43	1.40	1.35
41	Y	317	NEX	C30-C29	3.43	1.40	1.35
23	r	601	CLA	C4B-NB	3.42	1.42	1.37
23	S	610	CLA	C4B-NB	3.42	1.42	1.37
38	F	501	HEM	FE-NB	3.42	2.05	1.94
23	g	603	CLA	C4B-NB	3.42	1.42	1.37
23	R	612	CLA	C4B-NB	3.42	1.42	1.37
23	d	405	CLA	C4B-NB	3.41	1.42	1.37
41	S	617	NEX	C17-C1	3.41	1.60	1.53
25	b	618	BCR	C1-C6	-3.41	1.49	1.53
40	G	615	LUT	C30-C29	3.41	1.40	1.35
23	y	306	CLA	C4B-NB	3.41	1.42	1.37
41	S	617	NEX	C35-C15	3.41	1.41	1.32
40	G	616	LUT	C12-C13	3.41	1.53	1.45
40	y	316	LUT	C14-C13	3.41	1.40	1.35
23	n	611	CLA	C4B-NB	3.41	1.42	1.37
25	A	407	BCR	C1-C6	-3.40	1.49	1.53
23	r	612	CLA	C4B-NB	3.40	1.42	1.37
25	b	619	BCR	C1-C6	-3.40	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	Y	301	XAT	C35-C34	-3.40	1.32	1.43
40	Y	315	LUT	C14-C13	3.40	1.40	1.35
24	A	405	PHO	C4D-CHA	3.39	1.45	1.39
24	D	402	PHO	C4D-CHA	3.39	1.45	1.39
26	L	101	SQD	O47-C7	3.39	1.43	1.34
23	n	612	CLA	C4B-NB	3.39	1.42	1.37
23	y	314	CLA	C4B-NB	3.39	1.42	1.37
23	D	406	CLA	C4B-NB	3.39	1.41	1.37
23	s	610	CLA	C4B-NB	3.39	1.41	1.37
40	n	616	LUT	C30-C29	3.39	1.40	1.35
23	b	603	CLA	C4B-NB	3.38	1.41	1.37
41	G	617	NEX	C35-C15	3.38	1.40	1.32
26	L	101	SQD	O5-C1	3.38	1.50	1.41
40	g	616	LUT	C12-C13	3.38	1.53	1.45
23	s	613	CLA	C4B-NB	3.38	1.41	1.37
25	a	408	BCR	C1-C6	-3.38	1.49	1.53
25	k	101	BCR	C1-C6	-3.38	1.49	1.53
23	G	611	CLA	C4B-NB	3.38	1.41	1.37
40	N	615	LUT	C11-C10	3.38	1.53	1.43
23	D	405	CLA	C4B-NB	3.38	1.41	1.37
41	N	617	NEX	C16-C1	3.37	1.60	1.53
42	Y	301	XAT	C31-C32	3.37	1.43	1.34
41	R	618	NEX	C30-C29	3.37	1.40	1.35
23	S	608	CLA	C4B-NB	3.37	1.41	1.37
23	c	511	CLA	C4B-NB	3.37	1.41	1.37
23	s	609	CLA	C4B-NB	3.36	1.41	1.37
23	n	614	CLA	C4B-NB	3.36	1.41	1.37
40	g	615	LUT	C30-C29	3.36	1.40	1.35
23	s	603	CLA	C4B-NB	3.36	1.41	1.37
23	G	612	CLA	C4B-NB	3.36	1.41	1.37
23	S	613	CLA	C4B-NB	3.36	1.41	1.37
23	B	610	CLA	C4B-NB	3.36	1.41	1.37
23	N	614	CLA	C4B-NB	3.35	1.41	1.37
23	g	614	CLA	C4B-NB	3.35	1.41	1.37
41	g	617	NEX	C20-C13	3.35	1.57	1.50
40	G	615	LUT	C10-C9	3.35	1.40	1.35
23	C	506	CLA	C4B-NB	3.35	1.41	1.37
23	S	612	CLA	C4B-NB	3.35	1.41	1.37
41	s	617	NEX	C20-C13	3.35	1.57	1.50
23	b	601	CLA	C4B-NB	3.34	1.41	1.37
23	R	610	CLA	C4B-NB	3.34	1.41	1.37
42	y	302	XAT	C15-C14	-3.34	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	305	CLA	C4B-NB	3.34	1.41	1.37
23	G	604	CLA	C4B-NB	3.34	1.41	1.37
23	N	604	CLA	C4B-NB	3.34	1.41	1.37
40	s	614	LUT	C32-C33	3.34	1.53	1.45
23	Y	313	CLA	C4B-NB	3.34	1.41	1.37
23	b	615	CLA	C4B-NB	3.34	1.41	1.37
23	n	604	CLA	C4B-NB	3.34	1.41	1.37
23	c	506	CLA	C4B-NB	3.34	1.41	1.37
23	c	504	CLA	C4B-NB	3.33	1.41	1.37
23	C	501	CLA	C4B-NB	3.33	1.41	1.37
41	g	617	NEX	C16-C1	3.33	1.60	1.53
42	r	615	XAT	O24-C25	3.33	1.51	1.46
23	N	613	CLA	C4B-NB	3.33	1.41	1.37
23	B	602	CLA	C4B-NB	3.33	1.41	1.37
38	F	501	HEM	FE-ND	3.33	2.05	1.94
42	n	620	XAT	O24-C25	3.32	1.51	1.46
23	c	505	CLA	C4B-NB	3.32	1.41	1.37
23	s	602	CLA	C4B-NB	3.32	1.41	1.37
23	R	609	CLA	C4B-NB	3.32	1.41	1.37
23	g	612	CLA	C4B-NB	3.32	1.41	1.37
28	X	201	3PH	P-O11	3.32	1.70	1.60
23	Y	314	CLA	C4B-NB	3.32	1.41	1.37
42	R	615	XAT	C24-C23	3.32	1.57	1.52
42	N	619	XAT	O24-C25	3.31	1.51	1.46
23	c	501	CLA	C4B-NB	3.31	1.41	1.37
23	g	611	CLA	C4B-NB	3.31	1.41	1.37
42	r	615	XAT	C35-C34	-3.31	1.33	1.43
23	B	605	CLA	C4B-NB	3.31	1.41	1.37
42	R	615	XAT	O24-C25	3.31	1.51	1.46
23	b	609	CLA	C4B-NB	3.31	1.41	1.37
23	C	504	CLA	C4B-NB	3.31	1.41	1.37
23	r	608	CLA	C4B-NB	3.31	1.41	1.37
23	R	604	CLA	C4B-NB	3.30	1.41	1.37
23	n	613	CLA	C4B-NB	3.30	1.41	1.37
23	C	505	CLA	C4B-NB	3.30	1.41	1.37
23	s	611	CLA	C4B-NB	3.30	1.41	1.37
23	s	612	CLA	C4B-NB	3.30	1.41	1.37
30	r	616	LHG	P-O3	3.30	1.72	1.59
23	g	604	CLA	C4B-NB	3.30	1.41	1.37
41	n	618	NEX	C39-C29	3.30	1.57	1.50
23	S	602	CLA	C4B-NB	3.30	1.41	1.37
23	S	611	CLA	C4B-NB	3.30	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	507	CLA	C4B-NB	3.30	1.41	1.37
28	L	102	3PH	P-O11	3.30	1.70	1.60
23	S	603	CLA	C4B-NB	3.30	1.41	1.37
41	g	617	NEX	C19-C9	3.30	1.57	1.50
23	B	607	CLA	C4B-NB	3.30	1.41	1.37
42	R	615	XAT	C35-C34	-3.30	1.33	1.43
24	a	406	PHO	C4D-CHA	3.29	1.44	1.39
23	N	612	CLA	C4B-NB	3.29	1.41	1.37
23	R	608	CLA	C4B-NB	3.29	1.41	1.37
28	x	201	3PH	P-O11	3.29	1.70	1.60
23	a	407	CLA	C4B-NB	3.29	1.41	1.37
42	n	620	XAT	C30-C29	3.29	1.40	1.35
23	B	609	CLA	C4B-NB	3.29	1.41	1.37
23	C	507	CLA	C4B-NB	3.29	1.41	1.37
23	B	603	CLA	C4B-NB	3.29	1.41	1.37
23	R	611	CLA	C4B-NB	3.29	1.41	1.37
23	c	503	CLA	C4B-NB	3.29	1.41	1.37
23	r	611	CLA	C4B-NB	3.29	1.41	1.37
23	b	610	CLA	C4B-NB	3.28	1.41	1.37
23	y	304	CLA	C4B-NB	3.28	1.41	1.37
26	a	409	SQD	O47-C7	3.28	1.43	1.34
28	d	403	3PH	P-O11	3.28	1.70	1.60
23	C	510	CLA	C4B-NB	3.28	1.41	1.37
41	N	617	NEX	C39-C29	3.28	1.57	1.50
23	r	610	CLA	C4B-NB	3.28	1.41	1.37
25	Z	101	BCR	C30-C25	-3.28	1.49	1.53
23	C	503	CLA	C4B-NB	3.28	1.41	1.37
23	c	510	CLA	C4B-NB	3.28	1.41	1.37
23	R	602	CLA	C4B-NB	3.28	1.41	1.37
41	r	614	NEX	C16-C1	3.28	1.60	1.53
28	W	201	3PH	P-O11	3.28	1.70	1.60
23	b	612	CLA	C4B-NB	3.27	1.41	1.37
26	a	409	SQD	O5-C1	3.27	1.50	1.41
23	b	605	CLA	C4B-NB	3.27	1.41	1.37
28	T	101	3PH	P-O11	3.27	1.70	1.60
41	G	617	NEX	C40-C33	3.27	1.57	1.50
23	B	614	CLA	C4B-NB	3.27	1.41	1.37
25	z	101	BCR	C30-C25	-3.27	1.49	1.53
41	r	614	NEX	C19-C9	3.27	1.57	1.50
23	C	511	CLA	C4B-NB	3.27	1.41	1.37
23	A	402	CLA	C4B-NB	3.27	1.41	1.37
28	C	524	3PH	P-O11	3.27	1.70	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	g	613	CLA	C4B-NB	3.27	1.41	1.37
23	r	602	CLA	C4B-NB	3.27	1.41	1.37
41	R	618	NEX	C17-C1	3.27	1.60	1.53
23	b	613	CLA	C4B-NB	3.27	1.41	1.37
23	S	604	CLA	C4B-NB	3.27	1.41	1.37
23	B	613	CLA	C4B-NB	3.26	1.41	1.37
42	y	302	XAT	C35-C34	-3.26	1.33	1.43
23	Y	311	CLA	C4B-NB	3.26	1.41	1.37
41	Y	317	NEX	C16-C1	3.26	1.60	1.53
28	a	410	3PH	P-O11	3.26	1.70	1.60
23	C	502	CLA	C4B-NB	3.26	1.41	1.37
23	S	609	CLA	C4B-NB	3.26	1.41	1.37
23	B	606	CLA	C3B-C4B	3.26	1.50	1.42
23	b	606	CLA	C3B-C4B	3.26	1.50	1.42
40	S	614	LUT	C28-C27	3.26	1.40	1.32
40	S	615	LUT	C32-C33	3.26	1.52	1.45
23	y	312	CLA	C4B-NB	3.26	1.41	1.37
28	w	202	3PH	P-O11	3.26	1.70	1.60
23	r	604	CLA	C4B-NB	3.26	1.41	1.37
41	R	614	NEX	C16-C1	3.25	1.60	1.53
28	s	618	3PH	P-O11	3.25	1.70	1.60
41	n	618	NEX	C16-C1	3.25	1.60	1.53
23	b	608	CLA	C4B-NB	3.25	1.41	1.37
23	B	601	CLA	C4B-NB	3.25	1.41	1.37
23	G	603	CLA	C4B-NB	3.25	1.41	1.37
23	A	404	CLA	C4B-NB	3.25	1.41	1.37
23	G	613	CLA	C4B-NB	3.25	1.41	1.37
41	R	614	NEX	C19-C9	3.25	1.57	1.50
23	B	608	CLA	C4B-NB	3.25	1.41	1.37
41	S	617	NEX	C16-C1	3.25	1.60	1.53
23	C	512	CLA	C4B-NB	3.25	1.41	1.37
23	b	607	CLA	C4B-NB	3.25	1.41	1.37
23	c	502	CLA	C4B-NB	3.25	1.41	1.37
41	N	617	NEX	C22-C21	3.25	1.59	1.54
28	D	403	3PH	P-O11	3.25	1.70	1.60
41	g	617	NEX	C40-C33	3.24	1.57	1.50
41	n	618	NEX	C19-C9	3.24	1.57	1.50
23	C	509	CLA	C4B-NB	3.24	1.41	1.37
23	c	509	CLA	C4B-NB	3.24	1.41	1.37
41	s	617	NEX	C19-C9	3.24	1.57	1.50
40	s	614	LUT	C28-C27	3.24	1.40	1.32
23	B	616	CLA	C4B-NB	3.24	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	G	602	CLA	C4B-NB	3.24	1.41	1.37
42	R	615	XAT	C15-C14	-3.24	1.33	1.43
40	y	317	LUT	C12-C13	3.24	1.52	1.45
41	r	614	NEX	C40-C33	3.24	1.57	1.50
40	s	614	LUT	C8-C9	3.24	1.52	1.45
41	Y	317	NEX	C17-C1	3.24	1.60	1.53
41	R	618	NEX	C19-C9	3.23	1.57	1.50
26	A	408	SQD	O5-C1	3.23	1.50	1.41
23	g	602	CLA	C4B-NB	3.23	1.41	1.37
23	r	603	CLA	C4B-NB	3.23	1.41	1.37
23	s	604	CLA	C4B-NB	3.23	1.41	1.37
42	Y	301	XAT	C2-C1	3.23	1.59	1.54
42	r	615	XAT	C15-C14	-3.23	1.33	1.43
38	f	501	HEM	FE-NA	3.23	2.06	1.95
41	n	618	NEX	C22-C21	3.23	1.59	1.54
23	C	508	CLA	C4B-NB	3.23	1.41	1.37
41	S	617	NEX	C20-C13	3.23	1.57	1.50
42	r	615	XAT	C24-C23	3.23	1.57	1.52
23	y	305	CLA	C4B-NB	3.23	1.41	1.37
41	S	617	NEX	C19-C9	3.23	1.57	1.50
41	N	617	NEX	C19-C9	3.22	1.57	1.50
26	A	408	SQD	O47-C7	3.22	1.43	1.34
23	d	406	CLA	C4B-NB	3.22	1.41	1.37
23	A	406	CLA	C4B-NB	3.22	1.41	1.37
41	s	617	NEX	C16-C1	3.22	1.60	1.53
23	C	513	CLA	C4B-NB	3.22	1.41	1.37
23	a	405	CLA	C4B-NB	3.22	1.41	1.37
41	R	614	NEX	C40-C33	3.22	1.57	1.50
23	a	403	CLA	C4B-NB	3.22	1.41	1.37
23	c	512	CLA	C4B-NB	3.21	1.41	1.37
23	b	614	CLA	C4B-NB	3.21	1.41	1.37
23	B	604	CLA	C4B-NB	3.21	1.41	1.37
42	N	619	XAT	C11-C12	3.21	1.42	1.34
23	n	602	CLA	C4B-NB	3.21	1.41	1.37
23	n	603	CLA	C4B-NB	3.21	1.41	1.37
42	n	620	XAT	C11-C12	3.21	1.42	1.34
23	r	609	CLA	C4B-NB	3.21	1.41	1.37
28	A	410	3PH	P-O11	3.21	1.70	1.60
23	Y	303	CLA	C4B-NB	3.21	1.41	1.37
23	b	602	CLA	C4B-NB	3.21	1.41	1.37
23	b	616	CLA	C4B-NB	3.21	1.41	1.37
41	R	614	NEX	C39-C29	3.20	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	Y	317	NEX	C40-C33	3.20	1.57	1.50
23	R	603	CLA	C4B-NB	3.20	1.41	1.37
40	n	616	LUT	C12-C13	3.20	1.52	1.45
40	g	615	LUT	C14-C13	3.20	1.40	1.35
23	b	604	CLA	C4B-NB	3.20	1.41	1.37
25	H	501	BCR	C30-C25	-3.20	1.49	1.53
41	R	618	NEX	C40-C33	3.19	1.57	1.50
42	N	619	XAT	C31-C32	3.19	1.42	1.34
30	N	618	LHG	P-O3	3.19	1.72	1.59
25	h	501	BCR	C30-C25	-3.19	1.49	1.53
41	N	617	NEX	C40-C33	3.19	1.57	1.50
40	N	616	LUT	C26-C27	3.19	1.55	1.50
23	N	602	CLA	C4B-NB	3.19	1.41	1.37
23	B	612	CLA	C4B-NB	3.19	1.41	1.37
40	S	615	LUT	C11-C10	3.19	1.53	1.43
41	R	618	NEX	C16-C1	3.18	1.60	1.53
30	A	412	LHG	P-O3	3.18	1.72	1.59
25	b	617	BCR	C1-C6	-3.18	1.49	1.53
23	n	610	CLA	C4B-NB	3.18	1.41	1.37
40	S	615	LUT	C28-C27	3.18	1.39	1.32
23	s	609	CLA	C3B-C4B	3.18	1.50	1.42
30	n	619	LHG	P-O3	3.18	1.72	1.59
41	Y	317	NEX	C19-C9	3.18	1.57	1.50
42	n	617	XAT	O24-C25	3.18	1.50	1.46
41	n	618	NEX	C40-C33	3.18	1.57	1.50
42	G	619	XAT	C31-C32	3.18	1.42	1.34
40	Y	316	LUT	C12-C13	3.17	1.52	1.45
30	a	412	LHG	P-O3	3.17	1.72	1.59
23	N	610	CLA	C4B-NB	3.17	1.41	1.37
23	c	513	CLA	C4B-NB	3.17	1.41	1.37
23	g	610	CLA	C4B-NB	3.17	1.41	1.37
42	y	302	XAT	C2-C1	3.17	1.59	1.54
30	d	404	LHG	O7-C7	3.17	1.43	1.34
23	Y	304	CLA	C4B-NB	3.17	1.41	1.37
42	y	302	XAT	O24-C25	3.17	1.50	1.46
23	c	508	CLA	C4B-NB	3.16	1.41	1.37
23	N	603	CLA	C4B-NB	3.16	1.41	1.37
30	r	616	LHG	P-O6	3.16	1.72	1.59
23	A	403	CLA	C4B-NB	3.16	1.41	1.37
30	N	618	LHG	P-O6	3.15	1.72	1.59
40	s	614	LUT	C31-C30	3.15	1.53	1.43
23	G	610	CLA	C4B-NB	3.15	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	S	614	LUT	C11-C10	3.15	1.53	1.43
41	r	614	NEX	C20-C13	3.14	1.57	1.50
23	Y	310	CLA	C4B-NB	3.14	1.41	1.37
23	a	404	CLA	C4B-NB	3.14	1.41	1.37
26	M	101	SQD	O47-C45	-3.14	1.38	1.46
23	B	611	CLA	C4B-NB	3.14	1.41	1.37
25	C	514	BCR	C30-C25	-3.14	1.49	1.53
23	b	611	CLA	C4B-NB	3.14	1.41	1.37
30	R	616	LHG	P-O3	3.13	1.72	1.59
42	Y	301	XAT	O24-C25	3.13	1.50	1.46
23	y	311	CLA	C4B-NB	3.13	1.41	1.37
40	g	615	LUT	C10-C9	3.13	1.39	1.35
40	N	615	LUT	C26-C27	3.13	1.54	1.50
30	R	616	LHG	O7-C7	3.12	1.43	1.34
40	N	615	LUT	C28-C27	3.12	1.39	1.32
40	S	614	LUT	C32-C33	3.12	1.52	1.45
30	a	412	LHG	P-O6	3.12	1.71	1.59
42	G	619	XAT	O24-C25	3.12	1.50	1.46
26	L	101	SQD	O47-C45	-3.12	1.38	1.46
25	D	411	BCR	C30-C25	-3.11	1.49	1.53
30	Y	318	LHG	P-O6	3.11	1.71	1.59
30	N	618	LHG	O7-C7	3.11	1.43	1.34
25	Z	101	BCR	C1-C6	-3.11	1.49	1.53
41	N	617	NEX	C20-C13	3.11	1.57	1.50
40	R	613	LUT	C28-C27	3.10	1.39	1.32
40	N	616	LUT	C28-C27	3.10	1.39	1.32
30	G	618	LHG	P-O3	3.10	1.71	1.59
41	R	618	NEX	C39-C29	3.10	1.57	1.50
40	s	615	LUT	C28-C27	3.10	1.39	1.32
41	r	614	NEX	C39-C29	3.10	1.57	1.50
23	B	610	CLA	C3B-C4B	3.10	1.50	1.42
42	y	302	XAT	C31-C32	3.10	1.42	1.34
40	N	616	LUT	C11-C10	3.10	1.53	1.43
25	c	514	BCR	C30-C25	-3.10	1.49	1.53
40	r	613	LUT	C11-C10	3.09	1.53	1.43
30	S	616	LHG	P-O6	3.09	1.71	1.59
23	b	610	CLA	C3B-C4B	3.09	1.50	1.42
30	S	616	LHG	P-O3	3.08	1.71	1.59
40	N	616	LUT	C32-C33	3.08	1.52	1.45
41	n	618	NEX	C20-C13	3.08	1.57	1.50
23	Y	312	CLA	C3B-C4B	3.08	1.50	1.42
23	c	501	CLA	C3B-C4B	3.07	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	501	CLA	C3B-C4B	3.07	1.50	1.42
30	r	616	LHG	O7-C7	3.07	1.43	1.34
25	z	101	BCR	C1-C6	-3.07	1.49	1.53
40	R	613	LUT	C26-C27	3.07	1.54	1.50
25	a	408	BCR	C30-C25	-3.07	1.49	1.53
40	R	613	LUT	C11-C10	3.07	1.53	1.43
40	s	615	LUT	C11-C10	3.07	1.52	1.43
25	B	619	BCR	C1-C6	-3.06	1.49	1.53
38	F	501	HEM	FE-NA	3.06	2.05	1.95
23	G	612	CLA	C3B-C4B	3.06	1.49	1.42
38	F	501	HEM	CAB-C3B	3.06	1.55	1.47
26	M	101	SQD	C24-C23	3.06	1.59	1.50
23	y	313	CLA	C3B-C4B	3.06	1.49	1.42
38	F	501	HEM	CAC-C3C	3.05	1.55	1.47
25	D	411	BCR	C1-C6	-3.05	1.49	1.53
41	Y	317	NEX	C39-C29	3.05	1.57	1.50
30	s	616	LHG	P-O3	3.05	1.71	1.59
26	a	409	SQD	C24-C23	3.05	1.59	1.50
25	b	617	BCR	C30-C25	-3.05	1.49	1.53
40	S	615	LUT	C8-C9	3.05	1.52	1.45
38	f	501	HEM	CAC-C3C	3.04	1.55	1.47
23	r	601	CLA	C3B-C4B	3.04	1.49	1.42
30	S	616	LHG	O7-C7	3.04	1.42	1.34
23	b	610	CLA	C4D-ND	-3.04	1.33	1.37
30	d	408	LHG	P-O3	3.04	1.71	1.59
25	B	617	BCR	C1-C6	-3.04	1.49	1.53
38	f	501	HEM	CAB-C3B	3.04	1.55	1.47
40	N	615	LUT	C32-C33	3.04	1.52	1.45
30	Y	318	LHG	P-O3	3.03	1.71	1.59
42	R	615	XAT	C31-C32	3.03	1.42	1.34
26	L	101	SQD	C24-C23	3.03	1.59	1.50
23	G	614	CLA	C3B-C4B	3.03	1.49	1.42
40	Y	316	LUT	C28-C27	3.03	1.39	1.32
30	b	627	LHG	O7-C7	3.03	1.42	1.34
40	y	317	LUT	C28-C27	3.03	1.39	1.32
42	r	615	XAT	C31-C32	3.02	1.42	1.34
25	B	618	BCR	C30-C25	-3.02	1.49	1.53
40	s	615	LUT	C8-C9	3.02	1.52	1.45
23	R	601	CLA	C3B-C4B	3.02	1.49	1.42
23	B	611	CLA	C4D-ND	-3.02	1.33	1.37
40	r	613	LUT	C28-C27	3.02	1.39	1.32
25	A	407	BCR	C30-C25	-3.01	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	F	501	HEM	FE-NC	3.01	2.05	1.95
23	S	609	CLA	C3B-C4B	3.01	1.49	1.42
23	S	608	CLA	C3B-C4B	3.00	1.49	1.42
25	b	618	BCR	C30-C25	-3.00	1.49	1.53
26	A	408	SQD	C24-C23	3.00	1.59	1.50
41	R	614	NEX	C20-C13	3.00	1.57	1.50
23	s	610	CLA	C3B-C4B	3.00	1.49	1.42
40	G	615	LUT	C28-C27	3.00	1.39	1.32
30	g	618	LHG	P-O3	3.00	1.71	1.59
23	B	615	CLA	C3B-C4B	2.99	1.49	1.42
23	b	611	CLA	C4D-ND	-2.99	1.33	1.37
40	N	615	LUT	C8-C9	2.99	1.52	1.45
30	y	318	LHG	P-O3	2.99	1.71	1.59
30	s	616	LHG	P-O6	2.99	1.71	1.59
23	A	402	CLA	C4D-ND	-2.99	1.33	1.37
40	S	615	LUT	C31-C30	2.98	1.52	1.43
42	y	302	XAT	C28-C29	-2.98	1.39	1.45
23	d	406	CLA	C4D-ND	-2.98	1.33	1.37
25	B	617	BCR	C30-C25	-2.98	1.49	1.53
40	s	615	LUT	C32-C33	2.98	1.52	1.45
23	B	605	CLA	C4D-ND	-2.98	1.33	1.37
41	Y	317	NEX	C20-C13	2.98	1.57	1.50
30	R	616	LHG	P-O6	2.98	1.71	1.59
23	A	403	CLA	C4D-ND	-2.98	1.33	1.37
23	b	604	CLA	C4D-ND	-2.98	1.33	1.37
23	G	610	CLA	C3B-C4B	2.98	1.49	1.42
23	S	610	CLA	C3B-C4B	2.98	1.49	1.42
30	g	618	LHG	O7-C7	2.97	1.42	1.34
23	R	608	CLA	C3B-C4B	2.97	1.49	1.42
23	G	611	CLA	C3B-C4B	2.97	1.49	1.42
23	r	608	CLA	C3B-C4B	2.97	1.49	1.42
41	R	618	NEX	C20-C13	2.97	1.57	1.50
40	g	615	LUT	C28-C27	2.97	1.39	1.32
23	c	506	CLA	C4D-ND	-2.97	1.33	1.37
23	S	613	CLA	C4D-ND	-2.97	1.33	1.37
30	G	618	LHG	O7-C7	2.97	1.42	1.34
30	L	103	LHG	O7-C7	2.97	1.42	1.34
23	s	602	CLA	C3B-C4B	2.97	1.49	1.42
23	c	509	CLA	C4D-ND	-2.97	1.33	1.37
23	B	606	CLA	C4D-ND	-2.96	1.33	1.37
23	a	407	CLA	C4D-ND	-2.96	1.33	1.37
23	N	602	CLA	C3B-C4B	2.96	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	R	611	CLA	C3B-C4B	2.96	1.49	1.42
40	G	616	LUT	C28-C27	2.96	1.39	1.32
23	b	608	CLA	C4D-ND	-2.96	1.33	1.37
30	a	412	LHG	O7-C7	2.96	1.42	1.34
23	r	609	CLA	C3B-C4B	2.96	1.49	1.42
40	r	613	LUT	C8-C9	2.96	1.52	1.45
23	a	403	CLA	C4D-ND	-2.96	1.33	1.37
23	g	604	CLA	C4D-ND	-2.96	1.33	1.37
23	S	602	CLA	C3B-C4B	2.96	1.49	1.42
23	a	404	CLA	C4D-ND	-2.96	1.33	1.37
23	C	503	CLA	C4D-ND	-2.95	1.33	1.37
23	b	601	CLA	C3B-C4B	2.95	1.49	1.42
23	b	607	CLA	C3B-C4B	2.95	1.49	1.42
40	g	616	LUT	C28-C27	2.95	1.39	1.32
23	N	611	CLA	C3B-C4B	2.95	1.49	1.42
30	n	619	LHG	O7-C7	2.95	1.42	1.34
23	B	604	CLA	C4D-ND	-2.95	1.33	1.37
23	a	405	CLA	C4D-ND	-2.95	1.33	1.37
23	R	609	CLA	C3B-C4B	2.95	1.49	1.42
30	Y	318	LHG	O7-C7	2.95	1.42	1.34
23	B	610	CLA	C4D-ND	-2.95	1.33	1.37
23	B	608	CLA	C3B-C4B	2.95	1.49	1.42
23	y	304	CLA	C3B-C4B	2.95	1.49	1.42
40	n	616	LUT	C28-C27	2.95	1.39	1.32
23	a	403	CLA	C3B-C4B	2.95	1.49	1.42
40	s	615	LUT	C26-C27	2.95	1.54	1.50
23	c	513	CLA	C4D-ND	-2.95	1.33	1.37
23	R	612	CLA	C3B-C4B	2.95	1.49	1.42
23	g	603	CLA	C3B-C4B	2.94	1.49	1.42
23	Y	305	CLA	C4D-ND	-2.94	1.33	1.37
23	y	306	CLA	C4D-ND	-2.94	1.33	1.37
30	A	412	LHG	O7-C7	2.94	1.42	1.34
30	A	412	LHG	P-O6	2.94	1.71	1.59
23	r	603	CLA	C4D-ND	-2.94	1.33	1.37
23	A	406	CLA	C4D-ND	-2.94	1.33	1.37
23	C	509	CLA	C4D-ND	-2.94	1.33	1.37
40	S	614	LUT	C31-C30	2.94	1.52	1.43
23	b	608	CLA	C3B-C4B	2.94	1.49	1.42
23	s	608	CLA	C3B-C4B	2.94	1.49	1.42
23	g	610	CLA	C3B-C4B	2.94	1.49	1.42
23	C	501	CLA	C4D-ND	-2.94	1.33	1.37
23	c	503	CLA	C4D-ND	-2.94	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	502	CLA	C4D-ND	-2.94	1.33	1.37
23	B	607	CLA	C3B-C4B	2.93	1.49	1.42
23	g	602	CLA	C3B-C4B	2.93	1.49	1.42
30	n	619	LHG	P-O6	2.93	1.71	1.59
23	C	512	CLA	C3B-C4B	2.93	1.49	1.42
25	v	101	BCR	C30-C25	-2.93	1.49	1.53
23	Y	303	CLA	C3B-C4B	2.93	1.49	1.42
23	S	603	CLA	C3B-C4B	2.93	1.49	1.42
23	n	602	CLA	C3B-C4B	2.93	1.49	1.42
23	r	602	CLA	C3B-C4B	2.93	1.49	1.42
23	y	312	CLA	C4D-ND	-2.93	1.33	1.37
23	n	614	CLA	C3B-C4B	2.93	1.49	1.42
23	s	603	CLA	C3B-C4B	2.93	1.49	1.42
23	B	614	CLA	C4D-ND	-2.93	1.33	1.37
23	G	602	CLA	C3B-C4B	2.93	1.49	1.42
40	S	614	LUT	C8-C9	2.93	1.52	1.45
23	r	610	CLA	C3B-C4B	2.93	1.49	1.42
23	N	614	CLA	C3B-C4B	2.93	1.49	1.42
23	R	610	CLA	C3B-C4B	2.93	1.49	1.42
42	n	620	XAT	C28-C29	-2.93	1.39	1.45
23	B	612	CLA	C4D-ND	-2.93	1.33	1.37
23	R	612	CLA	C4D-ND	-2.93	1.33	1.37
23	D	406	CLA	C3B-C4B	2.93	1.49	1.42
23	b	602	CLA	C3B-C4B	2.93	1.49	1.42
23	D	406	CLA	C4D-ND	-2.92	1.33	1.37
23	b	616	CLA	C4D-ND	-2.92	1.33	1.37
40	N	616	LUT	C1-C6	2.92	1.57	1.53
23	c	510	CLA	C3B-C4B	2.92	1.49	1.42
23	y	315	CLA	C3B-C4B	2.92	1.49	1.42
40	R	613	LUT	C8-C9	2.92	1.52	1.45
23	R	602	CLA	C3B-C4B	2.92	1.49	1.42
23	g	612	CLA	C3B-C4B	2.92	1.49	1.42
23	R	602	CLA	C4D-ND	-2.92	1.33	1.37
23	r	612	CLA	C3B-C4B	2.92	1.49	1.42
23	Y	313	CLA	C3B-C4B	2.92	1.49	1.42
23	N	604	CLA	C3B-C4B	2.92	1.49	1.42
23	b	616	CLA	C3B-C4B	2.92	1.49	1.42
23	Y	312	CLA	C4D-ND	-2.92	1.33	1.37
30	L	103	LHG	P-O3	2.92	1.71	1.59
23	c	508	CLA	C3B-C4B	2.92	1.49	1.42
23	c	511	CLA	C3B-C4B	2.92	1.49	1.42
23	G	611	CLA	C4D-ND	-2.92	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	510	CLA	C3B-C4B	2.92	1.49	1.42
23	C	513	CLA	C4D-ND	-2.92	1.33	1.37
23	c	512	CLA	C3B-C4B	2.92	1.49	1.42
23	B	602	CLA	C3B-C4B	2.92	1.49	1.42
25	B	619	BCR	C30-C25	-2.91	1.49	1.53
23	b	614	CLA	C3B-C4B	2.91	1.49	1.42
23	r	604	CLA	C4D-ND	-2.91	1.33	1.37
30	y	318	LHG	P-O6	2.91	1.71	1.59
35	C	523	VIV	C10-C3	-2.91	1.46	1.51
23	B	608	CLA	C4D-ND	-2.91	1.33	1.37
23	N	612	CLA	C3B-C4B	2.91	1.49	1.42
23	Y	310	CLA	C3B-C4B	2.91	1.49	1.42
23	N	610	CLA	C3B-C4B	2.91	1.49	1.42
23	B	603	CLA	C4D-ND	-2.91	1.33	1.37
23	S	602	CLA	C4D-ND	-2.91	1.33	1.37
23	r	611	CLA	C3B-C4B	2.91	1.49	1.42
23	y	314	CLA	C4D-ND	-2.91	1.33	1.37
23	C	506	CLA	C4D-ND	-2.91	1.33	1.37
23	c	510	CLA	C4D-ND	-2.91	1.33	1.37
23	c	501	CLA	C4D-ND	-2.91	1.33	1.37
30	N	618	LHG	C6-C5	2.91	1.59	1.50
23	B	613	CLA	C3B-C4B	2.91	1.49	1.42
23	n	611	CLA	C3B-C4B	2.91	1.49	1.42
23	S	611	CLA	C4D-ND	-2.91	1.33	1.37
30	s	616	LHG	O7-C7	2.90	1.42	1.34
42	n	620	XAT	C31-C32	2.90	1.42	1.34
23	C	508	CLA	C4D-ND	-2.90	1.33	1.37
23	C	502	CLA	C4D-ND	-2.90	1.33	1.37
23	d	405	CLA	C4D-ND	-2.90	1.33	1.37
23	B	601	CLA	C3B-C4B	2.90	1.49	1.42
23	C	511	CLA	C3B-C4B	2.90	1.49	1.42
23	N	613	CLA	C4D-ND	-2.90	1.33	1.37
23	g	611	CLA	C3B-C4B	2.90	1.49	1.42
30	R	616	LHG	O8-C23	2.90	1.41	1.33
23	C	512	CLA	C4D-ND	-2.90	1.33	1.37
23	b	605	CLA	C4D-ND	-2.90	1.33	1.37
25	V	101	BCR	C30-C25	-2.90	1.49	1.53
23	n	604	CLA	C3B-C4B	2.90	1.49	1.42
23	b	606	CLA	C4D-ND	-2.90	1.33	1.37
23	B	616	CLA	C4D-ND	-2.90	1.33	1.37
23	D	405	CLA	C4D-ND	-2.90	1.33	1.37
23	B	602	CLA	C4D-ND	-2.90	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	N	602	CLA	C4D-ND	-2.90	1.33	1.37
23	c	507	CLA	C4D-ND	-2.90	1.33	1.37
23	c	513	CLA	C3B-C4B	2.90	1.49	1.42
23	c	504	CLA	C4D-ND	-2.89	1.33	1.37
23	s	602	CLA	C4D-ND	-2.89	1.33	1.37
23	c	511	CLA	C4D-ND	-2.89	1.33	1.37
30	n	619	LHG	O8-C23	2.89	1.41	1.33
30	D	404	LHG	O7-C7	2.89	1.42	1.34
23	Y	304	CLA	C4D-ND	-2.89	1.33	1.37
42	N	619	XAT	C24-C23	2.89	1.56	1.52
23	A	406	CLA	C3B-C4B	2.89	1.49	1.42
23	B	614	CLA	C3B-C4B	2.89	1.49	1.42
23	s	611	CLA	C3B-C4B	2.89	1.49	1.42
23	N	613	CLA	C3B-C4B	2.89	1.49	1.42
23	b	602	CLA	C4D-ND	-2.89	1.33	1.37
40	G	616	LUT	C8-C9	2.89	1.52	1.45
23	n	613	CLA	C3B-C4B	2.89	1.49	1.42
23	y	305	CLA	C4D-ND	-2.89	1.33	1.37
23	g	614	CLA	C3B-C4B	2.89	1.49	1.42
23	n	610	CLA	C3B-C4B	2.89	1.49	1.42
23	G	603	CLA	C3B-C4B	2.89	1.49	1.42
23	R	603	CLA	C3B-C4B	2.89	1.49	1.42
40	g	616	LUT	C8-C9	2.89	1.52	1.45
23	B	611	CLA	C3B-C4B	2.89	1.49	1.42
23	C	513	CLA	C3B-C4B	2.89	1.49	1.42
23	s	612	CLA	C3B-C4B	2.89	1.49	1.42
25	k	101	BCR	C30-C25	-2.89	1.49	1.53
23	g	613	CLA	C3B-C4B	2.89	1.49	1.42
23	B	616	CLA	C3B-C4B	2.89	1.49	1.42
42	r	615	XAT	C28-C29	-2.89	1.39	1.45
23	R	609	CLA	C4D-ND	-2.88	1.33	1.37
25	b	619	BCR	C30-C25	-2.88	1.49	1.53
23	R	601	CLA	C4D-ND	-2.88	1.33	1.37
23	b	612	CLA	C4D-ND	-2.88	1.33	1.37
23	Y	314	CLA	C3B-C4B	2.88	1.49	1.42
23	g	614	CLA	C4D-ND	-2.88	1.33	1.37
23	C	507	CLA	C4D-ND	-2.88	1.33	1.37
23	R	610	CLA	C4D-ND	-2.88	1.33	1.37
23	C	508	CLA	C3B-C4B	2.88	1.49	1.42
23	b	613	CLA	C3B-C4B	2.88	1.49	1.42
23	B	613	CLA	C4D-ND	-2.88	1.33	1.37
23	n	612	CLA	C3B-C4B	2.88	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	r	610	CLA	C4D-ND	-2.88	1.33	1.37
23	s	611	CLA	C4D-ND	-2.88	1.33	1.37
30	b	627	LHG	P-O3	2.88	1.71	1.59
30	D	404	LHG	P-O3	2.88	1.71	1.59
23	r	611	CLA	C4D-ND	-2.88	1.33	1.37
23	N	611	CLA	C4D-ND	-2.88	1.33	1.37
23	G	614	CLA	C4D-ND	-2.88	1.33	1.37
42	n	617	XAT	C31-C32	2.88	1.42	1.34
23	S	613	CLA	C3B-C4B	2.88	1.49	1.42
23	r	601	CLA	C4D-ND	-2.88	1.33	1.37
23	A	402	CLA	C3B-C4B	2.88	1.49	1.42
23	s	613	CLA	C3B-C4B	2.88	1.49	1.42
23	y	306	CLA	C3B-C4B	2.88	1.49	1.42
23	G	602	CLA	C4D-ND	-2.88	1.33	1.37
23	Y	311	CLA	C4D-ND	-2.88	1.33	1.37
23	Y	313	CLA	C4D-ND	-2.88	1.33	1.37
40	s	614	LUT	C22-C21	2.88	1.58	1.54
23	a	405	CLA	C3B-C4B	2.87	1.49	1.42
23	y	311	CLA	C3B-C4B	2.87	1.49	1.42
23	A	404	CLA	C4D-ND	-2.87	1.33	1.37
23	B	603	CLA	C3B-C4B	2.87	1.49	1.42
23	b	603	CLA	C3B-C4B	2.87	1.49	1.42
30	y	318	LHG	O8-C23	2.87	1.41	1.33
23	B	601	CLA	C4D-ND	-2.87	1.33	1.37
23	n	613	CLA	C4D-ND	-2.87	1.33	1.37
40	G	616	LUT	C11-C10	2.87	1.52	1.43
23	A	404	CLA	C3B-C4B	2.87	1.49	1.42
23	c	508	CLA	C4D-ND	-2.87	1.33	1.37
23	b	611	CLA	C3B-C4B	2.87	1.49	1.42
23	G	604	CLA	C4D-ND	-2.87	1.33	1.37
23	R	603	CLA	C4D-ND	-2.87	1.33	1.37
23	S	612	CLA	C3B-C4B	2.87	1.49	1.42
23	y	314	CLA	C3B-C4B	2.87	1.49	1.42
23	S	611	CLA	C3B-C4B	2.87	1.49	1.42
23	N	610	CLA	C4D-ND	-2.87	1.33	1.37
23	b	614	CLA	C4D-ND	-2.87	1.33	1.37
23	b	603	CLA	C4D-ND	-2.87	1.33	1.37
23	G	613	CLA	C4D-ND	-2.87	1.33	1.37
30	G	618	LHG	P-O6	2.87	1.70	1.59
23	c	512	CLA	C4D-ND	-2.86	1.33	1.37
23	A	403	CLA	C3B-C4B	2.86	1.49	1.42
30	r	616	LHG	C8-C7	2.86	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	n	602	CLA	C4D-ND	-2.86	1.33	1.37
23	S	612	CLA	C4D-ND	-2.86	1.33	1.37
30	g	618	LHG	O8-C23	2.86	1.41	1.33
23	Y	305	CLA	C3B-C4B	2.86	1.49	1.42
23	b	615	CLA	C4D-ND	-2.86	1.33	1.37
23	S	604	CLA	C3B-C4B	2.86	1.49	1.42
23	r	603	CLA	C3B-C4B	2.86	1.49	1.42
23	Y	310	CLA	C4D-ND	-2.86	1.33	1.37
23	g	604	CLA	C3B-C4B	2.86	1.49	1.42
23	b	609	CLA	C3B-C4B	2.86	1.49	1.42
23	b	613	CLA	C4D-ND	-2.86	1.33	1.37
23	n	603	CLA	C4D-ND	-2.86	1.33	1.37
42	n	617	XAT	C11-C12	2.86	1.41	1.34
23	b	612	CLA	C3B-C4B	2.86	1.49	1.42
23	g	612	CLA	C4D-ND	-2.86	1.33	1.37
23	C	504	CLA	C3B-C4B	2.86	1.49	1.42
40	g	616	LUT	C11-C10	2.86	1.52	1.43
23	r	608	CLA	C4D-ND	-2.86	1.33	1.37
40	s	615	LUT	C22-C21	2.86	1.58	1.54
23	B	612	CLA	C3B-C4B	2.86	1.49	1.42
23	r	604	CLA	C3B-C4B	2.86	1.49	1.42
23	r	612	CLA	C4D-ND	-2.86	1.33	1.37
23	s	613	CLA	C4D-ND	-2.86	1.33	1.37
23	g	613	CLA	C4D-ND	-2.86	1.33	1.37
23	s	604	CLA	C3B-C4B	2.86	1.49	1.42
40	n	616	LUT	C1-C6	2.85	1.57	1.53
30	y	318	LHG	O7-C7	2.85	1.42	1.34
23	c	504	CLA	C3B-C4B	2.85	1.49	1.42
40	R	613	LUT	C32-C33	2.85	1.52	1.45
23	y	311	CLA	C4D-ND	-2.85	1.33	1.37
23	Y	311	CLA	C3B-C4B	2.85	1.49	1.42
25	K	101	BCR	C30-C25	-2.85	1.49	1.53
30	g	618	LHG	P-O6	2.85	1.70	1.59
23	C	506	CLA	C3B-C4B	2.85	1.49	1.42
23	S	610	CLA	C4D-ND	-2.85	1.33	1.37
23	s	604	CLA	C4D-ND	-2.85	1.33	1.37
23	a	407	CLA	C3B-C4B	2.85	1.49	1.42
23	B	615	CLA	C4D-ND	-2.85	1.33	1.37
23	R	608	CLA	C4D-ND	-2.85	1.33	1.37
23	b	609	CLA	C4D-ND	-2.85	1.33	1.37
23	B	609	CLA	C4D-ND	-2.85	1.33	1.37
23	r	602	CLA	C4D-ND	-2.85	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	y	304	CLA	C4D-ND	-2.85	1.33	1.37
23	y	313	CLA	C4D-ND	-2.85	1.33	1.37
23	N	612	CLA	C4D-ND	-2.85	1.33	1.37
23	c	509	CLA	C3B-C4B	2.85	1.49	1.42
23	d	406	CLA	C3B-C4B	2.85	1.49	1.42
23	g	611	CLA	C4D-ND	-2.85	1.33	1.37
23	B	605	CLA	C3B-C4B	2.84	1.49	1.42
23	y	312	CLA	C3B-C4B	2.84	1.49	1.42
30	Y	318	LHG	C8-C7	2.84	1.59	1.50
23	y	305	CLA	C3B-C4B	2.84	1.49	1.42
30	d	408	LHG	O7-C7	2.84	1.42	1.34
23	C	510	CLA	C4D-ND	-2.84	1.33	1.37
23	n	612	CLA	C4D-ND	-2.84	1.33	1.37
23	B	609	CLA	C3B-C4B	2.84	1.49	1.42
30	d	404	LHG	C8-C7	2.84	1.59	1.50
23	c	506	CLA	C3B-C4B	2.84	1.49	1.42
23	b	615	CLA	C3B-C4B	2.84	1.49	1.42
23	N	603	CLA	C4D-ND	-2.84	1.33	1.37
30	R	616	LHG	C8-C7	2.84	1.59	1.50
40	G	616	LUT	C26-C27	2.84	1.54	1.50
23	a	404	CLA	C3B-C4B	2.84	1.49	1.42
30	N	618	LHG	O8-C23	2.83	1.41	1.33
23	g	602	CLA	C4D-ND	-2.83	1.33	1.37
23	C	511	CLA	C4D-ND	-2.83	1.33	1.37
23	C	505	CLA	C3B-C4B	2.83	1.49	1.42
30	d	404	LHG	P-O3	2.83	1.70	1.59
23	N	604	CLA	C4D-ND	-2.83	1.33	1.37
23	Y	304	CLA	C3B-C4B	2.83	1.49	1.42
23	c	502	CLA	C3B-C4B	2.83	1.49	1.42
40	s	614	LUT	C15-C14	2.83	1.52	1.43
23	G	603	CLA	C4D-ND	-2.83	1.33	1.37
40	S	615	LUT	C1-C6	2.83	1.57	1.53
30	S	616	LHG	O8-C23	2.83	1.41	1.33
23	R	604	CLA	C4D-ND	-2.83	1.33	1.37
23	G	610	CLA	C4D-ND	-2.83	1.33	1.37
23	C	504	CLA	C4D-ND	-2.83	1.33	1.37
30	r	616	LHG	O8-C23	2.82	1.41	1.33
42	n	620	XAT	C24-C23	2.82	1.56	1.52
23	R	611	CLA	C4D-ND	-2.82	1.33	1.37
30	s	616	LHG	O8-C23	2.82	1.41	1.33
40	N	616	LUT	C31-C30	2.82	1.52	1.43
40	Y	316	LUT	C26-C27	2.82	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	G	618	LHG	O8-C23	2.82	1.41	1.33
23	s	612	CLA	C4D-ND	-2.82	1.33	1.37
23	r	609	CLA	C4D-ND	-2.82	1.33	1.37
40	y	317	LUT	C26-C27	2.82	1.54	1.50
23	R	604	CLA	C3B-C4B	2.82	1.49	1.42
23	C	503	CLA	C3B-C4B	2.82	1.49	1.42
42	G	619	XAT	C24-C25	-2.82	1.48	1.52
30	g	618	LHG	C8-C7	2.81	1.58	1.50
23	S	604	CLA	C4D-ND	-2.81	1.33	1.37
23	G	613	CLA	C3B-C4B	2.81	1.49	1.42
23	g	603	CLA	C4D-ND	-2.81	1.33	1.37
23	C	502	CLA	C3B-C4B	2.81	1.49	1.42
30	S	616	LHG	C8-C7	2.81	1.58	1.50
23	G	604	CLA	C3B-C4B	2.81	1.49	1.42
23	c	505	CLA	C3B-C4B	2.80	1.49	1.42
23	C	509	CLA	C3B-C4B	2.80	1.49	1.42
23	n	611	CLA	C4D-ND	-2.80	1.33	1.37
23	G	612	CLA	C4D-ND	-2.80	1.33	1.37
23	s	603	CLA	C4D-ND	-2.80	1.33	1.37
23	s	608	CLA	C4D-ND	-2.80	1.33	1.37
30	Y	318	LHG	O8-C23	2.80	1.41	1.33
23	b	605	CLA	C3B-C4B	2.80	1.49	1.42
30	D	408	LHG	P-O3	2.80	1.70	1.59
40	N	615	LUT	C31-C30	2.80	1.52	1.43
23	n	610	CLA	C4D-ND	-2.80	1.33	1.37
23	c	503	CLA	C3B-C4B	2.80	1.49	1.42
30	a	412	LHG	O8-C23	2.80	1.41	1.33
23	Y	303	CLA	C4D-ND	-2.79	1.33	1.37
23	d	405	CLA	C3B-C4B	2.79	1.49	1.42
23	n	603	CLA	C3B-C4B	2.79	1.49	1.42
23	S	609	CLA	C4D-ND	-2.79	1.33	1.37
23	n	604	CLA	C4D-ND	-2.79	1.33	1.37
23	D	405	CLA	C3B-C4B	2.79	1.49	1.42
40	S	614	LUT	C1-C6	2.79	1.57	1.53
23	S	603	CLA	C4D-ND	-2.79	1.33	1.37
40	r	613	LUT	C15-C14	2.79	1.52	1.43
40	S	615	LUT	C5-C6	2.79	1.39	1.34
23	Y	314	CLA	C4D-ND	-2.79	1.33	1.37
30	L	103	LHG	O8-C23	2.79	1.41	1.33
30	b	627	LHG	C8-C7	2.79	1.58	1.50
30	D	404	LHG	C8-C7	2.78	1.58	1.50
23	s	610	CLA	C4D-ND	-2.78	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	503	CLA	C1B-C2B	2.78	1.49	1.43
30	b	627	LHG	O8-C23	2.78	1.41	1.33
23	B	604	CLA	C1B-C2B	2.78	1.49	1.43
23	B	607	CLA	C4D-ND	-2.78	1.33	1.37
23	y	315	CLA	C4D-ND	-2.78	1.33	1.37
30	G	618	LHG	C8-C7	2.77	1.58	1.50
23	b	604	CLA	C1B-C2B	2.77	1.49	1.43
30	N	618	LHG	C8-C7	2.77	1.58	1.50
30	L	103	LHG	P-O6	2.77	1.70	1.59
23	C	507	CLA	C3B-C4B	2.77	1.49	1.42
40	y	317	LUT	C8-C9	2.77	1.51	1.45
42	R	615	XAT	C28-C29	-2.77	1.40	1.45
23	b	607	CLA	C4D-ND	-2.77	1.33	1.37
42	N	619	XAT	C28-C29	-2.76	1.40	1.45
30	D	404	LHG	O8-C23	2.76	1.41	1.33
23	g	603	CLA	C1B-C2B	2.76	1.49	1.43
23	g	610	CLA	C4D-ND	-2.76	1.33	1.37
40	G	615	LUT	C22-C21	2.76	1.58	1.54
40	N	616	LUT	C8-C9	2.76	1.51	1.45
23	C	503	CLA	C1B-C2B	2.76	1.49	1.43
23	N	614	CLA	C4D-ND	-2.76	1.33	1.37
30	n	619	LHG	C8-C7	2.75	1.58	1.50
40	Y	316	LUT	C11-C10	2.75	1.52	1.43
23	N	603	CLA	C3B-C4B	2.75	1.49	1.42
40	y	317	LUT	C11-C10	2.75	1.52	1.43
40	r	613	LUT	C32-C33	2.75	1.51	1.45
23	N	603	CLA	C1B-C2B	2.75	1.49	1.43
40	R	613	LUT	C31-C30	2.75	1.52	1.43
23	c	505	CLA	C4D-ND	-2.75	1.33	1.37
23	B	605	CLA	C1B-C2B	2.75	1.49	1.43
30	b	627	LHG	P-O6	2.74	1.70	1.59
40	s	615	LUT	C31-C30	2.74	1.51	1.43
30	d	404	LHG	O8-C23	2.74	1.41	1.33
23	b	615	CLA	C1B-C2B	2.74	1.49	1.43
23	s	609	CLA	C4D-ND	-2.74	1.33	1.37
23	G	613	CLA	C1B-C2B	2.74	1.49	1.43
30	d	408	LHG	O8-C23	2.74	1.41	1.33
23	S	612	CLA	C1B-C2B	2.74	1.49	1.43
40	s	615	LUT	C1-C6	2.74	1.57	1.53
23	d	405	CLA	C1B-C2B	2.74	1.49	1.43
23	b	601	CLA	C4D-ND	-2.74	1.33	1.37
23	B	612	CLA	C1B-C2B	2.73	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	n	614	CLA	C4D-ND	-2.73	1.33	1.37
23	C	511	CLA	C1B-C2B	2.73	1.49	1.43
23	b	605	CLA	C1B-C2B	2.73	1.49	1.43
40	s	614	LUT	C11-C12	2.73	1.41	1.34
23	g	613	CLA	C1B-C2B	2.73	1.49	1.43
23	A	402	CLA	C1B-C2B	2.73	1.49	1.43
23	a	403	CLA	C1B-C2B	2.73	1.49	1.43
23	C	505	CLA	C1B-C2B	2.73	1.49	1.43
30	d	404	LHG	P-O6	2.73	1.70	1.59
23	b	613	CLA	C1B-C2B	2.73	1.49	1.43
40	N	615	LUT	C11-C12	2.73	1.41	1.34
40	R	613	LUT	C5-C6	2.73	1.39	1.34
30	y	318	LHG	C8-C7	2.73	1.58	1.50
23	S	608	CLA	C4D-ND	-2.73	1.33	1.37
23	c	507	CLA	C3B-C4B	2.72	1.49	1.42
40	n	616	LUT	C11-C10	2.72	1.51	1.43
30	d	408	LHG	P-O6	2.72	1.70	1.59
23	R	602	CLA	C1B-C2B	2.72	1.49	1.43
40	g	616	LUT	C5-C6	2.72	1.39	1.34
23	s	608	CLA	C1B-C2B	2.72	1.49	1.43
23	c	511	CLA	C1B-C2B	2.72	1.49	1.43
23	b	604	CLA	C3B-C4B	2.71	1.49	1.42
23	s	611	CLA	C1B-C2B	2.71	1.49	1.43
40	g	616	LUT	C26-C27	2.71	1.54	1.50
23	C	505	CLA	C4D-ND	-2.71	1.34	1.37
30	A	412	LHG	C8-C7	2.71	1.58	1.50
40	s	615	LUT	C5-C6	2.71	1.39	1.34
23	y	305	CLA	C1B-C2B	2.71	1.49	1.43
23	b	609	CLA	C1B-C2B	2.71	1.49	1.43
23	c	505	CLA	C1B-C2B	2.71	1.49	1.43
23	n	603	CLA	C1B-C2B	2.71	1.49	1.43
23	B	609	CLA	C1B-C2B	2.71	1.49	1.43
23	b	612	CLA	C1B-C2B	2.71	1.49	1.43
23	A	404	CLA	C1B-C2B	2.71	1.49	1.43
23	y	314	CLA	C1B-C2B	2.71	1.49	1.43
40	Y	316	LUT	C8-C9	2.70	1.51	1.45
23	g	611	CLA	C1B-C2B	2.70	1.49	1.43
23	b	607	CLA	C1B-C2B	2.70	1.49	1.43
40	n	616	LUT	C26-C27	2.70	1.54	1.50
23	C	502	CLA	C1B-C2B	2.70	1.49	1.43
23	R	611	CLA	C1B-C2B	2.70	1.49	1.43
23	B	604	CLA	C3B-C4B	2.70	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	r	611	CLA	C1B-C2B	2.70	1.49	1.43
23	r	602	CLA	C1B-C2B	2.70	1.49	1.43
23	g	602	CLA	C1B-C2B	2.70	1.49	1.43
23	a	405	CLA	C1B-C2B	2.70	1.49	1.43
30	d	408	LHG	C8-C7	2.70	1.58	1.50
23	Y	304	CLA	C1B-C2B	2.70	1.49	1.43
23	s	603	CLA	C1B-C2B	2.70	1.49	1.43
23	D	405	CLA	C1B-C2B	2.70	1.49	1.43
23	C	504	CLA	C1B-C2B	2.70	1.49	1.43
23	B	602	CLA	C1B-C2B	2.70	1.49	1.43
23	N	611	CLA	C1B-C2B	2.70	1.49	1.43
30	s	616	LHG	C8-C7	2.69	1.58	1.50
23	n	614	CLA	C1B-C2B	2.69	1.49	1.43
23	Y	313	CLA	C1B-C2B	2.69	1.49	1.43
40	N	616	LUT	C15-C14	2.69	1.51	1.43
30	r	616	LHG	C6-C5	2.69	1.59	1.50
23	c	502	CLA	C1B-C2B	2.69	1.49	1.43
23	c	513	CLA	C1B-C2B	2.69	1.49	1.43
23	s	612	CLA	C1B-C2B	2.69	1.49	1.43
40	N	615	LUT	C5-C6	2.69	1.39	1.34
23	G	611	CLA	C1B-C2B	2.69	1.49	1.43
23	R	603	CLA	C1B-C2B	2.68	1.49	1.43
23	n	613	CLA	C1B-C2B	2.68	1.49	1.43
23	S	611	CLA	C1B-C2B	2.68	1.49	1.43
23	G	602	CLA	C1B-C2B	2.68	1.49	1.43
23	B	613	CLA	C1B-C2B	2.68	1.49	1.43
23	G	603	CLA	C1B-C2B	2.68	1.49	1.43
23	S	602	CLA	C1B-C2B	2.68	1.49	1.43
23	R	612	CLA	C1B-C2B	2.68	1.49	1.43
23	S	603	CLA	C1B-C2B	2.68	1.49	1.43
40	y	317	LUT	C5-C6	2.68	1.39	1.34
23	C	509	CLA	C1B-C2B	2.68	1.49	1.43
23	c	504	CLA	C1B-C2B	2.68	1.49	1.43
23	n	612	CLA	C1B-C2B	2.68	1.49	1.43
23	y	304	CLA	C1B-C2B	2.68	1.49	1.43
40	S	615	LUT	C15-C14	2.68	1.51	1.43
40	y	316	LUT	C28-C27	2.68	1.38	1.32
23	n	611	CLA	C1B-C2B	2.68	1.49	1.43
30	A	412	LHG	O8-C23	2.68	1.41	1.33
23	N	613	CLA	C1B-C2B	2.68	1.49	1.43
23	r	612	CLA	C1B-C2B	2.68	1.49	1.43
30	S	616	LHG	C6-C5	2.68	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	r	608	CLA	C1B-C2B	2.67	1.49	1.43
23	N	602	CLA	C1B-C2B	2.67	1.49	1.43
23	R	610	CLA	C1B-C2B	2.67	1.49	1.43
23	a	404	CLA	C1B-C2B	2.67	1.49	1.43
23	Y	311	CLA	C1B-C2B	2.67	1.49	1.43
40	r	613	LUT	C26-C27	2.67	1.54	1.50
23	g	614	CLA	C1B-C2B	2.67	1.49	1.43
30	L	103	LHG	C8-C7	2.67	1.58	1.50
23	S	608	CLA	C1B-C2B	2.67	1.49	1.43
23	C	510	CLA	C1B-C2B	2.67	1.49	1.43
40	s	614	LUT	C5-C6	2.67	1.39	1.34
23	G	614	CLA	C1B-C2B	2.67	1.49	1.43
23	b	611	CLA	C1B-C2B	2.67	1.49	1.43
40	N	615	LUT	C1-C6	2.66	1.57	1.53
23	b	616	CLA	C1B-C2B	2.66	1.49	1.43
23	r	603	CLA	C1B-C2B	2.66	1.49	1.43
40	r	613	LUT	C5-C6	2.66	1.39	1.34
23	A	403	CLA	C1B-C2B	2.66	1.49	1.43
23	Y	303	CLA	C1B-C2B	2.66	1.49	1.43
23	N	610	CLA	C1B-C2B	2.66	1.49	1.43
23	c	508	CLA	C1B-C2B	2.66	1.49	1.43
40	S	614	LUT	C15-C14	2.66	1.51	1.43
23	b	602	CLA	C1B-C2B	2.66	1.49	1.43
23	r	609	CLA	C1B-C2B	2.66	1.49	1.43
23	c	507	CLA	C1B-C2B	2.66	1.49	1.43
23	R	608	CLA	C1B-C2B	2.65	1.49	1.43
40	Y	316	LUT	C5-C6	2.65	1.39	1.34
23	y	312	CLA	C1B-C2B	2.65	1.49	1.43
40	Y	315	LUT	C28-C27	2.65	1.38	1.32
23	N	614	CLA	C1B-C2B	2.65	1.49	1.43
23	c	509	CLA	C1B-C2B	2.65	1.49	1.43
23	a	407	CLA	C1B-C2B	2.65	1.49	1.43
23	B	614	CLA	C1B-C2B	2.65	1.49	1.43
30	n	619	LHG	C6-C5	2.65	1.58	1.50
23	n	602	CLA	C1B-C2B	2.65	1.49	1.43
23	S	613	CLA	C1B-C2B	2.65	1.49	1.43
23	s	610	CLA	C1B-C2B	2.65	1.49	1.43
40	s	614	LUT	C1-C6	2.65	1.57	1.53
30	D	404	LHG	P-O6	2.65	1.70	1.59
23	n	610	CLA	C1B-C2B	2.65	1.49	1.43
23	C	507	CLA	C1B-C2B	2.65	1.49	1.43
23	N	612	CLA	C1B-C2B	2.65	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	601	CLA	C1B-C2B	2.65	1.49	1.43
23	C	508	CLA	C1B-C2B	2.64	1.49	1.43
23	r	601	CLA	C1B-C2B	2.64	1.49	1.43
23	c	510	CLA	C1B-C2B	2.64	1.49	1.43
23	B	601	CLA	C1B-C2B	2.64	1.49	1.43
23	B	615	CLA	C1B-C2B	2.64	1.49	1.43
40	n	615	LUT	C28-C27	2.64	1.38	1.32
23	b	603	CLA	C1B-C2B	2.64	1.49	1.43
23	r	604	CLA	C1B-C2B	2.64	1.49	1.43
30	R	616	LHG	C6-C5	2.64	1.58	1.50
42	G	619	XAT	C24-C23	2.64	1.56	1.52
40	S	615	LUT	C11-C12	2.64	1.41	1.34
30	g	618	LHG	C6-C5	2.64	1.58	1.50
40	N	615	LUT	C15-C14	2.64	1.51	1.43
23	C	512	CLA	C1B-C2B	2.64	1.49	1.43
23	y	315	CLA	C1B-C2B	2.64	1.49	1.43
23	B	616	CLA	C1B-C2B	2.64	1.49	1.43
23	d	406	CLA	C1B-C2B	2.63	1.49	1.43
23	c	512	CLA	C1B-C2B	2.63	1.49	1.43
23	s	602	CLA	C1B-C2B	2.63	1.49	1.43
23	C	513	CLA	C1B-C2B	2.63	1.49	1.43
23	y	311	CLA	C1B-C2B	2.63	1.49	1.43
23	R	609	CLA	C1B-C2B	2.63	1.49	1.43
23	B	607	CLA	C1B-C2B	2.63	1.49	1.43
40	S	614	LUT	C11-C12	2.63	1.41	1.34
40	S	614	LUT	C5-C6	2.63	1.39	1.34
23	b	614	CLA	C1B-C2B	2.62	1.49	1.43
23	A	406	CLA	C1B-C2B	2.62	1.49	1.43
41	s	617	NEX	C40-C33	2.62	1.57	1.50
23	B	611	CLA	C1B-C2B	2.62	1.49	1.43
23	R	601	CLA	C1B-C2B	2.62	1.49	1.43
23	c	506	CLA	C1B-C2B	2.61	1.49	1.43
23	S	610	CLA	C1B-C2B	2.61	1.49	1.43
23	R	604	CLA	C1B-C2B	2.61	1.49	1.43
23	G	610	CLA	C1B-C2B	2.61	1.49	1.43
42	y	302	XAT	O4-C5	-2.61	1.42	1.46
40	G	616	LUT	C5-C6	2.61	1.38	1.34
23	C	501	CLA	C1B-C2B	2.61	1.49	1.43
23	g	604	CLA	C1B-C2B	2.61	1.49	1.43
23	s	613	CLA	C1B-C2B	2.61	1.49	1.43
30	y	318	LHG	C6-C5	2.61	1.58	1.50
23	B	603	CLA	C1B-C2B	2.61	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	r	615	XAT	C11-C12	2.61	1.41	1.34
23	G	604	CLA	C1B-C2B	2.61	1.49	1.43
30	N	618	LHG	C4-C5	2.61	1.58	1.50
40	N	616	LUT	C11-C12	2.61	1.41	1.34
40	R	613	LUT	C11-C12	2.60	1.41	1.34
30	a	412	LHG	C8-C7	2.60	1.58	1.50
23	D	406	CLA	C1B-C2B	2.60	1.49	1.43
23	C	506	CLA	C1B-C2B	2.60	1.49	1.43
23	Y	310	CLA	C1B-C2B	2.60	1.49	1.43
23	c	501	CLA	C1B-C2B	2.60	1.49	1.43
42	n	617	XAT	C24-C23	2.59	1.56	1.52
40	R	613	LUT	C15-C14	2.59	1.51	1.43
40	g	616	LUT	C1-C6	2.59	1.57	1.53
23	r	610	CLA	C1B-C2B	2.59	1.49	1.43
40	s	614	LUT	C28-C29	2.59	1.51	1.45
23	N	604	CLA	C1B-C2B	2.59	1.49	1.43
40	G	616	LUT	C32-C33	2.59	1.51	1.45
40	s	615	LUT	C11-C12	2.58	1.41	1.34
40	r	613	LUT	C11-C12	2.58	1.41	1.34
23	g	612	CLA	C1B-C2B	2.58	1.49	1.43
40	y	317	LUT	C32-C33	2.58	1.51	1.45
40	r	613	LUT	C31-C30	2.58	1.51	1.43
23	g	610	CLA	C1B-C2B	2.58	1.49	1.43
41	r	614	NEX	C37-C21	2.57	1.58	1.53
42	Y	301	XAT	O4-C5	-2.57	1.42	1.46
40	G	616	LUT	C1-C6	2.57	1.57	1.53
40	g	616	LUT	C32-C33	2.57	1.51	1.45
40	N	616	LUT	C5-C6	2.57	1.38	1.34
23	S	604	CLA	C1B-C2B	2.57	1.49	1.43
40	Y	316	LUT	C31-C30	2.56	1.51	1.43
40	y	316	LUT	C5-C6	2.56	1.38	1.34
23	Y	314	CLA	C1B-C2B	2.56	1.49	1.43
23	b	610	CLA	C1B-C2B	2.56	1.49	1.43
23	b	608	CLA	C1B-C2B	2.56	1.49	1.43
30	b	627	LHG	C6-C5	2.56	1.58	1.50
42	n	617	XAT	C28-C29	-2.56	1.40	1.45
23	n	604	CLA	C1B-C2B	2.56	1.49	1.43
30	d	408	LHG	C6-C5	2.56	1.58	1.50
23	Y	312	CLA	C1B-C2B	2.56	1.49	1.43
23	s	604	CLA	C1B-C2B	2.56	1.49	1.43
41	R	618	NEX	C37-C21	2.56	1.58	1.53
23	B	608	CLA	C1B-C2B	2.56	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	n	616	LUT	C5-C6	2.56	1.38	1.34
30	G	618	LHG	C6-C5	2.55	1.58	1.50
42	R	615	XAT	C11-C12	2.55	1.41	1.34
23	B	610	CLA	C1B-C2B	2.55	1.49	1.43
41	R	614	NEX	C37-C21	2.55	1.58	1.53
41	N	617	NEX	C38-C25	2.55	1.55	1.51
40	s	615	LUT	C15-C14	2.55	1.51	1.43
40	n	615	LUT	C5-C6	2.55	1.38	1.34
42	y	302	XAT	C24-C25	-2.54	1.48	1.52
30	L	103	LHG	C6-C5	2.54	1.58	1.50
40	Y	316	LUT	C32-C33	2.54	1.51	1.45
40	G	616	LUT	C11-C12	2.54	1.41	1.34
40	g	616	LUT	C11-C12	2.54	1.41	1.34
42	Y	301	XAT	C28-C29	-2.54	1.40	1.45
23	y	313	CLA	C1B-C2B	2.54	1.49	1.43
40	G	616	LUT	C31-C30	2.53	1.51	1.43
23	Y	305	CLA	C1B-C2B	2.53	1.49	1.43
40	y	317	LUT	C31-C30	2.53	1.51	1.43
35	C	523	VIV	O1-C9	-2.53	1.43	1.46
30	Y	318	LHG	C6-C5	2.53	1.58	1.50
41	Y	317	NEX	C37-C21	2.53	1.58	1.53
41	G	617	NEX	C38-C25	2.52	1.55	1.51
23	B	606	CLA	C1B-C2B	2.52	1.49	1.43
30	a	412	LHG	C6-C5	2.52	1.58	1.50
40	y	317	LUT	C1-C6	2.52	1.57	1.53
23	G	612	CLA	C1B-C2B	2.52	1.49	1.43
30	D	404	LHG	C6-C5	2.52	1.58	1.50
23	b	606	CLA	C1B-C2B	2.51	1.49	1.43
40	n	615	LUT	C12-C13	2.51	1.51	1.45
42	Y	301	XAT	C24-C23	2.51	1.55	1.52
41	r	614	NEX	C38-C25	2.51	1.55	1.51
40	g	616	LUT	C31-C30	2.51	1.51	1.43
41	G	617	NEX	C37-C21	2.51	1.58	1.53
41	g	617	NEX	C37-C21	2.50	1.58	1.53
23	y	306	CLA	C1B-C2B	2.50	1.49	1.43
41	N	617	NEX	C37-C21	2.50	1.58	1.53
30	d	404	LHG	C6-C5	2.50	1.58	1.50
41	g	617	NEX	C38-C25	2.50	1.55	1.51
41	n	618	NEX	C37-C21	2.49	1.58	1.53
33	C	515	DGD	O1G-C1G	-2.49	1.39	1.45
42	y	302	XAT	C24-C23	2.49	1.55	1.52
30	D	408	LHG	O7-C7	2.49	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	n	620	XAT	C4-C3	2.48	1.55	1.52
23	S	609	CLA	C1B-C2B	2.48	1.49	1.43
40	G	615	LUT	C26-C27	2.48	1.53	1.50
30	S	616	LHG	C4-C5	2.48	1.58	1.50
40	R	613	LUT	C1-C6	2.48	1.57	1.53
24	A	405	PHO	CMC-C2C	-2.47	1.46	1.50
42	N	619	XAT	C4-C3	2.47	1.55	1.52
41	R	614	NEX	C38-C25	2.47	1.55	1.51
42	y	302	XAT	C37-C21	2.47	1.58	1.53
42	r	615	XAT	C4-C3	2.47	1.55	1.52
40	n	616	LUT	C31-C30	2.46	1.51	1.43
40	n	616	LUT	C32-C33	2.46	1.51	1.45
42	n	617	XAT	O4-C5	-2.46	1.42	1.46
40	S	614	LUT	C28-C29	2.46	1.51	1.45
41	R	618	NEX	C38-C25	2.46	1.55	1.51
40	s	614	LUT	C31-C32	2.46	1.40	1.34
40	S	615	LUT	C28-C29	2.45	1.51	1.45
30	R	616	LHG	C24-C23	2.45	1.57	1.50
24	d	402	PHO	CMC-C2C	-2.45	1.46	1.50
30	y	318	LHG	C24-C23	2.45	1.57	1.50
30	A	412	LHG	C6-C5	2.45	1.58	1.50
23	s	609	CLA	CHC-C1C	2.45	1.43	1.38
41	n	618	NEX	C38-C25	2.45	1.55	1.51
42	G	619	XAT	O4-C5	-2.45	1.42	1.46
40	g	615	LUT	C26-C27	2.44	1.53	1.50
24	D	402	PHO	CMC-C2C	-2.44	1.46	1.50
40	n	616	LUT	C8-C9	2.44	1.51	1.45
42	R	615	XAT	C4-C3	2.44	1.55	1.52
40	Y	316	LUT	C1-C6	2.44	1.57	1.53
30	r	616	LHG	C4-C5	2.43	1.58	1.50
30	s	616	LHG	C6-C5	2.43	1.58	1.50
40	n	616	LUT	C11-C12	2.43	1.40	1.34
40	y	317	LUT	C11-C12	2.43	1.40	1.34
42	y	302	XAT	C17-C1	2.42	1.58	1.53
40	S	615	LUT	C31-C32	2.42	1.40	1.34
40	s	614	LUT	C35-C15	2.42	1.42	1.36
40	Y	316	LUT	C11-C12	2.42	1.40	1.34
40	y	316	LUT	C12-C13	2.42	1.51	1.45
40	Y	315	LUT	C5-C6	2.42	1.38	1.34
30	D	404	LHG	C24-C23	2.41	1.57	1.50
24	a	406	PHO	CMC-C2C	-2.41	1.46	1.50
30	g	618	LHG	C24-C23	2.41	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	515	DGD	O2G-C2G	-2.41	1.40	1.46
42	Y	301	XAT	C24-C25	-2.41	1.48	1.52
42	Y	301	XAT	C17-C1	2.40	1.58	1.53
42	G	619	XAT	C4-C5	-2.40	1.48	1.52
23	s	609	CLA	C1B-C2B	2.40	1.48	1.43
33	c	515	DGD	O2G-C2G	-2.40	1.40	1.46
40	S	614	LUT	C31-C32	2.40	1.40	1.34
24	a	406	PHO	CMD-C2D	-2.39	1.46	1.51
42	y	302	XAT	C4-C5	-2.39	1.48	1.52
40	g	615	LUT	C5-C6	2.38	1.38	1.34
30	N	618	LHG	C24-C23	2.38	1.57	1.50
42	N	619	XAT	C24-C25	-2.38	1.48	1.52
24	A	405	PHO	CMD-C2D	-2.38	1.46	1.51
42	n	617	XAT	C24-C25	-2.38	1.48	1.52
30	Y	318	LHG	C24-C23	2.38	1.57	1.50
30	Y	318	LHG	C4-C5	2.38	1.58	1.50
24	D	402	PHO	CMD-C2D	-2.38	1.46	1.51
42	n	620	XAT	C24-C25	-2.38	1.48	1.52
30	n	619	LHG	C24-C23	2.38	1.57	1.50
42	n	617	XAT	C4-C5	-2.37	1.48	1.52
30	s	616	LHG	C4-C5	2.37	1.58	1.50
39	G	607	CHL	C1B-NB	-2.37	1.34	1.37
40	G	616	LUT	C15-C14	2.37	1.50	1.43
30	s	616	LHG	C24-C23	2.37	1.57	1.50
39	G	620	CHL	C1B-NB	-2.37	1.34	1.37
40	S	614	LUT	C24-C25	2.36	1.36	1.33
30	r	616	LHG	C24-C23	2.36	1.57	1.50
40	R	613	LUT	C24-C25	2.36	1.36	1.33
30	S	616	LHG	C24-C23	2.36	1.57	1.50
40	Y	315	LUT	C12-C13	2.36	1.51	1.45
40	N	615	LUT	C24-C25	2.36	1.36	1.33
24	d	402	PHO	CMB-C2B	-2.36	1.46	1.51
40	r	613	LUT	C24-C25	2.35	1.36	1.33
39	R	606	CHL	C1B-NB	-2.35	1.34	1.37
30	d	408	LHG	C24-C23	2.35	1.57	1.50
40	N	615	LUT	C31-C32	2.35	1.40	1.34
23	S	609	CLA	CHC-C1C	2.34	1.43	1.38
40	g	616	LUT	C15-C14	2.34	1.50	1.43
24	d	402	PHO	CMD-C2D	-2.34	1.46	1.51
40	r	613	LUT	C1-C6	2.34	1.57	1.53
40	g	616	LUT	C24-C25	2.34	1.36	1.33
30	a	412	LHG	C4-C5	2.33	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	g	607	CHL	C1B-NB	-2.33	1.34	1.37
41	Y	317	NEX	C38-C25	2.33	1.55	1.51
24	A	405	PHO	CMB-C2B	-2.32	1.46	1.51
23	S	602	CLA	CHC-C1C	2.32	1.43	1.38
40	N	616	LUT	C31-C32	2.32	1.40	1.34
40	G	616	LUT	C24-C25	2.31	1.36	1.33
40	s	614	LUT	C8-C7	2.31	1.40	1.33
30	a	412	LHG	C24-C23	2.31	1.57	1.50
23	R	609	CLA	CHC-C1C	2.30	1.43	1.38
33	c	515	DGD	O1G-C1G	-2.30	1.39	1.45
40	s	615	LUT	C31-C32	2.30	1.40	1.34
39	n	607	CHL	C1B-NB	-2.30	1.35	1.37
39	Y	306	CHL	C1B-C2B	2.30	1.48	1.43
40	n	615	LUT	C15-C14	2.30	1.50	1.43
23	r	610	CLA	CHC-C1C	2.30	1.43	1.38
30	D	408	LHG	C8-C7	2.30	1.57	1.50
40	N	616	LUT	C24-C25	2.30	1.36	1.33
24	a	406	PHO	CMB-C2B	-2.30	1.46	1.51
30	G	618	LHG	C24-C23	2.30	1.57	1.50
40	R	613	LUT	C31-C32	2.30	1.40	1.34
23	s	603	CLA	CHC-C1C	2.30	1.43	1.38
23	C	510	CLA	CHC-C1C	2.29	1.43	1.38
30	A	412	LHG	C4-C5	2.29	1.57	1.50
39	g	605	CHL	C1B-NB	-2.29	1.35	1.37
40	S	615	LUT	C8-C7	2.29	1.40	1.33
23	n	610	CLA	CHC-C1C	2.29	1.43	1.38
40	N	616	LUT	C35-C15	2.29	1.41	1.36
41	Y	317	NEX	O24-C25	-2.29	1.42	1.46
23	c	510	CLA	CHC-C1C	2.29	1.43	1.38
23	r	609	CLA	CHC-C1C	2.29	1.43	1.38
23	B	606	CLA	CHC-C1C	2.29	1.43	1.38
40	S	615	LUT	C35-C15	2.28	1.41	1.36
40	S	614	LUT	C35-C15	2.28	1.41	1.36
23	B	601	CLA	CHC-C1C	2.28	1.43	1.38
23	R	610	CLA	CHC-C1C	2.28	1.43	1.38
24	d	402	PHO	C3D-C4D	2.28	1.44	1.41
23	R	601	CLA	CHC-C1C	2.28	1.43	1.38
24	D	402	PHO	CMB-C2B	-2.28	1.46	1.51
40	S	614	LUT	C8-C7	2.28	1.39	1.33
30	A	412	LHG	C24-C23	2.28	1.57	1.50
40	G	615	LUT	C5-C6	2.28	1.38	1.34
23	b	616	CLA	CHC-C1C	2.27	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	610	CLA	CHC-C1C	2.27	1.43	1.38
23	R	608	CLA	CHC-C1C	2.27	1.43	1.38
41	R	618	NEX	O24-C25	-2.27	1.43	1.46
23	c	511	CLA	CHC-C1C	2.27	1.43	1.38
23	N	610	CLA	CHC-C1C	2.27	1.43	1.38
30	y	318	LHG	C4-C5	2.27	1.57	1.50
40	s	615	LUT	C8-C7	2.27	1.39	1.33
23	g	602	CLA	CHC-C1C	2.27	1.43	1.38
23	s	602	CLA	CHC-C1C	2.27	1.43	1.38
40	N	615	LUT	C8-C7	2.27	1.39	1.33
23	N	604	CLA	CHC-C1C	2.27	1.43	1.38
23	d	405	CLA	CMD-C2D	-2.27	1.46	1.50
23	N	614	CLA	CHC-C1C	2.27	1.43	1.38
23	C	511	CLA	CHC-C1C	2.27	1.43	1.38
40	N	615	LUT	C35-C15	2.26	1.41	1.36
23	R	602	CLA	CHC-C1C	2.26	1.43	1.38
39	G	607	CHL	C1D-C2D	-2.26	1.40	1.45
41	G	617	NEX	C31-C32	2.26	1.40	1.34
24	a	406	PHO	CAC-C3C	-2.26	1.47	1.51
40	n	615	LUT	C30-C29	2.26	1.38	1.35
23	b	603	CLA	CHC-C1C	2.26	1.43	1.38
39	g	607	CHL	C1D-C2D	-2.26	1.40	1.45
23	n	602	CLA	CHC-C1C	2.26	1.43	1.38
39	G	620	CHL	C1D-C2D	-2.26	1.40	1.45
24	d	402	PHO	CAC-C3C	-2.26	1.47	1.51
23	G	602	CLA	CHC-C1C	2.26	1.43	1.38
23	b	614	CLA	CHC-C1C	2.26	1.43	1.38
23	c	505	CLA	CMD-C2D	-2.25	1.46	1.50
40	S	615	LUT	C22-C21	2.25	1.57	1.54
23	S	610	CLA	CHC-C1C	2.25	1.43	1.38
24	a	406	PHO	C4D-ND	-2.25	1.35	1.38
23	b	612	CLA	CHC-C1C	2.25	1.43	1.38
40	g	615	LUT	C1-C6	2.25	1.56	1.53
24	D	402	PHO	C4D-ND	-2.25	1.35	1.38
23	s	613	CLA	CHC-C1C	2.25	1.43	1.38
30	R	616	LHG	C4-C5	2.25	1.57	1.50
23	a	403	CLA	CHC-C1C	2.25	1.43	1.38
23	b	610	CLA	CHC-C1C	2.25	1.43	1.38
23	b	608	CLA	CHC-C1C	2.25	1.43	1.38
23	N	602	CLA	CHC-C1C	2.25	1.43	1.38
23	s	608	CLA	CHC-C1C	2.25	1.43	1.38
40	n	616	LUT	C15-C14	2.25	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	y	303	CHL	C1D-C2D	-2.25	1.40	1.45
23	a	407	CLA	CHC-C1C	2.25	1.43	1.38
39	N	607	CHL	C1B-NB	-2.25	1.35	1.37
40	S	615	LUT	C24-C25	2.25	1.35	1.33
30	D	408	LHG	C24-C23	2.25	1.57	1.50
23	n	614	CLA	CHC-C1C	2.24	1.43	1.38
24	A	405	PHO	C3D-C4D	2.24	1.44	1.41
23	n	604	CLA	CHC-C1C	2.24	1.43	1.38
40	g	616	LUT	C8-C7	2.24	1.39	1.33
24	A	405	PHO	CAC-C3C	-2.24	1.47	1.51
23	S	613	CLA	CHC-C1C	2.24	1.43	1.38
23	r	608	CLA	CHC-C1C	2.24	1.43	1.38
23	c	513	CLA	CHC-C1C	2.24	1.43	1.38
42	n	620	XAT	O4-C5	-2.24	1.43	1.46
40	s	615	LUT	C28-C29	2.24	1.50	1.45
39	g	619	CHL	C1B-NB	-2.24	1.35	1.37
41	S	617	NEX	C11-C12	2.24	1.40	1.34
23	B	614	CLA	CHC-C1C	2.24	1.43	1.38
23	b	613	CLA	CHC-C1C	2.24	1.43	1.38
23	r	601	CLA	CHC-C1C	2.24	1.43	1.38
23	b	601	CLA	CHC-C1C	2.24	1.43	1.38
23	g	614	CLA	CHC-C1C	2.24	1.43	1.38
42	G	619	XAT	C22-C21	2.24	1.58	1.54
23	B	603	CLA	CHC-C1C	2.24	1.43	1.38
23	n	613	CLA	CHC-C1C	2.24	1.43	1.38
40	G	616	LUT	C8-C7	2.24	1.39	1.33
42	N	619	XAT	O4-C5	-2.24	1.43	1.46
23	b	606	CLA	CHC-C1C	2.24	1.43	1.38
24	a	406	PHO	C3D-C4D	2.24	1.44	1.41
39	y	309	CHL	C1D-C2D	-2.24	1.40	1.45
23	B	613	CLA	CHC-C1C	2.24	1.43	1.38
23	R	611	CLA	CHC-C1C	2.24	1.43	1.38
41	r	614	NEX	O24-C25	-2.23	1.43	1.46
39	N	608	CHL	C1D-C2D	-2.23	1.40	1.45
40	y	317	LUT	C8-C7	2.23	1.39	1.33
23	G	614	CLA	CHC-C1C	2.23	1.43	1.38
23	y	312	CLA	CHC-C1C	2.23	1.43	1.38
23	S	603	CLA	CHC-C1C	2.23	1.43	1.38
23	y	311	CLA	CHC-C1C	2.23	1.43	1.38
41	N	617	NEX	O24-C25	-2.23	1.43	1.46
40	r	613	LUT	C8-C7	2.23	1.39	1.33
39	G	606	CHL	C1D-C2D	-2.23	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Y	307	CHL	C1D-C2D	-2.23	1.40	1.45
23	B	616	CLA	CHC-C1C	2.23	1.43	1.38
23	Y	314	CLA	CHC-C1C	2.23	1.43	1.38
39	N	607	CHL	C1D-C2D	-2.23	1.40	1.45
23	b	607	CLA	CHC-C1C	2.23	1.43	1.38
40	Y	315	LUT	C30-C29	2.23	1.38	1.35
23	y	304	CLA	CHC-C1C	2.23	1.43	1.38
23	y	314	CLA	CHC-C1C	2.23	1.43	1.38
40	N	616	LUT	C8-C7	2.23	1.39	1.33
40	R	613	LUT	C35-C15	2.23	1.41	1.36
40	y	316	LUT	C30-C29	2.23	1.38	1.35
40	y	317	LUT	C24-C25	2.23	1.35	1.33
39	g	605	CHL	C1D-C2D	-2.22	1.40	1.45
23	C	513	CLA	CHC-C1C	2.22	1.43	1.38
23	R	604	CLA	CHC-C1C	2.22	1.43	1.38
23	Y	303	CLA	CHC-C1C	2.22	1.43	1.38
23	y	315	CLA	CHC-C1C	2.22	1.43	1.38
39	r	606	CHL	C1B-NB	-2.22	1.35	1.37
23	B	609	CLA	CHC-C1C	2.22	1.43	1.38
23	r	611	CLA	CHC-C1C	2.22	1.43	1.38
40	R	613	LUT	C8-C7	2.22	1.39	1.33
40	n	616	LUT	C24-C25	2.22	1.35	1.33
23	s	610	CLA	CHC-C1C	2.22	1.43	1.38
24	A	405	PHO	C4D-ND	-2.22	1.35	1.38
26	L	101	SQD	O9-S	2.22	1.51	1.45
23	N	612	CLA	CHC-C1C	2.22	1.43	1.38
23	A	402	CLA	CHC-C1C	2.22	1.43	1.38
41	R	614	NEX	O24-C25	-2.22	1.43	1.46
23	B	612	CLA	CHC-C1C	2.22	1.43	1.38
23	r	602	CLA	CHC-C1C	2.22	1.43	1.38
23	Y	310	CLA	CHC-C1C	2.22	1.43	1.38
24	D	402	PHO	CAC-C3C	-2.22	1.47	1.51
40	r	613	LUT	C31-C32	2.22	1.40	1.34
23	c	509	CLA	CHC-C1C	2.22	1.43	1.38
40	N	615	LUT	C28-C29	2.22	1.50	1.45
39	G	601	CHL	C1B-C2B	2.22	1.48	1.43
23	Y	311	CLA	CHC-C1C	2.22	1.43	1.38
23	Y	313	CLA	CHC-C1C	2.22	1.43	1.38
23	C	505	CLA	CMD-C2D	-2.22	1.46	1.50
39	n	601	CHL	C1D-C2D	-2.21	1.41	1.45
23	B	608	CLA	CHC-C1C	2.21	1.43	1.38
23	Y	305	CLA	CHC-C1C	2.21	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	G	615	LUT	C17-C1	2.21	1.58	1.53
23	b	602	CLA	CHC-C1C	2.21	1.43	1.38
23	g	611	CLA	CHC-C1C	2.21	1.43	1.38
39	R	607	CHL	C1D-C2D	-2.21	1.41	1.45
23	N	611	CLA	CHC-C1C	2.21	1.43	1.38
23	R	612	CLA	CHC-C1C	2.21	1.43	1.38
23	C	509	CLA	CHC-C1C	2.21	1.43	1.38
40	s	615	LUT	C35-C15	2.21	1.41	1.36
23	G	610	CLA	CHC-C1C	2.21	1.43	1.38
23	S	608	CLA	CHC-C1C	2.21	1.43	1.38
39	g	609	CHL	C1D-C2D	-2.21	1.41	1.45
40	N	616	LUT	C28-C29	2.21	1.50	1.45
23	b	605	CLA	CHC-C1C	2.21	1.43	1.38
39	y	308	CHL	C1D-C2D	-2.21	1.41	1.45
23	b	607	CLA	CMD-C2D	-2.21	1.46	1.50
39	r	607	CHL	C1D-C2D	-2.21	1.41	1.45
39	r	607	CHL	C1B-NB	-2.21	1.35	1.37
23	D	405	CLA	CMD-C2D	-2.21	1.46	1.50
40	y	317	LUT	C31-C32	2.21	1.40	1.34
42	Y	301	XAT	C4-C5	-2.21	1.48	1.52
40	Y	316	LUT	C8-C7	2.21	1.39	1.33
40	Y	316	LUT	C31-C32	2.21	1.40	1.34
23	B	602	CLA	CHC-C1C	2.21	1.43	1.38
23	g	610	CLA	CHC-C1C	2.20	1.43	1.38
40	Y	315	LUT	C1-C6	2.20	1.56	1.53
39	g	606	CHL	C1D-C2D	-2.20	1.41	1.45
23	s	604	CLA	CHC-C1C	2.20	1.43	1.38
30	L	103	LHG	C24-C23	2.20	1.57	1.50
40	Y	316	LUT	C15-C14	2.20	1.50	1.43
40	y	317	LUT	C15-C14	2.20	1.50	1.43
23	b	609	CLA	CHC-C1C	2.20	1.43	1.38
23	C	503	CLA	CHC-C1C	2.20	1.43	1.38
23	g	612	CLA	CHC-C1C	2.20	1.43	1.38
23	s	612	CLA	CHC-C1C	2.20	1.43	1.38
39	Y	308	CHL	C1D-C2D	-2.20	1.41	1.45
23	C	508	CLA	CHC-C1C	2.20	1.43	1.38
23	R	603	CLA	CHC-C1C	2.20	1.43	1.38
23	r	612	CLA	CHC-C1C	2.20	1.43	1.38
30	n	619	LHG	C4-C5	2.20	1.57	1.50
39	N	601	CHL	C1D-C2D	-2.20	1.41	1.45
40	r	613	LUT	C35-C15	2.20	1.41	1.36
41	s	617	NEX	C11-C12	2.19	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	615	CLA	CHC-C1C	2.19	1.43	1.38
23	B	607	CLA	CHC-C1C	2.19	1.43	1.38
40	G	616	LUT	C31-C32	2.19	1.40	1.34
23	B	607	CLA	CMD-C2D	-2.19	1.46	1.50
39	r	605	CHL	C1D-C2D	-2.19	1.41	1.45
23	A	406	CLA	CHC-C1C	2.19	1.43	1.38
23	n	612	CLA	CHC-C1C	2.19	1.43	1.38
39	n	607	CHL	C1D-C2D	-2.19	1.41	1.45
23	g	604	CLA	CHC-C1C	2.19	1.43	1.38
39	Y	302	CHL	C1D-C2D	-2.19	1.41	1.45
42	r	615	XAT	O4-C5	-2.19	1.43	1.46
39	R	605	CHL	C1D-C2D	-2.19	1.41	1.45
26	a	409	SQD	O9-S	2.19	1.51	1.45
24	D	402	PHO	C3D-C4D	2.19	1.44	1.41
30	g	618	LHG	C4-C5	2.19	1.57	1.50
23	a	405	CLA	CHC-C1C	2.19	1.43	1.38
23	n	611	CLA	CHC-C1C	2.19	1.43	1.38
40	n	615	LUT	C1-C6	2.19	1.56	1.53
39	G	605	CHL	C1D-C2D	-2.19	1.41	1.45
23	Y	305	CLA	CMB-C2B	-2.19	1.46	1.50
39	g	619	CHL	C1D-C2D	-2.18	1.41	1.45
39	s	601	CHL	C1D-C2D	-2.18	1.41	1.45
23	C	512	CLA	CHC-C1C	2.18	1.43	1.38
23	G	611	CLA	CHC-C1C	2.18	1.43	1.38
23	G	612	CLA	CHC-C1C	2.18	1.43	1.38
40	g	615	LUT	C17-C1	2.18	1.58	1.53
23	A	404	CLA	CHC-C1C	2.18	1.43	1.38
39	s	607	CHL	C1D-C2D	-2.18	1.41	1.45
23	s	611	CLA	CHC-C1C	2.18	1.43	1.38
39	N	606	CHL	C1D-C2D	-2.18	1.41	1.45
23	r	604	CLA	CHC-C1C	2.18	1.43	1.38
23	G	603	CLA	CHC-C1C	2.18	1.43	1.38
23	S	604	CLA	CHC-C1C	2.18	1.43	1.38
26	A	408	SQD	O9-S	2.18	1.51	1.45
23	Y	312	CLA	CHC-C1C	2.18	1.42	1.38
26	M	101	SQD	O9-S	2.18	1.51	1.45
42	R	615	XAT	O4-C5	-2.18	1.43	1.46
39	N	609	CHL	C1D-C2D	-2.18	1.41	1.45
23	C	502	CLA	CHC-C1C	2.18	1.42	1.38
39	r	606	CHL	C1D-C2D	-2.18	1.41	1.45
23	N	613	CLA	CHC-C1C	2.17	1.42	1.38
39	S	606	CHL	C1D-C2D	-2.17	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	y	306	CLA	CMB-C2B	-2.17	1.46	1.50
39	N	601	CHL	C1B-C2B	2.17	1.48	1.43
39	S	607	CHL	C1D-C2D	-2.17	1.41	1.45
39	G	601	CHL	C1D-C2D	-2.17	1.41	1.45
23	b	612	CLA	CMD-C2D	-2.17	1.46	1.50
23	C	505	CLA	CHC-C1C	2.17	1.42	1.38
23	c	505	CLA	CHC-C1C	2.17	1.42	1.38
23	c	508	CLA	CHC-C1C	2.17	1.42	1.38
23	r	603	CLA	CHC-C1C	2.17	1.42	1.38
40	R	613	LUT	C17-C1	2.17	1.58	1.53
39	g	601	CHL	C1D-C2D	-2.17	1.41	1.45
23	C	504	CLA	CHC-C1C	2.17	1.42	1.38
23	g	613	CLA	CHC-C1C	2.17	1.42	1.38
39	G	608	CHL	C1D-C2D	-2.17	1.41	1.45
23	c	507	CLA	CHC-C1C	2.17	1.42	1.38
23	c	512	CLA	CHC-C1C	2.17	1.42	1.38
41	s	617	NEX	C32-C33	2.17	1.56	1.50
42	G	619	XAT	C28-C29	-2.17	1.41	1.45
39	S	605	CHL	C1D-C2D	-2.17	1.41	1.45
40	n	616	LUT	C8-C7	2.17	1.39	1.33
39	n	608	CHL	C1D-C2D	-2.17	1.41	1.45
23	S	611	CLA	CHC-C1C	2.17	1.42	1.38
23	d	406	CLA	CHC-C1C	2.17	1.42	1.38
39	R	606	CHL	C1D-C2D	-2.16	1.41	1.45
40	g	616	LUT	C31-C32	2.16	1.40	1.34
39	n	606	CHL	C1D-C2D	-2.16	1.41	1.45
23	C	507	CLA	CHC-C1C	2.16	1.42	1.38
23	G	604	CLA	CHC-C1C	2.16	1.42	1.38
40	Y	316	LUT	C24-C25	2.16	1.35	1.33
26	a	409	SQD	O7-S	2.16	1.51	1.45
39	g	608	CHL	C1D-C2D	-2.16	1.41	1.45
23	c	504	CLA	CHC-C1C	2.16	1.42	1.38
23	b	611	CLA	CHC-C1C	2.16	1.42	1.38
39	Y	309	CHL	C1D-C2D	-2.16	1.41	1.45
23	D	406	CLA	CHC-C1C	2.16	1.42	1.38
40	n	615	LUT	C17-C1	2.16	1.58	1.53
39	Y	306	CHL	C1D-C2D	-2.16	1.41	1.45
23	y	306	CLA	CHC-C1C	2.16	1.42	1.38
23	A	402	CLA	CMD-C2D	-2.16	1.46	1.50
30	b	627	LHG	C24-C23	2.16	1.57	1.50
39	S	601	CHL	C1D-C2D	-2.15	1.41	1.45
40	G	615	LUT	C1-C6	2.15	1.56	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	S	607	CHL	C3D-C4D	-2.15	1.39	1.44
23	A	403	CLA	CHC-C1C	2.15	1.42	1.38
23	b	615	CLA	CHC-C1C	2.15	1.42	1.38
23	B	605	CLA	CHC-C1C	2.15	1.42	1.38
39	s	605	CHL	C1D-C2D	-2.15	1.41	1.45
23	G	613	CLA	CHC-C1C	2.15	1.42	1.38
40	y	316	LUT	C1-C6	2.15	1.56	1.53
23	D	405	CLA	CHC-C1C	2.15	1.42	1.38
23	S	612	CLA	CHC-C1C	2.15	1.42	1.38
23	g	603	CLA	CHC-C1C	2.15	1.42	1.38
39	g	601	CHL	C1B-C2B	2.15	1.48	1.43
40	r	613	LUT	C17-C1	2.15	1.58	1.53
23	a	404	CLA	CHC-C1C	2.15	1.42	1.38
23	y	313	CLA	CHC-C1C	2.15	1.42	1.38
41	n	618	NEX	O24-C25	-2.14	1.43	1.46
39	s	606	CHL	C1D-C2D	-2.14	1.41	1.45
23	a	403	CLA	CMC-C2C	-2.14	1.46	1.50
40	n	615	LUT	C11-C12	2.14	1.40	1.34
39	y	307	CHL	C1B-C2B	2.14	1.48	1.43
23	g	604	CLA	CMB-C2B	-2.14	1.46	1.50
23	c	503	CLA	CHC-C1C	2.14	1.42	1.38
39	n	609	CHL	C1D-C2D	-2.14	1.41	1.45
23	c	501	CLA	CHC-C1C	2.14	1.42	1.38
23	B	611	CLA	CHC-C1C	2.14	1.42	1.38
23	c	506	CLA	CHC-C1C	2.14	1.42	1.38
23	C	506	CLA	CHC-C1C	2.13	1.42	1.38
26	M	101	SQD	O7-S	2.13	1.51	1.45
39	y	309	CHL	C3D-C4D	-2.13	1.39	1.44
23	c	502	CLA	CHC-C1C	2.13	1.42	1.38
23	n	603	CLA	CHC-C1C	2.13	1.42	1.38
40	n	616	LUT	C31-C32	2.13	1.40	1.34
39	y	310	CHL	C1D-C2D	-2.13	1.41	1.45
39	y	307	CHL	C1D-C2D	-2.13	1.41	1.45
23	C	506	CLA	CMB-C2B	-2.13	1.46	1.50
30	d	404	LHG	C24-C23	2.13	1.56	1.50
23	C	510	CLA	CMD-C2D	-2.13	1.46	1.50
33	H	502	DGD	O1G-C1G	-2.12	1.40	1.45
40	g	615	LUT	C22-C21	2.12	1.57	1.54
39	R	607	CHL	C1B-NB	-2.12	1.35	1.37
23	d	405	CLA	CHC-C1C	2.12	1.42	1.38
23	S	604	CLA	CMB-C2B	-2.12	1.46	1.50
39	s	605	CHL	C1B-C2B	2.12	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	G	618	LHG	C4-C5	2.12	1.57	1.50
39	n	601	CHL	C1B-C2B	2.12	1.48	1.43
39	S	607	CHL	C1B-C2B	2.12	1.48	1.43
23	R	604	CLA	CMB-C2B	-2.12	1.46	1.50
39	y	303	CHL	C1B-C2B	2.12	1.48	1.43
39	G	609	CHL	C1D-C2D	-2.12	1.41	1.45
23	A	402	CLA	CMC-C2C	-2.12	1.46	1.50
23	B	612	CLA	CMD-C2D	-2.12	1.46	1.50
23	C	501	CLA	CHC-C1C	2.12	1.42	1.38
39	G	605	CHL	C1B-C2B	2.12	1.48	1.43
23	a	403	CLA	CMD-C2D	-2.12	1.46	1.50
39	g	605	CHL	C1B-C2B	2.12	1.48	1.43
26	L	101	SQD	O7-S	2.12	1.51	1.45
39	S	605	CHL	C1B-C2B	2.11	1.48	1.43
39	S	601	CHL	C3D-C4D	-2.11	1.39	1.44
40	G	615	LUT	C31-C30	2.11	1.50	1.43
40	n	616	LUT	C17-C1	2.11	1.57	1.53
40	Y	316	LUT	C17-C1	2.11	1.57	1.53
40	y	317	LUT	C17-C1	2.11	1.57	1.53
41	g	617	NEX	C11-C12	2.11	1.40	1.34
39	N	605	CHL	C1D-C2D	-2.11	1.41	1.45
23	S	604	CLA	MG-NB	-2.11	2.01	2.05
26	A	408	SQD	O7-S	2.10	1.51	1.45
23	s	604	CLA	CMB-C2B	-2.10	1.46	1.50
33	d	411	DGD	O1G-C1G	-2.10	1.40	1.45
30	d	408	LHG	C4-C5	2.10	1.57	1.50
23	N	604	CLA	CMB-C2B	-2.10	1.46	1.50
39	y	308	CHL	C3D-C4D	-2.10	1.39	1.44
40	N	616	LUT	C17-C1	2.10	1.57	1.53
23	G	604	CLA	CMB-C2B	-2.10	1.46	1.50
39	s	601	CHL	C3D-C4D	-2.10	1.39	1.44
39	n	609	CHL	C1B-NB	-2.10	1.35	1.37
42	G	619	XAT	C11-C12	2.10	1.40	1.34
23	g	604	CLA	MG-NB	-2.10	2.01	2.05
39	y	303	CHL	C3D-C4D	-2.10	1.39	1.44
39	Y	308	CHL	C3D-C4D	-2.10	1.39	1.44
23	G	604	CLA	MG-NB	-2.10	2.01	2.05
23	y	306	CLA	MG-NB	-2.10	2.01	2.05
23	N	603	CLA	CHC-C1C	2.10	1.42	1.38
30	b	627	LHG	C4-C5	2.09	1.57	1.50
42	n	620	XAT	C2-C1	2.09	1.57	1.54
23	g	603	CLA	CMD-C2D	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	d	404	LHG	C4-C5	2.09	1.57	1.50
39	n	605	CHL	C1D-C2D	-2.09	1.41	1.45
39	G	609	CHL	C1B-NB	-2.09	1.35	1.37
23	B	604	CLA	CMD-C2D	-2.09	1.46	1.50
23	c	506	CLA	CMB-C2B	-2.09	1.46	1.50
39	Y	302	CHL	C3D-C4D	-2.09	1.39	1.44
23	y	305	CLA	CHC-C1C	2.09	1.42	1.38
23	b	605	CLA	CMC-C2C	-2.08	1.46	1.50
39	s	607	CHL	C3D-C4D	-2.08	1.39	1.44
23	n	604	CLA	CMB-C2B	-2.08	1.46	1.50
39	y	309	CHL	C1B-C2B	2.08	1.48	1.43
39	g	608	CHL	C3D-C4D	-2.08	1.39	1.44
23	g	612	CLA	CMD-C2D	-2.08	1.46	1.50
41	g	617	NEX	C31-C32	2.08	1.39	1.34
39	G	606	CHL	C1B-NB	-2.08	1.35	1.37
41	R	614	NEX	C11-C12	2.08	1.39	1.34
42	N	619	XAT	C37-C21	2.08	1.57	1.53
39	Y	307	CHL	C1B-C2B	2.08	1.48	1.43
23	c	510	CLA	CMD-C2D	-2.08	1.46	1.50
39	N	606	CHL	C3D-C4D	-2.08	1.39	1.44
41	g	617	NEX	O24-C25	-2.08	1.43	1.46
23	s	609	CLA	CMB-C2B	-2.08	1.46	1.50
39	N	609	CHL	C1B-NB	-2.08	1.35	1.37
39	y	310	CHL	C3D-C4D	-2.08	1.39	1.44
39	y	308	CHL	C1B-C2B	2.08	1.48	1.43
23	C	507	CLA	MG-NB	-2.08	2.01	2.05
23	Y	304	CLA	CHC-C1C	2.08	1.42	1.38
23	b	616	CLA	CMC-C2C	-2.07	1.46	1.50
40	R	613	LUT	C28-C29	2.07	1.50	1.45
23	B	616	CLA	CMC-C2C	-2.07	1.46	1.50
23	s	604	CLA	MG-NB	-2.07	2.01	2.05
40	y	316	LUT	C11-C10	2.07	1.49	1.43
39	G	608	CHL	C1B-C2B	2.07	1.48	1.43
39	R	607	CHL	C1B-C2B	2.07	1.48	1.43
23	n	603	CLA	CMD-C2D	-2.07	1.46	1.50
23	y	315	CLA	CMD-C2D	-2.07	1.46	1.50
23	R	604	CLA	MG-NB	-2.07	2.01	2.05
39	r	605	CHL	C3D-C4D	-2.07	1.39	1.44
39	S	605	CHL	C1B-NB	-2.07	1.35	1.37
23	N	604	CLA	MG-NB	-2.07	2.01	2.05
23	r	604	CLA	CMB-C2B	-2.07	1.46	1.50
39	n	608	CHL	C3D-C4D	-2.07	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	N	606	CHL	C1B-C2B	2.07	1.48	1.43
39	Y	309	CHL	C1B-NB	-2.07	1.35	1.37
39	n	609	CHL	C1B-C2B	2.06	1.48	1.43
40	N	615	LUT	C17-C1	2.06	1.57	1.53
40	s	615	LUT	C17-C1	2.06	1.57	1.53
23	b	606	CLA	CMC-C2C	-2.06	1.46	1.50
23	B	606	CLA	CMD-C2D	-2.06	1.46	1.50
23	C	501	CLA	CMD-C2D	-2.06	1.46	1.50
23	y	314	CLA	MG-NB	-2.06	2.01	2.05
40	S	615	LUT	C17-C1	2.06	1.57	1.53
40	Y	316	LUT	C22-C21	2.06	1.57	1.54
23	c	509	CLA	CMD-C2D	-2.06	1.46	1.50
41	G	617	NEX	O24-C25	-2.06	1.43	1.46
23	n	610	CLA	MG-NB	-2.06	2.01	2.05
39	g	608	CHL	C1B-C2B	2.06	1.48	1.43
23	n	604	CLA	MG-NB	-2.06	2.01	2.05
23	B	603	CLA	CMD-C2D	-2.06	1.46	1.50
23	n	604	CLA	CMD-C2D	-2.06	1.46	1.50
39	Y	302	CHL	C1B-C2B	2.06	1.48	1.43
39	R	607	CHL	C3D-C4D	-2.06	1.39	1.44
23	b	604	CLA	CMD-C2D	-2.06	1.46	1.50
39	s	607	CHL	C1B-C2B	2.06	1.48	1.43
40	s	614	LUT	C17-C1	2.06	1.57	1.53
23	Y	305	CLA	MG-NB	-2.06	2.01	2.05
23	b	608	CLA	CMD-C2D	-2.06	1.46	1.50
39	G	601	CHL	C3D-C4D	-2.06	1.39	1.44
39	G	620	CHL	C3D-C4D	-2.06	1.39	1.44
42	Y	301	XAT	C37-C21	2.06	1.57	1.53
23	c	513	CLA	CMD-C2D	-2.06	1.46	1.50
39	G	608	CHL	C3D-C4D	-2.06	1.39	1.44
40	y	316	LUT	C11-C12	2.06	1.39	1.34
23	g	611	CLA	MG-NB	-2.06	2.01	2.05
23	B	615	CLA	CMD-C2D	-2.06	1.46	1.50
23	b	606	CLA	CMD-C2D	-2.06	1.46	1.50
39	N	609	CHL	C1B-C2B	2.06	1.48	1.43
23	N	602	CLA	MG-NB	-2.06	2.01	2.05
39	n	608	CHL	C1B-NB	-2.06	1.35	1.37
40	G	615	LUT	C2-C3	2.06	1.55	1.52
23	b	604	CLA	CMB-C2B	-2.06	1.46	1.50
39	g	609	CHL	C1B-C2B	2.06	1.48	1.43
23	R	602	CLA	MG-NB	-2.05	2.01	2.05
23	Y	311	CLA	MG-NB	-2.05	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	r	607	CHL	C3D-C4D	-2.05	1.39	1.44
23	c	501	CLA	CMD-C2D	-2.05	1.46	1.50
23	B	605	CLA	CMD-C2D	-2.05	1.46	1.50
39	n	607	CHL	C3D-C4D	-2.05	1.39	1.44
23	N	603	CLA	MG-NB	-2.05	2.01	2.05
23	r	604	CLA	MG-NB	-2.05	2.01	2.05
23	R	603	CLA	CMD-C2D	-2.05	1.46	1.50
39	Y	309	CHL	C3D-C4D	-2.05	1.39	1.44
39	n	609	CHL	C3D-C4D	-2.05	1.39	1.44
23	D	405	CLA	MG-NB	-2.05	2.01	2.05
23	s	611	CLA	MG-NB	-2.05	2.01	2.05
23	b	603	CLA	CMD-C2D	-2.05	1.46	1.50
39	R	605	CHL	C1B-C2B	2.05	1.48	1.43
23	D	406	CLA	CMB-C2B	-2.05	1.46	1.50
23	y	312	CLA	MG-NB	-2.05	2.01	2.05
39	G	608	CHL	C1B-NB	-2.05	1.35	1.37
39	G	607	CHL	C3D-C4D	-2.04	1.39	1.44
42	n	620	XAT	C37-C21	2.04	1.57	1.53
23	C	510	CLA	MG-NB	-2.04	2.01	2.05
23	n	611	CLA	MG-NB	-2.04	2.01	2.05
23	r	610	CLA	MG-NB	-2.04	2.01	2.05
23	r	603	CLA	CMD-C2D	-2.04	1.46	1.50
23	Y	313	CLA	MG-NB	-2.04	2.01	2.05
40	S	614	LUT	C17-C1	2.04	1.57	1.53
39	N	608	CHL	C3D-C4D	-2.04	1.39	1.44
23	R	604	CLA	CMD-C2D	-2.04	1.46	1.50
39	G	609	CHL	C3D-C4D	-2.04	1.39	1.44
39	g	606	CHL	C1B-NB	-2.04	1.35	1.37
23	N	610	CLA	MG-NB	-2.04	2.01	2.05
39	r	606	CHL	C3D-C4D	-2.04	1.39	1.44
40	G	616	LUT	C35-C15	2.04	1.41	1.36
23	c	502	CLA	CMB-C2B	-2.04	1.46	1.50
23	B	606	CLA	CMC-C2C	-2.04	1.46	1.50
23	R	610	CLA	MG-NB	-2.04	2.01	2.05
23	c	506	CLA	MG-NB	-2.04	2.01	2.05
39	n	601	CHL	C3D-C4D	-2.04	1.39	1.44
39	g	601	CHL	C3D-C4D	-2.04	1.39	1.44
23	B	614	CLA	MG-NB	-2.04	2.01	2.05
23	r	611	CLA	MG-NB	-2.04	2.01	2.05
39	N	601	CHL	C1B-NB	-2.04	1.35	1.37
40	g	616	LUT	C35-C15	2.04	1.41	1.36
39	Y	308	CHL	C1B-C2B	2.04	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	n	606	CHL	C3D-C4D	-2.04	1.39	1.44
40	Y	315	LUT	C11-C12	2.04	1.39	1.34
39	s	606	CHL	C1B-NB	-2.04	1.35	1.37
23	C	513	CLA	CMD-C2D	-2.03	1.46	1.50
23	b	611	CLA	MG-NB	-2.03	2.01	2.05
39	R	605	CHL	C3D-C4D	-2.03	1.39	1.44
23	a	407	CLA	MG-NB	-2.03	2.01	2.05
23	b	610	CLA	CMD-C2D	-2.03	1.46	1.50
23	b	614	CLA	CMD-C2D	-2.03	1.46	1.50
23	a	404	CLA	MG-NB	-2.03	2.01	2.05
23	C	506	CLA	CMD-C2D	-2.03	1.46	1.50
39	N	609	CHL	C3D-C4D	-2.03	1.39	1.44
23	r	608	CLA	CMD-C2D	-2.03	1.46	1.50
23	r	603	CLA	MG-NB	-2.03	2.01	2.05
23	g	602	CLA	MG-NB	-2.03	2.01	2.05
39	r	607	CHL	C1B-C2B	2.03	1.48	1.43
23	A	403	CLA	CMD-C2D	-2.03	1.46	1.50
23	Y	314	CLA	CMB-C2B	-2.03	1.46	1.50
39	y	303	CHL	C1B-NB	-2.03	1.35	1.37
40	Y	315	LUT	C11-C10	2.03	1.49	1.43
23	y	311	CLA	CMB-C2B	-2.03	1.46	1.50
23	C	504	CLA	CMD-C2D	-2.03	1.46	1.50
39	N	607	CHL	C3D-C4D	-2.03	1.39	1.44
39	N	601	CHL	C3D-C4D	-2.03	1.39	1.44
39	N	605	CHL	C3D-C4D	-2.03	1.39	1.44
41	N	617	NEX	C11-C12	2.03	1.39	1.34
23	c	506	CLA	CMD-C2D	-2.03	1.46	1.50
23	n	610	CLA	CMD-C2D	-2.03	1.46	1.50
40	s	614	LUT	C24-C25	2.03	1.35	1.33
23	D	406	CLA	MG-NB	-2.03	2.01	2.05
23	b	603	CLA	CMB-C2B	-2.03	1.46	1.50
23	R	608	CLA	MG-NB	-2.03	2.01	2.05
39	y	310	CHL	C1B-C2B	2.03	1.48	1.43
23	N	604	CLA	CMD-C2D	-2.03	1.46	1.50
23	b	616	CLA	MG-NB	-2.03	2.01	2.05
23	r	602	CLA	MG-NB	-2.03	2.01	2.05
26	M	101	SQD	C8-C7	2.03	1.56	1.50
39	Y	307	CHL	C3D-C4D	-2.03	1.39	1.44
39	g	619	CHL	C3D-C4D	-2.03	1.39	1.44
23	B	609	CLA	MG-NB	-2.02	2.01	2.05
23	c	507	CLA	MG-NB	-2.02	2.01	2.05
23	Y	304	CLA	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	MG-NB	-2.02	2.01	2.05
23	N	611	CLA	MG-NB	-2.02	2.01	2.05
23	n	602	CLA	CMD-C2D	-2.02	1.46	1.50
39	r	605	CHL	C1B-NB	-2.02	1.35	1.37
23	B	604	CLA	CMB-C2B	-2.02	1.46	1.50
23	B	605	CLA	CMC-C2C	-2.02	1.46	1.50
23	G	602	CLA	CMD-C2D	-2.02	1.46	1.50
23	A	403	CLA	MG-NB	-2.02	2.01	2.05
39	r	605	CHL	C1B-C2B	2.02	1.48	1.43
23	B	608	CLA	CMB-C2B	-2.02	1.46	1.50
23	N	610	CLA	CMD-C2D	-2.02	1.46	1.50
39	g	609	CHL	C1B-NB	-2.02	1.35	1.37
23	C	511	CLA	MG-NB	-2.02	2.01	2.05
23	S	603	CLA	MG-NB	-2.02	2.01	2.05
40	N	616	LUT	C22-C21	2.02	1.57	1.54
23	G	603	CLA	CMD-C2D	-2.02	1.46	1.50
23	b	605	CLA	CMD-C2D	-2.02	1.46	1.50
23	n	612	CLA	CMD-C2D	-2.02	1.46	1.50
23	s	612	CLA	CMD-C2D	-2.02	1.46	1.50
39	Y	306	CHL	C3D-C4D	-2.02	1.39	1.44
39	n	605	CHL	C3D-C4D	-2.02	1.39	1.44
23	G	613	CLA	CMD-C2D	-2.02	1.46	1.50
23	R	611	CLA	CMD-C2D	-2.02	1.46	1.50
40	s	614	LUT	C35-C34	2.02	1.49	1.43
30	L	103	LHG	C4-C5	2.02	1.56	1.50
23	G	612	CLA	CMD-C2D	-2.02	1.46	1.50
23	c	504	CLA	CMD-C2D	-2.02	1.46	1.50
23	G	603	CLA	MG-NB	-2.02	2.01	2.05
39	S	607	CHL	C1B-NB	-2.02	1.35	1.37
23	b	615	CLA	CMD-C2D	-2.02	1.46	1.50
23	b	607	CLA	MG-NB	-2.02	2.01	2.05
23	g	614	CLA	MG-NB	-2.02	2.01	2.05
23	y	304	CLA	MG-NB	-2.02	2.01	2.05
23	n	614	CLA	CMD-C2D	-2.02	1.46	1.50
26	L	101	SQD	C8-C7	2.02	1.56	1.50
24	d	402	PHO	C4D-ND	-2.02	1.35	1.38
23	S	609	CLA	MG-NB	-2.02	2.01	2.05
23	C	505	CLA	MG-NB	-2.02	2.01	2.05
23	n	603	CLA	MG-NB	-2.02	2.01	2.05
23	A	404	CLA	CMD-C2D	-2.02	1.46	1.50
23	B	608	CLA	CMD-C2D	-2.02	1.46	1.50
39	y	307	CHL	C3D-C4D	-2.02	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	G	611	CLA	MG-NB	-2.02	2.01	2.05
23	n	602	CLA	MG-NB	-2.02	2.01	2.05
23	Y	314	CLA	CMD-C2D	-2.02	1.46	1.50
23	c	508	CLA	CMD-C2D	-2.02	1.46	1.50
23	s	602	CLA	CMD-C2D	-2.02	1.46	1.50
40	G	616	LUT	C17-C1	2.02	1.57	1.53
23	b	601	CLA	CMD-C2D	-2.02	1.46	1.50
38	f	501	HEM	CMB-C2B	2.02	1.55	1.50
23	B	608	CLA	MG-NB	-2.02	2.01	2.05
39	S	606	CHL	C3D-C4D	-2.02	1.39	1.44
39	g	606	CHL	C3D-C4D	-2.02	1.39	1.44
39	g	607	CHL	C1B-C2B	2.02	1.48	1.43
23	G	611	CLA	CMB-C2B	-2.02	1.46	1.50
23	S	612	CLA	CMD-C2D	-2.02	1.46	1.50
23	B	611	CLA	MG-NB	-2.02	2.01	2.05
39	R	606	CHL	C3D-C4D	-2.02	1.39	1.44
23	C	512	CLA	MG-NB	-2.02	2.01	2.05
23	C	506	CLA	MG-NB	-2.02	2.01	2.05
23	R	603	CLA	MG-NB	-2.02	2.01	2.05
23	b	614	CLA	MG-NB	-2.02	2.01	2.05
23	c	502	CLA	MG-NB	-2.02	2.01	2.05
23	G	602	CLA	MG-NB	-2.01	2.01	2.05
23	c	505	CLA	MG-NB	-2.01	2.01	2.05
23	R	601	CLA	CMD-C2D	-2.01	1.46	1.50
23	Y	310	CLA	MG-NB	-2.01	2.01	2.05
23	Y	314	CLA	MG-NB	-2.01	2.01	2.05
23	c	513	CLA	MG-NB	-2.01	2.01	2.05
23	C	502	CLA	CMB-C2B	-2.01	1.46	1.50
39	S	606	CHL	C1B-C2B	2.01	1.48	1.43
23	b	613	CLA	CMD-C2D	-2.01	1.46	1.50
23	c	501	CLA	CMB-C2B	-2.01	1.46	1.50
23	B	610	CLA	CMB-C2B	-2.01	1.46	1.50
39	n	606	CHL	C1B-C2B	2.01	1.48	1.43
23	a	404	CLA	CMD-C2D	-2.01	1.46	1.50
23	r	612	CLA	CMD-C2D	-2.01	1.46	1.50
23	R	612	CLA	MG-NB	-2.01	2.01	2.05
23	n	613	CLA	MG-NB	-2.01	2.01	2.05
40	y	317	LUT	C2-C3	2.01	1.55	1.52
23	s	603	CLA	CMD-C2D	-2.01	1.46	1.50
23	B	602	CLA	MG-NB	-2.01	2.01	2.05
23	S	611	CLA	MG-NB	-2.01	2.01	2.05
23	y	314	CLA	CMD-C2D	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	503	CLA	MG-NB	-2.01	2.01	2.05
39	s	606	CHL	C3D-C4D	-2.01	1.39	1.44
23	C	508	CLA	MG-NB	-2.01	2.01	2.05
23	S	602	CLA	CMD-C2D	-2.01	1.46	1.50
23	B	604	CLA	CHC-C1C	2.01	1.42	1.38
23	b	604	CLA	CHC-C1C	2.01	1.42	1.38
23	B	606	CLA	CMB-C2B	-2.01	1.46	1.50
23	B	614	CLA	CMD-C2D	-2.01	1.46	1.50
23	d	405	CLA	MG-NB	-2.01	2.01	2.05
41	n	618	NEX	C31-C32	2.01	1.39	1.34
23	N	603	CLA	CMD-C2D	-2.01	1.46	1.50
23	R	609	CLA	MG-NB	-2.01	2.01	2.05
23	y	315	CLA	CMB-C2B	-2.01	1.46	1.50
42	N	619	XAT	C2-C1	2.01	1.57	1.54
23	c	511	CLA	MG-NB	-2.01	2.01	2.05
23	s	609	CLA	MG-NB	-2.01	2.01	2.05
23	s	610	CLA	MG-NB	-2.01	2.01	2.05
23	C	502	CLA	MG-NB	-2.01	2.01	2.05
23	c	512	CLA	MG-NB	-2.01	2.01	2.05
23	s	603	CLA	MG-NB	-2.01	2.01	2.05
23	S	609	CLA	CMB-C2B	-2.01	1.46	1.50
23	d	406	CLA	MG-NB	-2.01	2.01	2.05
23	N	612	CLA	CMD-C2D	-2.01	1.46	1.50
23	N	612	CLA	MG-NB	-2.00	2.01	2.05
23	s	613	CLA	MG-NB	-2.00	2.01	2.05
23	B	603	CLA	CMB-C2B	-2.00	1.46	1.50
23	s	604	CLA	CMD-C2D	-2.00	1.46	1.50
30	D	404	LHG	C4-C5	2.00	1.56	1.50
39	n	605	CHL	C1B-C2B	2.00	1.48	1.43
23	b	611	CLA	CMC-C2C	-2.00	1.46	1.50
23	c	509	CLA	MG-NB	-2.00	2.01	2.05
23	y	311	CLA	MG-NB	-2.00	2.01	2.05
39	N	608	CHL	C1B-NB	-2.00	1.35	1.37
23	C	509	CLA	CMD-C2D	-2.00	1.46	1.50
23	a	404	CLA	CMB-C2B	-2.00	1.46	1.50
23	c	511	CLA	CMD-C2D	-2.00	1.46	1.50
23	r	608	CLA	MG-NB	-2.00	2.01	2.05
39	g	607	CHL	C3D-C4D	-2.00	1.39	1.44
23	c	507	CLA	CMD-C2D	-2.00	1.46	1.50
23	r	609	CLA	CMD-C2D	-2.00	1.46	1.50
23	Y	303	CLA	MG-NB	-2.00	2.01	2.05

All (2613) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	N	617	NEX	O24-C25-C24	23.84	131.29	113.38
41	n	618	NEX	O24-C25-C24	23.64	131.14	113.38
41	g	617	NEX	O24-C25-C24	23.37	130.94	113.38
41	R	618	NEX	O24-C25-C24	23.16	130.78	113.38
41	r	614	NEX	O24-C25-C24	23.13	130.76	113.38
41	R	614	NEX	O24-C25-C24	22.81	130.52	113.38
41	Y	317	NEX	O24-C25-C24	22.81	130.51	113.38
41	G	617	NEX	O24-C25-C24	22.71	130.44	113.38
42	n	620	XAT	C19-C9-C10	-13.64	103.81	122.92
42	N	619	XAT	C19-C9-C10	-13.42	104.12	122.92
42	n	617	XAT	C19-C9-C10	-12.09	105.99	122.92
42	r	615	XAT	C39-C29-C30	-12.08	106.00	122.92
42	R	615	XAT	C39-C29-C30	-12.07	106.02	122.92
42	G	619	XAT	C19-C9-C10	-11.96	106.16	122.92
42	y	302	XAT	C27-C28-C29	11.96	144.09	125.53
42	r	615	XAT	C19-C9-C10	-11.95	106.19	122.92
42	Y	301	XAT	C27-C28-C29	11.84	143.91	125.53
42	R	615	XAT	C19-C9-C10	-11.84	106.34	122.92
42	y	302	XAT	C20-C13-C14	-11.46	106.87	122.92
42	n	617	XAT	C27-C28-C29	11.42	143.25	125.53
39	N	605	CHL	C4A-NA-C1A	11.38	111.82	106.71
42	Y	301	XAT	C19-C9-C10	-11.25	107.17	122.92
39	Y	306	CHL	C4A-NA-C1A	11.19	111.74	106.71
42	y	302	XAT	C19-C9-C10	-11.19	107.25	122.92
42	Y	301	XAT	C20-C13-C14	-11.09	107.39	122.92
42	N	619	XAT	C20-C13-C14	-11.06	107.44	122.92
42	n	620	XAT	C20-C13-C14	-11.05	107.45	122.92
42	G	619	XAT	C27-C28-C29	10.99	142.58	125.53
42	N	619	XAT	C27-C28-C29	10.93	142.49	125.53
39	y	307	CHL	C4A-NA-C1A	10.93	111.62	106.71
42	n	620	XAT	C27-C28-C29	10.90	142.44	125.53
39	g	605	CHL	C4A-NA-C1A	10.79	111.56	106.71
39	G	605	CHL	C4A-NA-C1A	10.66	111.50	106.71
42	r	615	XAT	C20-C13-C14	-10.64	108.01	122.92
42	G	619	XAT	C39-C29-C30	-10.58	108.10	122.92
42	n	617	XAT	C20-C13-C14	-10.49	108.23	122.92
42	R	615	XAT	C20-C13-C14	-10.44	108.29	122.92
42	N	619	XAT	C39-C29-C30	-10.41	108.34	122.92
39	G	609	CHL	C4A-NA-C1A	10.33	111.35	106.71
42	r	615	XAT	C7-C8-C9	10.28	141.48	125.53
39	g	607	CHL	C4A-NA-C1A	10.24	111.31	106.71
39	n	605	CHL	C4A-NA-C1A	10.22	111.30	106.71
42	R	615	XAT	C7-C8-C9	10.18	141.33	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	G	607	CHL	C4A-NA-C1A	10.13	111.26	106.71
39	n	607	CHL	C4A-NA-C1A	10.05	111.22	106.71
39	G	620	CHL	C4A-NA-C1A	10.02	111.21	106.71
39	N	607	CHL	C4A-NA-C1A	9.96	111.19	106.71
39	N	601	CHL	C4A-NA-C1A	9.96	111.18	106.71
39	g	619	CHL	C4A-NA-C1A	9.93	111.17	106.71
39	g	609	CHL	C4A-NA-C1A	9.86	111.14	106.71
40	Y	315	LUT	C40-C33-C34	-9.85	109.13	122.92
42	G	619	XAT	C20-C13-C14	-9.84	109.13	122.92
39	S	605	CHL	C4A-NA-C1A	9.84	111.13	106.71
40	n	615	LUT	C40-C33-C34	-9.83	109.16	122.92
39	y	303	CHL	C4A-NA-C1A	9.82	111.12	106.71
39	R	607	CHL	C4A-NA-C1A	9.82	111.12	106.71
39	n	601	CHL	C4A-NA-C1A	9.79	111.11	106.71
40	y	316	LUT	C40-C33-C34	-9.79	109.22	122.92
39	g	606	CHL	C4A-NA-C1A	9.78	111.10	106.71
39	r	607	CHL	C4A-NA-C1A	9.72	111.07	106.71
39	G	601	CHL	C4A-NA-C1A	9.70	111.06	106.71
39	S	606	CHL	C4A-NA-C1A	9.67	111.06	106.71
42	n	620	XAT	C39-C29-C30	-9.67	109.38	122.92
42	n	617	XAT	C39-C29-C30	-9.65	109.40	122.92
39	G	606	CHL	C4A-NA-C1A	9.64	111.04	106.71
39	Y	302	CHL	C4A-NA-C1A	9.59	111.02	106.71
39	r	606	CHL	C4A-NA-C1A	9.59	111.02	106.71
39	R	606	CHL	C4A-NA-C1A	9.59	111.02	106.71
39	N	608	CHL	C4A-NA-C1A	9.58	111.01	106.71
39	Y	307	CHL	C4A-NA-C1A	9.56	111.01	106.71
39	n	608	CHL	C4A-NA-C1A	9.54	111.00	106.71
39	y	308	CHL	C4A-NA-C1A	9.54	111.00	106.71
39	Y	308	CHL	C4A-NA-C1A	9.52	110.98	106.71
39	s	605	CHL	C4A-NA-C1A	9.50	110.98	106.71
39	r	605	CHL	C4A-NA-C1A	9.50	110.97	106.71
42	Y	301	XAT	C39-C29-C30	-9.49	109.63	122.92
40	s	614	LUT	C40-C33-C34	-9.48	109.65	122.92
39	g	601	CHL	C4A-NA-C1A	9.47	110.96	106.71
39	N	609	CHL	C4A-NA-C1A	9.33	110.90	106.71
39	R	605	CHL	C4A-NA-C1A	9.31	110.89	106.71
39	y	309	CHL	C4A-NA-C1A	9.29	110.88	106.71
42	n	620	XAT	C28-C29-C30	9.29	133.19	118.94
39	n	609	CHL	C4A-NA-C1A	9.26	110.87	106.71
39	S	601	CHL	C4A-NA-C1A	9.23	110.86	106.71
40	Y	316	LUT	C40-C33-C34	-9.23	110.00	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	y	302	XAT	C39-C29-C30	-9.21	110.03	122.92
39	s	601	CHL	C4A-NA-C1A	9.19	110.84	106.71
40	y	317	LUT	C40-C33-C34	-9.19	110.05	122.92
39	s	606	CHL	C4A-NA-C1A	9.14	110.81	106.71
39	N	606	CHL	C4A-NA-C1A	9.09	110.79	106.71
40	S	615	LUT	C40-C33-C34	-9.08	110.20	122.92
39	Y	309	CHL	C4A-NA-C1A	9.08	110.79	106.71
40	S	614	LUT	C40-C33-C34	-9.06	110.23	122.92
40	n	616	LUT	C40-C33-C34	-9.05	110.25	122.92
39	S	607	CHL	C4A-NA-C1A	9.02	110.76	106.71
39	G	608	CHL	C4A-NA-C1A	9.01	110.76	106.71
40	N	615	LUT	C40-C33-C34	-9.01	110.30	122.92
40	g	616	LUT	C40-C33-C34	-9.00	110.32	122.92
40	G	616	LUT	C40-C33-C34	-8.99	110.33	122.92
40	r	613	LUT	C40-C33-C34	-8.98	110.34	122.92
40	s	615	LUT	C40-C33-C34	-8.97	110.36	122.92
39	y	310	CHL	C4A-NA-C1A	8.95	110.73	106.71
39	n	606	CHL	C4A-NA-C1A	8.94	110.72	106.71
39	s	607	CHL	C4A-NA-C1A	8.93	110.72	106.71
41	s	617	NEX	C12-C13-C14	8.92	132.63	118.94
40	g	615	LUT	C20-C13-C14	-8.86	110.52	122.92
42	R	615	XAT	C40-C33-C34	-8.75	110.67	122.92
40	n	615	LUT	C20-C13-C14	-8.72	110.71	122.92
42	r	615	XAT	C40-C33-C34	-8.69	110.75	122.92
39	g	608	CHL	C4A-NA-C1A	8.68	110.61	106.71
40	N	616	LUT	C40-C33-C34	-8.58	110.91	122.92
41	G	617	NEX	C28-C29-C30	8.43	131.88	118.94
42	y	302	XAT	C40-C33-C34	-8.42	111.13	122.92
41	N	617	NEX	C12-C13-C14	8.42	131.85	118.94
41	Y	317	NEX	C12-C13-C14	8.41	131.84	118.94
42	R	615	XAT	C27-C28-C29	8.40	138.56	125.53
41	r	614	NEX	C12-C13-C14	8.39	131.81	118.94
42	n	617	XAT	C40-C33-C34	-8.37	111.19	122.92
40	R	613	LUT	C40-C33-C34	-8.35	111.22	122.92
42	n	617	XAT	C28-C29-C30	8.34	131.74	118.94
42	N	619	XAT	C28-C29-C30	8.34	131.74	118.94
41	R	618	NEX	C12-C13-C14	8.34	131.73	118.94
41	g	617	NEX	C12-C13-C14	8.28	131.64	118.94
41	R	614	NEX	C12-C13-C14	8.26	131.61	118.94
42	G	619	XAT	C40-C33-C34	-8.25	111.37	122.92
41	Y	317	NEX	C40-C33-C34	-8.23	111.39	122.92
42	r	615	XAT	C27-C28-C29	8.21	138.27	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	N	617	NEX	C40-C33-C34	-8.19	111.46	122.92
41	R	618	NEX	C40-C33-C34	-8.17	111.48	122.92
42	N	619	XAT	C40-C33-C34	-8.16	111.49	122.92
41	n	618	NEX	C40-C33-C34	-8.15	111.50	122.92
41	g	617	NEX	C40-C33-C34	-8.14	111.53	122.92
41	S	617	NEX	C12-C13-C14	8.09	131.36	118.94
40	g	615	LUT	C40-C33-C34	-8.07	111.62	122.92
42	Y	301	XAT	C40-C33-C34	-8.05	111.64	122.92
41	R	614	NEX	C40-C33-C34	-8.04	111.66	122.92
41	n	618	NEX	C12-C13-C14	8.00	131.21	118.94
42	n	620	XAT	C40-C33-C34	-7.94	111.80	122.92
41	R	614	NEX	C20-C13-C14	-7.94	111.81	122.92
42	y	302	XAT	C28-C29-C30	7.93	131.10	118.94
41	r	614	NEX	C40-C33-C34	-7.90	111.85	122.92
40	R	613	LUT	C20-C13-C14	-7.89	111.87	122.92
40	G	615	LUT	C40-C33-C34	-7.80	111.99	122.92
42	Y	301	XAT	C28-C29-C30	7.80	130.91	118.94
40	N	616	LUT	C20-C13-C14	-7.79	112.01	122.92
41	Y	317	NEX	C20-C13-C14	-7.78	112.02	122.92
40	G	616	LUT	C20-C13-C14	-7.78	112.02	122.92
40	g	616	LUT	C20-C13-C14	-7.68	112.16	122.92
41	g	617	NEX	C28-C29-C30	7.63	130.65	118.94
41	G	617	NEX	C40-C33-C34	-7.63	112.24	122.92
40	n	616	LUT	C20-C13-C14	-7.59	112.30	122.92
40	Y	316	LUT	C20-C13-C14	-7.57	112.32	122.92
41	N	617	NEX	C17-C1-C6	-7.56	103.71	110.47
40	r	613	LUT	C20-C13-C14	-7.54	112.36	122.92
41	n	618	NEX	C17-C1-C6	-7.54	103.73	110.47
40	s	615	LUT	C20-C13-C14	-7.53	112.37	122.92
40	S	614	LUT	C20-C13-C14	-7.53	112.37	122.92
41	g	617	NEX	C20-C13-C14	-7.53	112.37	122.92
40	N	615	LUT	C19-C9-C8	-7.52	106.22	118.08
42	r	615	XAT	C32-C33-C34	7.51	130.46	118.94
41	Y	317	NEX	C17-C1-C6	-7.51	103.75	110.47
41	g	617	NEX	C17-C1-C6	-7.50	103.76	110.47
41	Y	317	NEX	C19-C9-C10	-7.49	112.43	122.92
42	y	302	XAT	C32-C33-C34	7.49	130.43	118.94
40	S	615	LUT	C20-C13-C14	-7.48	112.44	122.92
40	y	317	LUT	C20-C13-C14	-7.48	112.44	122.92
42	R	615	XAT	C32-C33-C34	7.46	130.40	118.94
40	N	615	LUT	C20-C13-C14	-7.45	112.49	122.92
42	G	619	XAT	C28-C29-C30	7.43	130.35	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	n	618	NEX	C20-C13-C14	-7.43	112.51	122.92
41	R	614	NEX	C17-C1-C6	-7.43	103.82	110.47
41	n	618	NEX	C19-C9-C10	-7.43	112.52	122.92
41	r	614	NEX	C20-C13-C14	-7.42	112.53	122.92
40	Y	315	LUT	C19-C9-C8	-7.42	106.39	118.08
41	r	614	NEX	C19-C9-C10	-7.41	112.54	122.92
41	S	617	NEX	C17-C1-C6	-7.41	103.84	110.47
41	s	617	NEX	C17-C1-C6	-7.40	103.85	110.47
42	Y	301	XAT	C32-C33-C34	7.40	130.29	118.94
41	Y	317	NEX	C2-C1-C6	7.37	116.38	109.21
41	r	614	NEX	C17-C1-C6	-7.37	103.88	110.47
41	N	617	NEX	C20-C13-C14	-7.33	112.65	122.92
40	y	316	LUT	C19-C9-C8	-7.31	106.56	118.08
42	G	619	XAT	O4-C5-C4	7.31	118.87	113.38
41	S	617	NEX	C35-C15-C14	7.30	132.90	123.25
41	R	618	NEX	C20-C13-C14	-7.26	112.76	122.92
23	b	604	CLA	C4A-NA-C1A	7.23	109.96	106.71
41	s	617	NEX	C20-C13-C14	-7.23	112.80	122.92
40	g	615	LUT	C7-C8-C9	7.21	137.13	126.23
23	B	604	CLA	C4A-NA-C1A	7.20	109.94	106.71
41	R	618	NEX	C17-C1-C6	-7.18	104.04	110.47
41	r	614	NEX	C39-C29-C28	-7.18	106.77	118.08
41	R	614	NEX	C39-C29-C28	-7.17	106.78	118.08
41	s	617	NEX	C19-C9-C10	-7.15	112.91	122.92
40	s	614	LUT	C20-C13-C14	-7.12	112.95	122.92
42	y	302	XAT	O4-C5-C4	7.12	118.73	113.38
42	y	302	XAT	C8-C9-C10	7.11	129.85	118.94
41	g	617	NEX	C19-C9-C10	-7.11	112.97	122.92
23	B	612	CLA	C4A-NA-C1A	7.10	109.90	106.71
23	a	403	CLA	C4A-NA-C1A	7.07	109.88	106.71
40	G	615	LUT	C7-C8-C9	7.06	136.91	126.23
23	A	402	CLA	C4A-NA-C1A	7.04	109.87	106.71
40	y	317	LUT	C19-C9-C8	-7.02	107.01	118.08
23	C	504	CLA	C4A-NA-C1A	7.02	109.86	106.71
42	G	619	XAT	C32-C33-C34	7.02	129.71	118.94
40	Y	316	LUT	C19-C9-C8	-7.02	107.02	118.08
41	n	618	NEX	C28-C29-C30	7.01	129.70	118.94
40	S	614	LUT	C19-C9-C8	-7.00	107.05	118.08
42	n	617	XAT	C32-C33-C34	6.97	129.64	118.94
23	d	406	CLA	C4A-NA-C1A	6.95	109.83	106.71
23	b	607	CLA	C4A-NA-C1A	6.94	109.83	106.71
23	c	507	CLA	C4A-NA-C1A	6.94	109.83	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	612	CLA	C4A-NA-C1A	6.93	109.82	106.71
23	R	608	CLA	C4A-NA-C1A	6.93	109.82	106.71
42	n	617	XAT	O4-C5-C4	6.92	118.58	113.38
23	c	504	CLA	C4A-NA-C1A	6.91	109.81	106.71
41	S	617	NEX	C19-C9-C10	-6.91	113.25	122.92
23	C	507	CLA	C4A-NA-C1A	6.90	109.81	106.71
23	c	503	CLA	C4A-NA-C1A	6.89	109.80	106.71
23	d	405	CLA	C4A-NA-C1A	6.88	109.80	106.71
41	R	614	NEX	C28-C29-C30	6.88	129.50	118.94
42	Y	301	XAT	O4-C5-C4	6.87	118.54	113.38
42	G	619	XAT	C7-C8-C9	6.87	136.19	125.53
23	b	615	CLA	C4A-NA-C1A	6.87	109.79	106.71
24	d	402	PHO	C4D-CHA-CBD	-6.86	105.42	108.52
23	C	502	CLA	C4A-NA-C1A	6.85	109.78	106.71
23	r	608	CLA	C4A-NA-C1A	6.85	109.78	106.71
40	R	613	LUT	C19-C9-C8	-6.84	107.29	118.08
23	c	511	CLA	C4A-NA-C1A	6.84	109.78	106.71
41	N	617	NEX	C39-C29-C28	-6.84	107.30	118.08
40	G	615	LUT	C20-C13-C14	-6.84	113.34	122.92
23	g	612	CLA	C4A-NA-C1A	6.84	109.78	106.71
41	n	618	NEX	C39-C29-C28	-6.83	107.31	118.08
23	B	607	CLA	C4A-NA-C1A	6.83	109.78	106.71
23	C	511	CLA	C4A-NA-C1A	6.82	109.77	106.71
23	C	503	CLA	C4A-NA-C1A	6.81	109.77	106.71
41	S	617	NEX	C20-C13-C14	-6.81	113.38	122.92
23	c	502	CLA	C4A-NA-C1A	6.81	109.77	106.71
40	N	615	LUT	C12-C13-C14	6.79	129.36	118.94
23	G	613	CLA	C4A-NA-C1A	6.79	109.76	106.71
23	S	612	CLA	C4A-NA-C1A	6.78	109.76	106.71
23	b	601	CLA	C4A-NA-C1A	6.78	109.76	106.71
23	g	613	CLA	C4A-NA-C1A	6.78	109.75	106.71
23	D	406	CLA	C4A-NA-C1A	6.78	109.75	106.71
41	g	617	NEX	C39-C29-C28	-6.77	107.41	118.08
23	r	611	CLA	C4A-NA-C1A	6.76	109.74	106.71
23	D	405	CLA	C4A-NA-C1A	6.74	109.73	106.71
23	b	605	CLA	C4A-NA-C1A	6.74	109.73	106.71
40	r	613	LUT	C7-C8-C9	6.73	136.40	126.23
41	R	618	NEX	C28-C29-C30	6.72	129.26	118.94
23	S	610	CLA	C4A-NA-C1A	6.72	109.73	106.71
41	Y	317	NEX	C39-C29-C28	-6.72	107.49	118.08
41	N	617	NEX	C28-C29-C30	6.72	129.25	118.94
23	s	612	CLA	C4A-NA-C1A	6.71	109.72	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	Y	301	XAT	C8-C9-C10	6.71	129.24	118.94
23	c	513	CLA	C4A-NA-C1A	6.70	109.72	106.71
42	n	617	XAT	C7-C8-C9	6.70	135.93	125.53
23	B	605	CLA	C4A-NA-C1A	6.70	109.72	106.71
23	y	314	CLA	C4A-NA-C1A	6.70	109.72	106.71
23	B	613	CLA	C4A-NA-C1A	6.70	109.72	106.71
41	R	618	NEX	C39-C29-C28	-6.68	107.55	118.08
23	r	602	CLA	C4A-NA-C1A	6.68	109.71	106.71
23	a	404	CLA	C4A-NA-C1A	6.68	109.71	106.71
23	N	603	CLA	C4A-NA-C1A	6.68	109.71	106.71
23	Y	304	CLA	C4A-NA-C1A	6.68	109.71	106.71
23	G	611	CLA	C4A-NA-C1A	6.67	109.71	106.71
23	c	506	CLA	C4A-NA-C1A	6.67	109.71	106.71
23	y	305	CLA	C4A-NA-C1A	6.67	109.71	106.71
23	b	613	CLA	C4A-NA-C1A	6.67	109.70	106.71
40	r	613	LUT	C19-C9-C8	-6.67	107.57	118.08
40	R	613	LUT	C7-C8-C9	6.67	136.31	126.23
23	C	506	CLA	C4A-NA-C1A	6.66	109.70	106.71
23	R	612	CLA	C4A-NA-C1A	6.66	109.70	106.71
23	n	613	CLA	C4A-NA-C1A	6.65	109.70	106.71
23	b	614	CLA	C4A-NA-C1A	6.65	109.69	106.71
23	s	610	CLA	C4A-NA-C1A	6.65	109.69	106.71
23	C	508	CLA	C4A-NA-C1A	6.65	109.69	106.71
23	g	611	CLA	C4A-NA-C1A	6.65	109.69	106.71
23	B	611	CLA	C4A-NA-C1A	6.64	109.69	106.71
23	R	602	CLA	C4A-NA-C1A	6.64	109.69	106.71
41	G	617	NEX	C39-C29-C28	-6.63	107.63	118.08
40	S	615	LUT	C19-C9-C8	-6.63	107.64	118.08
23	c	505	CLA	C4A-NA-C1A	6.62	109.68	106.71
41	G	617	NEX	C38-C25-C26	-6.62	111.17	122.26
23	B	615	CLA	C4A-NA-C1A	6.61	109.68	106.71
23	A	403	CLA	C4A-NA-C1A	6.61	109.68	106.71
23	S	611	CLA	C4A-NA-C1A	6.61	109.68	106.71
40	N	616	LUT	C7-C8-C9	6.60	136.22	126.23
23	B	614	CLA	C4A-NA-C1A	6.60	109.67	106.71
23	A	404	CLA	C4A-NA-C1A	6.60	109.67	106.71
23	s	611	CLA	C4A-NA-C1A	6.60	109.67	106.71
23	R	603	CLA	C4A-NA-C1A	6.60	109.67	106.71
23	B	616	CLA	C4A-NA-C1A	6.59	109.67	106.71
42	G	619	XAT	C20-C13-C12	6.59	128.46	118.08
23	R	611	CLA	C4A-NA-C1A	6.59	109.67	106.71
23	n	603	CLA	C4A-NA-C1A	6.59	109.67	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	G	610	CLA	C4A-NA-C1A	6.58	109.67	106.71
23	b	609	CLA	C4A-NA-C1A	6.58	109.67	106.71
23	c	510	CLA	C4A-NA-C1A	6.58	109.66	106.71
23	s	603	CLA	C4A-NA-C1A	6.58	109.66	106.71
23	S	604	CLA	C4A-NA-C1A	6.58	109.66	106.71
23	b	616	CLA	C4A-NA-C1A	6.57	109.66	106.71
23	r	604	CLA	C4A-NA-C1A	6.57	109.66	106.71
23	C	513	CLA	C4A-NA-C1A	6.57	109.66	106.71
23	c	501	CLA	C4A-NA-C1A	6.57	109.66	106.71
23	S	603	CLA	C4A-NA-C1A	6.56	109.66	106.71
23	G	602	CLA	C4A-NA-C1A	6.56	109.66	106.71
23	c	509	CLA	C4A-NA-C1A	6.56	109.66	106.71
23	C	505	CLA	C4A-NA-C1A	6.55	109.65	106.71
23	N	611	CLA	C4A-NA-C1A	6.55	109.65	106.71
41	Y	317	NEX	C28-C29-C30	6.55	129.00	118.94
23	r	603	CLA	C4A-NA-C1A	6.55	109.65	106.71
23	G	603	CLA	C4A-NA-C1A	6.55	109.65	106.71
23	Y	313	CLA	C4A-NA-C1A	6.55	109.65	106.71
41	r	614	NEX	C28-C29-C30	6.54	128.98	118.94
23	N	612	CLA	C4A-NA-C1A	6.53	109.64	106.71
23	C	509	CLA	C4A-NA-C1A	6.53	109.64	106.71
23	b	602	CLA	C4A-NA-C1A	6.53	109.64	106.71
23	C	512	CLA	C4A-NA-C1A	6.53	109.64	106.71
23	a	407	CLA	C4A-NA-C1A	6.53	109.64	106.71
23	b	603	CLA	C4A-NA-C1A	6.53	109.64	106.71
23	Y	303	CLA	C4A-NA-C1A	6.52	109.64	106.71
40	N	616	LUT	C19-C9-C8	-6.52	107.81	118.08
23	C	501	CLA	C4A-NA-C1A	6.52	109.64	106.71
23	N	613	CLA	C4A-NA-C1A	6.52	109.64	106.71
23	n	611	CLA	C4A-NA-C1A	6.52	109.64	106.71
23	Y	305	CLA	C4A-NA-C1A	6.51	109.64	106.71
23	s	604	CLA	C4A-NA-C1A	6.51	109.64	106.71
23	Y	311	CLA	C4A-NA-C1A	6.51	109.63	106.71
23	y	315	CLA	C4A-NA-C1A	6.51	109.63	106.71
23	n	604	CLA	C4A-NA-C1A	6.51	109.63	106.71
23	G	612	CLA	C4A-NA-C1A	6.50	109.63	106.71
23	g	604	CLA	C4A-NA-C1A	6.50	109.63	106.71
23	R	604	CLA	C4A-NA-C1A	6.50	109.63	106.71
23	g	610	CLA	C4A-NA-C1A	6.49	109.62	106.71
23	g	603	CLA	C4A-NA-C1A	6.48	109.62	106.71
23	r	612	CLA	C4A-NA-C1A	6.48	109.62	106.71
23	N	604	CLA	C4A-NA-C1A	6.48	109.62	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	n	602	CLA	C4A-NA-C1A	6.48	109.62	106.71
23	B	603	CLA	C4A-NA-C1A	6.47	109.62	106.71
23	y	304	CLA	C4A-NA-C1A	6.47	109.62	106.71
23	B	601	CLA	C4A-NA-C1A	6.47	109.61	106.71
23	g	602	CLA	C4A-NA-C1A	6.47	109.61	106.71
23	S	602	CLA	C4A-NA-C1A	6.46	109.61	106.71
23	b	611	CLA	C4A-NA-C1A	6.46	109.61	106.71
40	n	616	LUT	C7-C8-C9	6.46	135.99	126.23
23	B	609	CLA	C4A-NA-C1A	6.45	109.61	106.71
40	S	615	LUT	C7-C8-C9	6.45	135.98	126.23
41	n	618	NEX	C2-C1-C6	6.45	115.48	109.21
23	c	512	CLA	C4A-NA-C1A	6.45	109.60	106.71
23	c	508	CLA	C4A-NA-C1A	6.44	109.60	106.71
40	n	615	LUT	C19-C9-C8	-6.44	107.93	118.08
23	n	614	CLA	C4A-NA-C1A	6.44	109.60	106.71
23	B	602	CLA	C4A-NA-C1A	6.43	109.60	106.71
23	y	306	CLA	C4A-NA-C1A	6.43	109.60	106.71
23	A	406	CLA	C4A-NA-C1A	6.43	109.60	106.71
23	N	602	CLA	C4A-NA-C1A	6.43	109.59	106.71
23	a	405	CLA	C4A-NA-C1A	6.42	109.59	106.71
41	g	617	NEX	C38-C25-C26	-6.41	111.52	122.26
23	N	614	CLA	C4A-NA-C1A	6.41	109.59	106.71
41	S	617	NEX	C20-C13-C12	-6.39	108.00	118.08
23	C	510	CLA	C4A-NA-C1A	6.39	109.58	106.71
23	B	606	CLA	C4A-NA-C1A	6.38	109.58	106.71
23	s	602	CLA	C4A-NA-C1A	6.37	109.57	106.71
42	N	619	XAT	O4-C5-C4	6.36	118.16	113.38
23	G	604	CLA	C4A-NA-C1A	6.36	109.56	106.71
23	b	610	CLA	C4A-NA-C1A	6.35	109.56	106.71
23	r	601	CLA	C4A-NA-C1A	6.35	109.56	106.71
40	y	316	LUT	C20-C13-C14	-6.35	114.03	122.92
24	a	406	PHO	C4D-CHA-CBD	-6.34	105.65	108.52
23	n	612	CLA	C4A-NA-C1A	6.34	109.56	106.71
23	b	606	CLA	C4A-NA-C1A	6.33	109.55	106.71
23	g	614	CLA	C4A-NA-C1A	6.33	109.55	106.71
40	Y	315	LUT	C20-C13-C14	-6.33	114.06	122.92
23	Y	314	CLA	C4A-NA-C1A	6.33	109.55	106.71
42	r	615	XAT	C28-C29-C30	6.32	128.64	118.94
40	g	616	LUT	C19-C9-C8	-6.31	108.14	118.08
23	R	610	CLA	C4A-NA-C1A	6.30	109.54	106.71
23	y	312	CLA	C4A-NA-C1A	6.30	109.54	106.71
23	R	609	CLA	C4A-NA-C1A	6.29	109.53	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	G	616	LUT	C19-C9-C8	-6.29	108.17	118.08
23	r	609	CLA	C4A-NA-C1A	6.29	109.53	106.71
23	B	610	CLA	C4A-NA-C1A	6.28	109.53	106.71
23	Y	312	CLA	C4A-NA-C1A	6.27	109.52	106.71
40	Y	316	LUT	C7-C8-C9	6.27	135.71	126.23
24	A	405	PHO	C4D-CHA-CBD	-6.26	105.68	108.52
23	b	608	CLA	C4A-NA-C1A	6.26	109.52	106.71
41	N	617	NEX	C19-C9-C10	-6.26	114.15	122.92
23	R	601	CLA	C4A-NA-C1A	6.26	109.52	106.71
23	y	311	CLA	C4A-NA-C1A	6.25	109.52	106.71
41	R	614	NEX	C11-C10-C9	6.25	136.22	127.31
41	N	617	NEX	C38-C25-C26	-6.24	111.80	122.26
23	y	313	CLA	C4A-NA-C1A	6.24	109.51	106.71
42	n	620	XAT	O4-C5-C4	6.24	118.07	113.38
41	n	618	NEX	C38-C25-C26	-6.23	111.82	122.26
23	Y	310	CLA	C4A-NA-C1A	6.23	109.50	106.71
41	S	617	NEX	C11-C10-C9	6.22	136.19	127.31
41	R	618	NEX	C38-C25-C26	-6.22	111.84	122.26
40	s	614	LUT	C7-C8-C9	6.21	135.62	126.23
40	y	317	LUT	C7-C8-C9	6.20	135.61	126.23
40	G	616	LUT	C7-C8-C9	6.20	135.60	126.23
42	G	619	XAT	C26-C27-C28	6.20	139.10	125.99
42	R	615	XAT	C28-C29-C30	6.19	128.44	118.94
42	N	619	XAT	C32-C33-C34	6.19	128.44	118.94
23	B	608	CLA	C4A-NA-C1A	6.18	109.49	106.71
23	G	614	CLA	C4A-NA-C1A	6.18	109.48	106.71
40	g	616	LUT	C7-C8-C9	6.17	135.56	126.23
23	S	613	CLA	C4A-NA-C1A	6.17	109.48	106.71
40	s	615	LUT	C19-C9-C8	-6.15	108.39	118.08
23	n	610	CLA	C4A-NA-C1A	6.14	109.47	106.71
41	Y	317	NEX	C38-C25-C26	-6.14	111.97	122.26
40	n	616	LUT	C19-C9-C8	-6.13	108.42	118.08
40	N	616	LUT	C32-C33-C34	6.13	128.34	118.94
41	R	614	NEX	C38-C25-C26	-6.12	112.00	122.26
23	N	610	CLA	C4A-NA-C1A	6.11	109.45	106.71
41	Y	317	NEX	C20-C13-C12	-6.11	108.45	118.08
41	N	617	NEX	C11-C10-C9	6.11	136.03	127.31
24	D	402	PHO	C4D-CHA-CBD	-6.09	105.76	108.52
23	S	608	CLA	C4A-NA-C1A	6.09	109.44	106.71
23	s	608	CLA	C4A-NA-C1A	6.09	109.44	106.71
42	N	619	XAT	C7-C8-C9	6.09	134.98	125.53
40	s	614	LUT	C19-C9-C8	-6.07	108.51	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	r	614	NEX	C38-C25-C26	-6.05	112.12	122.26
41	R	618	NEX	C2-C1-C6	6.05	115.09	109.21
42	r	615	XAT	C38-C25-C24	6.05	121.08	114.28
41	R	614	NEX	C19-C9-C10	-6.04	114.46	122.92
23	r	610	CLA	C4A-NA-C1A	6.03	109.42	106.71
40	g	615	LUT	C19-C9-C8	-5.99	108.65	118.08
23	s	613	CLA	C4A-NA-C1A	5.98	109.39	106.71
41	n	618	NEX	C11-C10-C9	5.97	135.83	127.31
42	R	615	XAT	C38-C25-C24	5.97	120.99	114.28
40	y	316	LUT	C7-C8-C9	5.95	135.22	126.23
42	n	620	XAT	C32-C33-C34	5.94	128.06	118.94
41	R	618	NEX	C11-C10-C9	5.91	135.74	127.31
41	R	618	NEX	C19-C9-C10	-5.87	114.70	122.92
23	S	609	CLA	C4A-NA-C1A	5.87	109.34	106.71
41	g	617	NEX	C20-C13-C12	-5.86	108.84	118.08
40	N	615	LUT	C7-C8-C9	5.86	135.08	126.23
40	s	614	LUT	C12-C13-C14	5.85	127.92	118.94
42	n	617	XAT	C20-C13-C12	5.83	127.27	118.08
40	Y	315	LUT	C7-C8-C9	5.81	135.01	126.23
40	S	614	LUT	C7-C8-C9	5.81	135.01	126.23
23	s	609	CLA	C4A-NA-C1A	5.80	109.31	106.71
42	n	620	XAT	C7-C8-C9	5.78	134.50	125.53
42	r	615	XAT	C39-C29-C28	-5.78	108.97	118.08
41	R	614	NEX	C20-C13-C12	-5.68	109.12	118.08
40	n	615	LUT	C7-C8-C9	5.68	134.82	126.23
42	R	615	XAT	O4-C5-C4	5.65	117.63	113.38
41	S	617	NEX	C2-C1-C6	5.65	114.70	109.21
40	s	615	LUT	C12-C13-C14	5.64	127.59	118.94
41	s	617	NEX	C20-C13-C12	-5.64	109.20	118.08
40	N	615	LUT	C35-C15-C14	5.63	135.01	123.47
42	R	615	XAT	C39-C29-C28	-5.61	109.25	118.08
42	G	619	XAT	C18-C5-C6	-5.59	112.89	122.26
40	Y	316	LUT	C21-C26-C27	5.58	119.75	112.70
36	D	401	BCT	O2-C-O1	5.58	134.02	119.55
42	r	615	XAT	O4-C5-C4	5.58	117.57	113.38
42	R	615	XAT	C19-C9-C8	5.57	126.85	118.08
41	r	614	NEX	C20-C13-C12	-5.57	109.30	118.08
36	d	401	BCT	O2-C-O1	5.57	133.98	119.55
42	r	615	XAT	C19-C9-C8	5.55	126.82	118.08
42	N	619	XAT	C26-C27-C28	5.54	137.70	125.99
41	n	618	NEX	C20-C13-C12	-5.53	109.36	118.08
41	s	617	NEX	C2-C1-C6	5.53	114.58	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	n	617	XAT	C18-C5-C6	-5.52	113.00	122.26
40	y	317	LUT	C21-C26-C27	5.52	119.68	112.70
40	G	615	LUT	C19-C9-C8	-5.51	109.39	118.08
40	S	614	LUT	C12-C13-C14	5.49	127.36	118.94
41	g	617	NEX	C11-C10-C9	5.48	135.13	127.31
42	r	615	XAT	C18-C5-C6	-5.48	113.08	122.26
40	g	616	LUT	C12-C13-C14	5.47	127.33	118.94
42	n	620	XAT	C38-C25-C26	-5.46	113.11	122.26
40	S	615	LUT	C21-C26-C27	5.44	119.57	112.70
42	N	619	XAT	C38-C25-C26	-5.43	113.15	122.26
42	R	615	XAT	C18-C5-C6	-5.42	113.17	122.26
42	y	302	XAT	C38-C25-C24	5.41	120.37	114.28
42	R	615	XAT	C20-C13-C12	5.40	126.58	118.08
41	N	617	NEX	C20-C13-C12	-5.39	109.58	118.08
40	s	614	LUT	C8-C9-C10	5.39	127.21	118.94
42	n	620	XAT	C26-C27-C28	5.37	137.35	125.99
40	N	615	LUT	C35-C34-C33	5.37	134.97	127.31
41	s	617	NEX	C11-C10-C9	5.36	134.96	127.31
40	G	616	LUT	C12-C13-C14	5.36	127.16	118.94
42	R	615	XAT	C38-C25-C26	-5.34	113.31	122.26
42	N	619	XAT	C38-C25-C24	5.34	120.28	114.28
41	R	618	NEX	C20-C13-C12	-5.34	109.67	118.08
42	r	615	XAT	C20-C13-C12	5.33	126.48	118.08
41	Y	317	NEX	C11-C10-C9	5.33	134.92	127.31
40	G	615	LUT	C21-C26-C27	5.29	119.39	112.70
42	r	615	XAT	C38-C25-C26	-5.29	113.39	122.26
40	S	615	LUT	C32-C33-C34	5.28	127.04	118.94
41	N	617	NEX	C2-C1-C6	5.26	114.32	109.21
42	Y	301	XAT	C7-C8-C9	5.26	133.68	125.53
42	Y	301	XAT	C20-C13-C12	5.25	126.34	118.08
40	s	614	LUT	C21-C26-C27	5.22	119.30	112.70
42	N	619	XAT	C18-C5-C6	-5.21	113.52	122.26
42	n	620	XAT	C38-C25-C24	5.21	120.14	114.28
40	g	615	LUT	C21-C26-C27	5.21	119.28	112.70
42	n	620	XAT	C18-C5-C6	-5.18	113.58	122.26
41	R	614	NEX	C2-C1-C6	5.16	114.22	109.21
41	r	614	NEX	C11-C10-C9	5.15	134.66	127.31
40	S	615	LUT	C12-C13-C14	5.15	126.84	118.94
42	Y	301	XAT	C38-C25-C24	5.14	120.06	114.28
42	N	619	XAT	C20-C13-C12	5.11	126.13	118.08
40	r	613	LUT	C35-C15-C14	5.10	133.92	123.47
42	n	617	XAT	C26-C27-C28	5.09	136.75	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	n	605	CHL	C3B-C4B-NB	-5.08	105.80	110.52
40	N	616	LUT	C15-C35-C34	5.08	133.89	123.47
41	N	617	NEX	C39-C29-C30	-5.07	115.83	122.92
42	n	620	XAT	C20-C13-C12	5.05	126.04	118.08
40	N	616	LUT	C15-C14-C13	5.03	134.48	127.31
39	N	605	CHL	C3B-C4B-NB	-5.03	105.85	110.52
40	y	317	LUT	C12-C13-C14	5.02	126.65	118.94
40	s	615	LUT	C21-C26-C27	5.02	119.05	112.70
42	Y	301	XAT	C18-C5-C6	-5.01	113.86	122.26
40	s	615	LUT	C8-C9-C10	5.00	126.62	118.94
40	S	614	LUT	C32-C33-C34	5.00	126.61	118.94
40	g	616	LUT	C21-C26-C27	4.99	119.01	112.70
40	G	616	LUT	C21-C26-C27	4.99	119.01	112.70
41	n	618	NEX	C39-C29-C30	-4.98	115.94	122.92
42	G	619	XAT	C38-C25-C24	4.98	119.88	114.28
41	R	614	NEX	C39-C29-C30	-4.98	115.95	122.92
40	S	614	LUT	C21-C26-C27	4.96	118.97	112.70
40	n	615	LUT	C8-C9-C10	4.95	126.54	118.94
39	G	609	CHL	C3B-C4B-NB	-4.94	105.93	110.52
40	N	616	LUT	C21-C26-C27	4.93	118.94	112.70
40	S	615	LUT	C15-C35-C34	4.93	133.58	123.47
41	r	614	NEX	C2-C1-C6	4.93	114.00	109.21
41	r	614	NEX	C39-C29-C30	-4.92	116.04	122.92
40	S	615	LUT	C15-C14-C13	4.91	134.32	127.31
40	N	615	LUT	C21-C26-C27	4.91	118.91	112.70
42	N	619	XAT	O24-C25-C24	4.91	117.07	113.38
40	R	613	LUT	C32-C33-C34	4.90	126.46	118.94
40	n	616	LUT	C21-C26-C27	4.88	118.87	112.70
40	r	613	LUT	C32-C33-C34	4.88	126.43	118.94
41	G	617	NEX	C32-C33-C34	4.87	126.42	118.94
40	N	615	LUT	C8-C9-C10	4.87	126.41	118.94
42	r	615	XAT	C8-C9-C10	4.87	126.41	118.94
40	s	615	LUT	C7-C8-C9	4.87	133.59	126.23
40	S	614	LUT	C15-C35-C34	4.84	133.40	123.47
40	n	616	LUT	C12-C13-C14	4.82	126.34	118.94
40	Y	316	LUT	C12-C13-C14	4.82	126.34	118.94
42	R	615	XAT	C8-C9-C10	4.81	126.32	118.94
40	R	613	LUT	C15-C14-C13	4.80	134.16	127.31
42	R	615	XAT	O24-C25-C26	-4.78	55.01	58.96
40	R	613	LUT	C21-C26-C27	4.77	118.73	112.70
42	r	615	XAT	O24-C25-C26	-4.77	55.01	58.96
42	r	615	XAT	C26-C27-C28	4.76	136.06	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	Y	317	NEX	C32-C33-C34	4.76	126.25	118.94
42	Y	301	XAT	O24-C25-C26	-4.76	55.02	58.96
41	g	617	NEX	C39-C29-C30	-4.76	116.26	122.92
40	r	613	LUT	C21-C26-C27	4.75	118.71	112.70
42	y	302	XAT	C18-C5-C6	-4.75	114.30	122.26
40	N	616	LUT	C12-C13-C14	4.75	126.23	118.94
41	g	617	NEX	C2-C1-C6	4.74	113.81	109.21
42	G	619	XAT	C38-C25-C26	-4.73	114.34	122.26
42	y	302	XAT	C20-C13-C12	4.72	125.52	118.08
42	n	617	XAT	O24-C25-C26	-4.71	55.06	58.96
40	S	614	LUT	C8-C9-C10	4.70	126.16	118.94
33	C	515	DGD	O3G-C3G-C2G	-4.69	99.59	110.90
40	s	614	LUT	C15-C35-C34	4.68	133.06	123.47
40	s	615	LUT	C8-C7-C6	4.68	140.35	127.20
41	G	617	NEX	C39-C29-C30	-4.68	116.37	122.92
42	n	617	XAT	C38-C25-C24	4.67	119.53	114.28
39	Y	306	CHL	C3B-C4B-NB	-4.67	106.19	110.52
40	g	616	LUT	C8-C9-C10	4.66	126.09	118.94
42	n	617	XAT	C38-C25-C26	-4.66	114.45	122.26
39	y	307	CHL	C3B-C4B-NB	-4.66	106.19	110.52
40	G	616	LUT	C8-C9-C10	4.65	126.08	118.94
40	G	615	LUT	C32-C33-C34	4.65	126.08	118.94
39	s	601	CHL	C3B-C4B-NB	-4.65	106.20	110.52
40	R	613	LUT	C12-C13-C14	4.65	126.07	118.94
39	g	605	CHL	C3B-C4B-NB	-4.64	106.21	110.52
40	R	613	LUT	C15-C35-C34	4.64	132.97	123.47
42	n	617	XAT	C8-C9-C10	4.63	126.05	118.94
42	n	620	XAT	O24-C25-C24	4.63	116.86	113.38
42	n	620	XAT	O24-C25-C26	-4.63	55.13	58.96
40	g	615	LUT	C32-C33-C34	4.62	126.03	118.94
42	y	302	XAT	O24-C25-C26	-4.62	55.14	58.96
40	S	614	LUT	C15-C14-C13	4.61	133.89	127.31
39	G	606	CHL	C3B-C4B-NB	-4.61	106.24	110.52
39	g	606	CHL	C3B-C4B-NB	-4.60	106.25	110.52
42	n	620	XAT	C35-C34-C33	4.60	133.88	127.31
39	S	601	CHL	C3B-C4B-NB	-4.60	106.25	110.52
41	R	618	NEX	C32-C33-C34	4.59	125.98	118.94
39	G	605	CHL	C3B-C4B-NB	-4.58	106.27	110.52
40	s	614	LUT	C15-C14-C13	4.57	133.83	127.31
40	G	615	LUT	C12-C13-C14	4.56	125.94	118.94
40	Y	316	LUT	C32-C33-C34	4.56	125.94	118.94
42	N	619	XAT	O24-C25-C26	-4.55	55.19	58.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	c	515	DGD	O3G-C3G-C2G	-4.55	99.92	110.90
40	Y	316	LUT	C15-C35-C34	4.55	132.79	123.47
40	y	317	LUT	C32-C33-C34	4.54	125.92	118.94
39	N	605	CHL	CHD-C1D-ND	-4.54	120.28	124.45
42	R	615	XAT	C26-C27-C28	4.54	135.59	125.99
40	y	317	LUT	C15-C35-C34	4.53	132.76	123.47
40	s	615	LUT	C32-C33-C34	4.53	125.89	118.94
42	y	302	XAT	C38-C25-C26	-4.53	114.67	122.26
42	G	619	XAT	O24-C25-C24	4.51	116.77	113.38
42	G	619	XAT	O24-C25-C26	-4.51	55.22	58.96
40	s	614	LUT	C35-C34-C33	4.51	133.74	127.31
42	N	619	XAT	C35-C34-C33	4.51	133.74	127.31
42	G	619	XAT	C19-C9-C8	4.50	125.17	118.08
39	n	605	CHL	CHD-C1D-ND	-4.50	120.32	124.45
40	s	614	LUT	C35-C15-C14	4.50	132.69	123.47
40	S	614	LUT	C8-C7-C6	4.49	139.81	127.20
39	g	608	CHL	C3B-C4B-NB	-4.46	106.38	110.52
42	G	619	XAT	C8-C9-C10	4.42	125.72	118.94
40	G	616	LUT	C35-C15-C14	4.41	132.50	123.47
39	n	601	CHL	C3B-C4B-NB	-4.40	106.43	110.52
40	G	615	LUT	C1-C6-C5	-4.40	116.41	122.61
39	s	601	CHL	CHD-C1D-ND	-4.39	120.42	124.45
39	n	608	CHL	C3B-C4B-NB	-4.39	106.45	110.52
40	s	615	LUT	C15-C35-C34	4.37	132.44	123.47
39	G	609	CHL	CHD-C1D-ND	-4.37	120.43	124.45
40	n	616	LUT	C8-C9-C10	4.37	125.65	118.94
39	G	608	CHL	C3B-C4B-NB	-4.37	106.46	110.52
40	r	613	LUT	C15-C35-C34	4.37	132.42	123.47
39	Y	308	CHL	C3B-C4B-NB	-4.36	106.47	110.52
39	S	601	CHL	CHD-C1D-ND	-4.36	120.45	124.45
39	G	620	CHL	C3B-C4B-NB	-4.35	106.48	110.52
39	R	606	CHL	C3B-C4B-NB	-4.35	106.48	110.52
39	Y	306	CHL	CHD-C1D-ND	-4.35	120.46	124.45
39	n	601	CHL	CHD-C1D-ND	-4.35	120.46	124.45
39	y	307	CHL	CHD-C1D-ND	-4.35	120.46	124.45
39	N	601	CHL	C3B-C4B-NB	-4.35	106.48	110.52
40	y	317	LUT	C8-C7-C6	4.34	139.40	127.20
40	Y	316	LUT	C8-C7-C6	4.34	139.39	127.20
39	N	608	CHL	C3B-C4B-NB	-4.34	106.49	110.52
40	g	616	LUT	C35-C15-C14	4.33	132.35	123.47
41	n	618	NEX	C32-C33-C34	4.33	125.59	118.94
40	g	615	LUT	C15-C35-C34	4.33	132.35	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	G	607	CHL	C3B-C4B-NB	-4.32	106.50	110.52
39	y	308	CHL	C3B-C4B-NB	-4.32	106.50	110.52
39	r	607	CHL	C3B-C4B-NB	-4.32	106.50	110.52
40	y	317	LUT	C15-C14-C13	4.32	133.48	127.31
39	s	606	CHL	C3B-C4B-NB	-4.32	106.51	110.52
39	Y	306	CHL	C2B-C1B-NB	-4.31	107.34	110.23
39	Y	309	CHL	CHD-C1D-ND	-4.31	120.49	124.45
40	g	616	LUT	C32-C33-C34	4.31	125.56	118.94
39	s	607	CHL	C3B-C4B-NB	-4.31	106.52	110.52
39	g	609	CHL	C3B-C4B-NB	-4.31	106.52	110.52
40	S	615	LUT	C8-C9-C10	4.31	125.55	118.94
41	N	617	NEX	C32-C33-C34	4.31	125.55	118.94
40	G	616	LUT	C32-C33-C34	4.31	125.55	118.94
39	g	601	CHL	CHD-C1D-ND	-4.31	120.50	124.45
39	S	607	CHL	C3B-C4B-NB	-4.30	106.52	110.52
39	y	303	CHL	C3B-C4B-NB	-4.30	106.52	110.52
40	N	615	LUT	C8-C7-C6	4.30	139.29	127.20
39	g	619	CHL	C3B-C4B-NB	-4.30	106.53	110.52
41	Y	317	NEX	C39-C29-C30	-4.30	116.90	122.92
41	g	617	NEX	C32-C33-C34	4.30	125.53	118.94
39	s	607	CHL	CHD-C1D-ND	-4.29	120.51	124.45
39	g	608	CHL	CHD-C1D-ND	-4.29	120.51	124.45
40	s	615	LUT	C35-C15-C14	4.28	132.24	123.47
39	Y	302	CHL	C3B-C4B-NB	-4.28	106.55	110.52
40	n	615	LUT	C35-C15-C14	4.27	132.23	123.47
42	Y	301	XAT	C26-C27-C28	4.27	135.03	125.99
39	y	309	CHL	C3B-C4B-NB	-4.27	106.55	110.52
40	n	615	LUT	C32-C33-C34	4.27	125.49	118.94
40	n	616	LUT	C15-C14-C13	4.26	133.39	127.31
40	Y	316	LUT	C15-C14-C13	4.26	133.39	127.31
39	G	605	CHL	CHD-C1D-ND	-4.26	120.54	124.45
39	Y	309	CHL	C3B-C4B-NB	-4.26	106.56	110.52
39	n	605	CHL	C2B-C1B-NB	-4.26	107.38	110.23
39	R	607	CHL	C3B-C4B-NB	-4.26	106.56	110.52
41	R	618	NEX	C39-C29-C30	-4.26	116.96	122.92
39	r	606	CHL	C3B-C4B-NB	-4.26	106.56	110.52
39	n	606	CHL	C3B-C4B-NB	-4.25	106.57	110.52
39	S	606	CHL	C3B-C4B-NB	-4.25	106.57	110.52
39	G	601	CHL	CHD-C1D-ND	-4.25	120.55	124.45
39	R	605	CHL	C3B-C4B-NB	-4.24	106.58	110.52
39	Y	302	CHL	CHD-C1D-ND	-4.24	120.56	124.45
42	y	302	XAT	C7-C8-C9	4.24	132.11	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	n	606	CHL	CHD-C1D-ND	-4.24	120.56	124.45
39	n	609	CHL	CHD-C1D-ND	-4.24	120.56	124.45
40	s	614	LUT	C8-C7-C6	4.24	139.10	127.20
42	Y	301	XAT	C38-C25-C26	-4.24	115.16	122.26
39	Y	307	CHL	C3B-C4B-NB	-4.24	106.59	110.52
39	S	606	CHL	CHD-C1D-ND	-4.24	120.56	124.45
39	N	606	CHL	C3B-C4B-NB	-4.23	106.59	110.52
41	R	614	NEX	C32-C33-C34	4.23	125.44	118.94
39	n	607	CHL	C3B-C4B-NB	-4.23	106.59	110.52
39	G	608	CHL	CHD-C1D-ND	-4.23	120.57	124.45
39	r	605	CHL	CHD-C1D-ND	-4.23	120.57	124.45
39	y	310	CHL	CHD-C1D-ND	-4.23	120.57	124.45
40	N	616	LUT	C8-C9-C10	4.23	125.42	118.94
39	y	303	CHL	CHD-C1D-ND	-4.23	120.57	124.45
39	N	607	CHL	C3B-C4B-NB	-4.22	106.60	110.52
39	N	609	CHL	CHD-C1D-ND	-4.22	120.58	124.45
39	r	606	CHL	CHD-C1D-ND	-4.21	120.58	124.45
40	s	615	LUT	C15-C14-C13	4.20	133.30	127.31
39	N	601	CHL	CHD-C1D-ND	-4.19	120.60	124.45
40	n	616	LUT	C15-C35-C34	4.19	132.06	123.47
39	R	605	CHL	CHD-C1D-ND	-4.19	120.60	124.45
40	s	614	LUT	C32-C33-C34	4.19	125.37	118.94
39	R	606	CHL	CHD-C1D-ND	-4.19	120.61	124.45
39	g	605	CHL	CHD-C1D-ND	-4.19	120.61	124.45
39	g	601	CHL	C3B-C4B-NB	-4.18	106.63	110.52
42	R	615	XAT	O24-C25-C24	4.18	116.52	113.38
39	Y	307	CHL	CHD-C1D-ND	-4.18	120.61	124.45
39	G	620	CHL	CHD-C1D-ND	-4.18	120.61	124.45
41	r	614	NEX	C32-C33-C34	4.18	125.36	118.94
42	Y	301	XAT	C11-C12-C13	4.18	138.15	126.42
39	S	607	CHL	CHD-C1D-ND	-4.17	120.62	124.45
39	Y	308	CHL	CHD-C1D-ND	-4.17	120.62	124.45
39	G	601	CHL	C3B-C4B-NB	-4.17	106.65	110.52
40	g	616	LUT	C15-C35-C34	4.17	132.01	123.47
39	N	608	CHL	CHD-C1D-ND	-4.16	120.63	124.45
39	g	619	CHL	CHD-C1D-ND	-4.16	120.63	124.45
39	y	308	CHL	CHD-C1D-ND	-4.16	120.63	124.45
42	R	615	XAT	C11-C12-C13	4.16	138.10	126.42
39	y	309	CHL	CHD-C1D-ND	-4.16	120.64	124.45
39	s	605	CHL	CHD-C1D-ND	-4.15	120.64	124.45
39	n	608	CHL	CHD-C1D-ND	-4.15	120.64	124.45
39	N	606	CHL	CHD-C1D-ND	-4.15	120.64	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	G	616	LUT	C15-C35-C34	4.15	131.97	123.47
39	g	607	CHL	C3B-C4B-NB	-4.14	106.67	110.52
39	G	609	CHL	C2B-C1B-NB	-4.14	107.46	110.23
40	g	616	LUT	C8-C7-C6	4.14	138.82	127.20
42	r	615	XAT	C11-C12-C13	4.14	138.04	126.42
40	S	615	LUT	C8-C7-C6	4.13	138.81	127.20
40	y	317	LUT	C8-C9-C10	4.13	125.28	118.94
39	s	606	CHL	CHD-C1D-ND	-4.13	120.66	124.45
40	s	614	LUT	C31-C30-C29	4.13	133.20	127.31
39	G	607	CHL	CHD-C1D-ND	-4.13	120.66	124.45
39	S	605	CHL	CHD-C1D-ND	-4.12	120.67	124.45
39	N	607	CHL	CHD-C1D-ND	-4.12	120.67	124.45
39	R	607	CHL	CHD-C1D-ND	-4.12	120.67	124.45
39	g	606	CHL	CHD-C1D-ND	-4.12	120.67	124.45
39	y	310	CHL	C3B-C4B-NB	-4.12	106.70	110.52
39	G	606	CHL	CHD-C1D-ND	-4.12	120.67	124.45
26	L	101	SQD	O7-S-C6	4.12	111.83	106.94
40	G	616	LUT	C8-C7-C6	4.11	138.75	127.20
39	r	607	CHL	CHD-C1D-ND	-4.11	120.68	124.45
39	N	605	CHL	C2B-C1B-NB	-4.11	107.48	110.23
39	r	605	CHL	C3B-C4B-NB	-4.11	106.71	110.52
40	n	615	LUT	C15-C35-C34	4.10	131.88	123.47
39	s	605	CHL	C3B-C4B-NB	-4.10	106.71	110.52
40	Y	315	LUT	C35-C15-C14	4.10	131.87	123.47
40	y	316	LUT	C35-C15-C14	4.10	131.87	123.47
40	S	614	LUT	C35-C15-C14	4.10	131.86	123.47
40	n	616	LUT	C35-C15-C14	4.09	131.86	123.47
39	n	607	CHL	CHD-C1D-ND	-4.09	120.70	124.45
42	r	615	XAT	O24-C25-C24	4.07	116.44	113.38
42	y	302	XAT	C11-C12-C13	4.07	137.85	126.42
26	M	101	SQD	O7-S-C6	4.06	111.77	106.94
42	y	302	XAT	C26-C27-C28	4.06	134.58	125.99
40	Y	316	LUT	C8-C9-C10	4.05	125.16	118.94
40	n	616	LUT	C32-C33-C34	4.04	125.15	118.94
39	y	307	CHL	C2B-C1B-NB	-4.04	107.52	110.23
39	g	609	CHL	CHD-C1D-ND	-4.04	120.74	124.45
39	g	607	CHL	CHD-C1D-ND	-4.03	120.75	124.45
39	n	609	CHL	C3B-C4B-NB	-4.02	106.79	110.52
26	A	408	SQD	O47-C7-C8	3.99	120.10	111.50
39	S	605	CHL	C3B-C4B-NB	-3.98	106.82	110.52
41	s	617	NEX	C35-C15-C14	3.98	131.62	123.47
40	G	615	LUT	C15-C35-C34	3.98	131.62	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	M	101	SQD	O47-C7-C8	3.98	120.07	111.50
40	N	616	LUT	C8-C7-C6	3.98	138.37	127.20
39	N	609	CHL	C3B-C4B-NB	-3.98	106.83	110.52
40	S	615	LUT	C35-C15-C14	3.97	131.62	123.47
40	R	613	LUT	C35-C15-C14	3.97	131.60	123.47
26	a	409	SQD	O47-C7-C8	3.97	120.05	111.50
41	R	614	NEX	C35-C15-C14	3.94	131.55	123.47
23	r	610	CLA	O2D-CGD-O1D	-3.94	116.14	123.84
40	R	613	LUT	C8-C7-C6	3.93	138.24	127.20
40	s	615	LUT	C35-C34-C33	3.93	132.92	127.31
23	N	613	CLA	CAA-C2A-C3A	-3.93	102.02	112.78
40	r	613	LUT	C8-C7-C6	3.93	138.23	127.20
42	r	615	XAT	C10-C11-C12	3.92	135.46	123.22
40	r	613	LUT	C12-C13-C14	3.92	124.96	118.94
26	A	408	SQD	O9-S-C6	3.91	111.58	106.94
41	N	617	NEX	C35-C15-C14	3.90	131.47	123.47
40	r	613	LUT	C8-C9-C10	3.89	124.92	118.94
40	G	616	LUT	C35-C34-C33	3.89	132.87	127.31
26	L	101	SQD	O47-C7-C8	3.89	119.88	111.50
42	n	617	XAT	C10-C11-C12	3.89	135.34	123.22
41	g	617	NEX	C35-C15-C14	3.88	131.43	123.47
40	n	616	LUT	C35-C34-C33	3.88	132.85	127.31
40	N	616	LUT	C35-C15-C14	3.87	131.41	123.47
26	a	409	SQD	O7-S-C6	3.86	111.52	106.94
40	g	616	LUT	C35-C34-C33	3.85	132.81	127.31
40	y	317	LUT	C35-C15-C14	3.85	131.36	123.47
42	R	615	XAT	C10-C11-C12	3.84	135.20	123.22
42	y	302	XAT	C15-C14-C13	3.83	132.78	127.31
40	g	615	LUT	C1-C6-C5	-3.83	117.22	122.61
41	N	617	NEX	C5-C6-C1	-3.83	115.89	119.70
40	Y	316	LUT	C35-C15-C14	3.83	131.31	123.47
42	N	619	XAT	C11-C12-C13	3.83	137.17	126.42
41	S	617	NEX	C10-C11-C12	3.82	135.15	123.22
24	D	402	PHO	C2B-C1B-NB	-3.82	106.89	109.53
41	n	618	NEX	C35-C15-C14	3.81	131.27	123.47
24	A	405	PHO	C2B-C1B-NB	-3.80	106.90	109.53
39	n	605	CHL	C2A-C1A-CHA	3.80	130.51	123.86
26	a	409	SQD	O9-S-O7	-3.79	100.82	113.95
24	d	402	PHO	C2B-C1B-NB	-3.79	106.91	109.53
42	n	620	XAT	C11-C12-C13	3.79	137.06	126.42
41	r	614	NEX	C35-C15-C14	3.79	131.23	123.47
41	r	614	NEX	C5-C6-C1	-3.78	115.94	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	R	614	NEX	C10-C11-C12	3.78	135.02	123.22
40	G	616	LUT	C15-C14-C13	3.78	132.71	127.31
40	s	614	LUT	C10-C11-C12	3.78	135.00	123.22
40	s	615	LUT	C18-C5-C6	-3.77	120.30	124.53
40	G	616	LUT	C1-C6-C5	-3.76	117.31	122.61
40	n	616	LUT	C8-C7-C6	3.76	137.76	127.20
40	g	616	LUT	C15-C14-C13	3.75	132.67	127.31
26	A	408	SQD	O9-S-O7	-3.75	100.96	113.95
40	N	615	LUT	C31-C30-C29	3.75	132.66	127.31
26	L	101	SQD	O9-S-O7	-3.75	100.98	113.95
40	Y	315	LUT	C32-C33-C34	3.75	124.69	118.94
40	S	614	LUT	C35-C34-C33	3.74	132.65	127.31
40	R	613	LUT	C8-C9-C10	3.74	124.67	118.94
42	G	619	XAT	C11-C12-C13	3.73	136.91	126.42
39	n	609	CHL	CHC-C1C-NC	3.73	129.87	124.20
39	g	605	CHL	C2B-C1B-NB	-3.73	107.73	110.23
26	M	101	SQD	O9-S-C6	3.73	111.37	106.94
41	n	618	NEX	C10-C11-C12	3.72	134.84	123.22
39	N	609	CHL	CHC-C1C-NC	3.72	129.85	124.20
39	G	605	CHL	C2B-C1B-NB	-3.71	107.74	110.23
42	Y	301	XAT	C15-C14-C13	3.71	132.60	127.31
40	Y	315	LUT	C21-C26-C27	3.70	117.37	112.70
42	G	619	XAT	C35-C34-C33	3.70	132.58	127.31
39	Y	309	CHL	CHC-C1C-NC	3.69	129.80	124.20
41	R	614	NEX	C5-C6-C1	-3.69	116.03	119.70
41	N	617	NEX	C10-C11-C12	3.69	134.72	123.22
40	y	316	LUT	C32-C33-C34	3.68	124.59	118.94
39	R	607	CHL	CHC-C1C-NC	3.68	129.79	124.20
42	G	619	XAT	C10-C11-C12	3.68	134.70	123.22
39	G	601	CHL	CHC-C1C-NC	3.68	129.79	124.20
39	y	310	CHL	CHC-C1C-NC	3.67	129.77	124.20
25	b	617	BCR	C2-C1-C6	3.67	116.13	110.48
41	Y	317	NEX	C35-C15-C14	3.67	130.98	123.47
40	R	613	LUT	C35-C34-C33	3.66	132.54	127.31
40	g	616	LUT	C1-C6-C5	-3.66	117.46	122.61
41	n	618	NEX	C5-C6-C1	-3.66	116.06	119.70
39	g	601	CHL	CHC-C1C-NC	3.65	129.75	124.20
39	G	608	CHL	CHC-C1C-NC	3.65	129.74	124.20
40	y	316	LUT	C21-C26-C27	3.65	117.31	112.70
41	R	618	NEX	C35-C15-C14	3.65	130.94	123.47
39	s	607	CHL	CHC-C1C-NC	3.65	129.74	124.20
39	g	608	CHL	CHC-C1C-NC	3.63	129.72	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	406	PHO	C2B-C1B-NB	-3.63	107.02	109.53
40	n	616	LUT	C1-C6-C5	-3.63	117.50	122.61
39	r	605	CHL	CHC-C1C-NC	3.63	129.71	124.20
40	Y	315	LUT	C1-C6-C5	-3.63	117.51	122.61
40	G	615	LUT	C15-C14-C13	3.62	132.48	127.31
39	S	605	CHL	CHC-C1C-NC	3.62	129.70	124.20
39	g	619	CHL	CHC-C1C-NC	3.62	129.69	124.20
42	n	617	XAT	C19-C9-C8	3.62	123.78	118.08
39	r	607	CHL	CHC-C1C-NC	3.62	129.69	124.20
42	n	617	XAT	C35-C34-C33	3.61	132.47	127.31
39	S	606	CHL	CHC-C1C-NC	3.61	129.68	124.20
40	r	613	LUT	C35-C34-C33	3.61	132.46	127.31
26	A	408	SQD	O7-S-C6	3.60	111.22	106.94
39	g	608	CHL	C2B-C1B-NB	-3.60	107.82	110.23
39	R	605	CHL	CHC-C1C-NC	3.59	129.65	124.20
40	n	615	LUT	C21-C26-C27	3.59	117.23	112.70
26	M	101	SQD	O9-S-O7	-3.59	101.54	113.95
39	N	601	CHL	CHC-C1C-NC	3.58	129.64	124.20
39	G	607	CHL	CHC-C1C-NC	3.58	129.64	124.20
41	R	618	NEX	C10-C11-C12	3.58	134.39	123.22
39	s	605	CHL	CHC-C1C-NC	3.58	129.63	124.20
39	S	607	CHL	CHC-C1C-NC	3.58	129.63	124.20
39	g	606	CHL	CHC-C1C-NC	3.57	129.62	124.20
39	G	609	CHL	CHC-C1C-NC	3.57	129.62	124.20
39	n	607	CHL	CHC-C1C-NC	3.57	129.62	124.20
40	N	615	LUT	C32-C33-C34	3.57	124.42	118.94
39	g	607	CHL	CHC-C1C-NC	3.56	129.61	124.20
39	N	601	CHL	C2B-C1B-NB	-3.56	107.84	110.23
39	S	601	CHL	CHC-C1C-NC	3.56	129.61	124.20
39	n	608	CHL	CHC-C1C-NC	3.56	129.60	124.20
39	G	601	CHL	C2B-C1B-NB	-3.55	107.85	110.23
40	y	316	LUT	C1-C6-C5	-3.55	117.61	122.61
42	R	615	XAT	C17-C1-C6	3.55	119.64	110.05
42	r	615	XAT	C17-C1-C6	3.55	119.63	110.05
39	y	309	CHL	CHC-C1C-NC	3.55	129.59	124.20
39	g	605	CHL	CHC-C1C-NC	3.54	129.58	124.20
39	s	601	CHL	CHC-C1C-NC	3.54	129.58	124.20
39	Y	302	CHL	CHC-C1C-NC	3.54	129.58	124.20
39	y	303	CHL	CHC-C1C-NC	3.54	129.58	124.20
39	n	606	CHL	CHC-C1C-NC	3.54	129.57	124.20
39	Y	308	CHL	CHC-C1C-NC	3.54	129.57	124.20
39	N	608	CHL	CHC-C1C-NC	3.54	129.57	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	s	606	CHL	CHC-C1C-NC	3.53	129.57	124.20
42	n	620	XAT	C10-C11-C12	3.53	134.25	123.22
39	Y	307	CHL	CHC-C1C-NC	3.53	129.56	124.20
39	s	601	CHL	C2B-C1B-NB	-3.53	107.87	110.23
39	n	601	CHL	CHC-C1C-NC	3.53	129.55	124.20
39	N	606	CHL	CHC-C1C-NC	3.52	129.54	124.20
39	G	605	CHL	CHC-C1C-NC	3.52	129.54	124.20
39	R	605	CHL	C2B-C1B-NB	-3.51	107.88	110.23
25	B	618	BCR	C8-C7-C6	-3.51	121.09	127.09
39	G	606	CHL	CHC-C1C-NC	3.51	129.53	124.20
30	A	412	LHG	O7-C7-C8	3.51	119.06	111.50
39	y	308	CHL	CHC-C1C-NC	3.51	129.52	124.20
42	N	619	XAT	C8-C9-C10	3.50	124.32	118.94
26	L	101	SQD	O9-S-C6	3.50	111.10	106.94
41	g	617	NEX	C10-C11-C12	3.50	134.13	123.22
39	y	307	CHL	CHC-C1C-NC	3.50	129.51	124.20
39	S	601	CHL	C2B-C1B-NB	-3.49	107.89	110.23
40	N	616	LUT	C1-C6-C5	-3.49	117.70	122.61
39	G	620	CHL	CHC-C1C-NC	3.49	129.49	124.20
39	g	601	CHL	C2B-C1B-NB	-3.48	107.90	110.23
42	n	617	XAT	C11-C12-C13	3.48	136.19	126.42
42	Y	301	XAT	C19-C9-C8	3.47	123.55	118.08
39	N	605	CHL	CHC-C1C-NC	3.47	129.47	124.20
39	y	308	CHL	C2B-C1B-NB	-3.47	107.91	110.23
40	G	615	LUT	C8-C9-C10	3.47	124.26	118.94
39	n	601	CHL	C2B-C1B-NB	-3.47	107.91	110.23
40	S	615	LUT	C1-C6-C5	-3.46	117.74	122.61
40	y	316	LUT	C8-C9-C10	3.46	124.25	118.94
42	y	302	XAT	C37-C21-C26	3.46	119.37	110.05
39	r	606	CHL	CHC-C1C-NC	3.45	129.44	124.20
39	R	606	CHL	CHC-C1C-NC	3.45	129.44	124.20
42	N	619	XAT	C10-C11-C12	3.45	133.98	123.22
23	r	610	CLA	O2D-CGD-CBD	3.44	117.39	111.27
39	G	608	CHL	C2B-C1B-NB	-3.44	107.92	110.23
24	a	406	PHO	CMB-C2B-C3B	3.44	131.11	124.68
39	Y	306	CHL	CHC-C1C-NC	3.44	129.41	124.20
40	S	615	LUT	C35-C34-C33	3.43	132.21	127.31
40	r	613	LUT	C1-C6-C5	-3.43	117.78	122.61
25	B	617	BCR	C2-C1-C6	3.43	115.76	110.48
40	s	615	LUT	C1-C6-C5	-3.43	117.79	122.61
39	Y	308	CHL	C2B-C1B-NB	-3.42	107.94	110.23
39	N	607	CHL	CHC-C1C-NC	3.42	129.40	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	C	515	DGD	O6D-C1D-O3G	-3.42	101.87	109.97
39	S	607	CHL	C2B-C1B-NB	-3.42	107.94	110.23
39	y	309	CHL	C2B-C1B-NB	-3.42	107.94	110.23
42	n	620	XAT	C8-C9-C10	3.42	124.19	118.94
23	C	513	CLA	CAA-C2A-C3A	-3.42	103.42	112.78
41	s	617	NEX	C10-C11-C12	3.42	133.88	123.22
39	y	303	CHL	C2B-C1B-NB	-3.42	107.94	110.23
39	n	605	CHL	CHC-C1C-NC	3.41	129.38	124.20
40	y	316	LUT	C8-C7-C6	3.41	136.78	127.20
26	a	409	SQD	O9-S-C6	3.41	110.99	106.94
30	R	616	LHG	O7-C7-C8	3.40	118.83	111.50
40	g	615	LUT	C15-C14-C13	3.40	132.16	127.31
40	Y	315	LUT	C8-C9-C10	3.39	124.15	118.94
40	Y	316	LUT	C1-C6-C5	-3.39	117.84	122.61
40	R	613	LUT	C1-C6-C5	-3.39	117.84	122.61
39	s	607	CHL	C2B-C1B-NB	-3.39	107.96	110.23
42	y	302	XAT	C10-C11-C12	3.39	133.79	123.22
39	N	606	CHL	C2B-C1B-NB	-3.39	107.96	110.23
30	D	404	LHG	O7-C7-C8	3.38	118.78	111.50
42	G	619	XAT	C17-C1-C6	3.38	119.16	110.05
24	A	405	PHO	CMB-C2B-C3B	3.38	131.00	124.68
39	Y	307	CHL	C2B-C1B-NB	-3.38	107.97	110.23
40	n	615	LUT	C12-C13-C14	3.37	124.12	118.94
39	N	608	CHL	C2B-C1B-NB	-3.37	107.97	110.23
30	G	618	LHG	O7-C7-C8	3.36	118.75	111.50
40	s	615	LUT	C10-C11-C12	3.36	133.71	123.22
41	r	614	NEX	C10-C11-C12	3.36	133.70	123.22
40	N	615	LUT	C31-C32-C33	3.36	135.85	126.42
30	g	618	LHG	O7-C7-C8	3.36	118.73	111.50
40	Y	315	LUT	C8-C7-C6	3.36	136.62	127.20
40	r	613	LUT	C18-C5-C6	-3.35	120.76	124.53
39	g	607	CHL	CHB-C4A-NA	3.35	129.15	124.51
40	G	615	LUT	C35-C15-C14	3.34	130.32	123.47
30	s	616	LHG	O7-C7-C8	3.34	118.71	111.50
33	c	515	DGD	O6D-C1D-O3G	-3.34	102.06	109.97
26	a	409	SQD	O8-S-C6	3.34	111.07	105.74
30	d	404	LHG	O7-C7-C8	3.34	118.70	111.50
39	G	607	CHL	CHB-C4A-NA	3.34	129.13	124.51
39	g	609	CHL	C2B-C1B-NB	-3.33	108.00	110.23
39	s	605	CHL	C2B-C1B-NB	-3.33	108.00	110.23
39	N	607	CHL	CHB-C4A-NA	3.33	129.12	124.51
40	y	317	LUT	C1-C6-C5	-3.33	117.92	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	S	614	LUT	C1-C6-C5	-3.33	117.93	122.61
39	G	620	CHL	CHB-C4A-NA	3.32	129.11	124.51
42	n	620	XAT	C37-C21-C26	3.32	119.00	110.05
39	g	609	CHL	CHC-C1C-NC	3.32	129.24	124.20
41	Y	317	NEX	C10-C11-C12	3.32	133.56	123.22
42	Y	301	XAT	C37-C21-C26	3.31	118.99	110.05
39	n	606	CHL	C2B-C1B-NB	-3.31	108.01	110.23
24	d	402	PHO	CMB-C2B-C3B	3.31	130.86	124.68
40	S	615	LUT	C31-C30-C29	3.30	132.03	127.31
42	N	619	XAT	C11-C10-C9	3.30	132.02	127.31
24	D	402	PHO	CMB-C2B-C3B	3.30	130.85	124.68
42	n	617	XAT	C17-C1-C6	3.30	118.95	110.05
40	n	615	LUT	C1-C6-C5	-3.30	117.97	122.61
23	a	405	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
40	S	614	LUT	C10-C11-C12	3.29	133.48	123.22
33	d	411	DGD	O3G-C3G-C2G	-3.29	102.97	110.90
39	y	310	CHL	C2B-C1B-NB	-3.28	108.03	110.23
39	n	607	CHL	CHB-C4A-NA	3.28	129.05	124.51
41	s	617	NEX	C15-C35-C34	3.28	130.19	123.47
39	g	619	CHL	CHB-C4A-NA	3.28	129.04	124.51
42	n	620	XAT	C11-C10-C9	3.27	131.98	127.31
39	R	606	CHL	CHB-C4A-NA	3.27	129.04	124.51
23	A	404	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
39	n	607	CHL	C2B-C1B-NB	-3.27	108.04	110.23
42	Y	301	XAT	C10-C11-C12	3.27	133.42	123.22
42	N	619	XAT	C37-C21-C26	3.27	118.86	110.05
39	n	608	CHL	C2B-C1B-NB	-3.27	108.04	110.23
30	b	627	LHG	O7-C7-C8	3.26	118.53	111.50
39	Y	309	CHL	C2B-C1B-NB	-3.26	108.05	110.23
39	Y	302	CHL	C2B-C1B-NB	-3.26	108.05	110.23
42	G	619	XAT	C36-C21-C26	-3.26	101.25	110.05
39	r	605	CHL	C2B-C1B-NB	-3.25	108.05	110.23
40	N	616	LUT	C35-C34-C33	3.25	131.96	127.31
40	N	615	LUT	C15-C35-C34	3.25	130.14	123.47
42	n	617	XAT	O24-C25-C24	3.25	115.83	113.38
39	r	607	CHL	CHB-C4A-NA	3.25	129.00	124.51
30	a	412	LHG	O7-C7-C8	3.24	118.49	111.50
33	H	502	DGD	O3G-C3G-C2G	-3.23	103.10	110.90
39	r	606	CHL	CHB-C4A-NA	3.22	128.96	124.51
42	R	615	XAT	C15-C14-C13	3.22	131.90	127.31
40	y	317	LUT	C35-C34-C33	3.22	131.90	127.31
39	Y	309	CHL	CHB-C4A-NA	3.21	128.96	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	d	408	LHG	O7-C7-C8	3.21	118.42	111.50
40	s	614	LUT	C30-C31-C32	3.21	133.24	123.22
39	S	606	CHL	C2B-C1B-NB	-3.21	108.08	110.23
30	S	616	LHG	O7-C7-C8	3.20	118.40	111.50
31	C	518	LNL	C15-C14-C13	-3.20	96.29	112.02
30	r	616	LHG	O7-C7-C8	3.19	118.39	111.50
39	R	607	CHL	C2B-C1B-NB	-3.19	108.09	110.23
39	g	605	CHL	C4D-CHA-C1A	3.19	125.13	121.25
30	n	619	LHG	O7-C7-C8	3.19	118.38	111.50
39	G	609	CHL	C2A-C1A-CHA	3.18	129.42	123.86
39	n	609	CHL	CHB-C4A-NA	3.18	128.91	124.51
39	R	607	CHL	CHB-C4A-NA	3.18	128.91	124.51
30	L	103	LHG	O7-C7-C8	3.17	118.34	111.50
39	S	605	CHL	C2B-C1B-NB	-3.17	108.11	110.23
39	N	609	CHL	CHB-C4A-NA	3.17	128.90	124.51
39	G	606	CHL	C2B-C1B-NB	-3.17	108.11	110.23
39	g	607	CHL	C2B-C1B-NB	-3.16	108.11	110.23
42	G	619	XAT	C31-C30-C29	3.16	131.82	127.31
39	y	303	CHL	CHB-C4A-NA	3.16	128.88	124.51
40	G	616	LUT	C31-C30-C29	3.15	131.81	127.31
42	r	615	XAT	C15-C14-C13	3.15	131.81	127.31
39	g	609	CHL	CHB-C4A-NA	3.15	128.87	124.51
39	r	607	CHL	C2B-C1B-NB	-3.15	108.12	110.23
39	n	609	CHL	C2B-C1B-NB	-3.15	108.12	110.23
40	s	614	LUT	C1-C6-C5	-3.14	118.19	122.61
40	Y	316	LUT	C35-C34-C33	3.14	131.79	127.31
36	D	401	BCT	O3-C-O1	-3.14	111.41	119.55
23	y	312	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
31	C	519	LNL	C15-C14-C13	-3.14	96.58	112.02
40	N	615	LUT	C10-C11-C12	3.13	133.00	123.22
39	N	609	CHL	C2B-C1B-NB	-3.13	108.14	110.23
39	y	310	CHL	CHB-C4A-NA	3.13	128.83	124.51
40	g	616	LUT	C31-C30-C29	3.13	131.77	127.31
42	n	620	XAT	C31-C32-C33	3.12	135.19	126.42
40	N	616	LUT	C31-C32-C33	3.12	135.18	126.42
23	S	604	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
30	y	318	LHG	O7-C7-C8	3.12	118.22	111.50
39	s	606	CHL	CHB-C4A-NA	3.12	128.82	124.51
40	G	616	LUT	C10-C11-C12	3.11	132.94	123.22
40	y	317	LUT	C10-C11-C12	3.11	132.93	123.22
42	n	617	XAT	C37-C21-C26	3.11	118.44	110.05
39	Y	302	CHL	CHB-C4A-NA	3.11	128.81	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	d	401	BCT	O3-C-O1	-3.11	111.48	119.55
39	s	606	CHL	C2B-C1B-NB	-3.11	108.15	110.23
31	c	521	LNL	C15-C14-C13	-3.11	96.73	112.02
23	B	610	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
40	g	616	LUT	C10-C11-C12	3.10	132.90	123.22
40	n	615	LUT	C10-C11-C12	3.10	132.90	123.22
40	n	615	LUT	C8-C7-C6	3.10	135.91	127.20
40	Y	316	LUT	C10-C11-C12	3.10	132.90	123.22
39	G	620	CHL	C4D-CHA-C1A	3.10	125.02	121.25
23	r	602	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
39	S	605	CHL	CHB-C4A-NA	3.10	128.80	124.51
23	B	602	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
39	g	619	CHL	C4D-CHA-C1A	3.10	125.02	121.25
35	y	301	VIV	C10-C3-C4	-3.10	117.02	120.37
23	b	606	CLA	O2D-CGD-O1D	-3.10	117.79	123.84
23	B	601	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
23	C	505	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
23	B	606	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
31	i	101	LNL	C15-C14-C13	-3.09	96.81	112.02
40	R	613	LUT	C18-C5-C6	-3.09	121.06	124.53
41	Y	317	NEX	C35-C34-C33	-3.09	122.90	127.31
40	r	613	LUT	C31-C30-C29	3.08	131.71	127.31
23	c	505	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
39	G	607	CHL	C2B-C1B-NB	-3.08	108.17	110.23
39	G	605	CHL	C4D-CHA-C1A	3.08	124.99	121.25
39	r	606	CHL	C2B-C1B-NB	-3.07	108.17	110.23
39	S	606	CHL	CHB-C4A-NA	3.07	128.75	124.51
41	R	618	NEX	C35-C34-C33	-3.07	122.93	127.31
23	B	614	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
39	g	606	CHL	CHB-C4A-NA	3.06	128.75	124.51
39	N	607	CHL	C2B-C1B-NB	-3.06	108.18	110.23
39	Y	307	CHL	CHB-C4A-NA	3.06	128.75	124.51
31	c	519	LNL	C15-C14-C13	-3.06	96.95	112.02
23	a	407	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
40	G	615	LUT	C31-C32-C33	3.05	134.99	126.42
39	g	606	CHL	C2B-C1B-NB	-3.05	108.19	110.23
39	N	605	CHL	C4D-CHA-C1A	3.05	124.96	121.25
23	s	609	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
25	b	617	BCR	C15-C16-C17	-3.05	117.24	123.47
23	b	604	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
23	Y	311	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
23	b	610	CLA	O2D-CGD-O1D	-3.04	117.89	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	614	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
40	N	615	LUT	C1-C6-C5	-3.04	118.33	122.61
40	N	616	LUT	C31-C30-C29	3.04	131.65	127.31
40	S	615	LUT	C30-C31-C32	3.04	132.70	123.22
31	c	517	LNL	C15-C14-C13	-3.04	97.07	112.02
23	C	508	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
23	c	508	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
23	R	601	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
31	a	401	LNL	C15-C14-C13	-3.03	97.10	112.02
23	s	604	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
23	N	612	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
23	b	602	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
39	s	605	CHL	CHB-C4A-NA	3.02	128.69	124.51
23	A	406	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
39	S	606	CHL	C4D-CHA-C1A	3.02	124.92	121.25
23	B	604	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
31	c	522	LNL	C15-C14-C13	-3.02	97.16	112.02
39	n	608	CHL	CHB-C4A-NA	3.02	128.69	124.51
23	b	601	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
31	c	520	LNL	C15-C14-C13	-3.02	97.17	112.02
31	A	414	LNL	C15-C14-C13	-3.01	97.18	112.02
39	g	605	CHL	C2A-C1A-CHA	3.01	129.13	123.86
23	b	615	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
31	b	625	LNL	C15-C14-C13	-3.01	97.19	112.02
23	B	615	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
31	B	622	LNL	C15-C14-C13	-3.01	97.20	112.02
39	G	606	CHL	CHB-C4A-NA	3.01	128.68	124.51
23	A	403	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
23	b	612	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
31	C	521	LNL	C15-C14-C13	-3.01	97.21	112.02
23	a	404	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
39	N	608	CHL	CHB-C4A-NA	3.01	128.67	124.51
38	F	501	HEM	C4D-ND-C1D	3.00	108.18	105.07
41	g	617	NEX	C5-C4-C3	3.00	115.30	111.75
39	S	607	CHL	CHB-C4A-NA	3.00	128.66	124.51
31	a	413	LNL	C15-C14-C13	-3.00	97.24	112.02
23	b	616	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
41	g	617	NEX	C15-C35-C34	3.00	129.62	123.47
31	c	518	LNL	C15-C14-C13	-3.00	97.27	112.02
23	d	405	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
40	N	616	LUT	C18-C5-C6	-2.99	121.17	124.53
42	N	619	XAT	C17-C1-C6	2.99	118.13	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	y	308	CHL	CHB-C4A-NA	2.99	128.65	124.51
39	g	606	CHL	C4D-CHA-C1A	2.99	124.89	121.25
39	R	606	CHL	C4D-CHA-C1A	2.99	124.89	121.25
25	b	617	BCR	C15-C14-C13	-2.99	123.04	127.31
42	G	619	XAT	C15-C14-C13	2.99	131.57	127.31
23	B	612	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
39	n	601	CHL	CHB-C4A-NA	2.98	128.64	124.51
39	G	606	CHL	C4D-CHA-C1A	2.98	124.88	121.25
23	D	405	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
31	b	622	LNL	C15-C14-C13	-2.98	97.35	112.02
40	n	616	LUT	C31-C30-C29	2.98	131.56	127.31
23	g	612	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
23	s	613	CLA	CAA-C2A-C3A	-2.98	104.62	112.78
39	G	620	CHL	C2B-C1B-NB	-2.98	108.23	110.23
23	N	614	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
40	n	615	LUT	C16-C1-C6	-2.98	105.47	110.30
41	G	617	NEX	C34-C35-C15	2.97	130.22	123.42
40	S	614	LUT	C30-C31-C32	2.97	132.50	123.22
39	Y	306	CHL	C4D-CHA-C1A	2.97	124.87	121.25
23	B	616	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
23	Y	314	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
39	g	619	CHL	C2B-C1B-NB	-2.97	108.24	110.23
23	y	315	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
42	y	302	XAT	C19-C9-C8	2.97	122.76	118.08
39	N	607	CHL	C4D-CHA-C1A	2.97	124.87	121.25
39	Y	308	CHL	CHB-C4A-NA	2.97	128.62	124.51
39	g	601	CHL	CHB-C4A-NA	2.97	128.62	124.51
23	g	614	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
23	R	604	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
40	Y	315	LUT	C15-C35-C34	2.96	129.54	123.47
39	S	605	CHL	C4D-CHA-C1A	2.96	124.86	121.25
23	S	610	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
23	y	304	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
42	n	620	XAT	C17-C1-C6	2.96	118.03	110.05
23	r	604	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
40	y	316	LUT	C15-C35-C34	2.95	129.52	123.47
23	b	607	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
39	n	607	CHL	C4D-CHA-C1A	2.95	124.84	121.25
25	b	617	BCR	C11-C10-C9	-2.95	123.10	127.31
39	G	601	CHL	CHB-C4A-NA	2.95	128.59	124.51
40	S	614	LUT	C18-C5-C6	-2.95	121.21	124.53
39	S	601	CHL	C2A-C1A-CHA	2.95	129.02	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	y	307	CHL	C4D-CHA-C1A	2.95	124.84	121.25
23	n	612	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
40	R	613	LUT	C31-C30-C29	2.95	131.51	127.31
23	s	613	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
31	B	625	LNL	C15-C14-C13	-2.94	97.52	112.02
40	g	615	LUT	C35-C15-C14	2.94	129.51	123.47
39	s	605	CHL	C4D-CHA-C1A	2.94	124.83	121.25
23	B	607	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
23	C	507	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
23	R	602	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
39	G	608	CHL	CHB-C4A-NA	2.94	128.58	124.51
23	n	614	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
40	g	615	LUT	C31-C32-C33	2.94	134.68	126.42
39	y	309	CHL	CHB-C4A-NA	2.94	128.57	124.51
23	S	613	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
23	s	610	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
23	N	613	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
25	B	617	BCR	C11-C10-C9	-2.93	123.12	127.31
39	n	606	CHL	CHB-C4A-NA	2.93	128.57	124.51
39	Y	306	CHL	C2A-C1A-CHA	2.93	128.99	123.86
39	r	606	CHL	C4D-CHA-C1A	2.93	124.82	121.25
31	I	101	LNL	C15-C14-C13	-2.93	97.59	112.02
23	Y	303	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
23	r	610	CLA	C3B-C4B-NB	-2.93	107.80	110.52
23	b	610	CLA	C3B-C4B-NB	-2.93	107.80	110.52
31	C	517	LNL	C15-C14-C13	-2.93	97.61	112.02
39	N	606	CHL	CHB-C4A-NA	2.93	128.56	124.51
39	r	605	CHL	CHB-C4A-NA	2.92	128.55	124.51
23	C	501	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
30	N	618	LHG	O7-C7-C8	2.92	117.80	111.50
40	g	615	LUT	C16-C1-C6	-2.92	105.56	110.30
23	C	509	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
23	s	611	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
41	Y	317	NEX	C15-C35-C34	2.92	129.45	123.47
23	n	613	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
23	n	604	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
23	c	509	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
23	c	501	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
39	r	607	CHL	C4D-CHA-C1A	2.91	124.79	121.25
23	S	602	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
40	S	615	LUT	C10-C11-C12	2.91	132.29	123.22
40	n	616	LUT	C10-C11-C12	2.91	132.29	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	G	612	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
23	c	507	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
38	f	501	HEM	C4A-NA-C1A	2.91	108.19	105.35
23	R	610	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
39	S	601	CHL	C4D-CHA-C1A	2.90	124.78	121.25
30	Y	318	LHG	O7-C7-C8	2.90	117.76	111.50
23	R	611	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
42	y	302	XAT	C36-C21-C26	-2.90	102.21	110.05
31	C	522	LNL	C15-C14-C13	-2.90	97.74	112.02
31	b	623	LNL	C15-C14-C13	-2.90	97.74	112.02
39	r	605	CHL	C4D-CHA-C1A	2.90	124.78	121.25
42	r	615	XAT	C16-C1-C6	-2.90	102.22	110.05
23	N	604	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
23	G	614	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
31	A	413	LNL	C15-C14-C13	-2.89	97.77	112.02
23	c	511	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
39	N	605	CHL	C2A-C1A-CHA	2.89	128.92	123.86
39	g	608	CHL	CHB-C4A-NA	2.89	128.51	124.51
23	b	603	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
39	s	601	CHL	CHB-C4A-NA	2.89	128.51	124.51
40	s	615	LUT	C31-C30-C29	2.89	131.44	127.31
23	B	608	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
39	N	601	CHL	C4D-CHA-C1A	2.89	124.77	121.25
23	B	609	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
23	C	503	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
39	R	607	CHL	C4D-CHA-C1A	2.89	124.77	121.25
23	S	611	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
40	g	615	LUT	C8-C7-C6	2.89	135.32	127.20
23	C	511	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
39	y	307	CHL	C2A-C1A-CHA	2.89	128.91	123.86
23	R	612	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
40	s	614	LUT	C16-C1-C6	-2.88	105.62	110.30
23	s	608	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
39	s	606	CHL	C4D-CHA-C1A	2.88	124.76	121.25
39	g	608	CHL	C2A-C1A-CHA	2.88	128.90	123.86
23	B	603	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
39	g	605	CHL	CHB-C4A-NA	2.88	128.50	124.51
39	G	620	CHL	C2A-C1A-CHA	2.88	128.90	123.86
23	D	406	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
39	G	607	CHL	C4D-CHA-C1A	2.88	124.75	121.25
23	G	603	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
23	r	611	CLA	O2D-CGD-O1D	-2.88	118.21	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	R	615	XAT	C16-C1-C6	-2.88	102.28	110.05
23	c	502	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
23	b	605	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
23	g	603	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
23	r	612	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
38	F	501	HEM	C4A-NA-C1A	2.87	108.16	105.35
23	B	611	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
41	n	618	NEX	C15-C35-C34	2.87	129.36	123.47
39	N	601	CHL	CHB-C4A-NA	2.87	128.49	124.51
23	C	512	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
23	C	510	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
40	N	616	LUT	C10-C11-C12	2.87	132.18	123.22
23	Y	312	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
24	D	402	PHO	O1D-CGD-CBD	2.87	129.52	124.74
39	n	601	CHL	C2A-C1A-CHA	2.87	128.88	123.86
23	c	503	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
23	R	601	CLA	C3B-C4B-NB	-2.87	107.85	110.52
23	g	611	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
23	d	406	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
23	c	504	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
39	s	601	CHL	C2A-C1A-CHA	2.87	128.87	123.86
39	Y	306	CHL	CHB-C4A-NA	2.87	128.48	124.51
39	g	607	CHL	C4D-CHA-C1A	2.87	124.74	121.25
31	C	520	LNL	C15-C14-C13	-2.87	97.91	112.02
23	c	512	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
23	r	603	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
23	b	609	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
42	G	619	XAT	C37-C21-C26	2.86	117.78	110.05
25	B	618	BCR	C15-C16-C17	-2.86	117.61	123.47
23	r	601	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
23	B	610	CLA	C3B-C4B-NB	-2.86	107.86	110.52
39	G	605	CHL	C2A-C1A-CHA	2.86	128.86	123.86
23	R	603	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
40	y	317	LUT	C31-C30-C29	2.86	131.39	127.31
39	S	601	CHL	CHB-C4A-NA	2.86	128.47	124.51
23	b	611	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
23	C	502	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
23	b	608	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
23	c	510	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
23	y	313	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
23	C	504	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
31	B	624	LNL	C15-C14-C13	-2.86	97.96	112.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	y	305	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
23	B	601	CLA	C3B-C4B-NB	-2.86	107.87	110.52
39	R	605	CHL	C4D-CHA-C1A	2.86	124.72	121.25
23	n	602	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
40	G	615	LUT	C16-C1-C6	-2.85	105.67	110.30
39	R	605	CHL	CHB-C4A-NA	2.85	128.46	124.51
23	N	602	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
23	Y	304	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
23	S	603	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
39	G	605	CHL	CHB-C4A-NA	2.85	128.45	124.51
23	s	603	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
39	s	607	CHL	C4D-CHA-C1A	2.85	124.72	121.25
39	s	607	CHL	CHB-C4A-NA	2.85	128.45	124.51
40	G	615	LUT	C8-C7-C6	2.85	135.19	127.20
40	s	614	LUT	C18-C5-C6	-2.85	121.33	124.53
40	n	616	LUT	C31-C32-C33	2.84	134.40	126.42
23	S	609	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
40	G	616	LUT	C31-C32-C33	2.84	134.40	126.42
23	R	610	CLA	C3B-C4B-NB	-2.84	107.88	110.52
23	s	602	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
23	r	601	CLA	C3B-C4B-NB	-2.84	107.88	110.52
42	N	619	XAT	C31-C32-C33	2.84	134.39	126.42
40	R	613	LUT	C16-C1-C6	-2.84	105.70	110.30
23	y	311	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
42	n	617	XAT	C31-C30-C29	2.83	131.35	127.31
40	R	613	LUT	C30-C31-C32	2.83	132.05	123.22
23	Y	310	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
23	y	306	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
40	R	613	LUT	C10-C11-C12	2.83	132.05	123.22
23	b	606	CLA	C3B-C4B-NB	-2.83	107.89	110.52
23	R	609	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
24	A	405	PHO	O1D-CGD-CBD	2.83	129.45	124.74
39	N	605	CHL	CHB-C4A-NA	2.83	128.43	124.51
40	g	616	LUT	C31-C32-C33	2.83	134.36	126.42
23	b	611	CLA	C1-C2-C3	-2.83	121.15	126.04
23	B	606	CLA	C3B-C4B-NB	-2.83	107.89	110.52
23	b	601	CLA	C3B-C4B-NB	-2.83	107.89	110.52
23	G	602	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
26	L	101	SQD	O8-S-C6	2.83	110.24	105.74
39	n	608	CHL	C4D-CHA-C1A	2.83	124.69	121.25
41	R	614	NEX	C15-C35-C34	2.82	129.26	123.47
23	S	608	CLA	O2D-CGD-O1D	-2.82	118.32	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	n	610	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
41	s	617	NEX	C5-C6-C1	-2.82	116.89	119.70
39	G	609	CHL	CHB-C4A-NA	2.82	128.42	124.51
39	y	307	CHL	CHB-C4A-NA	2.82	128.42	124.51
41	R	618	NEX	C15-C35-C34	2.82	129.26	123.47
23	N	611	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
39	y	308	CHL	C4D-CHA-C1A	2.82	124.68	121.25
25	B	617	BCR	C15-C16-C17	-2.82	117.70	123.47
39	g	619	CHL	C2A-C1A-CHA	2.82	128.79	123.86
41	N	617	NEX	C15-C35-C34	2.82	129.24	123.47
23	g	610	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
40	Y	316	LUT	C31-C30-C29	2.82	131.33	127.31
39	N	608	CHL	C4D-CHA-C1A	2.82	124.68	121.25
39	S	607	CHL	C4D-CHA-C1A	2.81	124.67	121.25
23	c	513	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
24	d	402	PHO	O1D-CGD-CBD	2.81	129.42	124.74
23	N	603	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
23	Y	305	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
23	C	513	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
25	d	410	BCR	C24-C23-C22	-2.81	121.99	126.23
23	R	611	CLA	C3B-C4B-NB	-2.81	107.91	110.52
23	S	610	CLA	C3B-C4B-NB	-2.81	107.91	110.52
23	n	611	CLA	O2D-CGD-O1D	-2.80	118.35	123.84
23	r	609	CLA	O2D-CGD-O1D	-2.80	118.35	123.84
24	D	402	PHO	O2D-CGD-O1D	-2.80	118.36	123.84
40	s	615	LUT	C31-C32-C33	2.80	134.29	126.42
40	n	616	LUT	C18-C5-C6	-2.80	121.38	124.53
25	d	410	BCR	C33-C5-C6	-2.80	121.38	124.53
23	r	608	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	G	604	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
24	d	402	PHO	O2D-CGD-O1D	-2.80	118.37	123.84
39	Y	307	CHL	C4D-CHA-C1A	2.80	124.65	121.25
25	B	617	BCR	C15-C14-C13	-2.80	123.32	127.31
23	r	609	CLA	C3B-C4B-NB	-2.80	107.92	110.52
23	s	610	CLA	C3B-C4B-NB	-2.80	107.92	110.52
23	g	602	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
23	g	613	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
23	n	610	CLA	C3B-C4B-NB	-2.79	107.92	110.52
39	R	606	CHL	C2B-C1B-NB	-2.79	108.36	110.23
23	Y	313	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
23	S	608	CLA	C3B-C4B-NB	-2.79	107.93	110.52
23	N	610	CLA	O2D-CGD-O1D	-2.79	118.38	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	S	615	LUT	C18-C5-C6	-2.79	121.40	124.53
23	R	609	CLA	C3B-C4B-NB	-2.79	107.93	110.52
39	s	601	CHL	C4D-CHA-C1A	2.79	124.64	121.25
40	y	317	LUT	C16-C1-C6	-2.79	105.78	110.30
40	Y	316	LUT	C16-C1-C6	-2.78	105.78	110.30
23	G	611	CLA	C3B-C4B-NB	-2.78	107.94	110.52
40	r	613	LUT	C16-C1-C6	-2.78	105.79	110.30
38	f	501	HEM	C4D-ND-C1D	2.78	107.94	105.07
40	N	615	LUT	C18-C5-C6	-2.77	121.41	124.53
40	S	614	LUT	C16-C1-C6	-2.77	105.80	110.30
23	G	611	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
23	n	603	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
23	G	613	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
31	b	624	LNL	C15-C14-C13	-2.77	98.41	112.02
35	C	523	VIV	C12-C5-C4	-2.76	117.04	121.30
40	Y	316	LUT	C30-C31-C32	2.76	131.84	123.22
23	g	604	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
24	a	406	PHO	O1D-CGD-CBD	2.76	129.33	124.74
26	A	408	SQD	O8-S-C6	2.76	110.14	105.74
23	G	610	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
23	R	608	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
24	A	405	PHO	O2D-CGD-O1D	-2.75	118.45	123.84
42	Y	301	XAT	C16-C1-C6	-2.75	102.61	110.05
23	N	611	CLA	C3B-C4B-NB	-2.75	107.96	110.52
40	N	615	LUT	C16-C1-C6	-2.75	105.83	110.30
23	c	507	CLA	CHB-C4A-NA	2.75	128.32	124.51
25	b	618	BCR	C15-C16-C17	-2.75	117.83	123.47
42	n	620	XAT	C37-C21-C36	-2.75	103.31	107.37
23	s	612	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
39	N	601	CHL	C2A-C1A-CHA	2.75	128.67	123.86
39	G	601	CHL	C4D-CHA-C1A	2.75	124.60	121.25
42	N	619	XAT	C15-C14-C13	2.75	131.24	127.31
23	S	612	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
41	S	617	NEX	C5-C6-C1	-2.75	116.97	119.70
41	r	614	NEX	C15-C35-C34	2.75	129.10	123.47
40	N	616	LUT	C16-C1-C6	-2.74	105.85	110.30
24	a	406	PHO	O2D-CGD-O1D	-2.74	118.48	123.84
40	S	614	LUT	C31-C30-C29	2.74	131.22	127.31
23	S	613	CLA	CAA-C2A-C3A	-2.74	105.27	112.78
40	r	613	LUT	C30-C31-C32	2.74	131.77	123.22
39	G	606	CHL	C2A-C1A-CHA	2.74	128.65	123.86
39	R	605	CHL	C2A-C1A-CHA	2.74	128.65	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	g	612	CLA	CHB-C4A-NA	2.74	128.30	124.51
41	R	618	NEX	O24-C25-C38	-2.74	111.77	115.06
39	r	605	CHL	C2A-C1A-CHA	2.74	128.65	123.86
25	B	618	BCR	C15-C14-C13	-2.74	123.40	127.31
39	G	609	CHL	C4D-CHA-C1A	2.74	124.58	121.25
41	Y	317	NEX	C5-C6-C1	-2.74	116.98	119.70
23	y	315	CLA	C3B-C4B-NB	-2.74	107.98	110.52
39	g	609	CHL	C2A-C1A-CHA	2.74	128.64	123.86
40	y	317	LUT	C30-C31-C32	2.74	131.76	123.22
39	g	606	CHL	C2A-C1A-CHA	2.73	128.64	123.86
40	n	615	LUT	C18-C5-C6	-2.73	121.46	124.53
23	y	314	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
33	d	411	DGD	O6D-C1D-O3G	-2.73	103.50	109.97
39	N	608	CHL	C2A-C1A-CHA	2.73	128.64	123.86
40	s	615	LUT	C30-C31-C32	2.73	131.75	123.22
39	g	601	CHL	C2A-C1A-CHA	2.73	128.64	123.86
25	h	501	BCR	C24-C23-C22	-2.73	122.11	126.23
42	R	615	XAT	C37-C21-C26	2.73	117.42	110.05
40	y	317	LUT	C18-C5-C6	-2.73	121.46	124.53
40	G	615	LUT	C35-C34-C33	2.73	131.20	127.31
40	G	615	LUT	C10-C11-C12	2.73	131.73	123.22
39	G	601	CHL	C2A-C1A-CHA	2.73	128.63	123.86
39	R	606	CHL	C2A-C1A-CHA	2.73	128.63	123.86
23	G	612	CLA	C3B-C4B-NB	-2.73	107.99	110.52
40	Y	316	LUT	C18-C5-C6	-2.72	121.47	124.53
42	Y	301	XAT	C36-C21-C26	-2.72	102.69	110.05
40	N	615	LUT	C15-C14-C13	2.72	131.20	127.31
23	s	602	CLA	C3B-C4B-NB	-2.72	107.99	110.52
33	c	515	DGD	CDB-CCB-CBB	-2.72	100.60	114.42
40	G	615	LUT	C39-C29-C28	-2.72	113.79	118.08
23	C	507	CLA	C3B-C4B-NB	-2.72	107.99	110.52
41	g	617	NEX	C1-C2-C3	-2.72	107.50	113.64
23	D	406	CLA	C3B-C4B-NB	-2.72	107.99	110.52
40	S	615	LUT	C16-C1-C6	-2.72	105.89	110.30
39	G	607	CHL	C2A-C1A-CHA	2.72	128.61	123.86
39	Y	308	CHL	C4D-CHA-C1A	2.72	124.56	121.25
39	y	303	CHL	C4D-CHA-C1A	2.72	124.55	121.25
23	s	609	CLA	C3B-C4B-NB	-2.71	108.00	110.52
39	g	607	CHL	C2A-C1A-CHA	2.71	128.60	123.86
39	n	605	CHL	CHB-C4A-NA	2.71	128.26	124.51
25	d	410	BCR	C27-C26-C25	2.71	126.67	122.73
40	n	616	LUT	C16-C1-C6	-2.71	105.90	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L	101	SQD	O48-C23-C24	2.71	120.41	111.91
42	y	302	XAT	C16-C1-C6	-2.71	102.73	110.05
31	B	623	LNL	C15-C14-C13	-2.71	98.68	112.02
39	N	607	CHL	C2A-C1A-CHA	2.71	128.59	123.86
40	N	616	LUT	C30-C31-C32	2.71	131.66	123.22
23	N	610	CLA	C3B-C4B-NB	-2.71	108.00	110.52
33	d	411	DGD	CDB-CCB-CBB	-2.70	100.69	114.42
40	r	613	LUT	C10-C11-C12	2.70	131.65	123.22
33	H	502	DGD	CDB-CCB-CBB	-2.70	100.70	114.42
23	S	602	CLA	C3B-C4B-NB	-2.70	108.01	110.52
39	y	309	CHL	C2A-C1A-CHA	2.70	128.58	123.86
33	H	502	DGD	O6D-C1D-O3G	-2.70	103.58	109.97
39	n	606	CHL	C2A-C1A-CHA	2.70	128.58	123.86
25	H	501	BCR	C27-C26-C25	2.70	126.65	122.73
23	a	403	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
23	b	615	CLA	CHB-C4A-NA	2.70	128.24	124.51
33	C	515	DGD	CDB-CCB-CBB	-2.69	100.75	114.42
23	b	613	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
39	n	608	CHL	C2A-C1A-CHA	2.69	128.57	123.86
25	k	101	BCR	C24-C23-C22	-2.69	122.17	126.23
23	N	613	CLA	CHB-C4A-NA	2.69	128.24	124.51
39	Y	308	CHL	C2A-C1A-CHA	2.69	128.56	123.86
25	b	618	BCR	C15-C14-C13	-2.69	123.48	127.31
41	Y	317	NEX	C30-C31-C32	2.68	131.59	123.22
25	H	501	BCR	C24-C23-C22	-2.68	122.18	126.23
23	B	615	CLA	C3B-C4B-NB	-2.68	108.03	110.52
23	C	510	CLA	C3B-C4B-NB	-2.68	108.03	110.52
25	k	101	BCR	C15-C16-C17	-2.68	117.98	123.47
39	n	607	CHL	C2A-C1A-CHA	2.68	128.55	123.86
23	A	402	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
25	K	101	BCR	C24-C23-C22	-2.68	122.19	126.23
39	r	607	CHL	C2A-C1A-CHA	2.67	128.53	123.86
40	Y	315	LUT	C16-C1-C6	-2.67	105.96	110.30
41	r	614	NEX	O24-C25-C38	-2.67	111.85	115.06
25	h	501	BCR	C27-C26-C25	2.67	126.61	122.73
40	s	615	LUT	C16-C1-C6	-2.67	105.97	110.30
39	n	605	CHL	C4D-CHA-C1A	2.67	124.50	121.25
33	C	515	DGD	O5D-C6D-C5D	-2.67	104.11	109.05
39	y	309	CHL	C4D-CHA-C1A	2.67	124.50	121.25
23	Y	314	CLA	C3B-C4B-NB	-2.67	108.04	110.52
39	Y	307	CHL	C2A-C1A-CHA	2.67	128.52	123.86
23	C	507	CLA	CHB-C4A-NA	2.66	128.20	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	CHB-C4A-NA	2.66	128.20	124.51
23	Y	310	CLA	C3B-C4B-NB	-2.66	108.04	110.52
23	r	611	CLA	C3B-C4B-NB	-2.66	108.05	110.52
26	a	409	SQD	O48-C23-C24	2.66	120.26	111.91
42	Y	301	XAT	C17-C1-C6	2.66	117.23	110.05
26	M	101	SQD	O8-S-C6	2.66	109.98	105.74
23	B	615	CLA	CHB-C4A-NA	2.66	128.19	124.51
30	D	408	LHG	O7-C7-C8	2.66	117.23	111.50
42	r	615	XAT	C37-C21-C26	2.66	117.22	110.05
26	A	408	SQD	O48-C23-C24	2.66	120.24	111.91
39	y	310	CHL	C2A-C1A-CHA	2.65	128.50	123.86
23	d	406	CLA	CHB-C4A-NA	2.65	128.18	124.51
23	N	613	CLA	O2A-CGA-O1A	-2.65	116.90	123.59
23	s	603	CLA	C3B-C4B-NB	-2.65	108.06	110.52
23	B	614	CLA	C3B-C4B-NB	-2.65	108.06	110.52
39	s	605	CHL	C2A-C1A-CHA	2.65	128.49	123.86
39	G	608	CHL	C2A-C1A-CHA	2.64	128.48	123.86
23	B	605	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
40	g	616	LUT	C18-C5-C6	-2.64	121.56	124.53
23	b	614	CLA	C3B-C4B-NB	-2.64	108.06	110.52
23	c	510	CLA	C3B-C4B-NB	-2.64	108.06	110.52
40	s	614	LUT	C31-C32-C33	2.64	133.83	126.42
23	G	612	CLA	CHB-C4A-NA	2.64	128.16	124.51
39	n	601	CHL	C4D-CHA-C1A	2.64	124.46	121.25
23	s	608	CLA	C3B-C4B-NB	-2.64	108.07	110.52
23	g	612	CLA	C3B-C4B-NB	-2.64	108.07	110.52
26	M	101	SQD	O48-C23-C24	2.64	120.18	111.91
23	n	611	CLA	C3B-C4B-NB	-2.63	108.07	110.52
23	B	613	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
23	y	314	CLA	C3B-C4B-NB	-2.63	108.07	110.52
39	G	608	CHL	C4D-CHA-C1A	2.63	124.45	121.25
42	n	620	XAT	C15-C14-C13	2.63	131.06	127.31
39	g	609	CHL	C1-C2-C3	-2.63	121.50	126.04
23	G	602	CLA	C3B-C4B-NB	-2.63	108.08	110.52
23	y	311	CLA	C3B-C4B-NB	-2.63	108.08	110.52
39	s	607	CHL	C2A-C1A-CHA	2.62	128.44	123.86
25	v	101	BCR	C33-C5-C6	-2.62	121.58	124.53
41	N	617	NEX	O24-C25-C38	-2.62	111.91	115.06
39	n	609	CHL	C2A-C1A-CHA	2.62	128.44	123.86
40	g	615	LUT	C39-C29-C28	-2.62	113.95	118.08
39	g	601	CHL	C4D-CHA-C1A	2.62	124.44	121.25
25	K	101	BCR	C15-C16-C17	-2.62	118.11	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Y	311	CLA	C3B-C4B-NB	-2.62	108.08	110.52
40	r	613	LUT	C31-C32-C33	2.62	133.77	126.42
23	S	603	CLA	C3B-C4B-NB	-2.62	108.09	110.52
40	y	316	LUT	C16-C1-C6	-2.62	106.06	110.30
42	n	617	XAT	C15-C14-C13	2.61	131.04	127.31
23	D	406	CLA	CHB-C4A-NA	2.61	128.13	124.51
42	R	615	XAT	O4-C5-C6	-2.61	56.79	58.96
42	R	615	XAT	C31-C32-C33	2.61	133.76	126.42
39	N	606	CHL	C4D-CHA-C1A	2.61	124.43	121.25
42	Y	301	XAT	C35-C34-C33	2.61	131.04	127.31
40	R	613	LUT	C38-C25-C24	-2.61	117.97	123.56
42	N	619	XAT	C37-C21-C36	-2.61	103.52	107.37
39	N	609	CHL	C4D-CHA-C1A	2.61	124.43	121.25
42	r	615	XAT	O4-C5-C6	-2.61	56.80	58.96
23	B	601	CLA	CHB-C4A-NA	2.61	128.12	124.51
38	f	501	HEM	C1B-NB-C4B	2.61	107.77	105.07
23	g	610	CLA	C1-C2-C3	-2.61	121.53	126.04
41	n	618	NEX	O24-C25-C38	-2.61	111.93	115.06
23	n	614	CLA	C3B-C4B-NB	-2.60	108.10	110.52
40	y	317	LUT	C31-C32-C33	2.60	133.73	126.42
23	c	506	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
23	y	312	CLA	C3B-C4B-NB	-2.60	108.10	110.52
33	C	515	DGD	C3G-C2G-C1G	-2.60	105.63	111.79
23	C	501	CLA	CHB-C4A-NA	2.60	128.11	124.51
23	A	406	CLA	C3B-C4B-NB	-2.60	108.10	110.52
23	c	507	CLA	C3B-C4B-NB	-2.60	108.10	110.52
23	y	305	CLA	CHB-C4A-NA	2.60	128.11	124.51
41	Y	317	NEX	O24-C25-C38	-2.60	111.94	115.06
33	c	515	DGD	O5D-C6D-C5D	-2.60	104.24	109.05
38	F	501	HEM	C1B-NB-C4B	2.60	107.76	105.07
39	r	606	CHL	C2A-C1A-CHA	2.60	128.40	123.86
23	s	604	CLA	C3B-C4B-NB	-2.60	108.11	110.52
39	S	606	CHL	C2A-C1A-CHA	2.60	128.40	123.86
23	g	602	CLA	C3B-C4B-NB	-2.59	108.11	110.52
25	H	501	BCR	C33-C5-C6	-2.59	121.61	124.53
42	n	620	XAT	C35-C15-C14	2.59	128.78	123.47
23	r	608	CLA	CHB-C4A-NA	2.59	128.09	124.51
23	R	602	CLA	C3B-C4B-NB	-2.59	108.11	110.52
23	r	612	CLA	C3B-C4B-NB	-2.59	108.11	110.52
40	G	616	LUT	C16-C1-C6	-2.59	106.10	110.30
23	R	608	CLA	C3B-C4B-NB	-2.59	108.11	110.52
42	r	615	XAT	C31-C32-C33	2.59	133.69	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	501	CLA	CHB-C4A-NA	2.59	128.09	124.51
39	N	606	CHL	C2A-C1A-CHA	2.58	128.38	123.86
35	C	523	VIV	C11-C10-C3	2.58	115.80	111.75
41	N	617	NEX	C35-C34-C33	-2.58	123.62	127.31
23	b	612	CLA	C3B-C4B-NB	-2.58	108.12	110.52
39	Y	309	CHL	C4D-CHA-C1A	2.58	124.39	121.25
40	S	615	LUT	C31-C32-C33	2.58	133.67	126.42
23	C	506	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
23	R	608	CLA	CHB-C4A-NA	2.58	128.08	124.51
23	b	601	CLA	CHB-C4A-NA	2.58	128.08	124.51
23	r	602	CLA	C3B-C4B-NB	-2.58	108.12	110.52
23	B	601	CLA	CAA-C2A-C3A	-2.58	105.72	112.78
23	B	612	CLA	CHB-C4A-NA	2.58	128.08	124.51
40	g	615	LUT	C12-C13-C14	2.58	122.90	118.94
41	R	618	NEX	C30-C31-C32	2.58	131.26	123.22
40	y	316	LUT	C10-C11-C12	2.58	131.26	123.22
42	N	619	XAT	C35-C15-C14	2.57	128.75	123.47
40	y	317	LUT	C39-C29-C28	-2.57	114.02	118.08
23	N	602	CLA	C3B-C4B-NB	-2.57	108.13	110.52
23	R	612	CLA	C3B-C4B-NB	-2.57	108.13	110.52
40	Y	315	LUT	C10-C11-C12	2.57	131.25	123.22
25	z	101	BCR	C15-C16-C17	-2.57	118.20	123.47
42	y	302	XAT	C17-C1-C6	2.57	116.99	110.05
23	C	502	CLA	CHB-C4A-NA	2.57	128.07	124.51
39	y	308	CHL	C2A-C1A-CHA	2.57	128.35	123.86
25	h	501	BCR	C33-C5-C6	-2.57	121.64	124.53
23	G	614	CLA	C3B-C4B-NB	-2.57	108.13	110.52
23	S	603	CLA	CHB-C4A-NA	2.57	128.06	124.51
40	S	614	LUT	C31-C32-C33	2.57	133.62	126.42
25	V	101	BCR	C33-C5-C6	-2.56	121.65	124.53
23	a	407	CLA	CHB-C4A-NA	2.56	128.06	124.51
23	A	402	CLA	O2D-CGD-CBD	2.56	115.82	111.27
23	S	609	CLA	C3B-C4B-NB	-2.56	108.14	110.52
40	Y	315	LUT	C30-C31-C32	2.56	131.21	123.22
42	Y	301	XAT	C30-C31-C32	2.56	131.21	123.22
40	Y	316	LUT	C39-C29-C28	-2.56	114.05	118.08
40	R	613	LUT	C31-C32-C33	2.56	133.60	126.42
39	R	607	CHL	C2A-C1A-CHA	2.56	128.33	123.86
42	n	620	XAT	O4-C5-C6	-2.56	56.84	58.96
23	S	604	CLA	C3B-C4B-NB	-2.56	108.14	110.52
25	D	411	BCR	C15-C16-C17	-2.56	118.24	123.47
23	Y	313	CLA	C3B-C4B-NB	-2.55	108.14	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	G	603	CLA	CHB-C4A-NA	2.55	128.04	124.51
38	F	501	HEM	C4C-NC-C1C	2.55	107.85	105.35
23	a	403	CLA	O2D-CGD-CBD	2.55	115.80	111.27
23	b	608	CLA	C3B-C4B-NB	-2.55	108.15	110.52
23	C	501	CLA	C3B-C4B-NB	-2.55	108.15	110.52
23	n	613	CLA	C3B-C4B-NB	-2.55	108.15	110.52
40	Y	316	LUT	C31-C32-C33	2.55	133.58	126.42
40	y	316	LUT	C30-C31-C32	2.55	131.17	123.22
23	N	612	CLA	C3B-C4B-NB	-2.55	108.15	110.52
23	b	612	CLA	CHB-C4A-NA	2.55	128.04	124.51
23	g	603	CLA	CHB-C4A-NA	2.55	128.03	124.51
40	g	616	LUT	C30-C31-C32	2.55	131.17	123.22
23	S	612	CLA	CHB-C4A-NA	2.55	128.03	124.51
23	r	611	CLA	CHB-C4A-NA	2.54	128.03	124.51
25	Z	101	BCR	C27-C26-C25	2.54	126.42	122.73
23	Y	312	CLA	C3B-C4B-NB	-2.54	108.16	110.52
25	b	618	BCR	C27-C26-C25	2.54	126.42	122.73
25	b	619	BCR	C24-C23-C22	-2.54	122.39	126.23
23	s	609	CLA	CHB-C1B-NB	2.54	126.95	124.26
42	N	619	XAT	O4-C5-C6	-2.54	56.85	58.96
23	G	602	CLA	CHB-C4A-NA	2.54	128.03	124.51
23	b	607	CLA	CHB-C4A-NA	2.54	128.03	124.51
23	r	608	CLA	C3B-C4B-NB	-2.54	108.16	110.52
23	B	616	CLA	CHB-C4A-NA	2.54	128.03	124.51
23	y	313	CLA	C3B-C4B-NB	-2.54	108.16	110.52
23	s	611	CLA	CHB-C4A-NA	2.54	128.02	124.51
23	c	502	CLA	CHB-C4A-NA	2.54	128.02	124.51
39	Y	309	CHL	C2A-C1A-CHA	2.54	128.30	123.86
25	Z	101	BCR	C15-C16-C17	-2.54	118.28	123.47
40	n	615	LUT	C17-C1-C6	2.54	114.41	110.30
23	a	407	CLA	C3B-C4B-NB	-2.54	108.16	110.52
23	Y	304	CLA	CHB-C4A-NA	2.54	128.02	124.51
23	G	610	CLA	CMB-C2B-C1B	-2.54	121.51	125.37
23	n	603	CLA	CHB-C4A-NA	2.54	128.02	124.51
23	a	404	CLA	CHB-C4A-NA	2.53	128.02	124.51
23	b	613	CLA	CHB-C4A-NA	2.53	128.02	124.51
23	b	616	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	N	603	CLA	CHB-C4A-NA	2.53	128.01	124.51
39	S	605	CHL	C2A-C1A-CHA	2.53	128.29	123.86
25	z	101	BCR	C24-C23-C22	-2.53	122.41	126.23
40	S	614	LUT	C22-C23-C24	-2.53	108.86	111.74
23	B	604	CLA	CHB-C4A-NA	2.53	128.01	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	n	618	NEX	C35-C34-C33	-2.53	123.70	127.31
39	n	606	CHL	C4D-CHA-C1A	2.53	124.33	121.25
39	y	303	CHL	C2A-C1A-CHA	2.53	128.28	123.86
23	C	504	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	n	602	CLA	C3B-C4B-NB	-2.53	108.17	110.52
23	b	602	CLA	CHB-C4A-NA	2.53	128.01	124.51
40	G	616	LUT	C18-C5-C6	-2.53	121.69	124.53
40	G	616	LUT	C30-C31-C32	2.52	131.09	123.22
39	n	609	CHL	C4D-CHA-C1A	2.52	124.32	121.25
23	c	513	CLA	C3B-C4B-NB	-2.52	108.18	110.52
23	A	403	CLA	CHB-C4A-NA	2.52	128.00	124.51
23	n	603	CLA	C3B-C4B-NB	-2.52	108.18	110.52
23	y	304	CLA	C3B-C4B-NB	-2.52	108.18	110.52
24	A	405	PHO	C1C-C2C-C3C	-2.52	106.52	108.61
23	C	511	CLA	CHB-C4A-NA	2.52	128.00	124.51
23	N	602	CLA	CHB-C4A-NA	2.52	128.00	124.51
39	y	310	CHL	C4D-CHA-C1A	2.52	124.31	121.25
23	n	602	CLA	CHB-C4A-NA	2.52	128.00	124.51
40	g	616	LUT	C16-C1-C6	-2.52	106.21	110.30
25	v	101	BCR	C24-C23-C22	-2.52	122.43	126.23
25	B	618	BCR	C27-C26-C25	2.52	126.39	122.73
23	Y	303	CLA	C3B-C4B-NB	-2.52	108.18	110.52
23	S	610	CLA	CHB-C4A-NA	2.52	127.99	124.51
23	R	611	CLA	CHB-C4A-NA	2.52	127.99	124.51
23	S	604	CLA	CHB-C4A-NA	2.51	127.99	124.51
23	s	604	CLA	CHB-C4A-NA	2.51	127.99	124.51
23	C	508	CLA	CHB-C4A-NA	2.51	127.99	124.51
23	s	603	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	Y	303	CLA	CHB-C4A-NA	2.51	127.98	124.51
25	B	619	BCR	C24-C23-C22	-2.51	122.44	126.23
42	R	615	XAT	C35-C15-C14	2.51	128.62	123.47
23	c	504	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	C	503	CLA	C3B-C4B-NB	-2.51	108.19	110.52
42	r	615	XAT	C35-C15-C14	2.51	128.61	123.47
23	R	603	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	s	610	CLA	CHB-C4A-NA	2.51	127.98	124.51
25	z	101	BCR	C27-C26-C25	2.51	126.37	122.73
23	N	614	CLA	C3B-C4B-NB	-2.51	108.19	110.52
23	g	611	CLA	C3B-C4B-NB	-2.51	108.19	110.52
23	A	406	CLA	CHB-C4A-NA	2.51	127.98	124.51
39	N	609	CHL	C2A-C1A-CHA	2.51	128.24	123.86
40	Y	315	LUT	C35-C34-C33	2.50	130.88	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	c	515	DGD	C3G-C2G-C1G	-2.50	105.86	111.79
23	B	607	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	b	614	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	r	604	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	V	101	BCR	C24-C23-C22	-2.50	122.45	126.23
23	r	602	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	d	406	CLA	C3B-C4B-NB	-2.50	108.19	110.52
23	A	404	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	g	602	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	K	101	BCR	C33-C5-C6	-2.50	121.72	124.53
25	C	514	BCR	C15-C16-C17	-2.50	118.35	123.47
23	Y	312	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	b	604	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	B	608	CLA	C3B-C4B-NB	-2.50	108.20	110.52
23	N	613	CLA	C3B-C4B-NB	-2.50	108.20	110.52
25	Z	101	BCR	C24-C23-C22	-2.50	122.46	126.23
23	c	511	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	a	405	CLA	C3B-C4B-NB	-2.50	108.20	110.52
23	A	404	CLA	C3B-C4B-NB	-2.50	108.20	110.52
23	B	613	CLA	C3B-C4B-NB	-2.49	108.20	110.52
23	g	614	CLA	C3B-C4B-NB	-2.49	108.20	110.52
23	B	613	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	a	403	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	G	610	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	g	610	CLA	C3B-C4B-NB	-2.49	108.20	110.52
23	B	611	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	y	313	CLA	CHB-C4A-NA	2.49	127.95	124.51
40	y	316	LUT	C38-C25-C24	-2.49	118.24	123.56
23	c	503	CLA	CHB-C4A-NA	2.49	127.95	124.51
42	G	619	XAT	C31-C32-C33	2.49	133.40	126.42
23	r	604	CLA	C3B-C4B-NB	-2.49	108.21	110.52
25	c	514	BCR	C15-C16-C17	-2.49	118.38	123.47
23	y	304	CLA	CHB-C4A-NA	2.48	127.95	124.51
40	y	316	LUT	C18-C5-C6	-2.48	121.74	124.53
23	N	612	CLA	CHB-C4A-NA	2.48	127.94	124.51
23	n	612	CLA	CHB-C4A-NA	2.48	127.94	124.51
23	s	612	CLA	C3B-C4B-NB	-2.48	108.21	110.52
39	g	609	CHL	C4D-CHA-C1A	2.48	124.27	121.25
23	S	611	CLA	CHB-C4A-NA	2.48	127.94	124.51
40	G	615	LUT	C17-C1-C6	2.48	114.32	110.30
23	r	603	CLA	CHB-C4A-NA	2.48	127.94	124.51
23	a	405	CLA	CHB-C4A-NA	2.48	127.94	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	R	602	CLA	CHB-C4A-NA	2.48	127.94	124.51
23	C	503	CLA	CHB-C4A-NA	2.48	127.94	124.51
23	s	609	CLA	CMB-C2B-C1B	-2.48	121.60	125.37
40	g	615	LUT	C17-C1-C6	2.48	114.32	110.30
23	y	315	CLA	CHB-C4A-NA	2.48	127.94	124.51
40	Y	315	LUT	C38-C25-C24	-2.48	118.26	123.56
25	k	101	BCR	C33-C5-C6	-2.47	121.75	124.53
23	N	611	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	s	613	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	R	604	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	b	615	CLA	C3B-C4B-NB	-2.47	108.22	110.52
23	c	501	CLA	C3B-C4B-NB	-2.47	108.22	110.52
23	B	614	CLA	CHB-C4A-NA	2.47	127.93	124.51
24	a	406	PHO	C1C-C2C-C3C	-2.47	106.56	108.61
23	A	402	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	n	614	CLA	CHB-C4A-NA	2.47	127.93	124.51
39	s	606	CHL	C2A-C1A-CHA	2.47	128.18	123.86
23	b	606	CLA	O2A-CGA-O1A	-2.47	117.37	123.59
23	Y	311	CLA	CHB-C4A-NA	2.47	127.92	124.51
39	Y	302	CHL	C2A-C1A-CHA	2.47	128.17	123.86
23	S	602	CLA	CHB-C4A-NA	2.47	127.92	124.51
23	c	509	CLA	CHB-C4A-NA	2.47	127.92	124.51
23	c	510	CLA	CHB-C4A-NA	2.46	127.92	124.51
23	G	610	CLA	C3B-C4B-NB	-2.46	108.23	110.52
40	n	616	LUT	C30-C31-C32	2.46	130.90	123.22
23	n	611	CLA	CHB-C4A-NA	2.46	127.92	124.51
23	g	610	CLA	CHB-C4A-NA	2.46	127.92	124.51
25	c	514	BCR	C11-C10-C9	-2.46	123.80	127.31
41	r	614	NEX	C35-C34-C33	-2.46	123.80	127.31
23	S	613	CLA	CHB-C4A-NA	2.46	127.91	124.51
23	b	608	CLA	CHB-C4A-NA	2.46	127.91	124.51
23	s	611	CLA	C3B-C4B-NB	-2.46	108.24	110.52
23	n	613	CLA	CHB-C4A-NA	2.46	127.91	124.51
40	y	316	LUT	C35-C34-C33	2.45	130.81	127.31
23	R	612	CLA	CHB-C4A-NA	2.45	127.91	124.51
23	Y	314	CLA	CHB-C4A-NA	2.45	127.91	124.51
23	c	511	CLA	C3B-C4B-NB	-2.45	108.24	110.52
40	r	613	LUT	C3-C4-C5	2.45	116.74	111.85
23	C	513	CLA	C3B-C4B-NB	-2.45	108.24	110.52
23	s	612	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	s	602	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	G	603	CLA	C3B-C4B-NB	-2.45	108.24	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	Y	302	CHL	C4D-CHA-C1A	2.45	124.23	121.25
23	R	610	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	c	504	CLA	C3B-C4B-NB	-2.45	108.24	110.52
41	R	614	NEX	O24-C25-C38	-2.45	112.12	115.06
23	B	611	CLA	C3B-C4B-NB	-2.45	108.25	110.52
30	D	408	LHG	O8-C23-O10	-2.45	117.42	123.59
23	R	601	CLA	CHB-C4A-NA	2.45	127.89	124.51
23	c	508	CLA	CHB-C4A-NA	2.45	127.89	124.51
23	B	612	CLA	C3B-C4B-NB	-2.45	108.25	110.52
25	A	407	BCR	C15-C14-C13	-2.44	123.82	127.31
25	a	408	BCR	C15-C14-C13	-2.44	123.82	127.31
23	C	504	CLA	C3B-C4B-NB	-2.44	108.25	110.52
23	b	610	CLA	CHB-C4A-NA	2.44	127.89	124.51
23	b	611	CLA	C3B-C4B-NB	-2.44	108.25	110.52
41	g	617	NEX	C5-C6-C1	-2.44	117.27	119.70
23	b	603	CLA	CHB-C4A-NA	2.44	127.89	124.51
23	B	608	CLA	CHB-C4A-NA	2.44	127.88	124.51
23	B	603	CLA	CHB-C4A-NA	2.44	127.88	124.51
23	G	613	CLA	CHB-C4A-NA	2.44	127.88	124.51
23	g	610	CLA	CMB-C2B-C1B	-2.44	121.66	125.37
23	b	605	CLA	CHB-C4A-NA	2.44	127.88	124.51
23	b	611	CLA	CHB-C4A-NA	2.44	127.88	124.51
23	N	604	CLA	C3B-C4B-NB	-2.44	108.25	110.52
23	B	602	CLA	C1-C2-C3	-2.44	121.83	126.04
23	Y	310	CLA	CHB-C4A-NA	2.43	127.88	124.51
40	g	616	LUT	C38-C25-C24	-2.43	118.35	123.56
23	c	503	CLA	C3B-C4B-NB	-2.43	108.26	110.52
42	n	620	XAT	C16-C1-C6	-2.43	103.48	110.05
42	n	620	XAT	C31-C30-C29	2.43	130.78	127.31
41	Y	317	NEX	C19-C9-C8	-2.43	113.29	118.93
23	c	513	CLA	CHB-C4A-NA	2.43	127.88	124.51
25	C	514	BCR	C33-C5-C6	-2.43	121.80	124.53
25	b	617	BCR	C3-C4-C5	-2.43	109.74	114.08
23	C	510	CLA	CHB-C4A-NA	2.43	127.87	124.51
23	g	611	CLA	CHB-C4A-NA	2.43	127.87	124.51
23	R	609	CLA	CHB-C4A-NA	2.43	127.87	124.51
23	r	601	CLA	CHB-C4A-NA	2.43	127.87	124.51
23	g	613	CLA	CHB-C4A-NA	2.43	127.87	124.51
23	B	602	CLA	CHB-C4A-NA	2.42	127.86	124.51
23	N	604	CLA	CHB-C4A-NA	2.42	127.86	124.51
23	r	609	CLA	CHB-C4A-NA	2.42	127.86	124.51
23	B	606	CLA	CHB-C1B-NB	2.42	126.82	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	509	CLA	CHB-C4A-NA	2.42	127.86	124.51
25	C	514	BCR	C11-C10-C9	-2.42	123.86	127.31
40	R	613	LUT	C3-C4-C5	2.42	116.67	111.85
42	n	617	XAT	C35-C15-C14	2.42	128.43	123.47
42	N	619	XAT	C16-C1-C6	-2.42	103.52	110.05
23	B	616	CLA	C3B-C4B-NB	-2.42	108.27	110.52
30	D	408	LHG	O8-C23-C24	2.42	119.49	111.91
23	g	613	CLA	C3B-C4B-NB	-2.42	108.27	110.52
33	d	411	DGD	C1D-C2D-C3D	-2.42	104.96	110.00
23	G	604	CLA	CHB-C4A-NA	2.42	127.85	124.51
23	G	611	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	g	604	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	r	610	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	y	311	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	n	604	CLA	CHB-C4A-NA	2.41	127.84	124.51
23	G	604	CLA	C3B-C4B-NB	-2.41	108.28	110.52
23	S	611	CLA	C3B-C4B-NB	-2.41	108.28	110.52
23	B	605	CLA	CHB-C4A-NA	2.41	127.84	124.51
23	C	511	CLA	C3B-C4B-NB	-2.41	108.28	110.52
40	n	615	LUT	C38-C25-C24	-2.41	118.41	123.56
25	c	514	BCR	C33-C5-C6	-2.41	121.83	124.53
23	A	403	CLA	C3B-C4B-NB	-2.40	108.28	110.52
39	g	608	CHL	C4D-CHA-C1A	2.40	124.17	121.25
23	y	314	CLA	CHB-C4A-NA	2.40	127.83	124.51
23	b	616	CLA	C3B-C4B-NB	-2.40	108.29	110.52
25	b	619	BCR	C27-C26-C25	2.40	126.22	122.73
23	b	613	CLA	C3B-C4B-NB	-2.40	108.29	110.52
25	A	407	BCR	C15-C16-C17	-2.40	118.56	123.47
23	R	604	CLA	C3B-C4B-NB	-2.40	108.29	110.52
23	g	614	CLA	CHB-C4A-NA	2.40	127.83	124.51
39	S	607	CHL	C2A-C1A-CHA	2.40	128.05	123.86
23	g	604	CLA	C3B-C4B-NB	-2.40	108.29	110.52
23	N	610	CLA	CHB-C4A-NA	2.40	127.83	124.51
25	c	514	BCR	C7-C8-C9	-2.40	122.61	126.23
23	A	402	CLA	C3B-C4B-NB	-2.40	108.29	110.52
42	Y	301	XAT	C18-C5-C4	2.39	116.97	114.28
23	a	403	CLA	C3B-C4B-NB	-2.39	108.29	110.52
24	d	402	PHO	C1C-C2C-C3C	-2.39	106.62	108.61
23	B	610	CLA	CHB-C4A-NA	2.39	127.82	124.51
23	N	614	CLA	CHB-C4A-NA	2.39	127.82	124.51
23	B	605	CLA	C3B-C4B-NB	-2.39	108.30	110.52
25	D	411	BCR	C27-C26-C25	2.39	126.20	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	r	612	CLA	CHB-C4A-NA	2.39	127.82	124.51
23	G	610	CLA	C1-C2-C3	-2.39	121.91	126.04
23	D	405	CLA	CHB-C4A-NA	2.39	127.81	124.51
23	C	506	CLA	CHB-C4A-NA	2.39	127.81	124.51
23	y	312	CLA	CHB-C4A-NA	2.39	127.81	124.51
23	a	404	CLA	C3B-C4B-NB	-2.39	108.30	110.52
23	b	606	CLA	CHB-C1B-NB	2.39	126.78	124.26
23	c	506	CLA	CHB-C4A-NA	2.38	127.81	124.51
23	a	405	CLA	O2D-CGD-CBD	2.38	115.50	111.27
42	y	302	XAT	C18-C5-C4	2.38	116.96	114.28
23	n	610	CLA	CHB-C4A-NA	2.38	127.81	124.51
23	b	603	CLA	C3B-C4B-NB	-2.38	108.31	110.52
23	Y	313	CLA	CHB-C4A-NA	2.38	127.81	124.51
25	C	514	BCR	C7-C8-C9	-2.38	122.64	126.23
25	A	407	BCR	C11-C10-C9	-2.38	123.91	127.31
25	C	514	BCR	C27-C26-C25	2.38	126.19	122.73
23	B	603	CLA	C3B-C4B-NB	-2.38	108.31	110.52
23	b	607	CLA	C3B-C4B-NB	-2.38	108.31	110.52
40	G	616	LUT	C38-C25-C24	-2.38	118.47	123.56
23	n	604	CLA	C3B-C4B-NB	-2.38	108.31	110.52
24	D	402	PHO	C1C-C2C-C3C	-2.38	106.63	108.61
23	d	405	CLA	CHB-C4A-NA	2.38	127.80	124.51
25	c	514	BCR	C27-C26-C25	2.38	126.18	122.73
23	R	603	CLA	C3B-C4B-NB	-2.38	108.31	110.52
23	r	603	CLA	C3B-C4B-NB	-2.37	108.31	110.52
23	Y	305	CLA	CHB-C4A-NA	2.37	127.79	124.51
25	A	407	BCR	C33-C5-C6	-2.37	121.86	124.53
23	B	606	CLA	CHB-C4A-NA	2.37	127.79	124.51
23	C	513	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
25	a	408	BCR	C15-C16-C17	-2.37	118.61	123.47
35	y	301	VIV	C12-C5-C4	-2.37	117.64	121.30
42	n	617	XAT	C36-C21-C26	-2.37	103.64	110.05
23	b	609	CLA	CHB-C4A-NA	2.37	127.79	124.51
23	y	306	CLA	C3B-C4B-NB	-2.37	108.32	110.52
23	A	404	CLA	O2D-CGD-CBD	2.37	115.47	111.27
23	B	606	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
25	b	618	BCR	C33-C5-C6	-2.36	121.87	124.53
23	A	403	CLA	CHD-C1D-ND	-2.36	122.28	124.45
40	g	615	LUT	C8-C9-C10	2.36	122.56	118.94
40	G	615	LUT	C18-C5-C6	-2.36	121.88	124.53
23	G	614	CLA	CHB-C4A-NA	2.36	127.78	124.51
23	y	306	CLA	CHB-C4A-NA	2.36	127.78	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	508	CLA	C3B-C4B-NB	-2.36	108.33	110.52
25	B	619	BCR	C27-C26-C25	2.36	126.16	122.73
40	n	615	LUT	C30-C31-C32	2.36	130.58	123.22
25	B	617	BCR	C27-C26-C25	2.36	126.16	122.73
40	S	614	LUT	C3-C4-C5	2.35	116.54	111.85
23	S	612	CLA	C3B-C4B-NB	-2.35	108.33	110.52
25	a	408	BCR	C33-C5-C6	-2.35	121.89	124.53
23	b	601	CLA	C1-C2-C3	-2.35	122.95	126.75
41	r	614	NEX	C30-C31-C32	2.35	130.56	123.22
40	N	615	LUT	C30-C31-C32	2.35	130.55	123.22
40	g	615	LUT	C18-C5-C6	-2.35	121.89	124.53
42	Y	301	XAT	C31-C30-C29	2.35	130.66	127.31
23	b	602	CLA	C3B-C4B-NB	-2.35	108.34	110.52
33	H	502	DGD	C1D-C2D-C3D	-2.35	105.11	110.00
23	c	512	CLA	CHB-C4A-NA	2.35	127.76	124.51
23	C	502	CLA	C3B-C4B-NB	-2.35	108.34	110.52
41	R	614	NEX	C30-C31-C32	2.34	130.53	123.22
23	c	512	CLA	C3B-C4B-NB	-2.34	108.34	110.52
23	B	609	CLA	CHB-C4A-NA	2.34	127.75	124.51
23	s	608	CLA	CHB-C4A-NA	2.34	127.75	124.51
25	a	408	BCR	C27-C26-C25	2.34	126.13	122.73
41	N	617	NEX	C30-C31-C32	2.34	130.52	123.22
23	s	609	CLA	CHB-C4A-NA	2.34	127.74	124.51
23	Y	304	CLA	C3B-C4B-NB	-2.34	108.35	110.52
35	C	523	VIV	O1-C4-C3	2.34	124.79	122.36
41	s	617	NEX	C35-C34-C33	-2.33	123.95	127.30
23	C	512	CLA	CHB-C4A-NA	2.33	127.74	124.51
42	N	619	XAT	C36-C21-C26	-2.33	103.74	110.05
42	R	615	XAT	C31-C30-C29	2.33	130.64	127.31
23	g	610	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
23	B	602	CLA	C3B-C4B-NB	-2.33	108.35	110.52
26	A	408	SQD	O5-C5-C4	2.33	113.92	109.69
42	r	615	XAT	C31-C30-C29	2.33	130.63	127.31
23	a	404	CLA	CHD-C1D-ND	-2.33	122.32	124.45
38	f	501	HEM	C4C-NC-C1C	2.32	107.62	105.35
25	a	408	BCR	C11-C10-C9	-2.32	124.00	127.31
41	G	617	NEX	C14-C15-C35	2.32	131.38	125.55
23	Y	305	CLA	C3B-C4B-NB	-2.32	108.37	110.52
23	C	512	CLA	C3B-C4B-NB	-2.32	108.37	110.52
40	S	614	LUT	C38-C25-C24	-2.31	118.61	123.56
42	y	302	XAT	C30-C31-C32	2.31	130.43	123.22
23	N	604	CLA	CMB-C2B-C1B	-2.31	121.85	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	r	613	LUT	C4-C5-C6	2.31	126.00	120.85
23	B	604	CLA	C1-C2-C3	-2.31	122.05	126.04
40	s	615	LUT	C3-C4-C5	2.31	116.45	111.85
41	n	618	NEX	C30-C31-C32	2.31	130.42	123.22
23	c	502	CLA	C3B-C4B-NB	-2.31	108.38	110.52
40	s	614	LUT	C3-C4-C5	2.30	116.44	111.85
23	S	613	CLA	C3B-C4B-NB	-2.30	108.38	110.52
23	n	604	CLA	CMB-C2B-C1B	-2.30	121.86	125.37
23	y	315	CLA	C1-C2-C3	-2.30	122.06	126.04
23	B	607	CLA	C3B-C4B-NB	-2.30	108.38	110.52
41	R	614	NEX	C35-C34-C33	-2.30	124.03	127.31
40	S	614	LUT	C17-C1-C6	2.30	114.02	110.30
23	Y	310	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
41	g	617	NEX	O24-C25-C38	-2.29	112.31	115.06
25	k	101	BCR	C15-C14-C13	-2.29	124.04	127.31
23	S	609	CLA	CHB-C4A-NA	2.29	127.68	124.51
23	b	606	CLA	CHB-C4A-NA	2.29	127.68	124.51
23	C	509	CLA	C3B-C4B-NB	-2.29	108.39	110.52
28	T	101	3PH	O13-P-O11	-2.29	100.63	106.73
25	b	617	BCR	C27-C26-C25	2.29	126.06	122.73
40	N	615	LUT	C38-C25-C24	-2.29	118.66	123.56
23	b	605	CLA	C3B-C4B-NB	-2.29	108.39	110.52
25	A	407	BCR	C27-C26-C25	2.29	126.05	122.73
40	R	613	LUT	C39-C29-C28	-2.29	114.47	118.08
25	Z	101	BCR	C33-C5-C6	-2.29	121.96	124.53
23	g	613	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
23	C	508	CLA	C3B-C4B-NB	-2.28	108.40	110.52
33	C	515	DGD	C1D-C2D-C3D	-2.28	105.24	110.00
40	S	615	LUT	C38-C25-C24	-2.28	118.67	123.56
23	s	602	CLA	CHD-C1D-ND	-2.28	122.36	124.45
40	r	613	LUT	C38-C25-C24	-2.28	118.68	123.56
23	C	508	CLA	CMB-C2B-C1B	-2.28	121.90	125.37
42	n	617	XAT	C31-C32-C33	2.28	132.82	126.42
23	N	603	CLA	C3B-C4B-NB	-2.28	108.40	110.52
33	c	515	DGD	C1D-C2D-C3D	-2.28	105.25	110.00
42	G	619	XAT	C35-C15-C14	2.27	128.13	123.47
23	b	611	CLA	CHD-C1D-ND	-2.27	122.36	124.45
25	z	101	BCR	C33-C5-C6	-2.27	121.98	124.53
23	c	509	CLA	C3B-C4B-NB	-2.27	108.41	110.52
40	r	613	LUT	C17-C1-C6	2.27	113.98	110.30
42	R	615	XAT	C18-C5-C4	2.27	116.83	114.28
42	r	615	XAT	C18-C5-C4	2.27	116.83	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	y	306	CLA	CMB-C2B-C1B	-2.27	121.92	125.37
25	V	101	BCR	C27-C26-C25	2.27	126.02	122.73
23	b	604	CLA	C1-C2-C3	-2.27	122.12	126.04
23	b	609	CLA	C3B-C4B-NB	-2.27	108.41	110.52
23	B	611	CLA	CHD-C1D-ND	-2.26	122.37	124.45
23	S	609	CLA	CHB-C1B-NB	2.26	126.65	124.26
28	L	102	3PH	O13-P-O11	-2.26	100.72	106.73
24	A	405	PHO	C1-C2-C3	-2.26	122.14	126.04
40	Y	315	LUT	C18-C5-C6	-2.26	121.99	124.53
40	g	615	LUT	C38-C25-C24	-2.26	118.73	123.56
28	W	201	3PH	O13-P-O11	-2.25	100.74	106.73
40	S	615	LUT	C39-C29-C28	-2.25	114.53	118.08
25	b	619	BCR	C11-C10-C9	-2.25	124.10	127.31
38	f	501	HEM	C2A-C1A-NA	-2.25	107.63	110.15
23	N	613	CLA	C1-C2-C3	-2.25	122.16	126.04
40	N	616	LUT	C38-C25-C24	-2.24	118.76	123.56
25	c	514	BCR	C15-C14-C13	-2.24	124.11	127.31
25	K	101	BCR	C15-C14-C13	-2.24	124.11	127.31
23	s	613	CLA	C3B-C4B-NB	-2.24	108.44	110.52
23	y	311	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
30	S	616	LHG	O8-C23-C24	2.24	118.94	111.91
23	c	508	CLA	CMB-C2B-C1B	-2.24	121.96	125.37
23	N	610	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
38	F	501	HEM	C3D-C4D-ND	-2.24	107.67	110.17
23	G	613	CLA	C3B-C4B-NB	-2.24	108.44	110.52
25	v	101	BCR	C27-C26-C25	2.24	125.98	122.73
30	d	404	LHG	O8-C23-C24	2.24	118.92	111.91
28	A	410	3PH	O13-P-O11	-2.24	100.78	106.73
25	d	410	BCR	C11-C10-C9	-2.24	124.12	127.31
33	C	515	DGD	CFB-CEB-CDB	-2.23	103.08	114.42
28	C	524	3PH	O13-P-O11	-2.23	100.79	106.73
41	g	617	NEX	C30-C31-C32	2.23	130.19	123.22
25	d	410	BCR	C15-C16-C17	-2.23	118.90	123.47
23	n	610	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
23	C	510	CLA	CHD-C1D-ND	-2.23	122.41	124.45
40	N	615	LUT	C17-C1-C6	2.23	113.92	110.30
33	H	502	DGD	CBB-CAB-C9B	-2.23	103.11	114.42
42	N	619	XAT	C31-C30-C29	2.23	130.49	127.31
39	r	607	CHL	CAA-C2A-C1A	2.23	119.27	111.97
30	R	616	LHG	O8-C23-C24	2.23	118.90	111.91
23	Y	305	CLA	CMB-C2B-C1B	-2.23	121.98	125.37
33	d	411	DGD	C3G-C2G-C1G	-2.22	106.53	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	y	302	XAT	C31-C32-C33	2.22	132.66	126.42
41	G	617	NEX	C30-C31-C32	2.22	130.15	123.22
23	y	313	CLA	CHB-C1B-NB	2.22	126.61	124.26
23	b	611	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
40	G	615	LUT	C38-C25-C24	-2.22	118.82	123.56
23	a	407	CLA	C1-C2-C3	-2.22	122.21	126.04
23	b	606	CLA	CHD-C1D-ND	-2.21	122.42	124.45
23	G	614	CLA	CHD-C1D-ND	-2.21	122.42	124.45
23	N	604	CLA	CHD-C1D-ND	-2.21	122.42	124.45
23	R	604	CLA	CHD-C1D-ND	-2.21	122.42	124.45
23	y	306	CLA	CHD-C1D-ND	-2.21	122.42	124.45
23	c	505	CLA	CHB-C4A-NA	2.21	127.57	124.51
23	R	609	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
30	g	618	LHG	O8-C23-C24	2.21	118.84	111.91
23	b	615	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
39	R	607	CHL	C4B-CHC-C1C	-2.21	121.10	126.34
23	c	501	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
30	A	412	LHG	O8-C23-C24	2.21	118.83	111.91
23	a	407	CLA	CHD-C1D-ND	-2.21	122.43	124.45
23	B	609	CLA	C3B-C4B-NB	-2.21	108.47	110.52
25	z	101	BCR	C15-C14-C13	-2.21	124.16	127.31
23	S	613	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
23	B	608	CLA	CHD-C1D-ND	-2.20	122.43	124.45
23	S	608	CLA	CHB-C4A-NA	2.20	127.56	124.51
23	C	501	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
28	w	202	3PH	O13-P-O11	-2.20	100.87	106.73
23	y	312	CLA	CHD-C1D-ND	-2.20	122.43	124.45
23	g	603	CLA	C2D-C1D-ND	-2.20	108.48	110.10
30	Y	318	LHG	O8-C23-C24	2.20	118.81	111.91
40	s	614	LUT	C17-C1-C6	2.20	113.86	110.30
30	d	408	LHG	O8-C23-C24	2.20	118.81	111.91
33	H	502	DGD	C3G-C2G-C1G	-2.20	106.59	111.79
39	G	620	CHL	CHA-C1A-NA	-2.20	121.37	126.40
23	B	603	CLA	O2A-CGA-O1A	-2.19	118.05	123.59
23	r	609	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
23	r	602	CLA	O2D-CGD-CBD	2.19	115.17	111.27
23	n	602	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
25	D	411	BCR	C33-C5-C6	-2.19	122.07	124.53
25	b	619	BCR	C33-C5-C6	-2.19	122.07	124.53
23	b	613	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
23	Y	312	CLA	CHB-C1B-NB	2.19	126.57	124.26
42	y	302	XAT	C31-C30-C29	2.19	130.43	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	F	501	HEM	C2A-C1A-NA	-2.19	107.70	110.15
23	G	604	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
23	C	505	CLA	CHB-C4A-NA	2.19	127.54	124.51
23	N	604	CLA	CHB-C1B-NB	2.19	126.57	124.26
23	n	604	CLA	CHB-C1B-NB	2.18	126.57	124.26
23	N	602	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
23	s	613	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
41	s	617	NEX	C40-C33-C34	-2.18	111.09	122.73
23	c	512	CLA	CHD-C1D-ND	-2.18	122.45	124.45
40	y	316	LUT	C12-C13-C14	2.18	122.29	118.94
23	Y	311	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
25	C	514	BCR	C15-C14-C13	-2.18	124.20	127.31
40	R	613	LUT	C17-C1-C6	2.18	113.83	110.30
40	y	317	LUT	C38-C25-C24	-2.18	118.89	123.56
23	b	616	CLA	CHD-C1D-ND	-2.18	122.45	124.45
23	y	305	CLA	C3B-C4B-NB	-2.18	108.49	110.52
25	c	514	BCR	C24-C23-C22	-2.18	122.94	126.23
23	B	610	CLA	CHB-C1B-NB	2.18	126.56	124.26
40	Y	316	LUT	C38-C25-C24	-2.18	118.90	123.56
28	X	201	3PH	O13-P-O11	-2.18	100.94	106.73
39	g	605	CHL	CHA-C1A-NA	-2.18	121.41	126.40
33	c	515	DGD	CBB-CAB-C9B	-2.18	103.38	114.42
23	y	312	CLA	O2D-CGD-CBD	2.18	115.13	111.27
23	S	602	CLA	CHD-C1D-ND	-2.17	122.46	124.45
23	a	403	CLA	CMB-C2B-C1B	-2.17	122.06	125.37
23	B	602	CLA	CHD-C1D-ND	-2.17	122.46	124.45
40	s	615	LUT	C38-C25-C24	-2.17	118.91	123.56
23	s	604	CLA	CHB-C1B-NB	2.17	126.56	124.26
23	S	609	CLA	CMB-C2B-C1B	-2.17	122.06	125.37
23	b	602	CLA	CHD-C1D-ND	-2.17	122.46	124.45
23	y	312	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
23	D	406	CLA	CHD-C1D-ND	-2.17	122.46	124.45
23	S	612	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
39	g	619	CHL	CHA-C1A-NA	-2.17	121.43	126.40
33	C	515	DGD	CBB-CAB-C9B	-2.17	103.42	114.42
40	Y	315	LUT	C17-C1-C6	2.17	113.82	110.30
23	B	602	CLA	CMB-C2B-C1B	-2.17	122.07	125.37
23	a	404	CLA	C1-C2-C3	-2.17	122.29	126.04
23	B	606	CLA	CHD-C1D-ND	-2.17	122.46	124.45
23	B	610	CLA	CHD-C1D-ND	-2.17	122.46	124.45
23	b	610	CLA	CHB-C1B-NB	2.17	126.55	124.26
23	A	402	CLA	CMB-C2B-C1B	-2.17	122.07	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Y	305	CLA	CHD-C1D-ND	-2.16	122.47	124.45
23	c	510	CLA	CHD-C1D-ND	-2.16	122.47	124.45
40	s	614	LUT	C38-C25-C24	-2.16	118.93	123.56
30	a	412	LHG	O8-C23-C24	2.16	118.69	111.91
23	B	615	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
23	c	506	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
40	y	316	LUT	C17-C1-C6	2.16	113.80	110.30
41	S	617	NEX	C19-C9-C8	-2.16	113.93	118.93
35	y	301	VIV	C11-C10-C3	-2.16	108.38	111.75
23	n	613	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
30	r	616	LHG	O8-C23-C24	2.16	118.67	111.91
41	s	617	NEX	C19-C9-C8	-2.16	113.93	118.93
23	s	610	CLA	C1-C2-C3	-2.15	122.32	126.04
23	R	604	CLA	CMB-C2B-C1B	-2.15	122.09	125.37
23	s	612	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
40	S	615	LUT	C3-C4-C5	2.15	116.14	111.85
23	G	613	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
23	S	609	CLA	CHD-C1D-ND	-2.15	122.47	124.45
23	y	313	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
23	y	305	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
23	A	406	CLA	CHD-C1D-ND	-2.15	122.48	124.45
23	S	610	CLA	C1-C2-C3	-2.15	122.32	126.04
23	Y	305	CLA	CHB-C1B-NB	2.15	126.53	124.26
25	D	411	BCR	C24-C23-C22	-2.15	122.98	126.23
25	b	617	BCR	C24-C23-C22	-2.15	122.98	126.23
23	G	612	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
39	G	607	CHL	CHA-C1A-NA	-2.15	121.47	126.40
41	G	617	NEX	C38-C25-C24	-2.15	111.86	114.28
23	Y	313	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
25	C	514	BCR	C24-C23-C22	-2.15	122.99	126.23
23	S	604	CLA	CHB-C1B-NB	2.15	126.53	124.26
23	Y	305	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
39	r	607	CHL	C4B-CHC-C1C	-2.15	121.25	126.34
23	b	608	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
25	b	617	BCR	C8-C7-C6	-2.15	121.18	127.20
39	r	607	CHL	CHA-C1A-NA	-2.14	121.49	126.40
25	Z	101	BCR	C15-C14-C13	-2.14	124.25	127.31
42	Y	301	XAT	C11-C10-C9	2.14	130.37	127.31
23	b	608	CLA	CHD-C1D-ND	-2.14	122.48	124.45
23	n	604	CLA	CHD-C1D-ND	-2.14	122.48	124.45
23	A	403	CLA	C1-C2-C3	-2.14	122.34	126.04
23	C	512	CLA	C1-C2-C3	-2.14	122.34	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	618	BCR	C24-C23-C22	-2.14	123.00	126.23
41	R	614	NEX	C25-C24-C23	-2.14	108.51	112.75
25	k	101	BCR	C27-C26-C25	2.14	125.84	122.73
23	r	608	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
39	n	605	CHL	CHD-C1D-C2D	2.14	129.97	125.48
42	n	620	XAT	C36-C21-C26	-2.14	104.27	110.05
30	s	616	LHG	O8-C23-C24	2.14	118.62	111.91
23	b	604	CLA	C3B-C4B-NB	-2.14	108.53	110.52
23	g	604	CLA	CHD-C1D-ND	-2.14	122.49	124.45
23	G	613	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
23	B	612	CLA	C1-C2-C3	-2.14	122.35	126.04
33	c	515	DGD	CAB-C9B-C8B	-2.14	103.58	114.42
39	N	607	CHL	CHA-C1A-NA	-2.14	121.51	126.40
23	r	610	CLA	CHD-C1D-ND	-2.13	122.49	124.45
23	G	603	CLA	O2A-CGA-O1A	-2.13	118.20	123.59
42	y	302	XAT	O4-C5-C6	-2.13	57.19	58.96
23	C	511	CLA	CMB-C2B-C1B	-2.13	122.12	125.37
23	b	607	CLA	CMB-C2B-C1B	-2.13	122.12	125.37
30	N	618	LHG	O8-C23-C24	2.13	118.60	111.91
23	y	304	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
23	S	613	CLA	CHD-C1D-ND	-2.13	122.49	124.45
23	a	407	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
23	B	604	CLA	C3B-C4B-NB	-2.13	108.54	110.52
23	r	610	CLA	CHB-C1B-NB	2.13	126.51	124.26
23	r	604	CLA	CHD-C1D-ND	-2.13	122.50	124.45
23	G	610	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
23	d	405	CLA	C3B-C4B-NB	-2.13	108.54	110.52
23	y	314	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
23	B	616	CLA	CHD-C1D-ND	-2.13	122.50	124.45
23	G	602	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
23	g	612	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
39	g	607	CHL	CHA-C1A-NA	-2.13	121.52	126.40
23	b	606	CLA	C1-C2-C3	-2.13	122.36	126.04
23	s	613	CLA	CHD-C1D-ND	-2.13	122.50	124.45
23	c	512	CLA	C1-C2-C3	-2.13	122.36	126.04
33	C	515	DGD	C5B-C4B-C3B	-2.13	103.62	114.42
23	b	609	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
25	B	619	BCR	C33-C5-C6	-2.13	122.14	124.53
23	c	511	CLA	CMB-C2B-C1B	-2.12	122.13	125.37
23	C	506	CLA	C3B-C4B-NB	-2.12	108.54	110.52
23	R	603	CLA	CHD-C1D-ND	-2.12	122.50	124.45
39	n	605	CHL	CHA-C1A-NA	-2.12	121.53	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	y	306	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
23	b	612	CLA	C1-C2-C3	-2.12	122.37	126.04
41	N	617	NEX	C38-C25-C24	-2.12	111.89	114.28
23	B	608	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
23	d	406	CLA	CHD-C1D-ND	-2.12	122.50	124.45
23	R	601	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
23	R	612	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
23	y	311	CLA	C1-C2-C3	-2.12	122.38	126.04
40	R	613	LUT	C4-C5-C6	2.12	125.57	120.85
23	R	603	CLA	CMB-C2B-C1B	-2.12	122.14	125.37
39	R	606	CHL	CHA-C1A-NA	-2.12	121.55	126.40
42	y	302	XAT	C11-C10-C9	2.12	130.33	127.31
39	R	607	CHL	CAA-C2A-C1A	2.12	118.92	111.97
23	N	610	CLA	C1-C2-C3	-2.12	122.38	126.04
23	Y	303	CLA	C1-C2-C3	-2.12	122.38	126.04
30	D	404	LHG	O8-C23-C24	2.12	118.55	111.91
25	K	101	BCR	C27-C26-C25	2.12	125.81	122.73
23	G	604	CLA	CHD-C1D-ND	-2.12	122.51	124.45
23	s	609	CLA	CHD-C1D-ND	-2.12	122.51	124.45
23	Y	312	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
39	G	609	CHL	CHD-C1D-C2D	2.12	129.92	125.48
23	B	616	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
23	g	603	CLA	C3B-C4B-NB	-2.11	108.55	110.52
23	y	306	CLA	CHB-C1B-NB	2.11	126.50	124.26
35	y	301	VIV	O2-C7-C6	2.11	123.67	118.10
28	x	201	3PH	O13-P-O11	-2.11	101.11	106.73
40	y	317	LUT	C17-C1-C6	2.11	113.72	110.30
38	f	501	HEM	C3D-C4D-ND	-2.11	107.82	110.17
39	n	607	CHL	CHA-C1A-NA	-2.11	121.56	126.40
23	s	610	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
25	h	501	BCR	C38-C26-C25	-2.11	122.16	124.53
23	C	507	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
23	s	604	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
23	b	610	CLA	CHD-C1D-ND	-2.11	122.52	124.45
23	A	406	CLA	C1-C2-C3	-2.11	122.40	126.04
23	N	604	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
23	Y	310	CLA	C1-C2-C3	-2.11	122.40	126.04
23	c	502	CLA	CHD-C1D-ND	-2.11	122.52	124.45
28	s	618	3PH	O13-P-O11	-2.11	101.13	106.73
23	b	603	CLA	CHD-C1D-ND	-2.11	122.52	124.45
25	B	618	BCR	C11-C10-C9	-2.11	124.31	127.31
23	B	609	CLA	O2A-CGA-O1A	-2.11	118.28	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	618	BCR	C11-C10-C9	-2.10	124.31	127.31
41	g	617	NEX	C19-C9-C8	-2.10	114.05	118.93
23	B	603	CLA	CHD-C1D-ND	-2.10	122.52	124.45
23	c	508	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
39	N	605	CHL	CHD-C1D-C2D	2.10	129.89	125.48
30	y	318	LHG	O8-C23-C24	2.10	118.51	111.91
23	c	508	CLA	CHB-C1B-NB	2.10	126.48	124.26
33	C	515	DGD	CAB-C9B-C8B	-2.10	103.75	114.42
25	B	618	BCR	C24-C23-C22	-2.10	123.06	126.23
23	B	607	CLA	CMB-C2B-C1B	-2.10	122.17	125.37
23	Y	303	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
23	n	610	CLA	C1-C2-C3	-2.10	122.41	126.04
23	n	614	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
40	Y	315	LUT	C12-C13-C14	2.10	122.17	118.94
23	D	406	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
30	n	619	LHG	O8-C23-C24	2.10	118.50	111.91
23	b	603	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
41	r	614	NEX	C25-C24-C23	-2.10	108.59	112.75
23	r	603	CLA	CMB-C2B-C1B	-2.10	122.17	125.37
42	n	617	XAT	C12-C13-C14	2.10	122.16	118.94
23	g	602	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
23	y	311	CLA	CHB-C1B-NB	2.10	126.48	124.26
33	d	411	DGD	CBB-CAB-C9B	-2.10	103.78	114.42
25	H	501	BCR	C38-C26-C25	-2.10	122.17	124.53
39	r	607	CHL	C3A-C2A-C1A	2.10	104.48	101.34
23	A	406	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
23	D	405	CLA	C3B-C4B-NB	-2.10	108.57	110.52
23	g	604	CLA	CHB-C1B-NB	2.10	126.47	124.26
23	r	604	CLA	CHB-C1B-NB	2.10	126.47	124.26
42	R	615	XAT	C30-C31-C32	2.10	129.75	123.22
23	c	506	CLA	CHD-C1D-ND	-2.09	122.53	124.45
23	b	616	CLA	CMB-C2B-C1B	-2.09	122.18	125.37
23	B	607	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	B	611	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	b	601	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	C	506	CLA	CHD-C1D-ND	-2.09	122.53	124.45
39	g	609	CHL	CAA-C2A-C1A	2.09	118.83	111.97
23	C	508	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
39	S	607	CHL	CHA-C1A-NA	-2.09	121.61	126.40
23	Y	313	CLA	CHD-C1D-ND	-2.09	122.53	124.45
23	N	612	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	b	607	CLA	O2A-CGA-O1A	-2.09	118.31	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	g	617	NEX	C35-C34-C33	-2.09	124.33	127.31
39	G	607	CHL	C4B-CHC-C1C	-2.09	121.38	126.34
42	r	615	XAT	C30-C31-C32	2.09	129.74	123.22
23	d	406	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
23	Y	303	CLA	CHD-C1D-ND	-2.09	122.53	124.45
23	c	506	CLA	C3B-C4B-NB	-2.09	108.58	110.52
42	Y	301	XAT	O4-C5-C6	-2.09	57.23	58.96
23	R	610	CLA	CHD-C1D-ND	-2.09	122.53	124.45
23	s	608	CLA	CHD-C1D-ND	-2.09	122.53	124.45
39	Y	302	CHL	C1-C2-C3	-2.09	122.43	126.04
23	R	604	CLA	CHB-C1B-NB	2.09	126.47	124.26
25	B	617	BCR	C24-C23-C22	-2.09	123.08	126.23
23	S	603	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
28	D	403	3PH	O13-P-O11	-2.09	101.18	106.73
39	S	607	CHL	C4B-CHC-C1C	-2.09	121.39	126.34
30	b	627	LHG	O8-C23-C24	2.09	118.45	111.91
23	n	604	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
39	S	606	CHL	CHA-C1A-NA	-2.08	121.62	126.40
39	N	601	CHL	CHA-C1A-NA	-2.08	121.63	126.40
39	Y	308	CHL	C4B-CHC-C1C	-2.08	121.40	126.34
23	C	506	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
23	Y	311	CLA	CHD-C1D-ND	-2.08	122.54	124.45
23	n	602	CLA	CHD-C1D-ND	-2.08	122.54	124.45
23	r	601	CLA	CHB-C1B-NB	2.08	126.46	124.26
35	C	523	VIV	O2-C7-C6	2.08	123.58	118.10
23	y	315	CLA	CHD-C1D-ND	-2.08	122.54	124.45
39	S	605	CHL	C4B-CHC-C1C	-2.08	121.40	126.34
23	S	610	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
23	g	604	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
39	R	607	CHL	CHA-C1A-NA	-2.08	121.63	126.40
23	y	314	CLA	CHD-C1D-ND	-2.08	122.54	124.45
23	g	611	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
23	C	505	CLA	C1-C2-C3	-2.08	122.45	126.04
23	a	405	CLA	CHD-C1D-ND	-2.08	122.54	124.45
39	s	605	CHL	CHA-C1A-NA	-2.08	121.64	126.40
23	Y	310	CLA	CHB-C1B-NB	2.08	126.46	124.26
39	N	601	CHL	C4B-CHC-C1C	-2.08	121.41	126.34
39	G	605	CHL	CHA-C1A-NA	-2.08	121.64	126.40
23	Y	314	CLA	CHD-C1D-ND	-2.08	122.54	124.45
23	c	511	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
23	B	602	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
23	y	315	CLA	O2A-CGA-O1A	-2.08	118.35	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	s	601	CHL	CHD-C1D-C2D	2.08	129.84	125.48
39	N	609	CHL	C4B-CHC-C1C	-2.08	121.41	126.34
23	C	501	CLA	CHB-C1B-NB	2.08	126.46	124.26
23	b	602	CLA	CMB-C2B-C1B	-2.08	122.21	125.37
23	N	614	CLA	CHD-C1D-ND	-2.08	122.55	124.45
23	R	608	CLA	CHD-C1D-ND	-2.08	122.55	124.45
39	S	601	CHL	CHD-C1D-C2D	2.08	129.83	125.48
23	C	509	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
23	N	614	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
23	c	505	CLA	C3B-C4B-NB	-2.08	108.59	110.52
23	G	612	CLA	CHB-C1B-NB	2.07	126.45	124.26
30	G	618	LHG	O8-C23-C24	2.07	118.42	111.91
23	g	602	CLA	CHD-C1D-ND	-2.07	122.55	124.45
30	L	103	LHG	O8-C23-C24	2.07	118.42	111.91
23	R	601	CLA	CHB-C1B-NB	2.07	126.45	124.26
39	r	606	CHL	C3A-C2A-C1A	2.07	104.44	101.34
23	B	605	CLA	CHD-C1D-ND	-2.07	122.55	124.45
23	n	611	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
23	c	505	CLA	O2D-CGD-CBD	2.07	114.95	111.27
42	y	302	XAT	C37-C21-C36	-2.07	104.31	107.37
23	G	610	CLA	CMB-C2B-C3B	2.07	131.60	126.59
39	R	606	CHL	C3A-C2A-C1A	2.07	104.44	101.34
23	b	601	CLA	CHD-C1D-ND	-2.07	122.55	124.45
33	c	515	DGD	C5B-C4B-C3B	-2.07	103.92	114.42
23	R	610	CLA	CHB-C1B-NB	2.07	126.45	124.26
23	R	608	CLA	CMB-C2B-C1B	-2.07	122.22	125.37
28	d	403	3PH	O13-P-O11	-2.07	101.23	106.73
23	a	404	CLA	CMB-C2B-C1B	-2.07	122.22	125.37
40	S	614	LUT	C4-C5-C6	2.07	125.46	120.85
39	s	606	CHL	C4B-CHC-C1C	-2.07	121.43	126.34
23	g	613	CLA	C1-C2-C3	-2.07	122.47	126.04
39	G	601	CHL	C4B-CHC-C1C	-2.07	121.44	126.34
23	c	501	CLA	CHB-C1B-NB	2.07	126.44	124.26
39	n	609	CHL	C4B-CHC-C1C	-2.07	121.44	126.34
23	B	616	CLA	CMB-C2B-C1B	-2.07	122.22	125.37
39	S	601	CHL	CHA-C1A-NA	-2.07	121.67	126.40
39	G	605	CHL	CAA-C2A-C1A	2.07	118.75	111.97
39	N	609	CHL	CHC-C1C-C2C	-2.07	118.62	126.11
23	B	611	CLA	CMB-C2B-C1B	-2.07	122.22	125.37
40	r	613	LUT	C15-C14-C13	2.07	130.26	127.31
23	c	513	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
39	Y	306	CHL	CHD-C1D-C2D	2.07	129.81	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	Y	316	LUT	C17-C1-C6	2.06	113.65	110.30
40	g	615	LUT	C10-C11-C12	2.06	129.66	123.22
39	g	606	CHL	C3A-C2A-C1A	2.06	104.43	101.34
23	C	512	CLA	CHD-C1D-ND	-2.06	122.56	124.45
39	y	310	CHL	C4B-CHC-C1C	-2.06	121.44	126.34
39	N	608	CHL	CAA-C2A-C1A	2.06	118.74	111.97
40	G	615	LUT	C40-C33-C32	2.06	121.33	118.08
23	Y	314	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
23	c	505	CLA	C1-C2-C3	-2.06	122.47	126.04
23	S	602	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
39	s	606	CHL	CHA-C1A-NA	-2.06	121.67	126.40
23	r	611	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
23	r	609	CLA	CHD-C1D-ND	-2.06	122.56	124.45
39	Y	309	CHL	C4B-CHC-C1C	-2.06	121.45	126.34
42	G	619	XAT	C16-C1-C6	-2.06	104.48	110.05
23	S	604	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
23	b	608	CLA	CHB-C1B-NB	2.06	126.44	124.26
23	n	612	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
23	G	604	CLA	CHB-C1B-NB	2.06	126.44	124.26
40	n	615	LUT	C20-C13-C12	-2.06	114.83	118.08
25	a	408	BCR	C24-C23-C22	-2.06	123.12	126.23
23	b	614	CLA	CHD-C1D-ND	-2.06	122.56	124.45
39	r	606	CHL	CHA-C1A-NA	-2.06	121.68	126.40
23	y	312	CLA	CHB-C1B-NB	2.06	126.44	124.26
39	y	307	CHL	CHD-C1D-C2D	2.06	129.79	125.48
23	b	616	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
23	C	513	CLA	CMB-C2B-C1B	-2.06	122.24	125.37
23	S	611	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
40	s	615	LUT	C4-C5-C6	2.06	125.43	120.85
23	C	511	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
25	B	619	BCR	C2-C1-C6	2.06	113.65	110.48
23	y	306	CLA	C1-C2-C3	-2.05	122.49	126.04
39	g	607	CHL	C4B-CHC-C1C	-2.05	121.47	126.34
23	C	508	CLA	CHB-C1B-NB	2.05	126.43	124.26
23	Y	314	CLA	CHB-C1B-NB	2.05	126.43	124.26
23	C	503	CLA	CHD-C1D-ND	-2.05	122.57	124.45
39	n	601	CHL	CHD-C1D-C2D	2.05	129.79	125.48
40	s	614	LUT	C4-C5-C6	2.05	125.43	120.85
39	Y	309	CHL	CHD-C1D-C2D	2.05	129.79	125.48
39	G	608	CHL	C4B-CHC-C1C	-2.05	121.47	126.34
23	Y	310	CLA	CHD-C1D-ND	-2.05	122.57	124.45
23	s	603	CLA	O2A-CGA-O1A	-2.05	118.41	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	617	BCR	C3-C4-C5	-2.05	110.41	114.08
39	s	607	CHL	CHA-C1A-NA	-2.05	121.70	126.40
23	B	609	CLA	C1-C2-C3	-2.05	122.50	126.04
39	S	606	CHL	C4B-CHC-C1C	-2.05	121.47	126.34
25	d	410	BCR	C15-C14-C13	-2.05	124.38	127.31
23	C	502	CLA	CHD-C1D-ND	-2.05	122.57	124.45
23	c	513	CLA	CHD-C1D-ND	-2.05	122.57	124.45
23	n	614	CLA	CHD-C1D-ND	-2.05	122.57	124.45
39	G	605	CHL	C4B-CHC-C1C	-2.05	121.48	126.34
23	C	505	CLA	O2D-CGD-CBD	2.05	114.91	111.27
23	y	304	CLA	CHD-C1D-ND	-2.05	122.57	124.45
39	y	309	CHL	C4B-CHC-C1C	-2.05	121.48	126.34
23	n	602	CLA	C1-C2-C3	-2.05	122.50	126.04
23	N	602	CLA	CHD-C1D-ND	-2.05	122.57	124.45
39	R	605	CHL	CHA-C1A-NA	-2.05	121.71	126.40
23	r	603	CLA	CHD-C1D-ND	-2.05	122.57	124.45
40	N	615	LUT	C3-C4-C5	2.05	115.93	111.85
23	b	611	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
39	g	601	CHL	CHD-C1D-C2D	2.05	129.77	125.48
39	s	607	CHL	CHD-C1D-C2D	2.05	129.77	125.48
23	B	613	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
23	r	609	CLA	CHB-C1B-NB	2.05	126.42	124.26
39	s	607	CHL	C4B-CHC-C1C	-2.04	121.49	126.34
39	y	303	CHL	C4B-CHC-C1C	-2.04	121.49	126.34
39	G	606	CHL	CHA-C1A-NA	-2.04	121.72	126.40
39	s	601	CHL	CHA-C1A-NA	-2.04	121.72	126.40
39	y	310	CHL	CHD-C1D-C2D	2.04	129.77	125.48
39	Y	307	CHL	CHA-C1A-NA	-2.04	121.72	126.40
23	B	602	CLA	O2D-CGD-CBD	2.04	114.90	111.27
25	K	101	BCR	C11-C10-C9	-2.04	124.39	127.31
23	B	610	CLA	O2D-CGD-CBD	2.04	114.90	111.27
28	a	410	3PH	O13-P-O11	-2.04	101.30	106.73
39	R	607	CHL	CHC-C1C-C2C	-2.04	118.70	126.11
23	C	506	CLA	C1-C2-C3	-2.04	122.51	126.04
24	A	405	PHO	O2A-CGA-O1A	-2.04	118.44	123.59
23	R	611	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
23	b	612	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
39	s	605	CHL	C4B-CHC-C1C	-2.04	121.50	126.34
39	g	608	CHL	CHD-C1D-C2D	2.04	129.76	125.48
23	b	605	CLA	CHD-C1D-ND	-2.04	122.58	124.45
39	g	601	CHL	C4B-CHC-C1C	-2.04	121.50	126.34
23	B	612	CLA	O2A-CGA-O1A	-2.04	118.44	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	r	604	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
25	b	619	BCR	C15-C14-C13	-2.04	124.40	127.31
39	n	609	CHL	CHC-C1C-C2C	-2.04	118.72	126.11
39	r	605	CHL	CHA-C1A-NA	-2.04	121.73	126.40
23	N	603	CLA	C1-C2-C3	-2.04	122.52	126.04
23	B	601	CLA	CHD-C1D-ND	-2.04	122.58	124.45
23	r	608	CLA	CHD-C1D-ND	-2.04	122.58	124.45
42	n	617	XAT	C16-C1-C6	-2.04	104.54	110.05
42	Y	301	XAT	C25-C24-C23	-2.04	108.72	112.75
23	S	608	CLA	CHD-C1D-ND	-2.04	122.58	124.45
40	N	615	LUT	C4-C5-C6	2.04	125.39	120.85
23	G	611	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
23	G	602	CLA	CHD-C1D-ND	-2.04	122.58	124.45
39	G	601	CHL	CHD-C1D-C2D	2.04	129.75	125.48
39	n	606	CHL	CHD-C1D-C2D	2.04	129.75	125.48
40	n	616	LUT	C38-C25-C24	-2.04	119.20	123.56
39	g	619	CHL	C4B-CHC-C1C	-2.04	121.51	126.34
23	c	509	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
39	G	605	CHL	CHD-C1D-C2D	2.04	129.75	125.48
39	S	606	CHL	CHD-C1D-C2D	2.04	129.75	125.48
25	B	619	BCR	C15-C16-C17	-2.04	119.31	123.47
23	C	505	CLA	C3B-C4B-NB	-2.04	108.63	110.52
39	Y	302	CHL	CHD-C1D-C2D	2.03	129.75	125.48
23	A	403	CLA	CMB-C2B-C1B	-2.03	122.27	125.37
42	N	619	XAT	C39-C29-C28	-2.03	114.87	118.08
23	G	611	CLA	CHB-C1B-NB	2.03	126.41	124.26
38	f	501	HEM	C3B-C2B-C1B	2.03	108.00	106.49
39	g	606	CHL	CHA-C1A-NA	-2.03	121.74	126.40
25	D	411	BCR	C15-C14-C13	-2.03	124.41	127.31
25	B	617	BCR	C8-C7-C6	-2.03	121.49	127.20
39	n	609	CHL	CHD-C1D-C2D	2.03	129.74	125.48
39	g	606	CHL	CAA-C2A-C1A	2.03	118.63	111.97
23	g	614	CLA	CHD-C1D-ND	-2.03	122.59	124.45
23	c	502	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
23	g	610	CLA	CMB-C2B-C3B	2.03	131.51	126.59
23	s	609	CLA	CMB-C2B-C3B	2.03	131.51	126.59
23	B	608	CLA	CHB-C1B-NB	2.03	126.41	124.26
25	v	101	BCR	C16-C15-C14	-2.03	119.31	123.47
40	S	615	LUT	C4-C5-C6	2.03	125.37	120.85
39	y	308	CHL	CHA-C1A-NA	-2.03	121.75	126.40
23	G	602	CLA	C1-C2-C3	-2.03	122.53	126.04
23	Y	304	CLA	CHD-C1D-ND	-2.03	122.59	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	n	603	CLA	CHD-C1D-ND	-2.03	122.59	124.45
39	R	607	CHL	C3A-C2A-C1A	2.03	104.38	101.34
23	N	611	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
39	R	606	CHL	CHD-C1D-C2D	2.03	129.73	125.48
39	r	605	CHL	C4B-CHC-C1C	-2.03	121.53	126.34
23	g	603	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
39	S	605	CHL	CHA-C1A-NA	-2.03	121.76	126.40
25	D	411	BCR	C2-C1-C6	2.03	113.60	110.48
23	C	513	CLA	C1-C2-C3	-2.03	122.54	126.04
23	R	608	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
39	N	609	CHL	CHD-C1D-C2D	2.03	129.73	125.48
23	g	613	CLA	CHD-C1D-ND	-2.03	122.59	124.45
39	r	605	CHL	CHD-C1D-C2D	2.02	129.73	125.48
39	R	606	CHL	CAA-C2A-C1A	2.02	118.61	111.97
23	n	611	CLA	CHD-C1D-ND	-2.02	122.59	124.45
39	Y	302	CHL	C4B-CHC-C1C	-2.02	121.54	126.34
42	G	619	XAT	C12-C13-C14	2.02	122.05	118.94
39	R	605	CHL	CHD-C1D-C2D	2.02	129.72	125.48
23	N	610	CLA	CHD-C1D-ND	-2.02	122.59	124.45
23	y	305	CLA	CHD-C1D-ND	-2.02	122.59	124.45
39	R	605	CHL	C4B-CHC-C1C	-2.02	121.54	126.34
39	g	608	CHL	C4B-CHC-C1C	-2.02	121.54	126.34
23	S	609	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
39	r	606	CHL	CHD-C1D-C2D	2.02	129.72	125.48
23	r	602	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
39	n	608	CHL	CHA-C1A-NA	-2.02	121.77	126.40
23	N	603	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
35	y	301	VIV	C15-C16-C17	-2.02	108.62	112.74
23	N	610	CLA	CHB-C1B-NB	2.02	126.39	124.26
39	N	608	CHL	CHA-C1A-NA	-2.02	121.78	126.40
23	B	614	CLA	CHD-C1D-ND	-2.02	122.60	124.45
23	N	611	CLA	CHD-C1D-ND	-2.02	122.60	124.45
23	C	502	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
23	R	603	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
39	G	620	CHL	CHD-C1D-C2D	2.02	129.71	125.48
39	G	620	CHL	CAA-C2A-C1A	2.02	118.59	111.97
39	N	601	CHL	CHD-C1D-C2D	2.02	129.71	125.48
25	k	101	BCR	C11-C10-C9	-2.02	124.43	127.31
23	n	603	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
23	a	405	CLA	CHB-C1B-NB	2.02	126.39	124.26
40	Y	315	LUT	C3-C4-C5	2.02	115.87	111.85
40	N	616	LUT	C17-C1-C6	2.02	113.57	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	y	303	CHL	CHA-C1A-NA	-2.02	121.78	126.40
39	g	609	CHL	C3A-C2A-C1A	2.02	104.36	101.34
23	b	610	CLA	O2D-CGD-CBD	2.02	114.85	111.27
23	c	507	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
39	n	606	CHL	CHA-C1A-NA	-2.02	121.78	126.40
23	c	512	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
40	g	615	LUT	C40-C33-C32	2.01	121.25	118.08
23	b	614	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
39	G	608	CHL	CHD-C1D-C2D	2.01	129.71	125.48
23	A	404	CLA	CHD-C1D-ND	-2.01	122.60	124.45
23	C	509	CLA	CHD-C1D-ND	-2.01	122.60	124.45
23	r	603	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
23	b	611	CLA	CHB-C1B-NB	2.01	126.39	124.26
39	y	303	CHL	CHD-C1D-C2D	2.01	129.70	125.48
40	s	615	LUT	C17-C1-C6	2.01	113.56	110.30
23	B	609	CLA	CHD-C1D-ND	-2.01	122.61	124.45
23	c	511	CLA	CHD-C1D-ND	-2.01	122.61	124.45
25	V	101	BCR	C16-C15-C14	-2.01	119.36	123.47
23	g	614	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
23	c	508	CLA	CHD-C1D-ND	-2.01	122.61	124.45
23	r	612	CLA	CHD-C1D-ND	-2.01	122.61	124.45
42	Y	301	XAT	C31-C32-C33	2.01	132.06	126.42
39	g	605	CHL	C4B-CHC-C1C	-2.01	121.58	126.34
39	S	607	CHL	CHC-C1C-C2C	-2.01	118.83	126.11
23	Y	314	CLA	C1-C2-C3	-2.01	122.57	126.04
41	n	618	NEX	C38-C25-C24	-2.01	112.02	114.28
23	y	304	CLA	C1-C2-C3	-2.01	122.57	126.04
23	b	604	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
39	g	619	CHL	C3A-C2A-C1A	2.01	104.34	101.34
39	N	608	CHL	C4B-CHC-C1C	-2.01	121.58	126.34
33	d	411	DGD	C1E-O6E-C5E	2.01	117.63	113.69
23	b	609	CLA	CHD-C1D-ND	-2.01	122.61	124.45
23	s	604	CLA	CHD-C1D-ND	-2.01	122.61	124.45
39	N	606	CHL	C4B-CHC-C1C	-2.01	121.58	126.34
23	G	614	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
23	B	605	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
23	s	603	CLA	CHD-C1D-ND	-2.01	122.61	124.45
23	y	311	CLA	CHD-C1D-ND	-2.01	122.61	124.45
39	s	605	CHL	CHD-C1D-C2D	2.01	129.69	125.48
23	B	604	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
39	y	310	CHL	CHC-C1C-C2C	-2.00	118.84	126.11
39	g	605	CHL	CHD-C1D-C2D	2.00	129.68	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	503	CLA	CHD-C1D-ND	-2.00	122.61	124.45
23	c	512	CLA	CMB-C2B-C1B	-2.00	122.32	125.37
33	H	502	DGD	O3E-C3E-C2E	-2.00	105.72	110.35
24	d	402	PHO	O2A-CGA-O1A	-2.00	118.54	123.59
23	b	609	CLA	C1-C2-C3	-2.00	122.58	126.04
39	n	608	CHL	C4B-CHC-C1C	-2.00	121.59	126.34
23	r	604	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
39	N	606	CHL	CHA-C1A-NA	-2.00	121.82	126.40

There are no chirality outliers.

All (3750) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	403	CLA	C2A-CAA-CBA-CGA
23	A	403	CLA	CHA-CBD-CGD-O1D
23	A	403	CLA	CHA-CBD-CGD-O2D
23	B	601	CLA	C1A-C2A-CAA-CBA
23	B	601	CLA	CHA-CBD-CGD-O1D
23	B	601	CLA	CHA-CBD-CGD-O2D
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	602	CLA	CHA-CBD-CGD-O1D
23	B	602	CLA	CHA-CBD-CGD-O2D
23	B	603	CLA	C4-C3-C5-C6
23	B	605	CLA	CBD-CGD-O2D-CED
23	B	605	CLA	C4-C3-C5-C6
23	B	609	CLA	C1A-C2A-CAA-CBA
23	B	609	CLA	CHA-CBD-CGD-O1D
23	B	609	CLA	CHA-CBD-CGD-O2D
23	B	609	CLA	CBD-CGD-O2D-CED
23	B	611	CLA	C12-C13-C15-C16
23	B	612	CLA	C1A-C2A-CAA-CBA
23	B	612	CLA	C3A-C2A-CAA-CBA
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	B	614	CLA	C2-C3-C5-C6
23	B	614	CLA	C4-C3-C5-C6
23	C	501	CLA	CHA-CBD-CGD-O1D
23	C	501	CLA	CHA-CBD-CGD-O2D
23	C	501	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	C	513	CLA	C1A-C2A-CAA-CBA
23	G	604	CLA	CHA-CBD-CGD-O1D
23	G	604	CLA	CHA-CBD-CGD-O2D
23	G	610	CLA	CBD-CGD-O2D-CED
23	R	601	CLA	CHA-CBD-CGD-O1D
23	R	601	CLA	CHA-CBD-CGD-O2D
23	R	610	CLA	C1A-C2A-CAA-CBA
23	R	610	CLA	C3A-C2A-CAA-CBA
23	R	610	CLA	C2B-C3B-CAB-CBB
23	R	610	CLA	C4B-C3B-CAB-CBB
23	R	611	CLA	CBD-CGD-O2D-CED
23	R	612	CLA	CHA-CBD-CGD-O1D
23	R	612	CLA	CHA-CBD-CGD-O2D
23	S	603	CLA	C1A-C2A-CAA-CBA
23	S	603	CLA	C3A-C2A-CAA-CBA
23	S	604	CLA	CHA-CBD-CGD-O1D
23	S	604	CLA	CHA-CBD-CGD-O2D
23	S	609	CLA	C1A-C2A-CAA-CBA
23	S	609	CLA	C3A-C2A-CAA-CBA
23	S	611	CLA	CBD-CGD-O2D-CED
23	S	613	CLA	C1A-C2A-CAA-CBA
23	Y	310	CLA	CBD-CGD-O2D-CED
23	Y	314	CLA	C2B-C3B-CAB-CBB
23	Y	314	CLA	C4B-C3B-CAB-CBB
23	a	403	CLA	CBD-CGD-O2D-CED
23	a	404	CLA	CHA-CBD-CGD-O1D
23	a	404	CLA	CHA-CBD-CGD-O2D
23	b	601	CLA	C1A-C2A-CAA-CBA
23	b	601	CLA	C3A-C2A-CAA-CBA
23	b	602	CLA	C2-C3-C5-C6
23	b	602	CLA	C4-C3-C5-C6
23	b	605	CLA	CBD-CGD-O2D-CED
23	b	609	CLA	C1A-C2A-CAA-CBA
23	b	609	CLA	C3A-C2A-CAA-CBA
23	b	609	CLA	CHA-CBD-CGD-O1D
23	b	609	CLA	CHA-CBD-CGD-O2D
23	b	609	CLA	CBD-CGD-O2D-CED
23	b	612	CLA	C1A-C2A-CAA-CBA
23	b	612	CLA	C3A-C2A-CAA-CBA
23	b	613	CLA	C11-C12-C13-C14
23	b	614	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	b	614	CLA	CAD-CBD-CGD-O2D
23	c	501	CLA	CHA-CBD-CGD-O1D
23	c	501	CLA	CHA-CBD-CGD-O2D
23	c	501	CLA	CAD-CBD-CGD-O1D
23	c	501	CLA	C14-C13-C15-C16
23	c	503	CLA	CBD-CGD-O2D-CED
23	c	507	CLA	C2B-C3B-CAB-CBB
23	c	507	CLA	C4B-C3B-CAB-CBB
23	c	509	CLA	C6-C7-C8-C9
23	g	604	CLA	CHA-CBD-CGD-O1D
23	g	604	CLA	CHA-CBD-CGD-O2D
23	g	610	CLA	CBD-CGD-O2D-CED
23	n	614	CLA	CBD-CGD-O2D-CED
23	r	610	CLA	C1A-C2A-CAA-CBA
23	r	610	CLA	C3A-C2A-CAA-CBA
23	r	611	CLA	CBD-CGD-O2D-CED
23	r	612	CLA	C1A-C2A-CAA-CBA
23	r	612	CLA	C3A-C2A-CAA-CBA
23	r	612	CLA	CHA-CBD-CGD-O1D
23	r	612	CLA	CHA-CBD-CGD-O2D
23	s	602	CLA	C1A-C2A-CAA-CBA
23	s	602	CLA	C3A-C2A-CAA-CBA
23	s	602	CLA	C2-C3-C5-C6
23	s	602	CLA	C4-C3-C5-C6
23	s	604	CLA	CHA-CBD-CGD-O1D
23	s	604	CLA	CHA-CBD-CGD-O2D
23	s	609	CLA	C1A-C2A-CAA-CBA
23	s	609	CLA	C3A-C2A-CAA-CBA
23	s	609	CLA	CBD-CGD-O2D-CED
23	s	611	CLA	CBD-CGD-O2D-CED
23	s	613	CLA	C1A-C2A-CAA-CBA
23	y	315	CLA	C4B-C3B-CAB-CBB
25	B	617	BCR	C11-C12-C13-C14
25	B	617	BCR	C11-C12-C13-C35
25	B	617	BCR	C20-C21-C22-C37
25	B	617	BCR	C21-C22-C23-C24
25	B	618	BCR	C5-C6-C7-C8
25	C	514	BCR	C1-C6-C7-C8
25	C	514	BCR	C20-C21-C22-C37
25	H	501	BCR	C1-C6-C7-C8
25	H	501	BCR	C7-C8-C9-C34
25	K	101	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	b	617	BCR	C1-C6-C7-C8
25	b	618	BCR	C7-C8-C9-C34
25	b	619	BCR	C7-C8-C9-C10
25	b	619	BCR	C7-C8-C9-C34
25	c	514	BCR	C20-C21-C22-C37
25	d	410	BCR	C6-C7-C8-C9
25	h	501	BCR	C7-C8-C9-C34
25	k	101	BCR	C1-C6-C7-C8
25	v	101	BCR	C21-C22-C23-C24
26	A	408	SQD	C5-C6-S-O7
26	A	408	SQD	C5-C6-S-O8
26	A	408	SQD	C5-C6-S-O9
26	L	101	SQD	O5-C1-O6-C44
26	L	101	SQD	C8-C7-O47-C45
26	M	101	SQD	C2-C1-O6-C44
26	M	101	SQD	O5-C1-O6-C44
26	M	101	SQD	O5-C5-C6-S
27	A	409	LMG	C2-C1-O1-C7
27	A	409	LMG	O6-C1-O1-C7
27	C	525	LMG	C2-C1-O1-C7
27	C	525	LMG	O6-C1-O1-C7
27	c	523	LMG	C2-C1-O1-C7
27	c	523	LMG	O6-C1-O1-C7
28	D	403	3PH	C1-O11-P-O13
28	L	102	3PH	C1-O11-P-O13
28	L	102	3PH	C1-O11-P-O14
28	L	102	3PH	C1-O11-P-O12
28	L	102	3PH	O22-C21-O21-C2
28	T	101	3PH	C1-O11-P-O13
28	T	101	3PH	C1-O11-P-O14
28	T	101	3PH	O11-C1-C2-O21
28	T	101	3PH	O22-C21-O21-C2
28	X	201	3PH	C22-C21-O21-C2
28	s	618	3PH	C1-O11-P-O13
28	s	618	3PH	C1-O11-P-O14
28	s	618	3PH	C1-O11-P-O12
28	w	202	3PH	C1-O11-P-O13
28	w	202	3PH	C1-O11-P-O14
28	w	202	3PH	C1-O11-P-O12
28	x	201	3PH	O11-C1-C2-O21
28	x	201	3PH	C22-C21-O21-C2
29	A	411	PL9	C34-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
29	A	411	PL9	C43-C44-C46-C47
29	A	411	PL9	C45-C44-C46-C47
29	a	411	PL9	C29-C31-C32-C33
30	A	412	LHG	O1-C1-C2-C3
30	A	412	LHG	C3-O3-P-O5
30	A	412	LHG	C4-O6-P-O4
30	D	404	LHG	O1-C1-C2-C3
30	D	408	LHG	O1-C1-C2-C3
30	D	408	LHG	C4-O6-P-O4
30	G	618	LHG	C3-O3-P-O4
30	G	618	LHG	C3-O3-P-O5
30	L	103	LHG	O1-C1-C2-C3
30	L	103	LHG	C3-O3-P-O4
30	L	103	LHG	C3-O3-P-O5
30	L	103	LHG	C3-O3-P-O6
30	L	103	LHG	C4-O6-P-O3
30	L	103	LHG	C4-O6-P-O4
30	L	103	LHG	C4-O6-P-O5
30	N	618	LHG	O1-C1-C2-C3
30	N	618	LHG	C4-C5-O7-C7
30	N	618	LHG	O9-C7-O7-C5
30	N	618	LHG	C8-C7-O7-C5
30	R	616	LHG	O1-C1-C2-O2
30	R	616	LHG	O1-C1-C2-C3
30	R	616	LHG	C8-C7-O7-C5
30	S	616	LHG	O1-C1-C2-C3
30	S	616	LHG	O2-C2-C3-O3
30	S	616	LHG	C4-O6-P-O4
30	S	616	LHG	C4-O6-P-O5
30	Y	318	LHG	O1-C1-C2-O2
30	Y	318	LHG	O1-C1-C2-C3
30	Y	318	LHG	C1-C2-C3-O3
30	a	412	LHG	O1-C1-C2-C3
30	a	412	LHG	C3-O3-P-O4
30	a	412	LHG	C3-O3-P-O5
30	a	412	LHG	C3-O3-P-O6
30	b	627	LHG	O1-C1-C2-C3
30	b	627	LHG	C3-O3-P-O4
30	b	627	LHG	C4-O6-P-O3
30	b	627	LHG	C4-O6-P-O4
30	b	627	LHG	C4-O6-P-O5
30	d	404	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
30	d	404	LHG	C4-O6-P-O4
30	d	404	LHG	C4-O6-P-O5
30	d	408	LHG	O1-C1-C2-C3
30	d	408	LHG	C4-O6-P-O4
30	g	618	LHG	O2-C2-C3-O3
30	g	618	LHG	C3-O3-P-O5
30	g	618	LHG	O10-C23-O8-C6
30	g	618	LHG	C24-C23-O8-C6
30	n	619	LHG	O1-C1-C2-O2
30	n	619	LHG	O1-C1-C2-C3
30	r	616	LHG	O1-C1-C2-C3
30	s	616	LHG	O1-C1-C2-C3
30	s	616	LHG	O2-C2-C3-O3
30	s	616	LHG	C4-O6-P-O5
30	s	616	LHG	O7-C5-C6-O8
30	y	318	LHG	O1-C1-C2-O2
30	y	318	LHG	O1-C1-C2-C3
30	y	318	LHG	C1-C2-C3-O3
31	A	413	LNL	C9-C10-C11-C12
31	A	414	LNL	C15-C16-C17-C18
31	C	517	LNL	C13-C14-C15-C16
31	C	518	LNL	C15-C16-C17-C18
31	C	519	LNL	C15-C16-C17-C18
31	C	520	LNL	C9-C10-C11-C12
31	C	520	LNL	C13-C14-C15-C16
31	C	521	LNL	C15-C16-C17-C18
31	C	522	LNL	C13-C14-C15-C16
31	b	622	LNL	C15-C16-C17-C18
31	b	624	LNL	C10-C11-C12-C13
31	b	624	LNL	C15-C16-C17-C18
31	c	518	LNL	C9-C10-C11-C12
31	c	518	LNL	C15-C16-C17-C18
31	c	521	LNL	C9-C10-C11-C12
33	d	411	DGD	C2E-C1E-O5D-C6D
33	d	411	DGD	O6E-C1E-O5D-C6D
35	y	301	VIV	C16-C15-C9-O1
35	y	301	VIV	C16-C15-C9-C11
35	y	301	VIV	C16-C15-C9-C14
37	D	410	DGA	CB2-CB1-OG2-CG2
37	D	410	DGA	OG2-CG2-CG3-OXT
37	b	626	DGA	CB2-CB1-OG2-CG2
39	G	601	CHL	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
39	G	601	CHL	C4B-C3B-CAB-CBB
39	G	601	CHL	C1C-C2C-CMC-OMC
39	G	601	CHL	C3C-C2C-CMC-OMC
39	G	601	CHL	CHA-CBD-CGD-O1D
39	G	601	CHL	CHA-CBD-CGD-O2D
39	G	605	CHL	C1C-C2C-CMC-OMC
39	G	605	CHL	C3C-C2C-CMC-OMC
39	G	606	CHL	C1C-C2C-CMC-OMC
39	G	606	CHL	C3C-C2C-CMC-OMC
39	G	607	CHL	C1C-C2C-CMC-OMC
39	G	607	CHL	C3C-C2C-CMC-OMC
39	G	608	CHL	C1C-C2C-CMC-OMC
39	G	608	CHL	C3C-C2C-CMC-OMC
39	G	609	CHL	C1C-C2C-CMC-OMC
39	G	609	CHL	C3C-C2C-CMC-OMC
39	G	609	CHL	C2-C3-C5-C6
39	G	609	CHL	C4-C3-C5-C6
39	G	609	CHL	C6-C7-C8-C9
39	G	620	CHL	C3C-C2C-CMC-OMC
39	N	601	CHL	C1A-C2A-CAA-CBA
39	N	601	CHL	C3A-C2A-CAA-CBA
39	N	601	CHL	C1C-C2C-CMC-OMC
39	N	601	CHL	C3C-C2C-CMC-OMC
39	N	601	CHL	CHA-CBD-CGD-O1D
39	N	601	CHL	CHA-CBD-CGD-O2D
39	N	605	CHL	C1C-C2C-CMC-OMC
39	N	605	CHL	C3C-C2C-CMC-OMC
39	N	606	CHL	C1C-C2C-CMC-OMC
39	N	607	CHL	C4B-C3B-CAB-CBB
39	N	608	CHL	C3C-C2C-CMC-OMC
39	N	609	CHL	C1C-C2C-CMC-OMC
39	N	609	CHL	C3C-C2C-CMC-OMC
39	R	605	CHL	C1C-C2C-CMC-OMC
39	R	605	CHL	C3C-C2C-CMC-OMC
39	R	606	CHL	C3C-C2C-CMC-OMC
39	R	606	CHL	C14-C13-C15-C16
39	R	607	CHL	C1A-C2A-CAA-CBA
39	R	607	CHL	C1C-C2C-CMC-OMC
39	S	601	CHL	C1C-C2C-CMC-OMC
39	S	601	CHL	C3C-C2C-CMC-OMC
39	S	605	CHL	C1C-C2C-CMC-OMC
39	S	605	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
39	S	606	CHL	C3A-C2A-CAA-CBA
39	S	606	CHL	C2B-C3B-CAB-CBB
39	S	606	CHL	C4B-C3B-CAB-CBB
39	S	606	CHL	C1C-C2C-CMC-OMC
39	S	606	CHL	C3C-C2C-CMC-OMC
39	S	607	CHL	C1A-C2A-CAA-CBA
39	S	607	CHL	C3A-C2A-CAA-CBA
39	S	607	CHL	C2B-C3B-CAB-CBB
39	S	607	CHL	C4B-C3B-CAB-CBB
39	S	607	CHL	C1C-C2C-CMC-OMC
39	S	607	CHL	C3C-C2C-CMC-OMC
39	Y	302	CHL	C2B-C3B-CAB-CBB
39	Y	302	CHL	C4B-C3B-CAB-CBB
39	Y	302	CHL	C1C-C2C-CMC-OMC
39	Y	302	CHL	C3C-C2C-CMC-OMC
39	Y	302	CHL	C4-C3-C5-C6
39	Y	306	CHL	C1C-C2C-CMC-OMC
39	Y	306	CHL	C3C-C2C-CMC-OMC
39	Y	308	CHL	C1C-C2C-CMC-OMC
39	Y	308	CHL	C3C-C2C-CMC-OMC
39	Y	309	CHL	C1C-C2C-CMC-OMC
39	Y	309	CHL	C3C-C2C-CMC-OMC
39	g	601	CHL	C2B-C3B-CAB-CBB
39	g	601	CHL	C4B-C3B-CAB-CBB
39	g	601	CHL	C1C-C2C-CMC-OMC
39	g	601	CHL	C3C-C2C-CMC-OMC
39	g	601	CHL	CHA-CBD-CGD-O1D
39	g	601	CHL	CHA-CBD-CGD-O2D
39	g	605	CHL	C1C-C2C-CMC-OMC
39	g	605	CHL	C3C-C2C-CMC-OMC
39	g	606	CHL	C1C-C2C-CMC-OMC
39	g	606	CHL	C3C-C2C-CMC-OMC
39	g	607	CHL	C1C-C2C-CMC-OMC
39	g	607	CHL	C3C-C2C-CMC-OMC
39	g	607	CHL	C6-C7-C8-C9
39	g	608	CHL	C1A-C2A-CAA-CBA
39	g	608	CHL	C1C-C2C-CMC-OMC
39	g	608	CHL	C3C-C2C-CMC-OMC
39	g	608	CHL	CHA-CBD-CGD-O1D
39	g	608	CHL	CHA-CBD-CGD-O2D
39	g	609	CHL	C1A-C2A-CAA-CBA
39	g	609	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
39	g	609	CHL	CHA-CBD-CGD-O2D
39	g	619	CHL	C1C-C2C-CMC-OMC
39	g	619	CHL	C3C-C2C-CMC-OMC
39	n	601	CHL	C3C-C2C-CMC-OMC
39	n	601	CHL	CHA-CBD-CGD-O1D
39	n	601	CHL	CHA-CBD-CGD-O2D
39	n	605	CHL	C1C-C2C-CMC-OMC
39	n	605	CHL	C3C-C2C-CMC-OMC
39	n	606	CHL	C1C-C2C-CMC-OMC
39	n	607	CHL	C3C-C2C-CMC-OMC
39	n	608	CHL	C3C-C2C-CMC-OMC
39	n	609	CHL	C1C-C2C-CMC-OMC
39	n	609	CHL	C3C-C2C-CMC-OMC
39	r	605	CHL	C1C-C2C-CMC-OMC
39	r	605	CHL	C3C-C2C-CMC-OMC
39	r	606	CHL	C3C-C2C-CMC-OMC
39	r	607	CHL	C1A-C2A-CAA-CBA
39	r	607	CHL	C1C-C2C-CMC-OMC
39	s	601	CHL	C1C-C2C-CMC-OMC
39	s	601	CHL	C3C-C2C-CMC-OMC
39	s	601	CHL	C2-C3-C5-C6
39	s	605	CHL	C1A-C2A-CAA-CBA
39	s	605	CHL	C3A-C2A-CAA-CBA
39	s	605	CHL	C1C-C2C-CMC-OMC
39	s	605	CHL	C3C-C2C-CMC-OMC
39	s	606	CHL	C1C-C2C-CMC-OMC
39	s	606	CHL	C3C-C2C-CMC-OMC
39	s	607	CHL	C1C-C2C-CMC-OMC
39	s	607	CHL	C3C-C2C-CMC-OMC
39	y	303	CHL	C2B-C3B-CAB-CBB
39	y	303	CHL	C4B-C3B-CAB-CBB
39	y	303	CHL	C1C-C2C-CMC-OMC
39	y	303	CHL	C3C-C2C-CMC-OMC
39	y	303	CHL	C2-C3-C5-C6
39	y	303	CHL	C4-C3-C5-C6
39	y	307	CHL	C1C-C2C-CMC-OMC
39	y	307	CHL	C3C-C2C-CMC-OMC
39	y	308	CHL	C1C-C2C-CMC-OMC
39	y	309	CHL	C1C-C2C-CMC-OMC
39	y	309	CHL	C3C-C2C-CMC-OMC
39	y	310	CHL	C1C-C2C-CMC-OMC
39	y	310	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
40	G	615	LUT	C1-C6-C7-C8
40	G	615	LUT	C7-C8-C9-C10
40	G	615	LUT	C10-C11-C12-C13
40	G	615	LUT	C11-C12-C13-C14
40	G	615	LUT	C12-C13-C14-C15
40	G	615	LUT	C26-C27-C28-C29
40	G	615	LUT	C27-C28-C29-C30
40	G	615	LUT	C28-C29-C30-C31
40	G	615	LUT	C39-C29-C30-C31
40	G	615	LUT	C30-C31-C32-C33
40	G	615	LUT	C31-C32-C33-C34
40	G	615	LUT	C31-C32-C33-C40
40	G	616	LUT	C11-C10-C9-C8
40	G	616	LUT	C11-C10-C9-C19
40	G	616	LUT	C11-C12-C13-C20
40	G	616	LUT	C31-C32-C33-C40
40	N	615	LUT	C1-C6-C7-C8
40	N	615	LUT	C6-C7-C8-C9
40	N	615	LUT	C7-C8-C9-C10
40	N	615	LUT	C7-C8-C9-C19
40	N	615	LUT	C11-C10-C9-C19
40	N	615	LUT	C9-C10-C11-C12
40	N	615	LUT	C11-C12-C13-C20
40	N	615	LUT	C27-C28-C29-C39
40	N	615	LUT	C31-C32-C33-C40
40	N	616	LUT	C7-C8-C9-C10
40	N	616	LUT	C11-C10-C9-C19
40	N	616	LUT	C10-C11-C12-C13
40	N	616	LUT	C11-C12-C13-C14
40	N	616	LUT	C20-C13-C14-C15
40	N	616	LUT	C26-C27-C28-C29
40	N	616	LUT	C27-C28-C29-C39
40	N	616	LUT	C39-C29-C30-C31
40	R	613	LUT	C11-C10-C9-C19
40	R	613	LUT	C10-C11-C12-C13
40	R	613	LUT	C11-C12-C13-C14
40	R	613	LUT	C26-C27-C28-C29
40	R	613	LUT	C39-C29-C30-C31
40	R	613	LUT	C31-C32-C33-C34
40	S	614	LUT	C6-C7-C8-C9
40	S	614	LUT	C7-C8-C9-C10
40	S	614	LUT	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
40	S	614	LUT	C11-C10-C9-C19
40	S	614	LUT	C10-C11-C12-C13
40	S	614	LUT	C11-C12-C13-C20
40	S	614	LUT	C21-C26-C27-C28
40	S	614	LUT	C25-C26-C27-C28
40	S	614	LUT	C26-C27-C28-C29
40	S	614	LUT	C27-C28-C29-C30
40	S	614	LUT	C30-C31-C32-C33
40	S	615	LUT	C1-C6-C7-C8
40	S	615	LUT	C6-C7-C8-C9
40	S	615	LUT	C7-C8-C9-C19
40	S	615	LUT	C11-C10-C9-C19
40	S	615	LUT	C10-C11-C12-C13
40	S	615	LUT	C11-C12-C13-C20
40	S	615	LUT	C27-C28-C29-C30
40	S	615	LUT	C28-C29-C30-C31
40	S	615	LUT	C39-C29-C30-C31
40	S	615	LUT	C31-C32-C33-C34
40	Y	315	LUT	C6-C7-C8-C9
40	Y	315	LUT	C7-C8-C9-C19
40	Y	315	LUT	C11-C10-C9-C8
40	Y	315	LUT	C10-C11-C12-C13
40	Y	315	LUT	C27-C28-C29-C30
40	Y	315	LUT	C39-C29-C30-C31
40	Y	316	LUT	C6-C7-C8-C9
40	Y	316	LUT	C7-C8-C9-C19
40	Y	316	LUT	C11-C12-C13-C20
40	Y	316	LUT	C21-C26-C27-C28
40	Y	316	LUT	C25-C26-C27-C28
40	Y	316	LUT	C26-C27-C28-C29
40	Y	316	LUT	C27-C28-C29-C30
40	Y	316	LUT	C28-C29-C30-C31
40	Y	316	LUT	C39-C29-C30-C31
40	g	615	LUT	C7-C8-C9-C10
40	g	615	LUT	C11-C10-C9-C19
40	g	615	LUT	C11-C12-C13-C20
40	g	615	LUT	C20-C13-C14-C15
40	g	615	LUT	C26-C27-C28-C29
40	g	615	LUT	C27-C28-C29-C30
40	g	615	LUT	C28-C29-C30-C31
40	g	615	LUT	C39-C29-C30-C31
40	g	615	LUT	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
40	g	615	LUT	C30-C31-C32-C33
40	g	615	LUT	C31-C32-C33-C34
40	g	615	LUT	C31-C32-C33-C40
40	g	615	LUT	C40-C33-C34-C35
40	g	616	LUT	C1-C6-C7-C8
40	g	616	LUT	C11-C10-C9-C8
40	g	616	LUT	C11-C10-C9-C19
40	g	616	LUT	C11-C12-C13-C20
40	g	616	LUT	C39-C29-C30-C31
40	g	616	LUT	C31-C32-C33-C40
40	n	615	LUT	C20-C13-C14-C15
40	n	615	LUT	C14-C15-C35-C34
40	n	615	LUT	C26-C27-C28-C29
40	n	615	LUT	C27-C28-C29-C39
40	n	615	LUT	C28-C29-C30-C31
40	n	615	LUT	C30-C31-C32-C33
40	n	615	LUT	C31-C32-C33-C40
40	n	616	LUT	C7-C8-C9-C10
40	n	616	LUT	C11-C10-C9-C19
40	n	616	LUT	C10-C11-C12-C13
40	n	616	LUT	C11-C12-C13-C20
40	n	616	LUT	C20-C13-C14-C15
40	n	616	LUT	C26-C27-C28-C29
40	n	616	LUT	C27-C28-C29-C39
40	n	616	LUT	C31-C32-C33-C40
40	r	613	LUT	C11-C10-C9-C19
40	r	613	LUT	C11-C12-C13-C20
40	r	613	LUT	C26-C27-C28-C29
40	r	613	LUT	C27-C28-C29-C39
40	s	614	LUT	C1-C6-C7-C8
40	s	614	LUT	C5-C6-C7-C8
40	s	614	LUT	C6-C7-C8-C9
40	s	614	LUT	C9-C10-C11-C12
40	s	614	LUT	C11-C12-C13-C14
40	s	614	LUT	C26-C27-C28-C29
40	s	614	LUT	C27-C28-C29-C30
40	s	614	LUT	C39-C29-C30-C31
40	s	615	LUT	C5-C6-C7-C8
40	s	615	LUT	C6-C7-C8-C9
40	s	615	LUT	C7-C8-C9-C19
40	s	615	LUT	C11-C12-C13-C20
40	s	615	LUT	C31-C32-C33-C40

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Mol	Chain	Res	Type	Atoms
40	y	316	LUT	C6-C7-C8-C9
40	y	316	LUT	C7-C8-C9-C19
40	y	316	LUT	C11-C10-C9-C8
40	y	316	LUT	C10-C11-C12-C13
40	y	316	LUT	C27-C28-C29-C30
40	y	316	LUT	C39-C29-C30-C31
40	y	317	LUT	C6-C7-C8-C9
40	y	317	LUT	C7-C8-C9-C19
40	y	317	LUT	C11-C12-C13-C20
40	y	317	LUT	C21-C26-C27-C28
40	y	317	LUT	C25-C26-C27-C28
40	y	317	LUT	C26-C27-C28-C29
40	y	317	LUT	C27-C28-C29-C30
40	y	317	LUT	C28-C29-C30-C31
40	y	317	LUT	C39-C29-C30-C31
40	y	317	LUT	C31-C32-C33-C40
41	G	617	NEX	O24-C26-C27-C28
41	N	617	NEX	C20-C13-C14-C15
41	N	617	NEX	O24-C26-C27-C28
41	N	617	NEX	C27-C28-C29-C39
41	N	617	NEX	C39-C29-C30-C31
41	N	617	NEX	C40-C33-C34-C35
41	R	614	NEX	C7-C8-C9-C19
41	R	614	NEX	C9-C10-C11-C12
41	R	614	NEX	C11-C12-C13-C14
41	R	614	NEX	C12-C13-C14-C15
41	R	614	NEX	C14-C15-C35-C34
41	R	614	NEX	O24-C26-C27-C28
41	R	614	NEX	C27-C28-C29-C39
41	R	614	NEX	C31-C32-C33-C40
41	R	618	NEX	O24-C26-C27-C28
41	R	618	NEX	C27-C28-C29-C39
41	R	618	NEX	C29-C30-C31-C32
41	R	618	NEX	C40-C33-C34-C35
41	S	617	NEX	C20-C13-C14-C15
41	S	617	NEX	C13-C14-C15-C35
41	Y	317	NEX	C7-C8-C9-C19
41	Y	317	NEX	C11-C10-C9-C19
41	Y	317	NEX	C10-C11-C12-C13
41	Y	317	NEX	C11-C12-C13-C14
41	Y	317	NEX	C20-C13-C14-C15
41	Y	317	NEX	C14-C15-C35-C34

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Mol	Chain	Res	Type	Atoms
41	Y	317	NEX	O24-C26-C27-C28
41	Y	317	NEX	C40-C33-C34-C35
41	g	617	NEX	C11-C10-C9-C19
41	g	617	NEX	C11-C12-C13-C14
41	g	617	NEX	O24-C26-C27-C28
41	g	617	NEX	C29-C30-C31-C32
41	g	617	NEX	C31-C32-C33-C34
41	n	618	NEX	C7-C8-C9-C19
41	n	618	NEX	C11-C10-C9-C19
41	n	618	NEX	C11-C12-C13-C14
41	n	618	NEX	O24-C26-C27-C28
41	n	618	NEX	C27-C28-C29-C39
41	n	618	NEX	C39-C29-C30-C31
41	n	618	NEX	C40-C33-C34-C35
41	r	614	NEX	C11-C12-C13-C20
41	r	614	NEX	O24-C26-C27-C28
41	r	614	NEX	C27-C28-C29-C39
41	r	614	NEX	C31-C32-C33-C40
41	s	617	NEX	C40-C33-C34-C35
42	G	619	XAT	O4-C6-C7-C8
42	G	619	XAT	C7-C8-C9-C10
42	G	619	XAT	C31-C32-C33-C40
42	N	619	XAT	C7-C8-C9-C10
42	N	619	XAT	C11-C12-C13-C14
42	N	619	XAT	C31-C32-C33-C34
42	R	615	XAT	C11-C10-C9-C19
42	R	615	XAT	O24-C26-C27-C28
42	R	615	XAT	C26-C27-C28-C29
42	R	615	XAT	C27-C28-C29-C30
42	R	615	XAT	C27-C28-C29-C39
42	R	615	XAT	C39-C29-C30-C31
42	Y	301	XAT	O4-C6-C7-C8
42	Y	301	XAT	C31-C32-C33-C34
42	Y	301	XAT	C31-C32-C33-C40
42	n	617	XAT	O4-C6-C7-C8
42	n	617	XAT	C7-C8-C9-C19
42	n	617	XAT	C11-C10-C9-C19
42	n	617	XAT	C11-C12-C13-C14
42	n	620	XAT	O4-C6-C7-C8
42	n	620	XAT	C7-C8-C9-C10
42	n	620	XAT	C11-C12-C13-C14
42	r	615	XAT	C11-C10-C9-C19

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Mol	Chain	Res	Type	Atoms
42	r	615	XAT	O24-C26-C27-C28
42	r	615	XAT	C26-C27-C28-C29
42	r	615	XAT	C27-C28-C29-C30
42	r	615	XAT	C27-C28-C29-C39
42	r	615	XAT	C39-C29-C30-C31
42	y	302	XAT	O4-C6-C7-C8
42	y	302	XAT	C31-C32-C33-C34
42	y	302	XAT	C40-C33-C34-C35
23	R	611	CLA	O1D-CGD-O2D-CED
23	S	603	CLA	O1D-CGD-O2D-CED
23	s	603	CLA	O1D-CGD-O2D-CED
23	S	609	CLA	O1D-CGD-O2D-CED
23	r	611	CLA	O1D-CGD-O2D-CED
23	A	402	CLA	CBD-CGD-O2D-CED
23	N	611	CLA	CBD-CGD-O2D-CED
23	R	601	CLA	CBD-CGD-O2D-CED
23	S	603	CLA	CBD-CGD-O2D-CED
23	S	604	CLA	CBD-CGD-O2D-CED
23	S	609	CLA	CBD-CGD-O2D-CED
23	n	611	CLA	CBD-CGD-O2D-CED
23	s	602	CLA	CBD-CGD-O2D-CED
23	s	603	CLA	CBD-CGD-O2D-CED
23	s	604	CLA	CBD-CGD-O2D-CED
23	y	311	CLA	CBD-CGD-O2D-CED
24	d	402	PHO	CBD-CGD-O2D-CED
23	S	612	CLA	O1A-CGA-O2A-C1
23	S	613	CLA	O1A-CGA-O2A-C1
23	s	612	CLA	O1A-CGA-O2A-C1
23	s	613	CLA	O1A-CGA-O2A-C1
24	A	405	PHO	O1A-CGA-O2A-C1
30	G	618	LHG	O10-C23-O8-C6
30	n	619	LHG	O10-C23-O8-C6
23	R	601	CLA	O1D-CGD-O2D-CED
23	S	604	CLA	O1D-CGD-O2D-CED
33	d	411	DGD	C4D-C5D-C6D-O5D
23	B	605	CLA	O1D-CGD-O2D-CED
23	Y	310	CLA	O1D-CGD-O2D-CED
23	c	503	CLA	O1D-CGD-O2D-CED
23	g	610	CLA	O1D-CGD-O2D-CED
23	s	609	CLA	O1D-CGD-O2D-CED
23	y	311	CLA	O1D-CGD-O2D-CED
23	S	613	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	s	612	CLA	CBA-CGA-O2A-C1
24	A	405	PHO	CBA-CGA-O2A-C1
30	G	618	LHG	C24-C23-O8-C6
30	n	619	LHG	C24-C23-O8-C6
23	C	502	CLA	CBD-CGD-O2D-CED
23	G	614	CLA	CBD-CGD-O2D-CED
23	N	613	CLA	CBD-CGD-O2D-CED
23	N	614	CLA	CBD-CGD-O2D-CED
23	S	602	CLA	CBD-CGD-O2D-CED
23	c	502	CLA	CBD-CGD-O2D-CED
23	g	614	CLA	CBD-CGD-O2D-CED
24	D	402	PHO	CBD-CGD-O2D-CED
23	B	616	CLA	O1A-CGA-O2A-C1
23	G	611	CLA	O1A-CGA-O2A-C1
23	R	612	CLA	O1A-CGA-O2A-C1
23	S	603	CLA	O1A-CGA-O2A-C1
23	S	610	CLA	O1A-CGA-O2A-C1
23	Y	311	CLA	O1A-CGA-O2A-C1
23	b	613	CLA	O1A-CGA-O2A-C1
23	g	613	CLA	O1A-CGA-O2A-C1
23	n	614	CLA	O1A-CGA-O2A-C1
23	s	603	CLA	O1A-CGA-O2A-C1
23	s	610	CLA	O1A-CGA-O2A-C1
23	y	312	CLA	O1A-CGA-O2A-C1
28	s	618	3PH	O32-C31-O31-C3
30	D	408	LHG	O10-C23-O8-C6
30	N	618	LHG	O10-C23-O8-C6
30	d	408	LHG	O10-C23-O8-C6
23	G	610	CLA	O1D-CGD-O2D-CED
23	S	611	CLA	O1D-CGD-O2D-CED
23	b	605	CLA	O1D-CGD-O2D-CED
23	s	611	CLA	O1D-CGD-O2D-CED
23	B	609	CLA	O1D-CGD-O2D-CED
23	C	503	CLA	O1D-CGD-O2D-CED
23	b	609	CLA	O1D-CGD-O2D-CED
23	n	614	CLA	O1D-CGD-O2D-CED
23	B	607	CLA	CBD-CGD-O2D-CED
23	N	611	CLA	O1D-CGD-O2D-CED
26	M	101	SQD	O49-C7-O47-C45
28	X	201	3PH	O22-C21-O21-C2
28	x	201	3PH	O22-C21-O21-C2
30	R	616	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
37	D	410	DGA	OB1-CB1-OG2-CG2
37	b	626	DGA	OB1-CB1-OG2-CG2
23	B	602	CLA	C3-C5-C6-C7
23	B	616	CLA	C3-C5-C6-C7
23	C	511	CLA	C3-C5-C6-C7
23	G	613	CLA	C3-C5-C6-C7
23	S	610	CLA	C3-C5-C6-C7
23	b	604	CLA	C3-C5-C6-C7
23	s	602	CLA	C3-C5-C6-C7
23	s	609	CLA	C3-C5-C6-C7
23	s	610	CLA	C3-C5-C6-C7
23	y	306	CLA	C3-C5-C6-C7
23	y	315	CLA	C3-C5-C6-C7
24	A	405	PHO	C3-C5-C6-C7
24	a	406	PHO	C3-C5-C6-C7
39	n	609	CHL	C3-C5-C6-C7
23	G	611	CLA	CBA-CGA-O2A-C1
23	R	612	CLA	CBA-CGA-O2A-C1
23	S	603	CLA	CBA-CGA-O2A-C1
23	S	612	CLA	CBA-CGA-O2A-C1
23	n	614	CLA	CBA-CGA-O2A-C1
23	s	603	CLA	CBA-CGA-O2A-C1
23	s	613	CLA	CBA-CGA-O2A-C1
28	s	618	3PH	C32-C31-O31-C3
30	N	618	LHG	C24-C23-O8-C6
26	M	101	SQD	C8-C7-O47-C45
28	L	102	3PH	C22-C21-O21-C2
28	T	101	3PH	C22-C21-O21-C2
23	A	402	CLA	O1D-CGD-O2D-CED
23	a	403	CLA	O1D-CGD-O2D-CED
23	n	613	CLA	CBD-CGD-O2D-CED
23	B	616	CLA	C4-C3-C5-C6
23	R	604	CLA	C4-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6
23	r	604	CLA	C4-C3-C5-C6
23	B	603	CLA	C2-C3-C5-C6
23	B	605	CLA	C2-C3-C5-C6
39	Y	302	CHL	C2-C3-C5-C6
23	b	607	CLA	CBD-CGD-O2D-CED
23	n	610	CLA	CBD-CGD-O2D-CED
23	B	606	CLA	C2A-CAA-CBA-CGA
23	S	604	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
23	a	404	CLA	C2A-CAA-CBA-CGA
23	b	606	CLA	C2A-CAA-CBA-CGA
23	s	604	CLA	C2A-CAA-CBA-CGA
39	Y	308	CHL	C2A-CAA-CBA-CGA
23	R	601	CLA	O1A-CGA-O2A-C1
23	C	512	CLA	C3-C5-C6-C7
23	Y	305	CLA	C3-C5-C6-C7
23	Y	313	CLA	C3-C5-C6-C7
23	c	511	CLA	C3-C5-C6-C7
23	B	616	CLA	CBA-CGA-O2A-C1
23	N	614	CLA	CBA-CGA-O2A-C1
23	R	601	CLA	CBA-CGA-O2A-C1
23	S	610	CLA	CBA-CGA-O2A-C1
23	Y	311	CLA	CBA-CGA-O2A-C1
23	b	610	CLA	CBA-CGA-O2A-C1
23	b	613	CLA	CBA-CGA-O2A-C1
23	g	603	CLA	CBA-CGA-O2A-C1
23	g	613	CLA	CBA-CGA-O2A-C1
23	s	610	CLA	CBA-CGA-O2A-C1
23	y	312	CLA	CBA-CGA-O2A-C1
26	M	101	SQD	C24-C23-O48-C46
28	T	101	3PH	C32-C31-O31-C3
30	D	408	LHG	C24-C23-O8-C6
30	d	408	LHG	C24-C23-O8-C6
33	C	515	DGD	C4E-C5E-C6E-O5E
23	s	602	CLA	O1D-CGD-O2D-CED
23	N	602	CLA	CBD-CGD-O2D-CED
23	g	604	CLA	CBD-CGD-O2D-CED
26	L	101	SQD	O49-C7-O47-C45
33	H	502	DGD	C4E-C5E-C6E-O5E
33	c	515	DGD	C4E-C5E-C6E-O5E
23	A	402	CLA	O1A-CGA-O2A-C1
23	G	604	CLA	O1A-CGA-O2A-C1
23	a	403	CLA	O1A-CGA-O2A-C1
23	g	603	CLA	O1A-CGA-O2A-C1
23	g	604	CLA	O1A-CGA-O2A-C1
28	T	101	3PH	O32-C31-O31-C3
40	G	616	LUT	C9-C10-C11-C12
40	N	616	LUT	C29-C30-C31-C32
40	R	613	LUT	C29-C30-C31-C32
40	g	616	LUT	C9-C10-C11-C12
40	n	616	LUT	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
40	s	614	LUT	C29-C30-C31-C32
41	N	617	NEX	C9-C10-C11-C12
41	R	614	NEX	C13-C14-C15-C35
41	R	618	NEX	C9-C10-C11-C12
41	S	617	NEX	C9-C10-C11-C12
41	g	617	NEX	C9-C10-C11-C12
41	n	618	NEX	C9-C10-C11-C12
41	s	617	NEX	C9-C10-C11-C12
42	G	619	XAT	C9-C10-C11-C12
42	y	302	XAT	C33-C34-C35-C15
23	C	510	CLA	CBD-CGD-O2D-CED
23	D	406	CLA	CBD-CGD-O2D-CED
23	G	602	CLA	CBD-CGD-O2D-CED
23	N	610	CLA	CBD-CGD-O2D-CED
23	Y	305	CLA	CBD-CGD-O2D-CED
23	b	606	CLA	CBD-CGD-O2D-CED
23	c	510	CLA	CBD-CGD-O2D-CED
23	n	602	CLA	CBD-CGD-O2D-CED
23	s	604	CLA	O1D-CGD-O2D-CED
30	L	103	LHG	O2-C2-C3-O3
30	Y	318	LHG	O2-C2-C3-O3
30	a	412	LHG	O2-C2-C3-O3
30	y	318	LHG	O2-C2-C3-O3
23	c	504	CLA	C3-C5-C6-C7
23	y	314	CLA	C3-C5-C6-C7
23	d	406	CLA	CBA-CGA-O2A-C1
26	L	101	SQD	C24-C23-O48-C46
28	A	410	3PH	C32-C31-O31-C3
28	a	410	3PH	C32-C31-O31-C3
26	M	101	SQD	O10-C23-O48-C46
28	A	410	3PH	O32-C31-O31-C3
33	d	411	DGD	O6E-C5E-C6E-O5E
23	B	606	CLA	CBD-CGD-O2D-CED
23	G	612	CLA	CBD-CGD-O2D-CED
23	d	406	CLA	CBD-CGD-O2D-CED
31	b	622	LNL	C2-C3-C4-C5
28	a	410	3PH	O32-C31-O31-C3
30	D	408	LHG	C24-C25-C26-C27
30	b	627	LHG	C31-C32-C33-C34
31	C	521	LNL	C3-C4-C5-C6
31	C	521	LNL	C5-C6-C7-C8
23	n	611	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	d	402	PHO	O1D-CGD-O2D-CED
30	d	404	LHG	C31-C32-C33-C34
31	C	522	LNL	C2-C3-C4-C5
23	C	504	CLA	C3-C5-C6-C7
23	A	402	CLA	CBA-CGA-O2A-C1
23	G	604	CLA	CBA-CGA-O2A-C1
23	a	403	CLA	CBA-CGA-O2A-C1
23	g	604	CLA	CBA-CGA-O2A-C1
33	C	515	DGD	O6E-C5E-C6E-O5E
33	d	411	DGD	C4E-C5E-C6E-O5E
30	N	618	LHG	C5-C4-O6-P
23	b	610	CLA	O1A-CGA-O2A-C1
33	H	502	DGD	O6E-C5E-C6E-O5E
23	b	603	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
29	D	407	PL9	C12-C11-C9-C10
29	a	411	PL9	C40-C39-C41-C42
29	d	407	PL9	C12-C11-C9-C10
23	b	603	CLA	C2-C3-C5-C6
23	b	614	CLA	C2-C3-C5-C6
29	D	407	PL9	C12-C11-C9-C8
29	a	411	PL9	C38-C39-C41-C42
29	d	407	PL9	C12-C11-C9-C8
39	g	607	CHL	C2A-CAA-CBA-CGA
39	n	608	CHL	C2A-CAA-CBA-CGA
33	c	515	DGD	O6E-C5E-C6E-O5E
23	N	614	CLA	O1A-CGA-O2A-C1
27	r	617	LMG	O6-C1-O1-C7
29	A	411	PL9	C44-C46-C47-C48
29	a	411	PL9	C19-C21-C22-C23
29	a	411	PL9	C44-C46-C47-C48
23	N	612	CLA	CBA-CGA-O2A-C1
23	c	510	CLA	CBA-CGA-O2A-C1
31	B	622	LNL	C2-C3-C4-C5
23	d	406	CLA	O1A-CGA-O2A-C1
26	L	101	SQD	O10-C23-O48-C46
30	A	412	LHG	C1-C2-C3-O3
30	a	412	LHG	C1-C2-C3-O3
30	g	618	LHG	C1-C2-C3-O3
23	S	602	CLA	O1D-CGD-O2D-CED
24	D	402	PHO	O1D-CGD-O2D-CED
23	D	406	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	N	603	CLA	CBA-CGA-O2A-C1
23	S	611	CLA	CBA-CGA-O2A-C1
23	c	506	CLA	CBA-CGA-O2A-C1
23	g	611	CLA	CBA-CGA-O2A-C1
23	g	612	CLA	CBA-CGA-O2A-C1
23	n	603	CLA	CBA-CGA-O2A-C1
23	c	512	CLA	CBD-CGD-O2D-CED
40	S	615	LUT	C9-C10-C11-C12
42	n	617	XAT	C9-C10-C11-C12
23	s	610	CLA	C15-C16-C17-C18
31	A	413	LNL	C5-C6-C7-C8
23	C	502	CLA	O1D-CGD-O2D-CED
30	d	404	LHG	C33-C34-C35-C36
23	C	504	CLA	C5-C6-C7-C8
23	S	613	CLA	C10-C11-C12-C13
23	b	612	CLA	C15-C16-C17-C18
39	G	620	CHL	C10-C11-C12-C13
39	n	606	CHL	C10-C11-C12-C13
39	n	607	CHL	C5-C6-C7-C8
30	A	412	LHG	O2-C2-C3-O3
30	N	618	LHG	O2-C2-C3-O3
28	x	201	3PH	C26-C27-C28-C29
23	N	603	CLA	O1A-CGA-O2A-C1
23	c	506	CLA	O1A-CGA-O2A-C1
23	g	611	CLA	O1A-CGA-O2A-C1
23	g	612	CLA	O1A-CGA-O2A-C1
23	D	406	CLA	C4-C3-C5-C6
23	R	604	CLA	C2-C3-C5-C6
23	r	604	CLA	C2-C3-C5-C6
23	B	604	CLA	C6-C7-C8-C9
23	B	607	CLA	C11-C12-C13-C14
23	B	610	CLA	C11-C12-C13-C14
23	C	504	CLA	C11-C12-C13-C14
23	C	507	CLA	C14-C13-C15-C16
23	C	509	CLA	C6-C7-C8-C9
23	G	603	CLA	C11-C10-C8-C9
23	N	603	CLA	C11-C12-C13-C14
23	N	611	CLA	C11-C10-C8-C9
23	S	609	CLA	C6-C7-C8-C9
23	S	610	CLA	C6-C7-C8-C9
23	S	613	CLA	C11-C10-C8-C9
23	S	613	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	b	610	CLA	C11-C12-C13-C14
23	b	616	CLA	C11-C10-C8-C9
23	c	504	CLA	C11-C12-C13-C14
23	c	512	CLA	C6-C7-C8-C9
23	g	603	CLA	C11-C10-C8-C9
23	n	603	CLA	C11-C12-C13-C14
23	r	608	CLA	C11-C10-C8-C9
23	s	610	CLA	C6-C7-C8-C9
23	y	305	CLA	C11-C10-C8-C9
23	y	315	CLA	C11-C10-C8-C9
35	C	523	VIV	C21-C22-C23-C1
35	y	301	VIV	C21-C22-C23-C1
39	G	607	CHL	C6-C7-C8-C9
39	N	607	CHL	C6-C7-C8-C9
39	R	606	CHL	C6-C7-C8-C9
39	r	606	CHL	C11-C10-C8-C9
39	y	303	CHL	C6-C7-C8-C9
23	N	613	CLA	O1D-CGD-O2D-CED
23	c	502	CLA	O1D-CGD-O2D-CED
23	S	612	CLA	CBD-CGD-O2D-CED
23	g	612	CLA	CBD-CGD-O2D-CED
23	S	610	CLA	C15-C16-C17-C18
23	B	607	CLA	C2A-CAA-CBA-CGA
23	C	513	CLA	C2A-CAA-CBA-CGA
23	b	613	CLA	C2A-CAA-CBA-CGA
23	s	613	CLA	C2A-CAA-CBA-CGA
25	B	617	BCR	C7-C8-C9-C34
25	V	101	BCR	C37-C22-C23-C24
25	v	101	BCR	C37-C22-C23-C24
40	G	615	LUT	C7-C8-C9-C19
40	G	615	LUT	C11-C12-C13-C20
40	R	613	LUT	C11-C12-C13-C20
40	R	613	LUT	C27-C28-C29-C39
40	R	613	LUT	C31-C32-C33-C40
40	Y	315	LUT	C27-C28-C29-C39
40	Y	316	LUT	C31-C32-C33-C40
40	g	615	LUT	C27-C28-C29-C39
40	s	614	LUT	C7-C8-C9-C19
40	s	614	LUT	C11-C12-C13-C20
40	y	316	LUT	C27-C28-C29-C39
41	G	617	NEX	C27-C28-C29-C39
41	N	617	NEX	C11-C12-C13-C20

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Mol	Chain	Res	Type	Atoms
41	R	618	NEX	C11-C12-C13-C20
41	g	617	NEX	C31-C32-C33-C40
42	N	619	XAT	C7-C8-C9-C19
42	Y	301	XAT	C7-C8-C9-C19
42	Y	301	XAT	C11-C12-C13-C20
42	n	620	XAT	C7-C8-C9-C19
42	y	302	XAT	C31-C32-C33-C40
25	B	617	BCR	C7-C8-C9-C10
25	V	101	BCR	C21-C22-C23-C24
40	N	615	LUT	C11-C12-C13-C14
40	R	613	LUT	C27-C28-C29-C30
40	Y	316	LUT	C31-C32-C33-C34
40	s	614	LUT	C7-C8-C9-C10
40	s	614	LUT	C31-C32-C33-C34
40	s	615	LUT	C7-C8-C9-C10
40	y	317	LUT	C31-C32-C33-C34
41	N	617	NEX	C11-C12-C13-C14
41	R	618	NEX	C11-C12-C13-C14
41	s	617	NEX	C11-C12-C13-C14
42	Y	301	XAT	C7-C8-C9-C10
42	Y	301	XAT	C11-C12-C13-C14
42	y	302	XAT	C11-C12-C13-C14
30	A	412	LHG	C29-C30-C31-C32
30	D	404	LHG	C23-C24-C25-C26
31	C	521	LNL	C1-C2-C3-C4
23	n	603	CLA	O1A-CGA-O2A-C1
23	y	306	CLA	C13-C15-C16-C17
35	C	523	VIV	C23-C24-C25-C26
39	N	601	CHL	C5-C6-C7-C8
23	G	614	CLA	O1D-CGD-O2D-CED
30	N	618	LHG	C26-C27-C28-C29
23	n	604	CLA	CBD-CGD-O2D-CED
23	r	608	CLA	CBD-CGD-O2D-CED
23	g	614	CLA	O1D-CGD-O2D-CED
28	d	403	3PH	C32-C31-O31-C3
23	B	606	CLA	C13-C15-C16-C17
23	B	612	CLA	C15-C16-C17-C18
23	C	512	CLA	C5-C6-C7-C8
23	S	609	CLA	C5-C6-C7-C8
23	Y	310	CLA	C13-C15-C16-C17
23	c	504	CLA	C5-C6-C7-C8
23	c	510	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	y	313	CLA	C8-C10-C11-C12
35	C	523	VIV	C20-C21-C22-C23
39	n	609	CHL	C5-C6-C7-C8
27	B	620	LMG	C28-C29-C30-C31
31	B	625	LNL	C1-C2-C3-C4
31	b	622	LNL	C1-C2-C3-C4
31	c	522	LNL	C1-C2-C3-C4
33	d	411	DGD	C1B-C2B-C3B-C4B
23	B	604	CLA	C5-C6-C7-C8
23	C	510	CLA	C8-C10-C11-C12
23	C	510	CLA	C10-C11-C12-C13
23	C	510	CLA	C15-C16-C17-C18
23	D	405	CLA	C10-C11-C12-C13
23	N	611	CLA	C8-C10-C11-C12
23	b	604	CLA	C10-C11-C12-C13
23	b	615	CLA	C10-C11-C12-C13
23	c	510	CLA	C15-C16-C17-C18
23	s	609	CLA	C5-C6-C7-C8
23	s	613	CLA	C5-C6-C7-C8
23	y	311	CLA	C5-C6-C7-C8
35	C	523	VIV	C15-C16-C17-C18
39	G	601	CHL	C5-C6-C7-C8
39	g	609	CHL	C5-C6-C7-C8
30	A	412	LHG	O1-C1-C2-O2
30	a	412	LHG	O1-C1-C2-O2
30	s	616	LHG	O1-C1-C2-O2
30	D	408	LHG	C23-C24-C25-C26
30	G	618	LHG	C7-C8-C9-C10
30	r	616	LHG	C23-C24-C25-C26
30	s	616	LHG	C23-C24-C25-C26
31	B	622	LNL	C1-C2-C3-C4
31	b	625	LNL	C1-C2-C3-C4
31	c	521	LNL	C1-C2-C3-C4
32	B	621	PAM	C1-C2-C3-C4
33	H	502	DGD	C1B-C2B-C3B-C4B
23	N	612	CLA	CBD-CGD-O2D-CED
23	B	607	CLA	C13-C15-C16-C17
23	C	512	CLA	C8-C10-C11-C12
23	Y	312	CLA	C8-C10-C11-C12
23	b	613	CLA	C8-C10-C11-C12
39	Y	302	CHL	C5-C6-C7-C8
39	Y	307	CHL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
39	y	303	CHL	C5-C6-C7-C8
26	a	409	SQD	C14-C15-C16-C17
23	b	616	CLA	C8-C10-C11-C12
23	c	506	CLA	C15-C16-C17-C18
23	c	513	CLA	C10-C11-C12-C13
24	A	405	PHO	C13-C15-C16-C17
24	a	406	PHO	C13-C15-C16-C17
26	M	101	SQD	C23-C24-C25-C26
28	A	410	3PH	C21-C22-C23-C24
31	I	101	LNL	C1-C2-C3-C4
31	a	401	LNL	C1-C2-C3-C4
23	C	508	CLA	CBD-CGD-O2D-CED
23	C	512	CLA	CBD-CGD-O2D-CED
23	C	505	CLA	C5-C6-C7-C8
23	C	505	CLA	C15-C16-C17-C18
23	R	604	CLA	C5-C6-C7-C8
23	c	505	CLA	C5-C6-C7-C8
23	c	505	CLA	C15-C16-C17-C18
23	r	604	CLA	C5-C6-C7-C8
23	C	509	CLA	C6-C7-C8-C10
23	N	603	CLA	C11-C12-C13-C15
23	N	613	CLA	C12-C13-C15-C16
23	b	602	CLA	C11-C10-C8-C7
23	b	602	CLA	C12-C13-C15-C16
23	b	603	CLA	C11-C12-C13-C15
23	b	611	CLA	C12-C13-C15-C16
23	b	613	CLA	C11-C10-C8-C7
23	c	501	CLA	C12-C13-C15-C16
23	c	512	CLA	C11-C12-C13-C15
23	s	613	CLA	C11-C10-C8-C7
39	R	606	CHL	C12-C13-C15-C16
23	y	313	CLA	C3-C5-C6-C7
42	R	615	XAT	C13-C14-C15-C35
42	Y	301	XAT	C9-C10-C11-C12
42	r	615	XAT	C13-C14-C15-C35
42	y	302	XAT	C9-C10-C11-C12
23	B	610	CLA	C2A-CAA-CBA-CGA
23	R	604	CLA	C2A-CAA-CBA-CGA
23	S	612	CLA	C2A-CAA-CBA-CGA
23	b	607	CLA	C2A-CAA-CBA-CGA
23	r	604	CLA	C2A-CAA-CBA-CGA
23	s	612	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
23	N	614	CLA	O1D-CGD-O2D-CED
23	B	602	CLA	C8-C10-C11-C12
23	B	615	CLA	C10-C11-C12-C13
23	n	602	CLA	C5-C6-C7-C8
23	r	609	CLA	C5-C6-C7-C8
35	C	523	VIV	C18-C20-C21-C22
39	R	606	CHL	C5-C6-C7-C8
39	g	601	CHL	C5-C6-C7-C8
30	a	412	LHG	C33-C34-C35-C36
25	b	619	BCR	C6-C7-C8-C9
23	D	406	CLA	O1A-CGA-O2A-C1
23	N	612	CLA	O1A-CGA-O2A-C1
23	S	611	CLA	O1A-CGA-O2A-C1
23	d	405	CLA	C10-C11-C12-C13
39	G	601	CHL	C8-C10-C11-C12
29	A	411	PL9	C24-C26-C27-C28
29	a	411	PL9	C9-C11-C12-C13
25	B	617	BCR	C10-C11-C12-C13
25	V	101	BCR	C18-C19-C20-C21
25	v	101	BCR	C18-C19-C20-C21
40	Y	315	LUT	C30-C31-C32-C33
40	Y	316	LUT	C30-C31-C32-C33
40	n	616	LUT	C30-C31-C32-C33
40	r	613	LUT	C10-C11-C12-C13
40	s	614	LUT	C10-C11-C12-C13
40	s	614	LUT	C30-C31-C32-C33
40	y	316	LUT	C30-C31-C32-C33
40	y	317	LUT	C30-C31-C32-C33
42	N	619	XAT	C10-C11-C12-C13
42	n	620	XAT	C10-C11-C12-C13
30	g	618	LHG	C27-C28-C29-C30
30	d	404	LHG	O2-C2-C3-O3
30	n	619	LHG	O2-C2-C3-O3
23	B	603	CLA	C5-C6-C7-C8
23	B	612	CLA	C13-C15-C16-C17
23	Y	310	CLA	C5-C6-C7-C8
23	r	602	CLA	C5-C6-C7-C8
39	G	609	CHL	C5-C6-C7-C8
23	B	601	CLA	CBA-CGA-O2A-C1
23	b	616	CLA	CBA-CGA-O2A-C1
28	W	201	3PH	C3B-C3C-C3D-C3E
28	d	403	3PH	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
30	D	408	LHG	C7-C8-C9-C10
23	C	508	CLA	C5-C6-C7-C8
23	S	613	CLA	C13-C15-C16-C17
23	b	613	CLA	C10-C11-C12-C13
23	b	616	CLA	C5-C6-C7-C8
23	c	512	CLA	C5-C6-C7-C8
23	g	610	CLA	C5-C6-C7-C8
23	y	315	CLA	C5-C6-C7-C8
39	y	310	CHL	C8-C10-C11-C12
23	g	602	CLA	CBD-CGD-O2D-CED
23	c	510	CLA	O1A-CGA-O2A-C1
23	c	510	CLA	C8-C10-C11-C12
39	g	609	CHL	C8-C10-C11-C12
30	A	412	LHG	C3-O3-P-O6
30	A	412	LHG	C4-O6-P-O3
30	G	618	LHG	C3-O3-P-O6
30	R	616	LHG	C3-O3-P-O6
30	S	616	LHG	C4-O6-P-O3
30	b	627	LHG	C3-O3-P-O6
30	d	404	LHG	C4-O6-P-O3
30	g	618	LHG	C3-O3-P-O6
30	s	616	LHG	C4-O6-P-O3
26	L	101	SQD	C7-C8-C9-C10
23	r	602	CLA	C3-C5-C6-C7
39	G	607	CHL	C3-C5-C6-C7
23	C	513	CLA	CBA-CGA-O2A-C1
23	N	613	CLA	CBA-CGA-O2A-C1
23	c	511	CLA	CBA-CGA-O2A-C1
30	d	404	LHG	C24-C23-O8-C6
23	B	607	CLA	O1D-CGD-O2D-CED
27	b	628	LMG	C21-C22-C23-C24
23	n	613	CLA	O1D-CGD-O2D-CED
30	N	618	LHG	C1-C2-C3-O3
30	S	616	LHG	C1-C2-C3-O3
30	d	404	LHG	C1-C2-C3-O3
30	n	619	LHG	C1-C2-C3-O3
30	s	616	LHG	C1-C2-C3-O3
29	d	407	PL9	C15-C14-C16-C17
23	B	616	CLA	C2-C3-C5-C6
23	R	602	CLA	C13-C15-C16-C17
23	y	314	CLA	C5-C6-C7-C8
23	C	501	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
23	c	501	CLA	C2A-CAA-CBA-CGA
23	n	614	CLA	C2A-CAA-CBA-CGA
39	G	607	CHL	C2A-CAA-CBA-CGA
39	N	608	CHL	C2A-CAA-CBA-CGA
23	c	506	CLA	C16-C17-C18-C19
35	C	523	VIV	C25-C26-C27-C28
30	s	616	LHG	C24-C23-O8-C6
33	d	411	DGD	O6D-C5D-C6D-O5D
37	D	410	DGA	CB4-CB5-CB6-CB7
40	Y	316	LUT	C29-C30-C31-C32
41	N	617	NEX	C29-C30-C31-C32
42	R	615	XAT	C33-C34-C35-C15
42	Y	301	XAT	C33-C34-C35-C15
42	r	615	XAT	C9-C10-C11-C12
42	r	615	XAT	C33-C34-C35-C15
31	C	522	LNL	C1-C2-C3-C4
28	w	202	3PH	C34-C35-C36-C37
30	G	618	LHG	C34-C35-C36-C37
30	N	618	LHG	C12-C13-C14-C15
31	C	522	LNL	C3-C4-C5-C6
23	Y	314	CLA	CBD-CGD-O2D-CED
23	b	611	CLA	C15-C16-C17-C18
25	b	617	BCR	C20-C21-C22-C37
40	G	615	LUT	C11-C10-C9-C19
40	G	615	LUT	C40-C33-C34-C35
40	G	616	LUT	C20-C13-C14-C15
40	G	616	LUT	C39-C29-C30-C31
40	G	616	LUT	C40-C33-C34-C35
40	N	615	LUT	C40-C33-C34-C35
40	N	616	LUT	C40-C33-C34-C35
40	R	613	LUT	C20-C13-C14-C15
40	S	614	LUT	C20-C13-C14-C15
40	Y	315	LUT	C20-C13-C14-C15
40	g	616	LUT	C20-C13-C14-C15
40	g	616	LUT	C40-C33-C34-C35
40	n	615	LUT	C39-C29-C30-C31
40	n	616	LUT	C40-C33-C34-C35
40	r	613	LUT	C20-C13-C14-C15
40	r	613	LUT	C40-C33-C34-C35
40	s	614	LUT	C20-C13-C14-C15
40	s	614	LUT	C40-C33-C34-C35
40	s	615	LUT	C39-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
40	y	316	LUT	C20-C13-C14-C15
41	G	617	NEX	C39-C29-C30-C31
41	G	617	NEX	C40-C33-C34-C35
41	R	614	NEX	C39-C29-C30-C31
41	R	618	NEX	C20-C13-C14-C15
41	S	617	NEX	C11-C10-C9-C19
41	Y	317	NEX	C39-C29-C30-C31
41	g	617	NEX	C20-C13-C14-C15
41	g	617	NEX	C40-C33-C34-C35
41	n	618	NEX	C20-C13-C14-C15
41	r	614	NEX	C20-C13-C14-C15
41	r	614	NEX	C39-C29-C30-C31
41	s	617	NEX	C11-C10-C9-C19
41	s	617	NEX	C20-C13-C14-C15
42	G	619	XAT	C11-C10-C9-C19
42	G	619	XAT	C39-C29-C30-C31
42	N	619	XAT	C39-C29-C30-C31
42	R	615	XAT	C20-C13-C14-C15
42	Y	301	XAT	C11-C10-C9-C19
42	Y	301	XAT	C20-C13-C14-C15
42	Y	301	XAT	C40-C33-C34-C35
42	r	615	XAT	C20-C13-C14-C15
42	y	302	XAT	C11-C10-C9-C19
42	y	302	XAT	C20-C13-C14-C15
26	A	408	SQD	C30-C31-C32-C33
27	d	409	LMG	C18-C19-C20-C21
28	A	410	3PH	C3A-C3B-C3C-C3D
28	X	201	3PH	C25-C26-C27-C28
30	d	404	LHG	C26-C27-C28-C29
31	A	414	LNL	C2-C3-C4-C5
31	C	517	LNL	C2-C3-C4-C5
31	C	520	LNL	C2-C3-C4-C5
31	b	623	LNL	C3-C4-C5-C6
31	c	520	LNL	C5-C6-C7-C8
31	c	521	LNL	C2-C3-C4-C5
31	i	101	LNL	C4-C5-C6-C7
33	C	515	DGD	CAA-CBA-CCA-CDA
33	C	515	DGD	CCA-CDA-CEA-CFA
33	C	515	DGD	CBB-CCB-CDB-CEB
37	b	626	DGA	CBB-CCB-CDB-CEB
23	b	607	CLA	O1D-CGD-O2D-CED
23	g	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	A	408	SQD	C24-C23-O48-C46
26	A	408	SQD	C9-C10-C11-C12
27	A	409	LMG	C41-C42-C43-C44
27	R	617	LMG	C16-C17-C18-C19
28	C	524	3PH	C2E-C2F-C2G-C2H
28	C	524	3PH	C38-C39-C3A-C3B
28	D	403	3PH	C38-C39-C3A-C3B
28	L	102	3PH	C2A-C2B-C2C-C2D
30	R	616	LHG	C33-C34-C35-C36
30	Y	318	LHG	C34-C35-C36-C37
30	a	412	LHG	C12-C13-C14-C15
31	A	414	LNL	C3-C4-C5-C6
31	a	413	LNL	C5-C6-C7-C8
31	c	518	LNL	C5-C6-C7-C8
26	L	101	SQD	C46-C45-O47-C7
23	n	610	CLA	O1D-CGD-O2D-CED
23	A	403	CLA	C15-C16-C17-C18
23	C	512	CLA	C10-C11-C12-C13
23	C	512	CLA	C13-C15-C16-C17
23	C	513	CLA	C5-C6-C7-C8
23	a	404	CLA	C15-C16-C17-C18
23	y	315	CLA	CBD-CGD-O2D-CED
26	a	409	SQD	C11-C10-C9-C8
28	T	101	3PH	C38-C39-C3A-C3B
30	D	408	LHG	C11-C12-C13-C14
30	d	408	LHG	C12-C13-C14-C15
30	s	616	LHG	C9-C10-C11-C12
31	A	413	LNL	C3-C4-C5-C6
31	C	521	LNL	C2-C3-C4-C5
31	C	521	LNL	C4-C5-C6-C7
31	b	623	LNL	C5-C6-C7-C8
37	b	626	DGA	CAA-CBA-CCA-CDA
37	b	626	DGA	CDB-CEB-CFB-CGB
23	N	602	CLA	O1D-CGD-O2D-CED
27	b	620	LMG	C31-C32-C33-C34
27	r	617	LMG	C16-C17-C18-C19
28	A	410	3PH	C34-C35-C36-C37
37	D	410	DGA	CB7-CB8-CB9-CAB
30	D	404	LHG	O2-C2-C3-O3
27	A	409	LMG	C40-C41-C42-C43
28	W	201	3PH	C33-C34-C35-C36
30	y	318	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	b	616	CLA	C3-C5-C6-C7
30	d	404	LHG	C7-C8-C9-C10
23	C	510	CLA	O1D-CGD-O2D-CED
25	C	514	BCR	C20-C21-C22-C23
25	b	617	BCR	C11-C10-C9-C8
25	c	514	BCR	C20-C21-C22-C23
27	R	617	LMG	C2-C1-O1-C7
40	N	616	LUT	C11-C10-C9-C8
40	N	616	LUT	C12-C13-C14-C15
40	N	616	LUT	C28-C29-C30-C31
40	R	613	LUT	C28-C29-C30-C31
40	Y	315	LUT	C28-C29-C30-C31
40	Y	315	LUT	C32-C33-C34-C35
40	y	316	LUT	C28-C29-C30-C31
40	y	316	LUT	C32-C33-C34-C35
41	N	617	NEX	C32-C33-C34-C35
41	R	614	NEX	C11-C10-C9-C8
41	R	618	NEX	C11-C10-C9-C8
41	R	618	NEX	C28-C29-C30-C31
41	Y	317	NEX	C28-C29-C30-C31
41	g	617	NEX	C28-C29-C30-C31
41	r	614	NEX	C32-C33-C34-C35
42	R	615	XAT	C11-C10-C9-C8
42	Y	301	XAT	C11-C10-C9-C8
42	Y	301	XAT	C28-C29-C30-C31
42	Y	301	XAT	C32-C33-C34-C35
42	r	615	XAT	C11-C10-C9-C8
42	y	302	XAT	C11-C10-C9-C8
42	y	302	XAT	C32-C33-C34-C35
27	r	617	LMG	C31-C32-C33-C34
30	D	404	LHG	C30-C31-C32-C33
30	a	412	LHG	C24-C25-C26-C27
31	c	519	LNL	C5-C6-C7-C8
33	H	502	DGD	C9A-CAA-CBA-CCA
23	B	603	CLA	C15-C16-C17-C18
23	B	613	CLA	C16-C17-C18-C20
23	Y	304	CLA	C16-C17-C18-C20
23	y	305	CLA	C16-C17-C18-C20
23	N	610	CLA	O1D-CGD-O2D-CED
23	n	602	CLA	O1D-CGD-O2D-CED
23	S	613	CLA	C4-C3-C5-C6
29	D	407	PL9	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
29	D	407	PL9	C45-C44-C46-C47
39	G	620	CHL	C4-C3-C5-C6
39	g	607	CHL	C4-C3-C5-C6
28	A	410	3PH	C38-C39-C3A-C3B
28	C	524	3PH	C3E-C3F-C3G-C3H
28	d	403	3PH	C24-C25-C26-C27
28	w	202	3PH	C35-C36-C37-C38
30	D	404	LHG	C33-C34-C35-C36
30	d	408	LHG	C11-C12-C13-C14
29	a	411	PL9	C13-C14-C16-C17
29	d	407	PL9	C13-C14-C16-C17
23	B	611	CLA	C14-C13-C15-C16
23	B	613	CLA	C11-C12-C13-C14
23	N	603	CLA	C11-C10-C8-C9
23	R	608	CLA	C11-C12-C13-C14
23	c	506	CLA	C11-C12-C13-C14
23	c	511	CLA	C11-C12-C13-C14
23	g	611	CLA	C14-C13-C15-C16
24	A	405	PHO	C14-C13-C15-C16
35	y	301	VIV	C19-C18-C20-C21
39	n	607	CHL	C11-C10-C8-C9
31	B	623	LNL	C1-C2-C3-C4
26	A	408	SQD	C12-C13-C14-C15
28	W	201	3PH	C24-C25-C26-C27
30	r	616	LHG	C29-C30-C31-C32
30	y	318	LHG	C10-C11-C12-C13
30	y	318	LHG	C29-C30-C31-C32
31	C	519	LNL	C2-C3-C4-C5
31	a	401	LNL	C2-C3-C4-C5
33	H	502	DGD	C5B-C6B-C7B-C8B
33	H	502	DGD	C7B-C8B-C9B-CAB
33	d	411	DGD	C4A-C5A-C6A-C7A
23	b	605	CLA	C5-C6-C7-C8
23	N	613	CLA	C2A-CAA-CBA-CGA
23	S	613	CLA	C2A-CAA-CBA-CGA
39	G	606	CHL	C2A-CAA-CBA-CGA
23	b	616	CLA	O1A-CGA-O2A-C1
40	G	615	LUT	C27-C28-C29-C39
40	S	614	LUT	C27-C28-C29-C39
40	n	615	LUT	C11-C12-C13-C20
41	g	617	NEX	C11-C12-C13-C20
41	n	618	NEX	C11-C12-C13-C20

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Mol	Chain	Res	Type	Atoms
42	y	302	XAT	C7-C8-C9-C19
31	I	101	LNL	C3-C4-C5-C6
31	I	101	LNL	C5-C6-C7-C8
31	a	413	LNL	C2-C3-C4-C5
31	b	625	LNL	C2-C3-C4-C5
31	c	522	LNL	C5-C6-C7-C8
40	N	616	LUT	C27-C28-C29-C30
40	Y	316	LUT	C7-C8-C9-C10
40	y	317	LUT	C7-C8-C9-C10
42	R	615	XAT	C7-C8-C9-C10
42	n	617	XAT	C7-C8-C9-C10
42	r	615	XAT	C7-C8-C9-C10
42	y	302	XAT	C7-C8-C9-C10
23	b	609	CLA	C3-C5-C6-C7
39	g	607	CHL	C3-C5-C6-C7
30	Y	318	LHG	O9-C7-O7-C5
23	g	611	CLA	C15-C16-C17-C18
23	r	608	CLA	C13-C15-C16-C17
28	s	618	3PH	C22-C21-O21-C2
30	Y	318	LHG	C8-C7-O7-C5
30	y	318	LHG	C8-C7-O7-C5
27	R	617	LMG	C39-C40-C41-C42
28	a	410	3PH	C36-C37-C38-C39
31	I	101	LNL	C2-C3-C4-C5
31	a	401	LNL	C6-C7-C8-C9
26	M	101	SQD	C10-C11-C12-C13
27	B	620	LMG	C13-C14-C15-C16
27	R	617	LMG	C32-C33-C34-C35
28	W	201	3PH	C35-C36-C37-C38
28	s	618	3PH	C3A-C3B-C3C-C3D
30	D	408	LHG	C32-C33-C34-C35
30	N	618	LHG	C11-C12-C13-C14
31	B	623	LNL	C3-C4-C5-C6
31	c	518	LNL	C4-C5-C6-C7
31	i	101	LNL	C2-C3-C4-C5
33	d	411	DGD	C9B-CAB-CBB-CCB
37	b	626	DGA	CAB-CBB-CCB-CDB
23	B	601	CLA	C4B-C3B-CAB-CBB
23	C	507	CLA	C4B-C3B-CAB-CBB
23	r	610	CLA	C4B-C3B-CAB-CBB
39	G	607	CHL	C4B-C3B-CAB-CBB
39	G	620	CHL	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
39	N	601	CHL	C4B-C3B-CAB-CBB
39	N	605	CHL	C4B-C3B-CAB-CBB
39	N	608	CHL	C4B-C3B-CAB-CBB
39	R	607	CHL	C4B-C3B-CAB-CBB
39	Y	308	CHL	C4B-C3B-CAB-CBB
39	g	608	CHL	C4B-C3B-CAB-CBB
39	g	609	CHL	C4B-C3B-CAB-CBB
39	g	619	CHL	C4B-C3B-CAB-CBB
39	n	601	CHL	C4B-C3B-CAB-CBB
39	n	605	CHL	C4B-C3B-CAB-CBB
39	s	606	CHL	C4B-C3B-CAB-CBB
39	s	607	CHL	C4B-C3B-CAB-CBB
39	y	309	CHL	C4B-C3B-CAB-CBB
27	R	617	LMG	O6-C1-O1-C7
23	r	608	CLA	C15-C16-C17-C18
35	y	301	VIV	C15-C16-C17-C18
39	r	606	CHL	C8-C10-C11-C12
26	L	101	SQD	C30-C31-C32-C33
26	M	101	SQD	C14-C15-C16-C17
30	N	618	LHG	C32-C33-C34-C35
23	c	508	CLA	CBD-CGD-O2D-CED
23	y	306	CLA	CBD-CGD-O2D-CED
27	C	525	LMG	C36-C37-C38-C39
27	R	617	LMG	C30-C31-C32-C33
27	r	617	LMG	C23-C24-C25-C26
28	x	201	3PH	C34-C35-C36-C37
31	b	625	LNL	C4-C5-C6-C7
33	d	411	DGD	C4B-C5B-C6B-C7B
27	B	626	LMG	C28-C29-C30-C31
27	R	617	LMG	C28-C29-C30-C31
27	b	620	LMG	C28-C29-C30-C31
30	Y	318	LHG	C23-C24-C25-C26
23	b	608	CLA	C15-C16-C17-C18
39	G	601	CHL	C13-C15-C16-C17
23	C	513	CLA	O1A-CGA-O2A-C1
30	s	616	LHG	O10-C23-O8-C6
27	R	617	LMG	C36-C37-C38-C39
27	b	628	LMG	C16-C17-C18-C19
28	T	101	3PH	C2E-C2F-C2G-C2H
31	C	518	LNL	C5-C6-C7-C8
31	b	623	LNL	C2-C3-C4-C5
23	n	602	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
26	M	101	SQD	C15-C16-C17-C18
27	d	409	LMG	C19-C20-C21-C22
30	n	619	LHG	C29-C30-C31-C32
31	c	517	LNL	C2-C3-C4-C5
23	D	406	CLA	O1D-CGD-O2D-CED
23	G	602	CLA	O1D-CGD-O2D-CED
23	b	606	CLA	O1D-CGD-O2D-CED
23	c	510	CLA	O1D-CGD-O2D-CED
23	A	402	CLA	C3A-C2A-CAA-CBA
23	N	603	CLA	C3A-C2A-CAA-CBA
23	Y	304	CLA	C3A-C2A-CAA-CBA
23	a	403	CLA	C3A-C2A-CAA-CBA
23	g	603	CLA	C3A-C2A-CAA-CBA
23	n	603	CLA	C3A-C2A-CAA-CBA
23	r	601	CLA	C3A-C2A-CAA-CBA
23	s	608	CLA	C3A-C2A-CAA-CBA
24	D	402	PHO	C3A-C2A-CAA-CBA
40	G	615	LUT	C29-C30-C31-C32
41	Y	317	NEX	C9-C10-C11-C12
26	M	101	SQD	C25-C26-C27-C28
27	b	620	LMG	C38-C39-C40-C41
31	C	518	LNL	C4-C5-C6-C7
31	A	413	LNL	C1-C2-C3-C4
23	B	601	CLA	O1A-CGA-O2A-C1
30	d	404	LHG	O10-C23-O8-C6
23	Y	304	CLA	C16-C17-C18-C19
30	D	408	LHG	C28-C29-C30-C31
30	L	103	LHG	C16-C17-C18-C19
33	C	515	DGD	C8A-C9A-CAA-CBA
23	Y	305	CLA	O1D-CGD-O2D-CED
23	c	509	CLA	CBD-CGD-O2D-CED
30	D	408	LHG	C12-C13-C14-C15
31	B	625	LNL	C4-C5-C6-C7
33	C	515	DGD	C7A-C8A-C9A-CAA
40	G	615	LUT	C14-C15-C35-C34
40	R	613	LUT	C14-C15-C35-C34
23	g	603	CLA	C3-C5-C6-C7
28	C	524	3PH	C21-C22-C23-C24
30	n	619	LHG	C25-C26-C27-C28
31	b	623	LNL	C4-C5-C6-C7
29	d	407	PL9	C45-C44-C46-C47
39	N	606	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	C	511	CLA	CBA-CGA-O2A-C1
23	r	610	CLA	CBA-CGA-O2A-C1
23	S	613	CLA	C2-C3-C5-C6
29	D	407	PL9	C13-C14-C16-C17
39	N	606	CHL	C2-C3-C5-C6
39	g	607	CHL	C2-C3-C5-C6
39	g	619	CHL	C2-C3-C5-C6
30	a	412	LHG	C8-C7-O7-C5
28	s	618	3PH	C23-C24-C25-C26
33	C	515	DGD	C4B-C5B-C6B-C7B
30	D	408	LHG	O1-C1-C2-O2
30	L	103	LHG	O1-C1-C2-O2
30	N	618	LHG	O1-C1-C2-O2
30	S	616	LHG	O1-C1-C2-O2
30	b	627	LHG	O1-C1-C2-O2
30	d	404	LHG	O1-C1-C2-O2
30	d	408	LHG	O1-C1-C2-O2
30	r	616	LHG	O1-C1-C2-O2
26	A	408	SQD	C25-C26-C27-C28
27	w	201	LMG	C39-C40-C41-C42
30	D	408	LHG	C18-C19-C20-C21
30	n	619	LHG	C11-C10-C9-C8
31	a	413	LNL	C4-C5-C6-C7
33	d	411	DGD	C6A-C7A-C8A-C9A
33	d	411	DGD	C5B-C6B-C7B-C8B
23	N	613	CLA	O1A-CGA-O2A-C1
23	c	511	CLA	O1A-CGA-O2A-C1
23	y	305	CLA	C16-C17-C18-C19
23	B	601	CLA	C2B-C3B-CAB-CBB
23	C	507	CLA	C2B-C3B-CAB-CBB
23	r	610	CLA	C2B-C3B-CAB-CBB
23	y	315	CLA	C2B-C3B-CAB-CBB
30	b	627	LHG	O2-C2-C3-O3
39	G	607	CHL	C2B-C3B-CAB-CBB
39	G	620	CHL	C2B-C3B-CAB-CBB
39	N	601	CHL	C2B-C3B-CAB-CBB
39	N	605	CHL	C2B-C3B-CAB-CBB
39	N	607	CHL	C2B-C3B-CAB-CBB
39	N	608	CHL	C2B-C3B-CAB-CBB
39	R	607	CHL	C2B-C3B-CAB-CBB
39	Y	308	CHL	C2B-C3B-CAB-CBB
39	g	609	CHL	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
39	g	619	CHL	C2B-C3B-CAB-CBB
39	n	601	CHL	C2B-C3B-CAB-CBB
39	n	605	CHL	C2B-C3B-CAB-CBB
39	s	606	CHL	C2B-C3B-CAB-CBB
39	s	607	CHL	C2B-C3B-CAB-CBB
39	y	309	CHL	C2B-C3B-CAB-CBB
23	y	311	CLA	C8-C10-C11-C12
26	a	409	SQD	C11-C12-C13-C14
23	C	512	CLA	CBA-CGA-O2A-C1
23	N	611	CLA	CBA-CGA-O2A-C1
31	c	522	LNL	C3-C4-C5-C6
23	B	611	CLA	C8-C10-C11-C12
23	c	512	CLA	C10-C11-C12-C13
30	L	103	LHG	C1-C2-C3-O3
30	G	618	LHG	C24-C25-C26-C27
28	s	618	3PH	O22-C21-O21-C2
30	y	318	LHG	O9-C7-O7-C5
23	S	613	CLA	C2-C1-O2A-CGA
23	s	613	CLA	C2-C1-O2A-CGA
27	B	620	LMG	C31-C32-C33-C34
28	a	410	3PH	C38-C39-C3A-C3B
30	D	408	LHG	C29-C30-C31-C32
30	d	404	LHG	C13-C14-C15-C16
30	n	619	LHG	C10-C11-C12-C13
23	S	610	CLA	C5-C6-C7-C8
23	b	610	CLA	C15-C16-C17-C18
23	b	612	CLA	C13-C15-C16-C17
23	s	610	CLA	C5-C6-C7-C8
35	y	301	VIV	C18-C20-C21-C22
39	y	310	CHL	C5-C6-C7-C8
26	A	408	SQD	O10-C23-O48-C46
30	A	412	LHG	C26-C27-C28-C29
30	R	616	LHG	C31-C32-C33-C34
31	c	518	LNL	C1-C2-C3-C4
25	C	514	BCR	C5-C6-C7-C8
25	H	501	BCR	C5-C6-C7-C8
25	H	501	BCR	C23-C24-C25-C26
25	H	501	BCR	C23-C24-C25-C30
25	K	101	BCR	C5-C6-C7-C8
25	V	101	BCR	C1-C6-C7-C8
25	V	101	BCR	C5-C6-C7-C8
25	c	514	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	d	410	BCR	C1-C6-C7-C8
25	d	410	BCR	C5-C6-C7-C8
25	h	501	BCR	C1-C6-C7-C8
25	h	501	BCR	C5-C6-C7-C8
25	h	501	BCR	C23-C24-C25-C26
25	h	501	BCR	C23-C24-C25-C30
25	k	101	BCR	C5-C6-C7-C8
25	v	101	BCR	C1-C6-C7-C8
25	v	101	BCR	C5-C6-C7-C8
39	N	607	CHL	C3-C5-C6-C7
40	G	615	LUT	C5-C6-C7-C8
40	N	615	LUT	C5-C6-C7-C8
40	N	616	LUT	C1-C6-C7-C8
40	R	613	LUT	C1-C6-C7-C8
40	S	614	LUT	C1-C6-C7-C8
40	Y	315	LUT	C1-C6-C7-C8
40	g	615	LUT	C1-C6-C7-C8
40	n	615	LUT	C1-C6-C7-C8
40	n	616	LUT	C1-C6-C7-C8
40	r	613	LUT	C1-C6-C7-C8
40	s	615	LUT	C1-C6-C7-C8
40	y	316	LUT	C1-C6-C7-C8
28	C	524	3PH	C2B-C2C-C2D-C2E
30	y	318	LHG	C26-C27-C28-C29
23	R	610	CLA	CBA-CGA-O2A-C1
23	g	614	CLA	CBA-CGA-O2A-C1
39	R	606	CHL	C13-C15-C16-C17
39	g	619	CHL	C5-C6-C7-C8
28	a	410	3PH	C22-C21-O21-C2
26	L	101	SQD	C28-C29-C30-C31
28	L	102	3PH	C2D-C2E-C2F-C2G
30	G	618	LHG	C15-C16-C17-C18
31	A	414	LNL	C5-C6-C7-C8
33	C	515	DGD	C5A-C6A-C7A-C8A
33	H	502	DGD	CBA-CCA-CDA-CEA
33	c	515	DGD	C4B-C5B-C6B-C7B
26	M	101	SQD	C30-C31-C32-C33
28	d	403	3PH	C39-C3A-C3B-C3C
31	a	401	LNL	C15-C16-C17-C18
23	y	306	CLA	C15-C16-C17-C18
23	C	508	CLA	C4-C3-C5-C6
29	a	411	PL9	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
39	N	609	CHL	C4-C3-C5-C6
39	n	601	CHL	C4-C3-C5-C6
23	d	406	CLA	O1D-CGD-O2D-CED
23	B	613	CLA	C11-C12-C13-C15
23	C	506	CLA	C2-C3-C5-C6
23	C	513	CLA	C12-C13-C15-C16
23	D	406	CLA	C12-C13-C15-C16
23	G	610	CLA	C12-C13-C15-C16
23	N	603	CLA	C11-C10-C8-C7
23	R	608	CLA	C11-C12-C13-C15
23	Y	311	CLA	C11-C10-C8-C7
23	Y	313	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	c	501	CLA	C11-C10-C8-C7
23	c	506	CLA	C11-C12-C13-C15
23	c	509	CLA	C6-C7-C8-C10
23	c	511	CLA	C11-C12-C13-C15
23	c	512	CLA	C12-C13-C15-C16
23	y	305	CLA	C6-C7-C8-C10
23	y	306	CLA	C6-C7-C8-C10
23	y	312	CLA	C11-C10-C8-C7
23	y	314	CLA	C2-C3-C5-C6
29	d	407	PL9	C43-C44-C46-C47
35	y	301	VIV	C22-C23-C24-C25
39	G	620	CHL	C2-C3-C5-C6
23	s	613	CLA	C3-C5-C6-C7
23	C	512	CLA	O1A-CGA-O2A-C1
23	r	610	CLA	O1A-CGA-O2A-C1
40	n	615	LUT	C9-C10-C11-C12
42	R	615	XAT	C9-C10-C11-C12
35	C	523	VIV	C25-C26-C27-C29
31	C	519	LNL	C6-C7-C8-C9
31	b	622	LNL	C6-C7-C8-C9
30	a	412	LHG	O9-C7-O7-C5
23	B	607	CLA	CBA-CGA-O2A-C1
23	G	614	CLA	CBA-CGA-O2A-C1
23	c	512	CLA	CBA-CGA-O2A-C1
23	n	611	CLA	CBA-CGA-O2A-C1
30	R	616	LHG	C24-C23-O8-C6
30	D	404	LHG	C27-C28-C29-C30
30	L	103	LHG	C32-C33-C34-C35
31	C	522	LNL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	R	612	CLA	C2A-CAA-CBA-CGA
23	c	513	CLA	C2A-CAA-CBA-CGA
23	g	613	CLA	C2A-CAA-CBA-CGA
23	s	608	CLA	C2A-CAA-CBA-CGA
39	G	620	CHL	C2A-CAA-CBA-CGA
39	N	607	CHL	C2A-CAA-CBA-CGA
39	R	607	CHL	C2A-CAA-CBA-CGA
39	g	619	CHL	C2A-CAA-CBA-CGA
33	H	502	DGD	C4D-C5D-C6D-O5D
23	B	605	CLA	C5-C6-C7-C8
23	B	611	CLA	C15-C16-C17-C18
23	B	616	CLA	C5-C6-C7-C8
23	Y	313	CLA	C5-C6-C7-C8
27	d	409	LMG	C17-C18-C19-C20
28	A	410	3PH	C3D-C3E-C3F-C3G
30	S	616	LHG	C10-C11-C12-C13
31	C	520	LNL	C5-C6-C7-C8
23	B	606	CLA	O1D-CGD-O2D-CED
30	a	412	LHG	C25-C26-C27-C28
30	b	627	LHG	C28-C29-C30-C31
30	A	412	LHG	C23-C24-C25-C26
23	y	314	CLA	C8-C10-C11-C12
27	r	617	LMG	C32-C33-C34-C35
28	x	201	3PH	C38-C39-C3A-C3B
31	a	413	LNL	C3-C4-C5-C6
33	H	502	DGD	CBB-CCB-CDB-CEB
25	b	617	BCR	C6-C7-C8-C9
23	C	511	CLA	O1A-CGA-O2A-C1
23	N	611	CLA	O1A-CGA-O2A-C1
23	c	506	CLA	CBD-CGD-O2D-CED
23	Y	310	CLA	C8-C10-C11-C12
23	c	503	CLA	C5-C6-C7-C8
23	n	602	CLA	C10-C11-C12-C13
23	y	311	CLA	C13-C15-C16-C17
27	c	523	LMG	C32-C33-C34-C35
31	A	413	LNL	C2-C3-C4-C5
30	d	408	LHG	C7-C8-C9-C10
31	c	517	LNL	C1-C2-C3-C4
30	S	616	LHG	C8-C7-O7-C5
40	Y	315	LUT	C14-C15-C35-C34
40	y	316	LUT	C14-C15-C35-C34
41	n	618	NEX	C14-C15-C35-C34

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Mol	Chain	Res	Type	Atoms
23	b	613	CLA	CBD-CGD-O2D-CED
28	a	410	3PH	O22-C21-O21-C2
23	B	607	CLA	C3-C5-C6-C7
26	A	408	SQD	C15-C16-C17-C18
31	A	414	LNL	C4-C5-C6-C7
33	C	515	DGD	CEA-CFA-CGA-CHA
26	a	409	SQD	C2-C1-O6-C44
23	B	608	CLA	C15-C16-C17-C18
26	A	408	SQD	O6-C44-C45-O47
30	R	616	LHG	O7-C5-C6-O8
30	Y	318	LHG	O7-C5-C6-O8
30	d	404	LHG	O7-C5-C6-O8
26	A	408	SQD	C29-C30-C31-C32
28	T	101	3PH	C22-C23-C24-C25
23	c	506	CLA	C16-C17-C18-C20
26	A	408	SQD	C14-C15-C16-C17
27	r	617	LMG	C18-C19-C20-C21
28	W	201	3PH	C3A-C3B-C3C-C3D
33	C	515	DGD	C9A-CAA-CBA-CCA
23	C	512	CLA	C15-C16-C17-C18
31	a	413	LNL	C6-C7-C8-C9
31	b	625	LNL	C6-C7-C8-C9
23	C	506	CLA	C4-C3-C5-C6
23	Y	313	CLA	C4-C3-C5-C6
23	y	314	CLA	C4-C3-C5-C6
30	r	616	LHG	C7-C8-C9-C10
23	D	406	CLA	C2-C3-C5-C6
29	D	407	PL9	C43-C44-C46-C47
39	N	609	CHL	C2-C3-C5-C6
29	D	407	PL9	C4-C3-C7-C8
29	d	407	PL9	C4-C3-C7-C8
28	s	618	3PH	C35-C36-C37-C38
23	A	403	CLA	C14-C13-C15-C16
23	B	614	CLA	C11-C12-C13-C14
23	C	512	CLA	C11-C12-C13-C14
23	C	513	CLA	C14-C13-C15-C16
23	D	406	CLA	C14-C13-C15-C16
23	G	610	CLA	C14-C13-C15-C16
23	N	613	CLA	C14-C13-C15-C16
23	S	610	CLA	C14-C13-C15-C16
23	a	404	CLA	C14-C13-C15-C16
23	b	602	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
23	b	603	CLA	C11-C12-C13-C14
23	b	605	CLA	C14-C13-C15-C16
23	c	501	CLA	C11-C10-C8-C9
23	d	405	CLA	C11-C12-C13-C14
23	s	610	CLA	C14-C13-C15-C16
23	s	613	CLA	C14-C13-C15-C16
23	y	305	CLA	C6-C7-C8-C9
23	y	313	CLA	C14-C13-C15-C16
28	C	524	3PH	C3D-C3E-C3F-C3G
30	S	616	LHG	C18-C19-C20-C21
23	Y	312	CLA	C3-C5-C6-C7
39	y	303	CHL	C3-C5-C6-C7
23	B	603	CLA	C2A-CAA-CBA-CGA
23	B	616	CLA	C2A-CAA-CBA-CGA
23	b	603	CLA	C2A-CAA-CBA-CGA
27	w	201	LMG	C37-C38-C39-C40
28	D	403	3PH	C24-C25-C26-C27
30	G	618	LHG	C11-C10-C9-C8
30	a	412	LHG	C29-C30-C31-C32
37	b	626	DGA	CA2-CA1-OG1-CG1
25	b	617	BCR	C7-C8-C9-C34
42	N	619	XAT	C31-C32-C33-C40
23	G	612	CLA	O1D-CGD-O2D-CED
23	c	506	CLA	C5-C6-C7-C8
26	L	101	SQD	C11-C12-C13-C14
27	b	620	LMG	C13-C14-C15-C16
25	b	617	BCR	C21-C22-C23-C24
25	c	514	BCR	C7-C8-C9-C10
23	R	610	CLA	O1A-CGA-O2A-C1
23	g	614	CLA	O1A-CGA-O2A-C1
23	A	402	CLA	C1A-C2A-CAA-CBA
23	A	403	CLA	C1A-C2A-CAA-CBA
23	A	406	CLA	C1A-C2A-CAA-CBA
23	C	501	CLA	C1A-C2A-CAA-CBA
23	N	603	CLA	C1A-C2A-CAA-CBA
23	N	610	CLA	C1A-C2A-CAA-CBA
23	Y	304	CLA	C1A-C2A-CAA-CBA
23	a	403	CLA	C1A-C2A-CAA-CBA
23	a	404	CLA	C1A-C2A-CAA-CBA
23	c	501	CLA	C1A-C2A-CAA-CBA
23	g	603	CLA	C1A-C2A-CAA-CBA
23	n	603	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	r	601	CLA	C1A-C2A-CAA-CBA
23	s	608	CLA	C1A-C2A-CAA-CBA
23	y	315	CLA	C1A-C2A-CAA-CBA
39	G	608	CHL	C1A-C2A-CAA-CBA
39	G	609	CHL	C1A-C2A-CAA-CBA
39	s	607	CHL	C1A-C2A-CAA-CBA
23	B	613	CLA	C16-C17-C18-C19
30	S	616	LHG	O9-C7-O7-C5
31	C	521	LNL	C7-C8-C9-C10
40	y	317	LUT	C29-C30-C31-C32
42	R	615	XAT	C29-C30-C31-C32
23	C	503	CLA	C5-C6-C7-C8
23	C	507	CLA	C8-C10-C11-C12
23	a	404	CLA	C13-C15-C16-C17
30	D	408	LHG	C4-O6-P-O3
28	d	403	3PH	C31-C32-C33-C34
23	Y	304	CLA	C3-C5-C6-C7
23	A	403	CLA	C13-C15-C16-C17
23	B	610	CLA	C15-C16-C17-C18
23	b	609	CLA	C15-C16-C17-C18
39	r	606	CHL	C5-C6-C7-C8
27	R	617	LMG	C29-C28-O8-C9
28	T	101	3PH	O11-C1-C2-C3
28	w	202	3PH	O11-C1-C2-C3
28	x	201	3PH	O11-C1-C2-C3
28	A	410	3PH	C3C-C3D-C3E-C3F
31	c	522	LNL	C2-C3-C4-C5
27	B	626	LMG	O6-C5-C6-O5
31	c	519	LNL	C6-C7-C8-C9
32	b	621	PAM	C6-C7-C8-C9
30	L	103	LHG	C14-C15-C16-C17
27	c	523	LMG	O6-C5-C6-O5
30	G	618	LHG	C1-C2-C3-O3
23	g	610	CLA	C4-C3-C5-C6
39	g	619	CHL	C4-C3-C5-C6
30	Y	318	LHG	C33-C34-C35-C36
31	c	521	LNL	C5-C6-C7-C8
27	b	628	LMG	O6-C5-C6-O5
31	B	625	LNL	C2-C3-C4-C5
31	C	518	LNL	C2-C3-C4-C5
31	b	624	LNL	C2-C3-C4-C5
31	C	519	LNL	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
23	c	512	CLA	O1A-CGA-O2A-C1
30	n	619	LHG	C15-C16-C17-C18
23	c	513	CLA	C11-C12-C13-C14
23	S	612	CLA	O1D-CGD-O2D-CED
26	L	101	SQD	C27-C28-C29-C30
26	L	101	SQD	C32-C33-C34-C35
26	M	101	SQD	O6-C44-C45-C46
26	M	101	SQD	C44-C45-C46-O48
30	A	412	LHG	C4-C5-C6-O8
30	D	408	LHG	C4-C5-C6-O8
30	d	408	LHG	C4-C5-C6-O8
30	s	616	LHG	C4-C5-C6-O8
37	D	410	DGA	OG1-CG1-CG2-CG3
23	Y	305	CLA	C5-C6-C7-C8
30	d	408	LHG	C31-C32-C33-C34
33	C	515	DGD	C7B-C8B-C9B-CAB
23	n	611	CLA	O1A-CGA-O2A-C1
30	R	616	LHG	O10-C23-O8-C6
26	A	408	SQD	C19-C20-C21-C22
26	M	101	SQD	C31-C32-C33-C34
23	r	608	CLA	O1D-CGD-O2D-CED
23	G	614	CLA	O1A-CGA-O2A-C1
27	b	628	LMG	O6-C1-O1-C7
29	a	411	PL9	C14-C16-C17-C18
31	c	517	LNL	C4-C5-C6-C7
23	g	613	CLA	CBD-CGD-O2D-CED
30	D	404	LHG	O1-C1-C2-O2
39	S	607	CHL	O2A-C1-C2-C3
28	T	101	3PH	C32-C33-C34-C35
33	H	502	DGD	C2B-C3B-C4B-C5B
37	b	626	DGA	CA9-CAA-CBA-CCA
23	B	602	CLA	C10-C11-C12-C13
31	C	517	LNL	C1-C2-C3-C4
31	a	413	LNL	C1-C2-C3-C4
28	W	201	3PH	C26-C27-C28-C29
26	A	408	SQD	C8-C7-O47-C45
35	y	301	VIV	C20-C21-C22-C23
25	h	501	BCR	C16-C17-C18-C36
40	S	615	LUT	C20-C13-C14-C15
41	R	618	NEX	C39-C29-C30-C31
41	r	614	NEX	C11-C10-C9-C19
42	N	619	XAT	C11-C10-C9-C19

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Mol	Chain	Res	Type	Atoms
42	n	620	XAT	C11-C10-C9-C19
39	G	607	CHL	C4-C3-C5-C6
39	y	310	CHL	C4-C3-C5-C6
23	c	512	CLA	O1D-CGD-O2D-CED
23	B	612	CLA	CBA-CGA-O2A-C1
23	b	612	CLA	CBA-CGA-O2A-C1
27	C	525	LMG	O6-C5-C6-O5
28	W	201	3PH	C25-C26-C27-C28
33	H	502	DGD	C6B-C7B-C8B-C9B
23	C	509	CLA	CBD-CGD-O2D-CED
23	Y	303	CLA	C15-C16-C17-C18
23	n	610	CLA	C13-C15-C16-C17
37	b	626	DGA	CB6-CB7-CB8-CB9
23	B	602	CLA	C2A-CAA-CBA-CGA
23	Y	313	CLA	C2A-CAA-CBA-CGA
23	N	610	CLA	C15-C16-C17-C18
23	y	304	CLA	C15-C16-C17-C18
26	A	408	SQD	C10-C11-C12-C13
31	C	520	LNL	C4-C5-C6-C7
23	N	612	CLA	O1D-CGD-O2D-CED
23	n	604	CLA	O1D-CGD-O2D-CED
28	T	101	3PH	C1-O11-P-O12
28	a	410	3PH	C1-O11-P-O12
40	N	615	LUT	C26-C27-C28-C29
23	s	609	CLA	C2C-C3C-CAC-CBC
26	L	101	SQD	C9-C10-C11-C12
30	L	103	LHG	C15-C16-C17-C18
30	a	412	LHG	C31-C32-C33-C34
23	b	607	CLA	CBA-CGA-O2A-C1
26	a	409	SQD	C24-C23-O48-C46
23	B	607	CLA	O1A-CGA-O2A-C1
28	A	410	3PH	O11-C1-C2-O21
30	d	404	LHG	O6-C4-C5-O7
27	b	628	LMG	O8-C28-C29-C30
30	n	619	LHG	C9-C10-C11-C12
23	g	612	CLA	O1D-CGD-O2D-CED
37	b	626	DGA	OA1-CA1-OG1-CG1
32	b	621	PAM	C3-C4-C5-C6
23	c	506	CLA	C13-C15-C16-C17
40	S	615	LUT	C11-C10-C9-C8
42	y	302	XAT	C28-C29-C30-C31
28	a	410	3PH	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
23	C	513	CLA	CAA-CBA-CGA-O2A
28	W	201	3PH	O21-C2-C3-O31
30	y	318	LHG	O7-C5-C6-O8
26	a	409	SQD	C15-C16-C17-C18
23	c	507	CLA	C13-C15-C16-C17
23	C	508	CLA	O1D-CGD-O2D-CED
31	c	519	LNL	C1-C2-C3-C4
23	d	406	CLA	C5-C6-C7-C8
23	B	604	CLA	C6-C7-C8-C10
23	B	604	CLA	C11-C10-C8-C7
23	B	611	CLA	C6-C7-C8-C10
23	B	614	CLA	C11-C12-C13-C15
23	B	615	CLA	C12-C13-C15-C16
23	B	616	CLA	C6-C7-C8-C10
23	C	501	CLA	C11-C10-C8-C7
23	C	512	CLA	C11-C12-C13-C15
23	D	406	CLA	C11-C10-C8-C7
23	D	406	CLA	C11-C12-C13-C15
23	G	613	CLA	C11-C12-C13-C15
23	R	608	CLA	C12-C13-C15-C16
23	S	602	CLA	C11-C10-C8-C7
23	S	610	CLA	C6-C7-C8-C10
23	S	610	CLA	C11-C10-C8-C7
23	S	610	CLA	C12-C13-C15-C16
23	Y	303	CLA	C6-C7-C8-C10
23	Y	305	CLA	C11-C12-C13-C15
23	Y	312	CLA	C11-C10-C8-C7
23	a	407	CLA	C11-C10-C8-C7
23	b	603	CLA	C6-C7-C8-C10
23	b	604	CLA	C11-C10-C8-C7
23	b	614	CLA	C6-C7-C8-C10
23	c	512	CLA	C11-C10-C8-C7
23	d	405	CLA	C11-C12-C13-C15
23	n	603	CLA	C11-C12-C13-C15
23	s	610	CLA	C6-C7-C8-C10
23	s	610	CLA	C11-C10-C8-C7
23	s	610	CLA	C12-C13-C15-C16
23	y	304	CLA	C6-C7-C8-C10
23	y	305	CLA	C11-C10-C8-C7
23	y	311	CLA	C11-C12-C13-C15
23	y	313	CLA	C12-C13-C15-C16
23	y	314	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	y	315	CLA	C11-C12-C13-C15
35	y	301	VIV	C16-C17-C18-C20
35	y	301	VIV	C21-C22-C23-C24
39	G	620	CHL	C12-C13-C15-C16
39	N	606	CHL	C6-C7-C8-C10
39	R	606	CHL	C6-C7-C8-C10
39	g	607	CHL	C6-C7-C8-C10
39	n	601	CHL	C6-C7-C8-C10
39	r	606	CHL	C11-C10-C8-C7
33	H	502	DGD	O2G-C1B-C2B-C3B
23	B	614	CLA	C3-C5-C6-C7
24	D	402	PHO	C3-C5-C6-C7
23	B	603	CLA	C11-C10-C8-C9
23	B	604	CLA	C11-C10-C8-C9
23	B	605	CLA	C14-C13-C15-C16
23	B	608	CLA	C11-C12-C13-C14
23	B	616	CLA	C6-C7-C8-C9
23	C	501	CLA	C11-C10-C8-C9
23	C	502	CLA	C6-C7-C8-C9
23	C	507	CLA	C11-C12-C13-C14
23	D	405	CLA	C11-C12-C13-C14
23	D	406	CLA	C11-C10-C8-C9
23	D	406	CLA	C11-C12-C13-C14
23	G	613	CLA	C11-C12-C13-C14
23	R	608	CLA	C14-C13-C15-C16
23	R	609	CLA	C11-C12-C13-C14
23	S	602	CLA	C11-C10-C8-C9
23	b	603	CLA	C6-C7-C8-C9
23	b	604	CLA	C11-C10-C8-C9
23	b	608	CLA	C11-C12-C13-C14
23	b	614	CLA	C11-C10-C8-C9
23	c	502	CLA	C6-C7-C8-C9
23	c	512	CLA	C14-C13-C15-C16
23	g	611	CLA	C11-C12-C13-C14
23	r	609	CLA	C11-C12-C13-C14
23	y	304	CLA	C6-C7-C8-C9
23	y	306	CLA	C11-C10-C8-C9
23	y	314	CLA	C11-C12-C13-C14
23	y	314	CLA	C14-C13-C15-C16
23	y	315	CLA	C11-C12-C13-C14
24	a	406	PHO	C14-C13-C15-C16
35	y	301	VIV	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
39	N	606	CHL	C6-C7-C8-C9
39	n	601	CHL	C6-C7-C8-C9
27	c	523	LMG	C31-C32-C33-C34
32	B	621	PAM	C4-C5-C6-C7
23	a	404	CLA	CBA-CGA-O2A-C1
23	b	602	CLA	C13-C15-C16-C17
23	y	314	CLA	C2A-CAA-CBA-CGA
39	r	607	CHL	C2A-CAA-CBA-CGA
30	b	627	LHG	C35-C36-C37-C38
33	H	502	DGD	CCB-CDB-CEB-CFB
23	g	602	CLA	O1D-CGD-O2D-CED
25	d	410	BCR	C7-C8-C9-C34
40	N	616	LUT	C31-C32-C33-C40
23	b	613	CLA	C16-C17-C18-C20
28	A	410	3PH	C22-C23-C24-C25
28	T	101	3PH	C37-C38-C39-C3A
25	d	410	BCR	C7-C8-C9-C10
40	N	616	LUT	C31-C32-C33-C34
42	G	619	XAT	C27-C28-C29-C30
42	G	619	XAT	C31-C32-C33-C34
28	W	201	3PH	C28-C29-C2A-C2B
39	Y	302	CHL	C3-C5-C6-C7
30	D	404	LHG	C1-C2-C3-O3
23	n	603	CLA	C8-C10-C11-C12
39	G	620	CHL	C5-C6-C7-C8
23	B	612	CLA	O1A-CGA-O2A-C1
28	L	102	3PH	C35-C36-C37-C38
30	g	618	LHG	C10-C11-C12-C13
33	H	502	DGD	C4B-C5B-C6B-C7B
25	Z	101	BCR	C22-C23-C24-C25
24	A	405	PHO	CBD-CGD-O2D-CED
30	S	616	LHG	C30-C31-C32-C33
33	H	502	DGD	C5A-C6A-C7A-C8A
23	D	406	CLA	C4B-C3B-CAB-CBB
23	N	611	CLA	C4B-C3B-CAB-CBB
23	Y	311	CLA	C4B-C3B-CAB-CBB
23	b	601	CLA	C4B-C3B-CAB-CBB
23	n	611	CLA	C4B-C3B-CAB-CBB
39	G	605	CHL	C4B-C3B-CAB-CBB
39	G	608	CHL	C4B-C3B-CAB-CBB
39	g	605	CHL	C4B-C3B-CAB-CBB
39	g	607	CHL	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
39	n	608	CHL	C4B-C3B-CAB-CBB
39	r	607	CHL	C4B-C3B-CAB-CBB
39	s	601	CHL	C4B-C3B-CAB-CBB
23	c	513	CLA	C11-C12-C13-C15
30	N	618	LHG	O6-C4-C5-C6
30	n	619	LHG	O6-C4-C5-C6
30	Y	318	LHG	C7-C8-C9-C10
23	C	512	CLA	O1D-CGD-O2D-CED
23	A	403	CLA	CBA-CGA-O2A-C1
23	n	604	CLA	CBA-CGA-O2A-C1
23	b	616	CLA	CBD-CGD-O2D-CED
23	B	607	CLA	C10-C11-C12-C13
23	s	613	CLA	C13-C15-C16-C17
30	a	412	LHG	C27-C28-C29-C30
23	G	610	CLA	C4-C3-C5-C6
39	G	607	CHL	C2-C3-C5-C6
39	y	310	CHL	C2-C3-C5-C6
33	c	515	DGD	C5A-C6A-C7A-C8A
23	n	610	CLA	C5-C6-C7-C8
23	b	612	CLA	O1A-CGA-O2A-C1
23	G	610	CLA	C5-C6-C7-C8
28	W	201	3PH	C32-C31-O31-C3
33	H	502	DGD	CDB-CEB-CFB-CGB
23	y	306	CLA	O1D-CGD-O2D-CED
23	B	609	CLA	C3A-C2A-CAA-CBA
23	y	315	CLA	C3A-C2A-CAA-CBA
39	G	601	CHL	C3A-C2A-CAA-CBA
39	R	607	CHL	C3A-C2A-CAA-CBA
39	g	608	CHL	C3A-C2A-CAA-CBA
39	g	609	CHL	C3A-C2A-CAA-CBA
39	r	607	CHL	C3A-C2A-CAA-CBA
39	s	606	CHL	C3A-C2A-CAA-CBA
39	y	303	CHL	C3A-C2A-CAA-CBA
23	N	610	CLA	C5-C6-C7-C8
31	c	519	LNL	C2-C3-C4-C5
31	i	101	LNL	C5-C6-C7-C8
41	Y	317	NEX	C13-C14-C15-C35
42	N	619	XAT	C9-C10-C11-C12
42	r	615	XAT	C29-C30-C31-C32
23	Y	314	CLA	O1D-CGD-O2D-CED
23	C	506	CLA	CBA-CGA-O2A-C1
23	B	611	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	A	408	SQD	O6-C44-C45-C46
27	c	523	LMG	O1-C7-C8-C9
30	a	412	LHG	C4-C5-C6-O8
30	d	404	LHG	C4-C5-C6-O8
30	g	618	LHG	C14-C15-C16-C17
23	c	512	CLA	C3-C5-C6-C7
27	b	628	LMG	C33-C34-C35-C36
23	y	315	CLA	C4-C3-C5-C6
39	r	606	CHL	C4-C3-C5-C6
23	c	508	CLA	O1D-CGD-O2D-CED
33	C	515	DGD	C2B-C3B-C4B-C5B
23	G	613	CLA	CBD-CGD-O2D-CED
30	a	412	LHG	C9-C10-C11-C12
30	n	619	LHG	C31-C32-C33-C34
23	y	315	CLA	O1D-CGD-O2D-CED
30	y	318	LHG	C4-O6-P-O3
31	A	413	LNL	C10-C11-C12-C13
31	A	413	LNL	C13-C14-C15-C16
31	A	414	LNL	C9-C10-C11-C12
31	B	622	LNL	C13-C14-C15-C16
31	B	624	LNL	C13-C14-C15-C16
31	C	517	LNL	C12-C13-C14-C15
31	C	518	LNL	C9-C10-C11-C12
31	C	521	LNL	C10-C11-C12-C13
31	C	522	LNL	C9-C10-C11-C12
31	a	401	LNL	C12-C13-C14-C15
31	a	413	LNL	C9-C10-C11-C12
31	b	622	LNL	C12-C13-C14-C15
31	b	623	LNL	C10-C11-C12-C13
31	b	623	LNL	C13-C14-C15-C16
31	b	624	LNL	C13-C14-C15-C16
31	b	625	LNL	C12-C13-C14-C15
31	c	518	LNL	C10-C11-C12-C13
31	c	518	LNL	C12-C13-C14-C15
31	c	520	LNL	C10-C11-C12-C13
31	c	522	LNL	C9-C10-C11-C12
31	i	101	LNL	C9-C10-C11-C12
39	N	606	CHL	C3C-C2C-CMC-OMC
39	R	607	CHL	C3C-C2C-CMC-OMC
39	n	606	CHL	C3C-C2C-CMC-OMC
39	r	607	CHL	C3C-C2C-CMC-OMC
39	y	308	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
26	a	409	SQD	C10-C11-C12-C13
23	y	306	CLA	C2A-CAA-CBA-CGA
31	b	622	LNL	C3-C4-C5-C6
30	R	616	LHG	O6-C4-C5-O7
30	n	619	LHG	O6-C4-C5-O7
26	A	408	SQD	O49-C7-O47-C45
23	C	504	CLA	CBA-CGA-O2A-C1
23	b	607	CLA	O1A-CGA-O2A-C1
26	a	409	SQD	O10-C23-O48-C46
23	B	616	CLA	C13-C15-C16-C17
23	R	609	CLA	C5-C6-C7-C8
33	d	411	DGD	O2G-C1B-C2B-C3B
23	b	601	CLA	C2B-C3B-CAB-CBB
23	n	611	CLA	C2B-C3B-CAB-CBB
39	G	605	CHL	C2B-C3B-CAB-CBB
39	G	608	CHL	C2B-C3B-CAB-CBB
39	g	607	CHL	C2B-C3B-CAB-CBB
39	g	608	CHL	C2B-C3B-CAB-CBB
39	r	607	CHL	C2B-C3B-CAB-CBB
28	D	403	3PH	C36-C37-C38-C39
33	C	515	DGD	C2A-C3A-C4A-C5A
33	d	411	DGD	C3A-C4A-C5A-C6A
37	D	410	DGA	CCA-CDA-CEA-CFA
23	b	611	CLA	C8-C10-C11-C12
23	a	404	CLA	O1A-CGA-O2A-C1
23	S	609	CLA	C3-C5-C6-C7
30	b	627	LHG	C11-C12-C13-C14
30	b	627	LHG	C16-C17-C18-C19
27	A	409	LMG	O1-C7-C8-O7
27	C	525	LMG	O1-C7-C8-O7
27	c	523	LMG	O1-C7-C8-O7
28	C	524	3PH	O21-C2-C3-O31
28	D	403	3PH	O21-C2-C3-O31
30	D	408	LHG	O7-C5-C6-O8
37	D	410	DGA	OG1-CG1-CG2-OG2
23	y	306	CLA	C10-C11-C12-C13
30	N	618	LHG	C27-C28-C29-C30
31	C	519	LNL	C5-C6-C7-C8
31	c	518	LNL	C3-C4-C5-C6
40	S	615	LUT	C29-C30-C31-C32
23	N	610	CLA	C16-C17-C18-C20
23	R	603	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	S	612	CLA	C6-C7-C8-C10
23	b	613	CLA	C16-C17-C18-C19
23	r	603	CLA	C11-C12-C13-C14
23	Y	303	CLA	C10-C11-C12-C13
37	D	410	DGA	CG1-CG2-CG3-OXT
26	M	101	SQD	C11-C10-C9-C8
30	r	616	LHG	C24-C25-C26-C27
31	a	401	LNL	C3-C4-C5-C6
33	c	515	DGD	CDB-CEB-CFB-CGB
24	a	406	PHO	C4-C3-C5-C6
23	C	502	CLA	C2-C1-O2A-CGA
23	G	611	CLA	C2-C1-O2A-CGA
23	S	612	CLA	C2-C1-O2A-CGA
23	c	502	CLA	C2-C1-O2A-CGA
23	r	603	CLA	C2-C1-O2A-CGA
23	s	603	CLA	C2-C1-O2A-CGA
23	s	612	CLA	C2-C1-O2A-CGA
39	n	606	CHL	C2-C1-O2A-CGA
39	y	303	CHL	C2-C1-O2A-CGA
31	c	520	LNL	C3-C4-C5-C6
23	B	603	CLA	C6-C7-C8-C9
23	B	605	CLA	C11-C12-C13-C14
23	C	508	CLA	C11-C10-C8-C9
23	C	511	CLA	C6-C7-C8-C9
23	R	608	CLA	C11-C10-C8-C9
23	Y	303	CLA	C6-C7-C8-C9
23	Y	312	CLA	C14-C13-C15-C16
23	b	605	CLA	C11-C10-C8-C9
23	b	613	CLA	C11-C10-C8-C9
23	c	507	CLA	C11-C10-C8-C9
23	c	512	CLA	C11-C12-C13-C14
23	n	602	CLA	C11-C10-C8-C9
23	s	613	CLA	C11-C12-C13-C14
35	C	523	VIV	C1-C23-C24-C25
27	B	626	LMG	C32-C33-C34-C35
30	r	616	LHG	C9-C10-C11-C12
30	L	103	LHG	C10-C11-C12-C13
31	c	520	LNL	C4-C5-C6-C7
23	b	611	CLA	C13-C15-C16-C17
23	b	612	CLA	C10-C11-C12-C13
24	A	405	PHO	C5-C6-C7-C8
24	D	402	PHO	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	Y	318	LHG	C5-C4-O6-P
39	s	601	CHL	C4-C3-C5-C6
33	c	515	DGD	C4A-C5A-C6A-C7A
23	B	607	CLA	C16-C17-C18-C20
23	G	611	CLA	O2A-C1-C2-C3
25	A	407	BCR	C1-C6-C7-C8
25	A	407	BCR	C5-C6-C7-C8
25	B	618	BCR	C23-C24-C25-C26
25	B	618	BCR	C23-C24-C25-C30
25	B	619	BCR	C23-C24-C25-C26
25	B	619	BCR	C23-C24-C25-C30
25	C	514	BCR	C23-C24-C25-C26
25	C	514	BCR	C23-C24-C25-C30
25	D	411	BCR	C23-C24-C25-C26
25	D	411	BCR	C23-C24-C25-C30
25	K	101	BCR	C23-C24-C25-C26
25	K	101	BCR	C23-C24-C25-C30
25	a	408	BCR	C1-C6-C7-C8
25	a	408	BCR	C5-C6-C7-C8
25	a	408	BCR	C23-C24-C25-C26
25	b	617	BCR	C5-C6-C7-C8
25	b	618	BCR	C1-C6-C7-C8
25	b	618	BCR	C5-C6-C7-C8
25	b	618	BCR	C23-C24-C25-C26
25	b	618	BCR	C23-C24-C25-C30
25	b	619	BCR	C23-C24-C25-C26
25	c	514	BCR	C5-C6-C7-C8
25	c	514	BCR	C23-C24-C25-C26
25	c	514	BCR	C23-C24-C25-C30
25	k	101	BCR	C23-C24-C25-C26
25	k	101	BCR	C23-C24-C25-C30
40	G	616	LUT	C1-C6-C7-C8
27	A	409	LMG	C33-C34-C35-C36
27	B	626	LMG	C18-C19-C20-C21
41	R	614	NEX	C11-C12-C13-C20
41	s	617	NEX	C11-C12-C13-C20
30	S	616	LHG	C29-C30-C31-C32
23	s	611	CLA	CBA-CGA-O2A-C1
25	C	514	BCR	C7-C8-C9-C10
41	s	617	NEX	C32-C33-C34-C35
42	r	615	XAT	C11-C12-C13-C14
31	C	518	LNL	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
23	c	509	CLA	O1D-CGD-O2D-CED
23	y	315	CLA	C8-C10-C11-C12
28	a	410	3PH	C29-C2A-C2B-C2C
28	w	202	3PH	C29-C2A-C2B-C2C
31	B	624	LNL	C2-C3-C4-C5
23	B	604	CLA	C3-C5-C6-C7
23	r	604	CLA	C3-C5-C6-C7
31	A	413	LNL	C15-C16-C17-C18
31	B	622	LNL	C15-C16-C17-C18
31	B	623	LNL	C15-C16-C17-C18
31	B	624	LNL	C15-C16-C17-C18
31	B	625	LNL	C15-C16-C17-C18
31	C	520	LNL	C15-C16-C17-C18
31	I	101	LNL	C15-C16-C17-C18
31	a	413	LNL	C15-C16-C17-C18
31	b	623	LNL	C15-C16-C17-C18
31	b	625	LNL	C15-C16-C17-C18
31	c	517	LNL	C15-C16-C17-C18
31	c	519	LNL	C15-C16-C17-C18
31	c	521	LNL	C15-C16-C17-C18
31	i	101	LNL	C15-C16-C17-C18
23	B	604	CLA	C10-C11-C12-C13
23	c	506	CLA	O1D-CGD-O2D-CED
27	b	628	LMG	C18-C19-C20-C21
28	T	101	3PH	C2A-C2B-C2C-C2D
23	y	304	CLA	C10-C11-C12-C13
28	X	201	3PH	O11-C1-C2-C3
28	d	403	3PH	O11-C1-C2-C3
30	a	412	LHG	O6-C4-C5-C6
39	N	607	CHL	C4-C3-C5-C6
23	B	603	CLA	C6-C7-C8-C10
23	B	603	CLA	C11-C10-C8-C7
23	B	605	CLA	C11-C12-C13-C15
23	B	605	CLA	C12-C13-C15-C16
23	B	608	CLA	C11-C12-C13-C15
23	B	612	CLA	C12-C13-C15-C16
23	C	507	CLA	C11-C12-C13-C15
23	C	508	CLA	C2-C3-C5-C6
23	C	508	CLA	C11-C10-C8-C7
23	C	511	CLA	C6-C7-C8-C10
23	D	405	CLA	C11-C12-C13-C15
23	N	611	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
23	N	613	CLA	C11-C12-C13-C15
23	R	608	CLA	C11-C10-C8-C7
23	R	609	CLA	C11-C12-C13-C15
23	S	609	CLA	C6-C7-C8-C10
23	Y	303	CLA	C11-C12-C13-C15
23	Y	312	CLA	C12-C13-C15-C16
23	b	608	CLA	C11-C12-C13-C15
23	b	612	CLA	C12-C13-C15-C16
23	b	613	CLA	C11-C12-C13-C15
23	b	614	CLA	C11-C10-C8-C7
23	b	615	CLA	C12-C13-C15-C16
23	c	507	CLA	C11-C10-C8-C7
23	c	511	CLA	C6-C7-C8-C10
23	g	603	CLA	C11-C10-C8-C7
23	g	611	CLA	C11-C12-C13-C15
23	g	611	CLA	C12-C13-C15-C16
23	n	602	CLA	C11-C10-C8-C7
23	n	603	CLA	C12-C13-C15-C16
23	r	609	CLA	C11-C12-C13-C15
23	y	304	CLA	C11-C12-C13-C15
23	y	306	CLA	C11-C10-C8-C7
23	y	306	CLA	C12-C13-C15-C16
23	y	314	CLA	C6-C7-C8-C10
23	y	314	CLA	C11-C12-C13-C15
35	C	523	VIV	C21-C22-C23-C24
35	C	523	VIV	C22-C23-C24-C25
39	G	609	CHL	C6-C7-C8-C10
39	g	609	CHL	C6-C7-C8-C10
39	r	606	CHL	C2-C3-C5-C6
26	A	408	SQD	C27-C28-C29-C30
24	a	406	PHO	C15-C16-C17-C18
25	V	101	BCR	C19-C20-C21-C22
42	Y	301	XAT	C29-C30-C31-C32
42	n	620	XAT	C9-C10-C11-C12
42	y	302	XAT	C13-C14-C15-C35
23	S	612	CLA	C6-C7-C8-C9
31	C	522	LNL	C6-C7-C8-C9
27	C	525	LMG	C31-C32-C33-C34
23	c	504	CLA	CBA-CGA-O2A-C1
30	L	103	LHG	C29-C30-C31-C32
31	c	519	LNL	C4-C5-C6-C7
23	B	612	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	Y	305	CLA	C2A-CAA-CBA-CGA
25	H	501	BCR	C16-C17-C18-C36
25	b	617	BCR	C11-C10-C9-C34
28	D	403	3PH	C1-O11-P-O14
40	Y	316	LUT	C11-C10-C9-C19
40	s	615	LUT	C40-C33-C34-C35
40	y	317	LUT	C11-C10-C9-C19
33	H	502	DGD	C1A-C2A-C3A-C4A
23	G	602	CLA	C3-C5-C6-C7
23	N	610	CLA	C16-C17-C18-C19
23	R	610	CLA	C16-C17-C18-C20
23	B	608	CLA	CBA-CGA-O2A-C1
23	b	608	CLA	CBA-CGA-O2A-C1
23	r	601	CLA	CBA-CGA-O2A-C1
31	a	401	LNL	C5-C6-C7-C8
23	B	601	CLA	CAD-CBD-CGD-O2D
23	B	603	CLA	CAD-CBD-CGD-O2D
23	G	614	CLA	CAD-CBD-CGD-O2D
23	Y	305	CLA	CAD-CBD-CGD-O2D
23	Y	310	CLA	CAD-CBD-CGD-O2D
23	Y	312	CLA	CAD-CBD-CGD-O2D
23	c	513	CLA	CAD-CBD-CGD-O2D
23	g	610	CLA	CAD-CBD-CGD-O2D
23	g	611	CLA	CAD-CBD-CGD-O2D
23	g	614	CLA	CAD-CBD-CGD-O2D
23	n	604	CLA	CAD-CBD-CGD-O2D
23	r	609	CLA	CAD-CBD-CGD-O2D
23	s	609	CLA	CAD-CBD-CGD-O2D
23	y	306	CLA	CAD-CBD-CGD-O2D
23	y	311	CLA	CAD-CBD-CGD-O2D
23	y	313	CLA	CAD-CBD-CGD-O2D
24	a	406	PHO	CAD-CBD-CGD-O2D
26	M	101	SQD	C46-C45-O47-C7
30	Y	318	LHG	C4-C5-O7-C7
39	S	605	CHL	CAD-CBD-CGD-O2D
39	s	605	CHL	CAD-CBD-CGD-O2D
23	b	615	CLA	C13-C15-C16-C17
39	r	607	CHL	C5-C6-C7-C8
25	z	101	BCR	C22-C23-C24-C25
40	G	615	LUT	C6-C7-C8-C9
23	S	609	CLA	C4-C3-C5-C6
23	b	607	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
23	y	313	CLA	C16-C17-C18-C20
28	W	201	3PH	C3D-C3E-C3F-C3G
39	y	310	CHL	C10-C11-C12-C13
39	N	607	CHL	C2-C3-C5-C6
26	L	101	SQD	C44-C45-C46-O48
27	A	409	LMG	C7-C8-C9-O8
27	C	525	LMG	O1-C7-C8-C9
28	W	201	3PH	C1-C2-C3-O31
28	a	410	3PH	C1-C2-C3-O31
30	G	618	LHG	C2-C3-O3-P
23	A	403	CLA	O1A-CGA-O2A-C1
27	r	617	LMG	C14-C15-C16-C17
28	X	201	3PH	C23-C24-C25-C26
31	B	622	LNL	C5-C6-C7-C8
28	X	201	3PH	O11-C1-C2-O21
28	d	403	3PH	O11-C1-C2-O21
30	N	618	LHG	O6-C4-C5-O7
23	B	604	CLA	C8-C10-C11-C12
23	B	614	CLA	C15-C16-C17-C18
23	N	603	CLA	C8-C10-C11-C12
23	b	606	CLA	C8-C10-C11-C12
39	Y	302	CHL	C8-C10-C11-C12
23	R	604	CLA	C3-C5-C6-C7
23	G	612	CLA	O2A-C1-C2-C3
23	R	601	CLA	O2A-C1-C2-C3
23	R	612	CLA	O2A-C1-C2-C3
23	S	611	CLA	O2A-C1-C2-C3
23	r	601	CLA	O2A-C1-C2-C3
41	R	618	NEX	C14-C15-C35-C34
26	L	101	SQD	C29-C30-C31-C32
30	L	103	LHG	C25-C26-C27-C28
33	H	502	DGD	CAB-CBB-CCB-CDB
30	G	618	LHG	O2-C2-C3-O3
23	A	404	CLA	CHA-CBD-CGD-O1D
23	B	607	CLA	CHA-CBD-CGD-O1D
23	B	612	CLA	CHA-CBD-CGD-O1D
23	C	502	CLA	CHA-CBD-CGD-O1D
23	C	502	CLA	CHA-CBD-CGD-O2D
23	C	506	CLA	CHA-CBD-CGD-O1D
23	C	510	CLA	CHA-CBD-CGD-O1D
23	C	513	CLA	CHA-CBD-CGD-O1D
23	C	513	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	N	614	CLA	CHA-CBD-CGD-O1D
23	N	614	CLA	CHA-CBD-CGD-O2D
23	S	602	CLA	CHA-CBD-CGD-O1D
23	S	602	CLA	CHA-CBD-CGD-O2D
23	S	603	CLA	CHA-CBD-CGD-O1D
23	S	603	CLA	CHA-CBD-CGD-O2D
23	Y	314	CLA	CHA-CBD-CGD-O1D
23	b	601	CLA	CHA-CBD-CGD-O1D
23	b	601	CLA	CHA-CBD-CGD-O2D
23	b	607	CLA	CHA-CBD-CGD-O1D
23	b	612	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O2D
23	c	502	CLA	CHA-CBD-CGD-O1D
23	c	502	CLA	CHA-CBD-CGD-O2D
23	c	506	CLA	CHA-CBD-CGD-O1D
23	c	506	CLA	CHA-CBD-CGD-O2D
23	n	614	CLA	CHA-CBD-CGD-O1D
23	n	614	CLA	CHA-CBD-CGD-O2D
23	r	602	CLA	CHA-CBD-CGD-O1D
23	r	602	CLA	CHA-CBD-CGD-O2D
23	s	603	CLA	CHA-CBD-CGD-O1D
23	s	603	CLA	CHA-CBD-CGD-O2D
23	y	315	CLA	CHA-CBD-CGD-O1D
23	C	506	CLA	O1A-CGA-O2A-C1
23	n	604	CLA	O1A-CGA-O2A-C1
23	r	601	CLA	O1A-CGA-O2A-C1
28	C	524	3PH	C24-C25-C26-C27
28	D	403	3PH	C3C-C3D-C3E-C3F
30	N	618	LHG	C11-C10-C9-C8
40	N	616	LUT	C32-C33-C34-C35
40	g	615	LUT	C32-C33-C34-C35
26	M	101	SQD	C27-C28-C29-C30
28	T	101	3PH	C3C-C3D-C3E-C3F
26	L	101	SQD	O47-C45-C46-O48
28	w	202	3PH	O21-C2-C3-O31
30	A	412	LHG	O7-C5-C6-O8
30	a	412	LHG	O7-C5-C6-O8
30	n	619	LHG	O7-C5-C6-O8
26	a	409	SQD	C13-C14-C15-C16
23	B	608	CLA	O1A-CGA-O2A-C1
23	C	504	CLA	O1A-CGA-O2A-C1
27	R	617	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
23	y	305	CLA	CAA-CBA-CGA-O2A
23	R	603	CLA	C11-C12-C13-C15
23	c	512	CLA	C16-C17-C18-C20
23	r	610	CLA	C16-C17-C18-C20
23	b	613	CLA	O1D-CGD-O2D-CED
26	a	409	SQD	C9-C10-C11-C12
28	C	524	3PH	C22-C23-C24-C25
30	s	616	LHG	C24-C25-C26-C27
31	i	101	LNL	C3-C4-C5-C6
33	C	515	DGD	C6B-C7B-C8B-C9B
31	B	623	LNL	C6-C7-C8-C9
28	C	524	3PH	C23-C24-C25-C26
23	b	608	CLA	O1A-CGA-O2A-C1
23	s	611	CLA	O1A-CGA-O2A-C1
28	W	201	3PH	O32-C31-O31-C3
29	a	411	PL9	C4-C3-C7-C8
23	N	604	CLA	CBA-CGA-O2A-C1
23	B	607	CLA	C6-C7-C8-C9
23	C	511	CLA	C11-C12-C13-C14
23	s	613	CLA	C11-C10-C8-C9
24	d	402	PHO	C6-C7-C8-C9
35	y	301	VIV	C1-C23-C24-C25
39	G	620	CHL	C11-C12-C13-C14
23	c	504	CLA	O1A-CGA-O2A-C1
23	g	613	CLA	O1D-CGD-O2D-CED
26	a	409	SQD	C5-C6-S-O8
23	r	608	CLA	C16-C17-C18-C20
30	L	103	LHG	C28-C29-C30-C31
23	B	614	CLA	C2A-CAA-CBA-CGA
23	b	616	CLA	C2A-CAA-CBA-CGA
23	b	616	CLA	C13-C15-C16-C17
33	d	411	DGD	CDB-CEB-CFB-CGB
25	V	101	BCR	C36-C18-C19-C20
40	s	614	LUT	C31-C32-C33-C40
41	Y	317	NEX	C11-C12-C13-C20
42	G	619	XAT	C7-C8-C9-C19
30	D	408	LHG	C33-C34-C35-C36
30	D	408	LHG	C35-C36-C37-C38
30	r	616	LHG	C28-C29-C30-C31
25	V	101	BCR	C17-C18-C19-C20
25	b	617	BCR	C7-C8-C9-C10
40	n	615	LUT	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
41	n	618	NEX	C31-C32-C33-C34
23	a	407	CLA	C1A-C2A-CAA-CBA
23	n	610	CLA	C1A-C2A-CAA-CBA
39	G	605	CHL	C1A-C2A-CAA-CBA
39	S	606	CHL	C1A-C2A-CAA-CBA
39	n	605	CHL	C1A-C2A-CAA-CBA
39	y	310	CHL	C1A-C2A-CAA-CBA
23	r	603	CLA	C11-C12-C13-C15
35	y	301	VIV	C25-C26-C27-C29
23	y	304	CLA	C13-C15-C16-C17
23	y	306	CLA	C5-C6-C7-C8
23	r	601	CLA	C2-C1-O2A-CGA
23	B	611	CLA	CBA-CGA-O2A-C1
23	c	513	CLA	CBA-CGA-O2A-C1
30	n	619	LHG	C14-C15-C16-C17
25	B	617	BCR	C9-C10-C11-C12
30	d	408	LHG	C4-O6-P-O3
28	X	201	3PH	C38-C39-C3A-C3B
23	y	305	CLA	CBD-CGD-O2D-CED
28	A	410	3PH	C28-C29-C2A-C2B
31	B	624	LNL	C4-C5-C6-C7
23	n	602	CLA	C4-C3-C5-C6
30	A	412	LHG	C2-C3-O3-P
30	Y	318	LHG	C2-C3-O3-P
30	a	412	LHG	C2-C3-O3-P
30	a	412	LHG	C5-C4-O6-P
30	r	616	LHG	C2-C3-O3-P
30	s	616	LHG	C5-C4-O6-P
30	y	318	LHG	C5-C4-O6-P
23	C	509	CLA	O1D-CGD-O2D-CED
23	y	315	CLA	C2-C3-C5-C6
30	b	627	LHG	C25-C26-C27-C28
31	A	413	LNL	C4-C5-C6-C7
23	B	615	CLA	C4B-C3B-CAB-CBB
23	G	611	CLA	C4B-C3B-CAB-CBB
23	G	612	CLA	C4B-C3B-CAB-CBB
23	G	614	CLA	C4B-C3B-CAB-CBB
23	R	601	CLA	C4B-C3B-CAB-CBB
23	R	611	CLA	C4B-C3B-CAB-CBB
23	R	612	CLA	C4B-C3B-CAB-CBB
23	S	608	CLA	C4B-C3B-CAB-CBB
23	S	610	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	r	612	CLA	C4B-C3B-CAB-CBB
23	s	608	CLA	C4B-C3B-CAB-CBB
23	s	610	CLA	C4B-C3B-CAB-CBB
30	A	412	LHG	C3-O3-P-O4
30	A	412	LHG	C4-O6-P-O5
30	D	408	LHG	C4-O6-P-O5
30	R	616	LHG	C3-O3-P-O5
30	d	408	LHG	C4-O6-P-O5
30	g	618	LHG	C3-O3-P-O4
30	s	616	LHG	C4-O6-P-O4
30	y	318	LHG	C4-O6-P-O4
39	Y	306	CHL	C4B-C3B-CAB-CBB
39	Y	309	CHL	C4B-C3B-CAB-CBB
39	n	607	CHL	C4B-C3B-CAB-CBB
39	r	606	CHL	C4B-C3B-CAB-CBB
39	y	307	CHL	C4B-C3B-CAB-CBB
23	B	607	CLA	C16-C17-C18-C19
23	R	602	CLA	C16-C17-C18-C20
23	Y	305	CLA	C16-C17-C18-C20
28	C	524	3PH	C2D-C2E-C2F-C2G
23	b	605	CLA	C15-C16-C17-C18
23	C	502	CLA	CBA-CGA-O2A-C1
23	c	502	CLA	CBA-CGA-O2A-C1
28	D	403	3PH	O11-C1-C2-C3
30	R	616	LHG	O6-C4-C5-C6
26	a	409	SQD	C17-C18-C19-C20
27	A	409	LMG	C37-C38-C39-C40
30	D	408	LHG	C26-C27-C28-C29
30	n	619	LHG	C19-C20-C21-C22
28	T	101	3PH	C2D-C2E-C2F-C2G
23	G	613	CLA	C2A-CAA-CBA-CGA
23	B	613	CLA	C15-C16-C17-C18
30	a	412	LHG	C32-C33-C34-C35
23	g	611	CLA	C16-C17-C18-C20
23	B	609	CLA	CAD-CBD-CGD-O1D
23	C	502	CLA	CAD-CBD-CGD-O1D
23	C	506	CLA	CAD-CBD-CGD-O1D
23	G	604	CLA	CAD-CBD-CGD-O1D
23	S	603	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
23	c	502	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	g	604	CLA	CAD-CBD-CGD-O1D
23	n	614	CLA	CAD-CBD-CGD-O1D
23	s	603	CLA	CAD-CBD-CGD-O1D
23	y	315	CLA	CAD-CBD-CGD-O1D
39	g	609	CHL	CAD-CBD-CGD-O1D
41	S	617	NEX	C7-C8-C9-C10
24	A	405	PHO	C15-C16-C17-C18
37	D	410	DGA	CB5-CB6-CB7-CB8
23	N	604	CLA	O1A-CGA-O2A-C1
26	L	101	SQD	C12-C13-C14-C15
23	S	612	CLA	C5-C6-C7-C8
23	g	611	CLA	C13-C15-C16-C17
27	w	201	LMG	C36-C37-C38-C39
28	X	201	3PH	C29-C2A-C2B-C2C
23	b	616	CLA	O1D-CGD-O2D-CED
30	D	408	LHG	C14-C15-C16-C17
23	G	613	CLA	O1D-CGD-O2D-CED
28	D	403	3PH	C35-C36-C37-C38
23	d	406	CLA	C16-C17-C18-C19
23	r	602	CLA	C16-C17-C18-C20
23	s	609	CLA	C4-C3-C5-C6
23	B	601	CLA	C3A-C2A-CAA-CBA
23	B	607	CLA	C11-C10-C8-C7
23	C	505	CLA	C6-C7-C8-C10
23	C	509	CLA	C11-C10-C8-C7
23	D	406	CLA	C6-C7-C8-C10
23	G	610	CLA	C11-C12-C13-C15
23	S	613	CLA	C12-C13-C15-C16
23	Y	310	CLA	C11-C12-C13-C15
23	Y	312	CLA	C11-C12-C13-C15
23	Y	313	CLA	C6-C7-C8-C10
23	b	606	CLA	C6-C7-C8-C10
23	c	505	CLA	C6-C7-C8-C10
23	c	509	CLA	C11-C10-C8-C7
23	g	613	CLA	C6-C7-C8-C10
23	r	602	CLA	C11-C12-C13-C15
23	y	305	CLA	C12-C13-C15-C16
28	D	403	3PH	O11-C1-C2-O21
28	a	410	3PH	O11-C1-C2-O21
28	w	202	3PH	O11-C1-C2-O21
35	C	523	VIV	C16-C17-C18-C20
39	G	607	CHL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
39	N	607	CHL	C6-C7-C8-C10
28	X	201	3PH	C33-C34-C35-C36
33	c	515	DGD	CCB-CDB-CEB-CFB
23	c	513	CLA	O1A-CGA-O2A-C1
27	b	628	LMG	C29-C30-C31-C32
41	Y	317	NEX	C29-C30-C31-C32
26	L	101	SQD	C25-C26-C27-C28
30	D	404	LHG	C7-C8-C9-C10
30	R	616	LHG	C23-C24-C25-C26
28	a	410	3PH	C22-C23-C24-C25
30	D	408	LHG	C27-C28-C29-C30
23	C	502	CLA	O1A-CGA-O2A-C1
23	s	609	CLA	C4C-C3C-CAC-CBC
23	c	511	CLA	CBD-CGD-O2D-CED
23	G	602	CLA	C2A-CAA-CBA-CGA
23	g	602	CLA	C2A-CAA-CBA-CGA
30	a	412	LHG	C11-C10-C9-C8
31	c	521	LNL	C3-C4-C5-C6
30	N	618	LHG	C7-C8-C9-C10
27	B	626	LMG	O8-C28-C29-C30
26	A	408	SQD	C44-C45-C46-O48
27	A	409	LMG	O1-C7-C8-C9
28	W	201	3PH	C29-C2A-C2B-C2C
30	G	618	LHG	C4-C5-C6-O8
30	R	616	LHG	C4-C5-C6-O8
30	Y	318	LHG	C4-C5-C6-O8
30	n	619	LHG	C4-C5-C6-O8
39	G	620	CHL	C1C-C2C-CMC-OMC
39	N	608	CHL	C1C-C2C-CMC-OMC
39	R	606	CHL	C1C-C2C-CMC-OMC
39	n	601	CHL	C1C-C2C-CMC-OMC
39	n	607	CHL	C1C-C2C-CMC-OMC
39	n	608	CHL	C1C-C2C-CMC-OMC
39	r	606	CHL	C1C-C2C-CMC-OMC
26	A	408	SQD	O47-C45-C46-O48
26	L	101	SQD	O6-C44-C45-O47
26	M	101	SQD	O47-C45-C46-O48
30	G	618	LHG	O7-C5-C6-O8
30	d	408	LHG	O7-C5-C6-O8
31	B	623	LNL	C5-C6-C7-C8
31	C	517	LNL	C6-C7-C8-C9
27	r	617	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
23	c	502	CLA	O1A-CGA-O2A-C1
28	w	202	3PH	C38-C39-C3A-C3B
30	b	627	LHG	C10-C11-C12-C13
27	R	617	LMG	C15-C16-C17-C18
28	w	202	3PH	C2C-C2D-C2E-C2F
27	B	626	LMG	C14-C15-C16-C17
33	c	515	DGD	C6B-C7B-C8B-C9B
24	a	406	PHO	C2-C3-C5-C6
23	s	611	CLA	O2A-C1-C2-C3
23	B	615	CLA	C5-C6-C7-C8
23	B	602	CLA	C11-C12-C13-C14
23	B	611	CLA	C6-C7-C8-C9
23	C	503	CLA	C6-C7-C8-C9
23	N	613	CLA	C11-C12-C13-C14
23	R	609	CLA	C14-C13-C15-C16
23	Y	303	CLA	C11-C12-C13-C14
23	Y	311	CLA	C11-C12-C13-C14
23	b	615	CLA	C14-C13-C15-C16
23	c	503	CLA	C6-C7-C8-C9
23	c	511	CLA	C6-C7-C8-C9
23	c	512	CLA	C11-C10-C8-C9
23	g	610	CLA	C11-C12-C13-C14
23	n	603	CLA	C14-C13-C15-C16
23	y	304	CLA	C11-C12-C13-C14
23	y	304	CLA	C14-C13-C15-C16
23	y	314	CLA	C6-C7-C8-C9
39	n	607	CHL	C6-C7-C8-C9
24	A	405	PHO	O1D-CGD-O2D-CED
23	B	611	CLA	O1A-CGA-O2A-C1
23	N	604	CLA	CBD-CGD-O2D-CED
26	A	408	SQD	C26-C27-C28-C29
26	a	409	SQD	C16-C17-C18-C19
33	H	502	DGD	O6E-C1E-O5D-C6D
25	v	101	BCR	C19-C20-C21-C22
27	w	201	LMG	C11-C12-C13-C14
33	c	515	DGD	C3A-C4A-C5A-C6A
23	R	610	CLA	C16-C17-C18-C19
23	c	512	CLA	C16-C17-C18-C19
31	c	520	LNL	C2-C3-C4-C5
28	x	201	3PH	C2B-C2C-C2D-C2E
30	s	616	LHG	C18-C19-C20-C21
23	D	406	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	G	614	CLA	C2B-C3B-CAB-CBB
23	N	611	CLA	C2B-C3B-CAB-CBB
23	R	611	CLA	C2B-C3B-CAB-CBB
23	S	608	CLA	C2B-C3B-CAB-CBB
23	Y	311	CLA	C2B-C3B-CAB-CBB
23	s	608	CLA	C2B-C3B-CAB-CBB
39	R	606	CHL	C2B-C3B-CAB-CBB
39	g	605	CHL	C2B-C3B-CAB-CBB
39	n	608	CHL	C2B-C3B-CAB-CBB
39	s	601	CHL	C2B-C3B-CAB-CBB
39	y	310	CHL	C2B-C3B-CAB-CBB
30	d	404	LHG	C14-C15-C16-C17
23	b	607	CLA	C13-C15-C16-C17
40	G	615	LUT	C20-C13-C14-C15
28	x	201	3PH	C29-C2A-C2B-C2C
30	N	618	LHG	C31-C32-C33-C34
28	T	101	3PH	C2F-C2G-C2H-C2I
28	W	201	3PH	C36-C37-C38-C39
30	d	404	LHG	C35-C36-C37-C38
39	n	601	CHL	C2-C3-C5-C6
39	n	607	CHL	C10-C11-C12-C13
27	r	617	LMG	C11-C12-C13-C14
28	C	524	3PH	C33-C34-C35-C36
28	d	403	3PH	C34-C35-C36-C37
30	r	616	LHG	C11-C10-C9-C8
30	r	616	LHG	C31-C32-C33-C34
31	c	518	LNL	C2-C3-C4-C5
30	s	616	LHG	C13-C14-C15-C16
23	A	404	CLA	C1-C2-C3-C4
23	B	601	CLA	C1-C2-C3-C4
23	G	604	CLA	C1-C2-C3-C4
23	G	611	CLA	C1-C2-C3-C4
23	G	612	CLA	C1-C2-C3-C4
23	G	614	CLA	C1-C2-C3-C4
23	N	604	CLA	C1-C2-C3-C4
23	N	612	CLA	C1-C2-C3-C4
23	R	611	CLA	C1-C2-C3-C4
23	S	603	CLA	C1-C2-C3-C4
23	S	604	CLA	C1-C2-C3-C4
23	a	405	CLA	C1-C2-C3-C4
23	g	604	CLA	C1-C2-C3-C4
23	g	612	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
23	g	614	CLA	C1-C2-C3-C4
23	n	604	CLA	C1-C2-C3-C4
23	n	612	CLA	C1-C2-C3-C4
23	n	614	CLA	C1-C2-C3-C4
23	r	601	CLA	C1-C2-C3-C4
23	r	611	CLA	C1-C2-C3-C4
23	r	612	CLA	C1-C2-C3-C4
23	s	603	CLA	C1-C2-C3-C4
23	s	608	CLA	C1-C2-C3-C4
39	G	606	CHL	C1-C2-C3-C4
39	G	608	CHL	C1-C2-C3-C4
39	N	605	CHL	C1-C2-C3-C4
39	S	605	CHL	C1-C2-C3-C4
39	S	606	CHL	C1-C2-C3-C4
39	Y	308	CHL	C1-C2-C3-C4
39	g	606	CHL	C1-C2-C3-C4
39	g	608	CHL	C1-C2-C3-C4
39	n	608	CHL	C1-C2-C3-C4
39	r	605	CHL	C1-C2-C3-C4
39	y	308	CHL	C1-C2-C3-C4
39	y	309	CHL	C1-C2-C3-C4
28	a	410	3PH	C28-C29-C2A-C2B
31	I	101	LNL	C4-C5-C6-C7
28	A	410	3PH	O11-C1-C2-C3
30	d	404	LHG	O6-C4-C5-C6
30	r	616	LHG	O6-C4-C5-C6
23	S	602	CLA	C2A-CAA-CBA-CGA
23	b	602	CLA	C2A-CAA-CBA-CGA
23	b	614	CLA	C2A-CAA-CBA-CGA
23	n	602	CLA	C2A-CAA-CBA-CGA
37	b	626	DGA	CA6-CA7-CA8-CA9
30	y	318	LHG	C24-C23-O8-C6
23	B	610	CLA	C2-C1-O2A-CGA
23	C	504	CLA	C2-C1-O2A-CGA
23	R	603	CLA	C2-C1-O2A-CGA
23	b	608	CLA	C2-C1-O2A-CGA
23	c	504	CLA	C2-C1-O2A-CGA
39	Y	307	CHL	C2-C1-O2A-CGA
39	r	605	CHL	C2-C1-O2A-CGA
31	B	623	LNL	C4-C5-C6-C7
23	r	608	CLA	C16-C17-C18-C19
27	b	620	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
28	T	101	3PH	C35-C36-C37-C38
23	B	601	CLA	CAA-CBA-CGA-O2A
30	y	318	LHG	O10-C23-O8-C6
23	a	407	CLA	C3-C5-C6-C7
28	s	618	3PH	C2-C1-O11-P
30	S	616	LHG	C5-C4-O6-P
40	S	615	LUT	C26-C27-C28-C29
40	s	615	LUT	C26-C27-C28-C29
37	b	626	DGA	CEA-CFA-CGA-CHA
40	r	613	LUT	C9-C10-C11-C12
23	s	604	CLA	O1A-CGA-O2A-C1
30	a	412	LHG	O6-C4-C5-O7
23	c	501	CLA	C16-C17-C18-C20
23	r	610	CLA	C16-C17-C18-C19
23	y	311	CLA	C16-C17-C18-C20
23	Y	303	CLA	C13-C15-C16-C17
23	S	604	CLA	O2A-C1-C2-C3
39	N	608	CHL	O2A-C1-C2-C3
23	r	602	CLA	C4-C3-C5-C6
25	A	407	BCR	C23-C24-C25-C26
25	A	407	BCR	C23-C24-C25-C30
25	D	411	BCR	C1-C6-C7-C8
25	D	411	BCR	C5-C6-C7-C8
25	Z	101	BCR	C23-C24-C25-C26
25	Z	101	BCR	C23-C24-C25-C30
25	a	408	BCR	C23-C24-C25-C30
25	b	619	BCR	C23-C24-C25-C30
25	d	410	BCR	C23-C24-C25-C26
25	d	410	BCR	C23-C24-C25-C30
25	z	101	BCR	C23-C24-C25-C26
25	z	101	BCR	C23-C24-C25-C30
23	g	610	CLA	C2-C3-C5-C6
28	T	101	3PH	C39-C3A-C3B-C3C
23	C	501	CLA	CBA-CGA-O2A-C1
23	s	604	CLA	CBA-CGA-O2A-C1
27	c	523	LMG	O8-C28-C29-C30
23	n	613	CLA	C15-C16-C17-C18
23	g	613	CLA	C16-C17-C18-C20
23	s	612	CLA	C6-C7-C8-C10
30	D	408	LHG	C8-C7-O7-C5
31	c	517	LNL	C7-C8-C9-C10
26	L	101	SQD	C2-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
33	H	502	DGD	C2E-C1E-O5D-C6D
40	n	615	LUT	C12-C13-C14-C15
40	n	616	LUT	C28-C29-C30-C31
42	n	620	XAT	C11-C10-C9-C8
26	M	101	SQD	O6-C44-C45-O47
27	A	409	LMG	O7-C8-C9-O8
30	D	408	LHG	C3-O3-P-O6
30	N	618	LHG	C4-O6-P-O3
30	Y	318	LHG	C4-O6-P-O3
30	d	408	LHG	C3-O3-P-O6
30	n	619	LHG	C4-O6-P-O3
31	C	517	LNL	C15-C16-C17-C18
31	C	522	LNL	C15-C16-C17-C18
39	n	606	CHL	C5-C6-C7-C8
30	N	618	LHG	C15-C16-C17-C18
30	g	618	LHG	C32-C33-C34-C35
24	D	402	PHO	CHA-CBD-CGD-O2D
24	d	402	PHO	CHA-CBD-CGD-O1D
24	d	402	PHO	CHA-CBD-CGD-O2D
31	B	623	LNL	C2-C3-C4-C5
23	y	305	CLA	O1D-CGD-O2D-CED
28	D	403	3PH	C1-C2-C3-O31
30	y	318	LHG	C4-C5-C6-O8
23	B	602	CLA	C11-C10-C8-C7
23	B	602	CLA	C11-C12-C13-C15
23	B	607	CLA	C6-C7-C8-C10
23	C	503	CLA	C6-C7-C8-C10
23	C	510	CLA	C11-C12-C13-C15
23	n	602	CLA	C2-C3-C5-C6
23	r	602	CLA	C6-C7-C8-C10
23	y	315	CLA	C12-C13-C15-C16
26	A	408	SQD	C11-C10-C9-C8
31	a	401	LNL	C4-C5-C6-C7
26	a	409	SQD	C23-C24-C25-C26
28	s	618	3PH	C34-C35-C36-C37
23	B	607	CLA	C11-C10-C8-C9
23	B	615	CLA	C14-C13-C15-C16
23	G	610	CLA	C11-C12-C13-C14
23	S	610	CLA	C11-C10-C8-C9
23	Y	311	CLA	C11-C10-C8-C9
23	Y	312	CLA	C11-C12-C13-C14
23	Y	313	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	a	407	CLA	C11-C10-C8-C9
23	b	602	CLA	C14-C13-C15-C16
23	b	606	CLA	C6-C7-C8-C9
23	n	603	CLA	C11-C10-C8-C9
23	r	602	CLA	C11-C12-C13-C14
23	s	610	CLA	C11-C10-C8-C9
23	y	306	CLA	C14-C13-C15-C16
23	y	311	CLA	C11-C12-C13-C14
39	G	620	CHL	C14-C13-C15-C16
39	g	609	CHL	C6-C7-C8-C9
23	b	605	CLA	C13-C15-C16-C17
25	b	617	BCR	C9-C10-C11-C12
40	Y	315	LUT	C13-C14-C15-C35
40	y	316	LUT	C13-C14-C15-C35
23	Y	305	CLA	C16-C17-C18-C19
23	g	611	CLA	C16-C17-C18-C19
28	T	101	3PH	C29-C2A-C2B-C2C
23	b	614	CLA	C8-C10-C11-C12
23	s	612	CLA	C5-C6-C7-C8
23	b	601	CLA	C2A-CAA-CBA-CGA
37	b	626	DGA	CA5-CA6-CA7-CA8
25	d	410	BCR	C11-C12-C13-C35
40	n	616	LUT	C7-C8-C9-C19
30	b	627	LHG	C5-C4-O6-P
30	y	318	LHG	C2-C3-O3-P
42	R	615	XAT	C11-C12-C13-C14
30	Y	318	LHG	C30-C31-C32-C33
23	N	614	CLA	O2A-C1-C2-C3
23	n	611	CLA	O2A-C1-C2-C3
29	A	411	PL9	C26-C27-C28-C29
29	a	411	PL9	C36-C37-C38-C39
23	C	511	CLA	CBD-CGD-O2D-CED
23	G	610	CLA	C2-C3-C5-C6
23	R	602	CLA	C16-C17-C18-C19
23	r	602	CLA	C16-C17-C18-C19
23	Y	313	CLA	CBA-CGA-O2A-C1
23	y	314	CLA	CBA-CGA-O2A-C1
29	D	407	PL9	C2-C3-C7-C8
29	d	407	PL9	C2-C3-C7-C8
23	C	501	CLA	O1A-CGA-O2A-C1
32	B	621	PAM	O1-C1-C2-C3
28	W	201	3PH	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
39	R	607	CHL	C5-C6-C7-C8
23	Y	313	CLA	O1A-CGA-O2A-C1
23	G	613	CLA	CBA-CGA-O2A-C1
31	C	520	LNL	C7-C8-C9-C10
23	r	601	CLA	C4B-C3B-CAB-CBB
39	R	605	CHL	C4B-C3B-CAB-CBB
39	R	606	CHL	C4B-C3B-CAB-CBB
39	S	601	CHL	C4B-C3B-CAB-CBB
39	y	310	CHL	C4B-C3B-CAB-CBB
23	R	610	CLA	C2A-CAA-CBA-CGA
23	r	610	CLA	C2A-CAA-CBA-CGA
23	d	406	CLA	C16-C17-C18-C20
31	C	522	LNL	O2-C1-C2-C3
40	N	616	LUT	C9-C10-C11-C12
40	N	616	LUT	C33-C34-C35-C15
40	R	613	LUT	C33-C34-C35-C15
29	a	411	PL9	C39-C41-C42-C43
23	G	613	CLA	O1A-CGA-O2A-C1
23	y	314	CLA	O1A-CGA-O2A-C1
40	g	615	LUT	C10-C11-C12-C13
41	s	617	NEX	C10-C11-C12-C13
42	y	302	XAT	C10-C11-C12-C13
23	b	605	CLA	C8-C10-C11-C12
30	D	404	LHG	C29-C30-C31-C32
30	r	616	LHG	C30-C31-C32-C33
23	n	610	CLA	C16-C17-C18-C20
23	N	610	CLA	C4-C3-C5-C6
23	b	604	CLA	C4-C3-C5-C6
23	a	404	CLA	CBD-CGD-O2D-CED
23	B	602	CLA	C2-C3-C5-C6
23	c	510	CLA	C2-C3-C5-C6
31	C	517	LNL	C7-C8-C9-C10
23	B	613	CLA	C13-C15-C16-C17
23	C	507	CLA	C10-C11-C12-C13
23	b	608	CLA	C13-C15-C16-C17
23	B	608	CLA	C2-C1-O2A-CGA
39	N	606	CHL	C2-C1-O2A-CGA
39	g	607	CHL	C2-C1-O2A-CGA
39	n	609	CHL	C2-C1-O2A-CGA
28	W	201	3PH	C34-C35-C36-C37
30	L	103	LHG	C11-C12-C13-C14
23	C	502	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
30	g	618	LHG	C29-C30-C31-C32
23	C	505	CLA	C2A-CAA-CBA-CGA
23	c	505	CLA	C2A-CAA-CBA-CGA
23	n	613	CLA	C2A-CAA-CBA-CGA
23	r	602	CLA	C2A-CAA-CBA-CGA
23	y	304	CLA	C2A-CAA-CBA-CGA
27	d	409	LMG	O1-C7-C8-O7
28	A	410	3PH	O21-C2-C3-O31
39	n	607	CHL	C2A-CAA-CBA-CGA
33	c	515	DGD	C2A-C3A-C4A-C5A
23	g	613	CLA	C15-C16-C17-C18
28	C	524	3PH	C2C-C2D-C2E-C2F
33	C	515	DGD	C3A-C4A-C5A-C6A
30	r	616	LHG	C5-C4-O6-P
26	L	101	SQD	C15-C16-C17-C18
23	B	607	CLA	C3A-C2A-CAA-CBA
23	D	405	CLA	C3A-C2A-CAA-CBA
23	R	604	CLA	C3A-C2A-CAA-CBA
23	S	613	CLA	C3A-C2A-CAA-CBA
23	N	604	CLA	O1D-CGD-O2D-CED
31	B	624	LNL	C7-C8-C9-C10
31	c	520	LNL	C7-C8-C9-C10
23	s	604	CLA	O2A-C1-C2-C3
25	D	411	BCR	C9-C10-C11-C12
25	d	410	BCR	C19-C20-C21-C22
41	n	618	NEX	C29-C30-C31-C32
23	B	602	CLA	C4-C3-C5-C6
23	G	613	CLA	C4-C3-C5-C6
23	c	510	CLA	C4-C3-C5-C6
28	a	410	3PH	C3B-C3C-C3D-C3E
23	G	613	CLA	C2-C3-C5-C6
30	b	627	LHG	C34-C35-C36-C37
23	B	602	CLA	C6-C7-C8-C9
23	B	605	CLA	C11-C10-C8-C9
23	C	507	CLA	C11-C10-C8-C9
23	D	405	CLA	C14-C13-C15-C16
23	G	603	CLA	C6-C7-C8-C9
23	R	603	CLA	C6-C7-C8-C9
23	Y	310	CLA	C11-C12-C13-C14
23	b	602	CLA	C11-C12-C13-C14
23	b	605	CLA	C11-C12-C13-C14
23	b	607	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	s	613	CLA	C6-C7-C8-C9
23	y	312	CLA	C11-C12-C13-C14
23	y	315	CLA	C6-C7-C8-C9
24	a	406	PHO	C6-C7-C8-C9
39	Y	302	CHL	C14-C13-C15-C16
39	Y	307	CHL	C14-C13-C15-C16
39	g	619	CHL	C14-C13-C15-C16
28	A	410	3PH	C2C-C2D-C2E-C2F
31	b	624	LNL	C4-C5-C6-C7
26	M	101	SQD	C12-C13-C14-C15
30	A	412	LHG	C27-C28-C29-C30
23	c	511	CLA	O1D-CGD-O2D-CED
27	d	409	LMG	O1-C7-C8-C9
30	r	616	LHG	C4-C5-C6-O8
30	D	408	LHG	O9-C7-O7-C5
27	B	620	LMG	C14-C15-C16-C17
31	a	413	LNL	C7-C8-C9-C10
23	C	507	CLA	C2A-CAA-CBA-CGA
23	N	604	CLA	C2A-CAA-CBA-CGA
23	c	507	CLA	C2A-CAA-CBA-CGA
23	Y	310	CLA	C16-C17-C18-C20
23	g	613	CLA	C16-C17-C18-C19
23	s	612	CLA	C6-C7-C8-C9
39	R	607	CHL	O2A-C1-C2-C3
39	r	607	CHL	O2A-C1-C2-C3
23	B	608	CLA	C13-C15-C16-C17
23	y	306	CLA	C8-C10-C11-C12
25	V	101	BCR	C7-C8-C9-C34
25	v	101	BCR	C36-C18-C19-C20
41	S	617	NEX	C11-C12-C13-C20
27	b	620	LMG	C17-C18-C19-C20
41	G	617	NEX	C31-C32-C33-C34
30	a	412	LHG	C28-C29-C30-C31
30	y	318	LHG	C4-C5-O7-C7
23	D	405	CLA	C1A-C2A-CAA-CBA
23	S	602	CLA	C1A-C2A-CAA-CBA
23	Y	310	CLA	C1A-C2A-CAA-CBA
23	d	405	CLA	C1A-C2A-CAA-CBA
23	g	610	CLA	C1A-C2A-CAA-CBA
23	n	614	CLA	C1A-C2A-CAA-CBA
39	G	601	CHL	C1A-C2A-CAA-CBA
39	N	605	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
39	n	606	CHL	C1A-C2A-CAA-CBA
27	b	620	LMG	C20-C21-C22-C23
23	C	506	CLA	C6-C7-C8-C9
23	B	607	CLA	C11-C12-C13-C15
23	B	610	CLA	C11-C12-C13-C15
23	C	509	CLA	C11-C12-C13-C15
23	C	511	CLA	C11-C12-C13-C15
23	C	512	CLA	C12-C13-C15-C16
23	G	613	CLA	C12-C13-C15-C16
23	b	603	CLA	C11-C10-C8-C7
23	b	607	CLA	C11-C10-C8-C7
23	b	610	CLA	C11-C12-C13-C15
23	b	616	CLA	C11-C10-C8-C7
23	c	502	CLA	C11-C10-C8-C7
23	c	503	CLA	C6-C7-C8-C10
23	c	506	CLA	C12-C13-C15-C16
23	c	509	CLA	C11-C12-C13-C15
23	c	510	CLA	C11-C12-C13-C15
23	n	603	CLA	C11-C10-C8-C7
23	r	608	CLA	C12-C13-C15-C16
39	r	606	CHL	C6-C7-C8-C10
28	W	201	3PH	C39-C3A-C3B-C3C
30	A	412	LHG	C24-C25-C26-C27
30	g	618	LHG	C12-C13-C14-C15
31	A	414	LNL	C12-C13-C14-C15
31	B	623	LNL	C9-C10-C11-C12
31	B	624	LNL	C12-C13-C14-C15
31	C	517	LNL	C9-C10-C11-C12
31	C	521	LNL	C13-C14-C15-C16
31	I	101	LNL	C9-C10-C11-C12
31	b	622	LNL	C9-C10-C11-C12
31	b	624	LNL	C9-C10-C11-C12
31	c	519	LNL	C9-C10-C11-C12
31	i	101	LNL	C10-C11-C12-C13
28	C	524	3PH	C37-C38-C39-C3A
23	b	608	CLA	C16-C17-C18-C20
23	y	304	CLA	C16-C17-C18-C20
23	N	602	CLA	C2A-CAA-CBA-CGA
23	R	602	CLA	C2A-CAA-CBA-CGA
23	Y	303	CLA	C2A-CAA-CBA-CGA
23	n	604	CLA	C2A-CAA-CBA-CGA
23	C	513	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
26	A	408	SQD	C31-C32-C33-C34
30	G	618	LHG	C31-C32-C33-C34
30	Y	318	LHG	C11-C10-C9-C8
23	n	612	CLA	O2A-C1-C2-C3
23	B	614	CLA	C8-C10-C11-C12
28	L	102	3PH	C2F-C2G-C2H-C2I
30	L	103	LHG	O6-C4-C5-C6
23	a	403	CLA	C5-C6-C7-C8
31	b	623	LNL	O2-C1-C2-C3
28	s	618	3PH	C36-C37-C38-C39
30	N	618	LHG	C19-C20-C21-C22
23	n	610	CLA	C4-C3-C5-C6
23	A	402	CLA	C5-C6-C7-C8
23	c	511	CLA	C8-C10-C11-C12
23	B	615	CLA	C2B-C3B-CAB-CBB
23	G	611	CLA	C2B-C3B-CAB-CBB
23	G	612	CLA	C2B-C3B-CAB-CBB
23	R	601	CLA	C2B-C3B-CAB-CBB
23	R	612	CLA	C2B-C3B-CAB-CBB
23	S	610	CLA	C2B-C3B-CAB-CBB
23	g	614	CLA	C2B-C3B-CAB-CBB
23	r	601	CLA	C2B-C3B-CAB-CBB
23	r	612	CLA	C2B-C3B-CAB-CBB
23	s	610	CLA	C2B-C3B-CAB-CBB
39	R	605	CHL	C2B-C3B-CAB-CBB
39	S	601	CHL	C2B-C3B-CAB-CBB
39	Y	306	CHL	C2B-C3B-CAB-CBB
39	Y	309	CHL	C2B-C3B-CAB-CBB
39	n	607	CHL	C2B-C3B-CAB-CBB
39	n	609	CHL	C2B-C3B-CAB-CBB
39	r	606	CHL	C2B-C3B-CAB-CBB
39	y	307	CHL	C2B-C3B-CAB-CBB
28	A	410	3PH	C36-C37-C38-C39
23	c	501	CLA	CBA-CGA-O2A-C1
32	B	621	PAM	O2-C1-C2-C3
39	s	607	CHL	O2A-C1-C2-C3
23	C	513	CLA	CAA-CBA-CGA-O1A
25	h	501	BCR	C16-C17-C18-C19
40	n	615	LUT	C32-C33-C34-C35
40	r	613	LUT	C12-C13-C14-C15
41	N	617	NEX	C28-C29-C30-C31
41	R	614	NEX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
41	r	614	NEX	C28-C29-C30-C31
31	b	624	LNL	O1-C1-C2-C3
31	c	522	LNL	O2-C1-C2-C3
28	X	201	3PH	C39-C3A-C3B-C3C
23	C	511	CLA	O1D-CGD-O2D-CED
26	a	409	SQD	O6-C44-C45-O47
28	L	102	3PH	O21-C2-C3-O31
30	r	616	LHG	O7-C5-C6-O8
28	d	403	3PH	C32-C33-C34-C35
42	N	619	XAT	C29-C30-C31-C32
31	C	521	LNL	O2-C1-C2-C3
40	r	613	LUT	C6-C7-C8-C9
23	B	606	CLA	C16-C17-C18-C20
26	M	101	SQD	C16-C17-C18-C19
31	C	517	LNL	C3-C4-C5-C6
39	N	606	CHL	C5-C6-C7-C8
33	d	411	DGD	C6B-C7B-C8B-C9B
23	a	404	CLA	O1D-CGD-O2D-CED
30	b	627	LHG	C1-C2-C3-O3
31	C	521	LNL	O1-C1-C2-C3
31	C	522	LNL	O1-C1-C2-C3
31	b	623	LNL	O1-C1-C2-C3
29	D	407	PL9	C40-C39-C41-C42
39	n	609	CHL	C4-C3-C5-C6
28	d	403	3PH	C23-C24-C25-C26
23	R	601	CLA	C2-C1-O2A-CGA
23	Y	305	CLA	C2-C1-O2A-CGA
39	G	609	CHL	C2-C1-O2A-CGA
39	N	608	CHL	C2-C1-O2A-CGA
39	g	601	CHL	C2-C1-O2A-CGA
40	S	615	LUT	C30-C31-C32-C33
31	c	522	LNL	O1-C1-C2-C3
30	d	408	LHG	C23-C24-C25-C26
23	Y	303	CLA	C14-C13-C15-C16
23	b	606	CLA	C14-C13-C15-C16
23	c	511	CLA	C11-C10-C8-C9
23	g	613	CLA	C6-C7-C8-C9
23	r	603	CLA	C6-C7-C8-C9
23	y	306	CLA	C11-C12-C13-C14
37	D	410	DGA	CBB-CAB-CB9-CB8
33	d	411	DGD	C9A-CAA-CBA-CCA
23	B	606	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	b	612	CLA	C8-C10-C11-C12
28	a	410	3PH	C27-C28-C29-C2A
39	g	606	CHL	C2A-CAA-CBA-CGA
23	c	511	CLA	C16-C17-C18-C20
39	n	605	CHL	C2-C1-O2A-CGA
25	B	617	BCR	C1-C6-C7-C8
25	B	617	BCR	C23-C24-C25-C30
25	B	619	BCR	C1-C6-C7-C8
25	B	619	BCR	C5-C6-C7-C8
25	V	101	BCR	C23-C24-C25-C26
25	V	101	BCR	C23-C24-C25-C30
25	Z	101	BCR	C1-C6-C7-C8
25	Z	101	BCR	C5-C6-C7-C8
25	b	617	BCR	C23-C24-C25-C30
25	b	619	BCR	C1-C6-C7-C8
25	v	101	BCR	C23-C24-C25-C26
25	v	101	BCR	C23-C24-C25-C30
25	z	101	BCR	C1-C6-C7-C8
25	z	101	BCR	C5-C6-C7-C8
26	a	409	SQD	C24-C25-C26-C27
30	n	619	LHG	C26-C27-C28-C29
40	Y	315	LUT	C9-C10-C11-C12
40	s	615	LUT	C29-C30-C31-C32
41	G	617	NEX	C29-C30-C31-C32
26	L	101	SQD	C13-C14-C15-C16
23	B	604	CLA	C4-C3-C5-C6
23	Y	311	CLA	C4-C3-C5-C6
23	b	614	CLA	C5-C6-C7-C8
23	c	513	CLA	C5-C6-C7-C8
23	Y	311	CLA	C2-C3-C5-C6
23	r	602	CLA	C2-C3-C5-C6
23	s	610	CLA	C2-C3-C5-C6
26	A	408	SQD	O47-C7-C8-C9
31	B	625	LNL	O1-C1-C2-C3
23	b	607	CLA	C8-C10-C11-C12
31	b	625	LNL	O1-C1-C2-C3
31	c	519	LNL	O1-C1-C2-C3
23	c	501	CLA	O1A-CGA-O2A-C1
28	D	403	3PH	O31-C31-C32-C33
27	R	617	LMG	C31-C32-C33-C34
28	C	524	3PH	C2A-C2B-C2C-C2D
23	c	502	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
32	B	621	PAM	C7-C8-C9-C10
23	B	611	CLA	C13-C15-C16-C17
23	C	509	CLA	C13-C15-C16-C17
23	c	509	CLA	C13-C15-C16-C17
30	r	616	LHG	O6-C4-C5-O7
31	B	624	LNL	O1-C1-C2-C3
31	b	625	LNL	O2-C1-C2-C3
31	c	519	LNL	O2-C1-C2-C3
23	r	601	CLA	C2A-CAA-CBA-CGA
28	X	201	3PH	C35-C36-C37-C38
23	g	614	CLA	C4B-C3B-CAB-CBB
23	y	312	CLA	C4B-C3B-CAB-CBB
39	N	609	CHL	C4B-C3B-CAB-CBB
39	n	609	CHL	C4B-C3B-CAB-CBB
31	c	519	LNL	C3-C4-C5-C6
28	a	410	3PH	O11-C1-C2-C3
30	Y	318	LHG	O6-C4-C5-C6
23	B	606	CLA	C4-C3-C5-C6
23	a	407	CLA	C4-C3-C5-C6
29	A	411	PL9	C40-C39-C41-C42
29	d	407	PL9	C40-C39-C41-C42
23	C	502	CLA	C11-C10-C8-C7
23	C	503	CLA	C12-C13-C15-C16
23	R	609	CLA	C12-C13-C15-C16
23	b	605	CLA	C11-C12-C13-C15
23	c	503	CLA	C12-C13-C15-C16
23	g	610	CLA	C11-C12-C13-C15
39	G	620	CHL	C11-C12-C13-C15
39	Y	309	CHL	C2-C3-C5-C6
39	n	609	CHL	C2-C3-C5-C6
31	C	517	LNL	O1-C1-C2-C3
23	C	510	CLA	CBA-CGA-O2A-C1
23	n	613	CLA	CBA-CGA-O2A-C1
23	B	602	CLA	C15-C16-C17-C18
23	C	506	CLA	C5-C6-C7-C8
41	g	617	NEX	C13-C14-C15-C35
42	G	619	XAT	C29-C30-C31-C32
27	B	626	LMG	O1-C7-C8-O7
28	a	410	3PH	O21-C2-C3-O31
30	A	412	LHG	O9-C7-O7-C5
28	w	202	3PH	C2D-C2E-C2F-C2G
30	g	618	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
23	b	603	CLA	C13-C15-C16-C17
31	b	624	LNL	O2-C1-C2-C3
23	N	612	CLA	O2A-C1-C2-C3
23	S	603	CLA	O2A-C1-C2-C3
39	G	608	CHL	O2A-C1-C2-C3
39	S	605	CHL	O2A-C1-C2-C3
39	Y	308	CHL	O2A-C1-C2-C3
23	c	512	CLA	CAA-CBA-CGA-O2A
24	D	402	PHO	O1A-CGA-O2A-C1
23	b	610	CLA	C2A-CAA-CBA-CGA
23	n	610	CLA	C16-C17-C18-C19
30	G	618	LHG	C16-C17-C18-C19
24	D	402	PHO	CBA-CGA-O2A-C1
23	C	510	CLA	O1A-CGA-O2A-C1
28	a	410	3PH	C1-O11-P-O14
31	B	622	LNL	C4-C5-C6-C7
41	g	617	NEX	C39-C29-C30-C31
23	N	612	CLA	CAA-CBA-CGA-O2A
23	d	405	CLA	CAA-CBA-CGA-O2A
28	W	201	3PH	O21-C21-C22-C23
31	C	518	LNL	O1-C1-C2-C3
23	S	609	CLA	C2-C3-C5-C6
28	C	524	3PH	C31-C32-C33-C34
23	b	607	CLA	C16-C17-C18-C19
23	C	512	CLA	CAA-CBA-CGA-O2A
30	L	103	LHG	O7-C7-C8-C9
30	N	618	LHG	O8-C23-C24-C25
23	B	609	CLA	C6-C7-C8-C9
23	B	615	CLA	C11-C10-C8-C9
23	C	505	CLA	C6-C7-C8-C9
23	C	509	CLA	C11-C10-C8-C9
23	C	511	CLA	C11-C10-C8-C9
23	D	406	CLA	C6-C7-C8-C9
23	b	605	CLA	C6-C7-C8-C9
23	c	505	CLA	C6-C7-C8-C9
23	c	509	CLA	C11-C10-C8-C9
23	r	602	CLA	C6-C7-C8-C9
23	y	305	CLA	C14-C13-C15-C16
23	y	306	CLA	C6-C7-C8-C9
23	y	312	CLA	C11-C10-C8-C9
35	C	523	VIV	C16-C17-C18-C19
39	G	609	CHL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	n	613	CLA	O1A-CGA-O2A-C1
31	I	101	LNL	C6-C7-C8-C9
28	W	201	3PH	C37-C38-C39-C3A
28	s	618	3PH	C37-C38-C39-C3A
27	w	201	LMG	C15-C16-C17-C18
30	L	103	LHG	C17-C18-C19-C20
30	s	616	LHG	C29-C30-C31-C32
23	Y	314	CLA	C3A-C2A-CAA-CBA
23	b	607	CLA	C3A-C2A-CAA-CBA
23	d	405	CLA	C3A-C2A-CAA-CBA
23	r	604	CLA	C3A-C2A-CAA-CBA
39	G	608	CHL	C3A-C2A-CAA-CBA
39	G	609	CHL	C3A-C2A-CAA-CBA
39	Y	302	CHL	C3A-C2A-CAA-CBA
39	s	607	CHL	C3A-C2A-CAA-CBA
28	w	202	3PH	O21-C21-C22-C23
31	A	414	LNL	C7-C8-C9-C10
31	B	625	LNL	C7-C8-C9-C10
31	C	522	LNL	C7-C8-C9-C10
31	b	623	LNL	C7-C8-C9-C10
31	b	624	LNL	C7-C8-C9-C10
31	i	101	LNL	C7-C8-C9-C10
33	C	515	DGD	C8B-C9B-CAB-CBB
23	A	404	CLA	CAD-CBD-CGD-O2D
23	B	606	CLA	CAD-CBD-CGD-O2D
23	B	616	CLA	CAD-CBD-CGD-O2D
23	C	501	CLA	CAD-CBD-CGD-O2D
23	C	503	CLA	CAD-CBD-CGD-O2D
23	C	507	CLA	CAD-CBD-CGD-O2D
23	C	509	CLA	CAD-CBD-CGD-O2D
23	C	510	CLA	CAD-CBD-CGD-O2D
23	G	610	CLA	CAD-CBD-CGD-O2D
23	G	611	CLA	CAD-CBD-CGD-O2D
23	N	604	CLA	CAD-CBD-CGD-O2D
23	N	610	CLA	CAD-CBD-CGD-O2D
23	N	613	CLA	CAD-CBD-CGD-O2D
23	R	604	CLA	CAD-CBD-CGD-O2D
23	R	609	CLA	CAD-CBD-CGD-O2D
23	S	609	CLA	CAD-CBD-CGD-O2D
23	S	610	CLA	CAD-CBD-CGD-O2D
23	S	613	CLA	CAD-CBD-CGD-O2D
23	Y	304	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	b	603	CLA	CAD-CBD-CGD-O2D
23	b	606	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CAD-CBD-CGD-O2D
23	c	501	CLA	CAD-CBD-CGD-O2D
23	c	507	CLA	CAD-CBD-CGD-O2D
23	c	509	CLA	CAD-CBD-CGD-O2D
23	c	510	CLA	CAD-CBD-CGD-O2D
23	g	603	CLA	CAD-CBD-CGD-O2D
23	n	610	CLA	CAD-CBD-CGD-O2D
23	r	610	CLA	CAD-CBD-CGD-O2D
23	s	610	CLA	CAD-CBD-CGD-O2D
23	s	613	CLA	CAD-CBD-CGD-O2D
23	y	305	CLA	CAD-CBD-CGD-O2D
24	A	405	PHO	CAD-CBD-CGD-O2D
30	y	318	LHG	C6-C5-O7-C7
39	G	605	CHL	CAD-CBD-CGD-O2D
39	G	607	CHL	CAD-CBD-CGD-O2D
39	N	607	CHL	CAD-CBD-CGD-O2D
39	g	605	CHL	CAD-CBD-CGD-O2D
39	g	607	CHL	CAD-CBD-CGD-O2D
39	n	607	CHL	CAD-CBD-CGD-O2D
23	B	608	CLA	C16-C17-C18-C20
23	Y	310	CLA	C16-C17-C18-C19
23	b	608	CLA	C16-C17-C18-C19
28	L	102	3PH	C29-C2A-C2B-C2C
40	g	615	LUT	C9-C10-C11-C12
40	y	316	LUT	C9-C10-C11-C12
27	B	620	LMG	C20-C21-C22-C23
23	N	612	CLA	C2-C1-O2A-CGA
23	S	609	CLA	C2-C1-O2A-CGA
24	a	406	PHO	C2-C1-O2A-CGA
39	N	609	CHL	C2-C1-O2A-CGA
31	B	623	LNL	O1-C1-C2-C3
31	a	401	LNL	O1-C1-C2-C3
31	C	520	LNL	C1-C2-C3-C4
23	R	611	CLA	CAA-CBA-CGA-O2A
23	c	510	CLA	CAA-CBA-CGA-O2A
28	C	524	3PH	O21-C21-C22-C23
30	b	627	LHG	O7-C7-C8-C9
27	b	628	LMG	O10-C28-C29-C30
23	Y	305	CLA	CBA-CGA-O2A-C1
23	b	606	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	B	625	LNL	O2-C1-C2-C3
31	I	101	LNL	O1-C1-C2-C3
31	c	518	LNL	O1-C1-C2-C3
23	D	405	CLA	CAA-CBA-CGA-O2A
27	C	525	LMG	O8-C28-C29-C30
30	R	616	LHG	O8-C23-C24-C25
23	Y	304	CLA	O1A-CGA-O2A-C1
25	v	101	BCR	C17-C18-C19-C20
40	Y	315	LUT	C31-C32-C33-C34
40	y	316	LUT	C31-C32-C33-C34
42	N	619	XAT	C27-C28-C29-C30
31	B	622	LNL	C7-C8-C9-C10
31	c	519	LNL	C7-C8-C9-C10
30	b	627	LHG	C11-C10-C9-C8
26	L	101	SQD	O6-C44-C45-C46
42	N	619	XAT	O4-C6-C7-C8
42	N	619	XAT	O24-C26-C27-C28
42	n	620	XAT	O24-C26-C27-C28
23	s	608	CLA	O1A-CGA-O2A-C1
28	X	201	3PH	C26-C27-C28-C29
37	D	410	DGA	CB6-CB7-CB8-CB9
30	L	103	LHG	O6-C4-C5-O7
23	r	601	CLA	CAA-CBA-CGA-O2A
33	C	515	DGD	C1B-C2B-C3B-C4B
23	R	611	CLA	O2A-C1-C2-C3
23	r	611	CLA	O2A-C1-C2-C3
23	s	608	CLA	O2A-C1-C2-C3
31	C	517	LNL	O2-C1-C2-C3
23	Y	304	CLA	O2A-C1-C2-C3
24	a	406	PHO	O2A-C1-C2-C3
39	G	620	CHL	O2A-C1-C2-C3
39	g	607	CHL	O2A-C1-C2-C3
39	g	619	CHL	O2A-C1-C2-C3
28	L	102	3PH	C37-C38-C39-C3A
23	Y	304	CLA	C2A-CAA-CBA-CGA
30	D	408	LHG	C19-C20-C21-C22
23	C	510	CLA	CAA-CBA-CGA-O2A
28	A	410	3PH	O21-C21-C22-C23
39	g	609	CHL	CAA-CBA-CGA-O2A
33	H	502	DGD	O1B-C1B-C2B-C3B
31	B	624	LNL	O2-C1-C2-C3
31	c	518	LNL	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
31	a	401	LNL	C7-C8-C9-C10
31	b	622	LNL	C7-C8-C9-C10
31	c	518	LNL	C7-C8-C9-C10
23	R	608	CLA	C16-C17-C18-C19
23	y	313	CLA	C16-C17-C18-C19
27	B	620	LMG	C17-C18-C19-C20
27	b	628	LMG	C28-C29-C30-C31
26	A	408	SQD	C17-C18-C19-C20
23	Y	305	CLA	O1A-CGA-O2A-C1
23	A	402	CLA	CHA-CBD-CGD-O1D
23	A	402	CLA	CHA-CBD-CGD-O2D
23	B	607	CLA	CHA-CBD-CGD-O2D
23	B	612	CLA	CHA-CBD-CGD-O2D
23	B	615	CLA	CHA-CBD-CGD-O1D
23	B	615	CLA	CHA-CBD-CGD-O2D
23	C	505	CLA	CHA-CBD-CGD-O1D
23	C	506	CLA	CHA-CBD-CGD-O2D
23	C	512	CLA	CHA-CBD-CGD-O1D
23	G	603	CLA	CHA-CBD-CGD-O2D
23	G	612	CLA	CHA-CBD-CGD-O1D
23	G	612	CLA	CHA-CBD-CGD-O2D
23	N	602	CLA	CHA-CBD-CGD-O2D
23	R	602	CLA	CHA-CBD-CGD-O1D
23	R	602	CLA	CHA-CBD-CGD-O2D
23	S	611	CLA	CHA-CBD-CGD-O1D
23	S	611	CLA	CHA-CBD-CGD-O2D
23	Y	303	CLA	CHA-CBD-CGD-O1D
23	Y	303	CLA	CHA-CBD-CGD-O2D
23	Y	314	CLA	CHA-CBD-CGD-O2D
23	a	403	CLA	CHA-CBD-CGD-O1D
23	a	403	CLA	CHA-CBD-CGD-O2D
23	b	602	CLA	CHA-CBD-CGD-O1D
23	b	602	CLA	CHA-CBD-CGD-O2D
23	b	607	CLA	CHA-CBD-CGD-O2D
23	b	612	CLA	CHA-CBD-CGD-O2D
23	b	615	CLA	CHA-CBD-CGD-O1D
23	b	615	CLA	CHA-CBD-CGD-O2D
23	c	505	CLA	CHA-CBD-CGD-O1D
23	c	512	CLA	CHA-CBD-CGD-O1D
23	g	612	CLA	CHA-CBD-CGD-O2D
23	n	602	CLA	CHA-CBD-CGD-O2D
23	n	612	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	s	602	CLA	CHA-CBD-CGD-O1D
23	s	611	CLA	CHA-CBD-CGD-O1D
23	s	611	CLA	CHA-CBD-CGD-O2D
23	y	304	CLA	CHA-CBD-CGD-O1D
23	y	304	CLA	CHA-CBD-CGD-O2D
23	y	315	CLA	CHA-CBD-CGD-O2D
39	Y	302	CHL	CHA-CBD-CGD-O1D
39	Y	302	CHL	CHA-CBD-CGD-O2D
39	y	303	CHL	CHA-CBD-CGD-O1D
39	y	303	CHL	CHA-CBD-CGD-O2D
31	I	101	LNL	O2-C1-C2-C3
31	a	401	LNL	O2-C1-C2-C3
23	s	610	CLA	C4-C3-C5-C6
23	B	613	CLA	CAA-CBA-CGA-O2A
39	R	607	CHL	CAA-CBA-CGA-O2A
23	b	606	CLA	C2-C3-C5-C6
28	a	410	3PH	C2E-C2F-C2G-C2H
30	A	412	LHG	C9-C10-C11-C12
23	C	511	CLA	C8-C10-C11-C12
30	y	318	LHG	O6-C4-C5-C6
25	H	501	BCR	C16-C17-C18-C19
40	Y	315	LUT	C12-C13-C14-C15
40	y	316	LUT	C12-C13-C14-C15
41	G	617	NEX	C28-C29-C30-C31
41	n	618	NEX	C28-C29-C30-C31
27	A	409	LMG	C11-C12-C13-C14
28	x	201	3PH	C2C-C2D-C2E-C2F
23	y	304	CLA	C16-C17-C18-C19
23	C	501	CLA	CAA-CBA-CGA-O2A
23	G	611	CLA	CAA-CBA-CGA-O2A
23	R	610	CLA	CAA-CBA-CGA-O2A
23	r	610	CLA	CAA-CBA-CGA-O2A
28	a	410	3PH	O31-C31-C32-C33
39	S	601	CHL	CAA-CBA-CGA-O2A
39	r	607	CHL	CAA-CBA-CGA-O2A
27	D	409	LMG	O1-C7-C8-O7
23	Y	304	CLA	CBA-CGA-O2A-C1
28	x	201	3PH	C3B-C3C-C3D-C3E
31	C	518	LNL	O2-C1-C2-C3
39	r	606	CHL	C4C-C3C-CAC-CBC
23	R	612	CLA	CAA-CBA-CGA-O2A
23	c	501	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
23	r	611	CLA	CAA-CBA-CGA-O2A
39	s	601	CHL	CAA-CBA-CGA-O2A
23	y	315	CLA	C2A-CAA-CBA-CGA
31	C	520	LNL	O1-C1-C2-C3
24	D	402	PHO	CHA-CBD-CGD-O1D
23	B	605	CLA	C8-C10-C11-C12
23	C	504	CLA	C8-C10-C11-C12
23	g	602	CLA	C10-C11-C12-C13
23	s	608	CLA	CBA-CGA-O2A-C1
30	D	408	LHG	C25-C26-C27-C28
23	Y	304	CLA	CAA-CBA-CGA-O2A
39	g	607	CHL	CAA-CBA-CGA-O2A
23	S	610	CLA	C2-C3-C5-C6
23	Y	314	CLA	C6-C7-C8-C10
23	s	609	CLA	C2-C3-C5-C6
23	y	312	CLA	C2-C3-C5-C6
31	b	625	LNL	C7-C8-C9-C10
23	B	610	CLA	CAA-CBA-CGA-O2A
23	g	603	CLA	CAA-CBA-CGA-O2A
33	c	515	DGD	O2G-C1B-C2B-C3B
39	G	608	CHL	CAA-CBA-CGA-O2A
23	C	509	CLA	C11-C12-C13-C14
23	G	613	CLA	C14-C13-C15-C16
23	b	603	CLA	C11-C10-C8-C9
23	c	502	CLA	C11-C10-C8-C9
23	c	509	CLA	C11-C12-C13-C14
23	n	610	CLA	C11-C12-C13-C14
23	r	608	CLA	C14-C13-C15-C16
23	r	609	CLA	C14-C13-C15-C16
23	y	313	CLA	C11-C10-C8-C9
39	N	609	CHL	C11-C10-C8-C9
39	n	609	CHL	C6-C7-C8-C9
23	N	612	CLA	CAA-CBA-CGA-O1A
41	N	617	NEX	C33-C34-C35-C15
42	y	302	XAT	C29-C30-C31-C32
23	D	405	CLA	C15-C16-C17-C18
23	b	602	CLA	C10-C11-C12-C13
23	b	605	CLA	C10-C11-C12-C13
39	y	308	CHL	C2B-C3B-CAB-CBB
23	S	608	CLA	O2A-C1-C2-C3
39	N	605	CHL	O2A-C1-C2-C3
39	S	606	CHL	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
39	r	605	CHL	O2A-C1-C2-C3
26	A	408	SQD	C18-C19-C20-C21
26	M	101	SQD	C28-C29-C30-C31
42	y	302	XAT	C14-C15-C35-C34
38	F	501	HEM	CAA-CBA-CGA-O2A
27	R	617	LMG	C35-C36-C37-C38
30	n	619	LHG	O7-C7-C8-C9
26	a	409	SQD	C4-C5-C6-S
23	B	606	CLA	C16-C17-C18-C19
23	r	604	CLA	C6-C7-C8-C10
31	C	520	LNL	C3-C4-C5-C6
30	A	412	LHG	C8-C7-O7-C5
23	b	608	CLA	C2A-CAA-CBA-CGA
23	D	405	CLA	CAA-CBA-CGA-O1A
30	L	103	LHG	C13-C14-C15-C16
23	b	610	CLA	CAA-CBA-CGA-O2A
31	I	101	LNL	C7-C8-C9-C10
23	R	604	CLA	C6-C7-C8-C10
23	Y	303	CLA	C16-C17-C18-C20
28	D	403	3PH	C23-C24-C25-C26
29	D	407	PL9	C38-C39-C41-C42
28	x	201	3PH	C39-C3A-C3B-C3C
30	R	616	LHG	C28-C29-C30-C31
31	B	623	LNL	O2-C1-C2-C3
23	g	603	CLA	CAA-CBA-CGA-O1A
30	L	103	LHG	O9-C7-C8-C9
33	c	515	DGD	O1B-C1B-C2B-C3B
39	G	609	CHL	C10-C11-C12-C13
28	L	102	3PH	C2C-C2D-C2E-C2F
23	A	404	CLA	C1A-C2A-CAA-CBA
23	B	607	CLA	C1A-C2A-CAA-CBA
23	G	602	CLA	C1A-C2A-CAA-CBA
23	N	611	CLA	C1A-C2A-CAA-CBA
23	R	604	CLA	C1A-C2A-CAA-CBA
23	Y	314	CLA	C1A-C2A-CAA-CBA
23	b	607	CLA	C1A-C2A-CAA-CBA
23	r	604	CLA	C1A-C2A-CAA-CBA
23	r	609	CLA	C1A-C2A-CAA-CBA
23	y	311	CLA	C1A-C2A-CAA-CBA
39	N	606	CHL	C1A-C2A-CAA-CBA
39	r	605	CHL	C1A-C2A-CAA-CBA
39	s	606	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
39	y	303	CHL	C1A-C2A-CAA-CBA
23	A	402	CLA	C16-C17-C18-C20
23	C	512	CLA	CAA-CBA-CGA-O1A
23	d	405	CLA	CAA-CBA-CGA-O1A
39	g	609	CHL	CAA-CBA-CGA-O1A
38	F	501	HEM	CAD-CBD-CGD-O2D
23	B	605	CLA	C13-C15-C16-C17
23	R	611	CLA	CAA-CBA-CGA-O1A
23	c	512	CLA	CAA-CBA-CGA-O1A
27	C	525	LMG	O10-C28-C29-C30
30	N	618	LHG	O10-C23-C24-C25
30	b	627	LHG	O9-C7-C8-C9
30	g	618	LHG	C13-C14-C15-C16
27	B	626	LMG	O1-C7-C8-C9
39	G	605	CHL	CAA-CBA-CGA-O2A
23	C	503	CLA	C8-C10-C11-C12
23	B	608	CLA	C2A-CAA-CBA-CGA
23	c	510	CLA	C2A-CAA-CBA-CGA
23	s	602	CLA	C2A-CAA-CBA-CGA
33	H	502	DGD	CCA-CDA-CEA-CFA
33	H	502	DGD	C8B-C9B-CAB-CBB
23	B	608	CLA	C16-C17-C18-C19
27	b	620	LMG	C10-C11-C12-C13
23	c	510	CLA	CAA-CBA-CGA-O1A
28	W	201	3PH	O22-C21-C22-C23
28	w	202	3PH	O22-C21-C22-C23
39	r	607	CHL	CAA-CBA-CGA-O1A
27	c	523	LMG	C35-C36-C37-C38
31	C	517	LNL	C4-C5-C6-C7
27	r	617	LMG	C29-C30-C31-C32
28	C	524	3PH	C35-C36-C37-C38
23	Y	310	CLA	C4-C3-C5-C6
39	Y	309	CHL	C4-C3-C5-C6
23	S	602	CLA	CAA-CBA-CGA-O2A
28	W	201	3PH	O31-C31-C32-C33
28	x	201	3PH	C33-C34-C35-C36
23	R	610	CLA	CAA-CBA-CGA-O1A
23	r	611	CLA	CAA-CBA-CGA-O1A
30	n	619	LHG	O9-C7-C8-C9
31	i	101	LNL	O1-C1-C2-C3
32	b	621	PAM	C7-C8-C9-C10
23	b	609	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	A	404	CLA	C4B-C3B-CAB-CBB
23	C	501	CLA	C4B-C3B-CAB-CBB
30	D	408	LHG	C3-O3-P-O4
39	y	308	CHL	C4B-C3B-CAB-CBB
23	B	610	CLA	C16-C17-C18-C20
23	a	403	CLA	C16-C17-C18-C20
39	g	605	CHL	C2-C1-O2A-CGA
23	B	613	CLA	CAA-CBA-CGA-O1A
23	G	611	CLA	CAA-CBA-CGA-O1A
23	r	610	CLA	CAA-CBA-CGA-O1A
39	G	608	CHL	CAA-CBA-CGA-O1A
23	s	603	CLA	O2A-C1-C2-C3
27	r	617	LMG	O7-C10-C11-C12
23	Y	303	CLA	C8-C10-C11-C12
40	S	614	LUT	C5-C6-C7-C8
40	g	615	LUT	C5-C6-C7-C8
27	R	617	LMG	C42-C43-C44-C45
23	B	614	CLA	C13-C15-C16-C17
23	c	508	CLA	C5-C6-C7-C8
23	C	501	CLA	CAA-CBA-CGA-O1A
23	c	501	CLA	CAA-CBA-CGA-O1A
23	r	601	CLA	CAA-CBA-CGA-O1A
28	A	410	3PH	O22-C21-C22-C23
28	C	524	3PH	O22-C21-C22-C23
28	a	410	3PH	O32-C31-C32-C33
39	S	601	CHL	CAA-CBA-CGA-O1A
23	R	601	CLA	CAA-CBA-CGA-O2A
23	R	603	CLA	CAA-CBA-CGA-O2A
28	w	202	3PH	C3A-C3B-C3C-C3D
30	y	318	LHG	C27-C28-C29-C30
31	C	520	LNL	O2-C1-C2-C3
27	B	620	LMG	C12-C13-C14-C15
23	B	610	CLA	CAA-CBA-CGA-O1A
23	Y	304	CLA	CAA-CBA-CGA-O1A
33	d	411	DGD	O1B-C1B-C2B-C3B
39	R	606	CHL	C4C-C3C-CAC-CBC
23	Y	313	CLA	C13-C15-C16-C17
33	C	515	DGD	O1B-C1B-C2B-C3B
29	d	407	PL9	C38-C39-C41-C42
23	B	607	CLA	CAD-CBD-CGD-O1D
23	B	612	CLA	CAD-CBD-CGD-O1D
23	C	504	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	C	512	CLA	CAD-CBD-CGD-O1D
23	Y	314	CLA	CAD-CBD-CGD-O1D
23	b	605	CLA	CAD-CBD-CGD-O1D
23	b	607	CLA	CAD-CBD-CGD-O1D
23	b	612	CLA	CAD-CBD-CGD-O1D
23	c	504	CLA	CAD-CBD-CGD-O1D
23	c	505	CLA	CAD-CBD-CGD-O1D
23	c	512	CLA	CAD-CBD-CGD-O1D
26	A	408	SQD	O5-C5-C6-S
28	w	202	3PH	C31-C32-C33-C34
23	C	510	CLA	CAA-CBA-CGA-O1A
39	R	607	CHL	CAA-CBA-CGA-O1A
28	L	102	3PH	C25-C26-C27-C28
26	a	409	SQD	O47-C7-C8-C9
39	S	605	CHL	CAA-CBA-CGA-O2A
39	n	606	CHL	CAA-CBA-CGA-O2A
33	H	502	DGD	O6D-C5D-C6D-O5D
30	r	616	LHG	O2-C2-C3-O3
23	C	502	CLA	C11-C10-C8-C9
23	Y	314	CLA	C6-C7-C8-C9
23	Y	314	CLA	C11-C12-C13-C14
23	b	611	CLA	C14-C13-C15-C16
39	N	609	CHL	C14-C13-C15-C16
30	r	616	LHG	O9-C7-O7-C5
28	A	410	3PH	C2D-C2E-C2F-C2G
38	F	501	HEM	CAA-CBA-CGA-O1A
38	f	501	HEM	CAA-CBA-CGA-O2A
23	R	612	CLA	CAA-CBA-CGA-O1A
39	s	601	CHL	CAA-CBA-CGA-O1A
23	c	507	CLA	CBA-CGA-O2A-C1
30	Y	318	LHG	C24-C23-O8-C6
23	Y	312	CLA	CAA-CBA-CGA-O2A
23	s	603	CLA	CAA-CBA-CGA-O2A
23	S	603	CLA	C2A-CAA-CBA-CGA
23	y	306	CLA	CBA-CGA-O2A-C1
23	S	611	CLA	CAA-CBA-CGA-O2A
30	G	618	LHG	O7-C7-C8-C9
39	Y	308	CHL	CAA-CBA-CGA-O2A
23	b	611	CLA	C10-C11-C12-C13
23	c	503	CLA	C8-C10-C11-C12
33	c	515	DGD	C5B-C6B-C7B-C8B
23	A	403	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	S	610	CLA	C4-C3-C5-C6
23	C	507	CLA	C12-C13-C15-C16
23	N	610	CLA	C2-C3-C5-C6
23	N	611	CLA	C6-C7-C8-C10
23	N	613	CLA	C3A-C2A-CAA-CBA
23	Y	314	CLA	C11-C12-C13-C15
23	b	604	CLA	C2-C3-C5-C6
23	b	610	CLA	C11-C10-C8-C7
23	c	504	CLA	C11-C12-C13-C15
23	c	512	CLA	C6-C7-C8-C10
23	g	610	CLA	C12-C13-C15-C16
23	n	610	CLA	C11-C12-C13-C15
23	r	609	CLA	C12-C13-C15-C16
23	s	613	CLA	C3A-C2A-CAA-CBA
23	y	306	CLA	C11-C12-C13-C15
23	y	313	CLA	C11-C10-C8-C7
35	y	301	VIV	C17-C18-C20-C21
39	y	303	CHL	C11-C12-C13-C15
39	g	607	CHL	CAA-CBA-CGA-O1A
39	n	606	CHL	CAA-CBA-CGA-O1A
26	L	101	SQD	C11-C10-C9-C8
28	w	202	3PH	C27-C28-C29-C2A
23	r	603	CLA	CAA-CBA-CGA-O2A
28	T	101	3PH	O21-C21-C22-C23
30	Y	318	LHG	O8-C23-C24-C25
37	b	626	DGA	OG2-CB1-CB2-CB3
31	c	521	LNL	C7-C8-C9-C10
41	g	617	NEX	C27-C28-C29-C30
42	G	619	XAT	C11-C12-C13-C14
23	n	612	CLA	CAA-CBA-CGA-O1A
39	G	605	CHL	CAA-CBA-CGA-O1A
31	A	413	LNL	O1-C1-C2-C3
40	g	616	LUT	C29-C30-C31-C32
42	Y	301	XAT	C13-C14-C15-C35
27	d	409	LMG	C32-C33-C34-C35
23	B	602	CLA	CAA-CBA-CGA-O2A
23	N	603	CLA	CAA-CBA-CGA-O2A
23	N	613	CLA	CAA-CBA-CGA-O2A
23	s	611	CLA	CAA-CBA-CGA-O2A
39	N	608	CHL	CAA-CBA-CGA-O2A
23	g	602	CLA	C8-C10-C11-C12
23	y	306	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	b	627	LHG	C17-C18-C19-C20
23	R	601	CLA	CAA-CBA-CGA-O1A
27	b	628	LMG	C15-C16-C17-C18
23	B	605	CLA	C10-C11-C12-C13
23	c	505	CLA	O1A-CGA-O2A-C1
23	n	612	CLA	CAA-CBA-CGA-O2A
30	s	616	LHG	O8-C23-C24-C25
39	g	608	CHL	CAA-CBA-CGA-O2A
23	D	406	CLA	C10-C11-C12-C13
23	S	602	CLA	CAA-CBA-CGA-O1A
23	S	611	CLA	CAA-CBA-CGA-O1A
23	b	610	CLA	CAA-CBA-CGA-O1A
23	s	603	CLA	CAA-CBA-CGA-O1A
28	W	201	3PH	O32-C31-C32-C33
23	Y	310	CLA	C2A-CAA-CBA-CGA
23	b	610	CLA	C16-C17-C18-C20
27	C	525	LMG	C34-C35-C36-C37
23	s	613	CLA	C15-C16-C17-C18
30	G	618	LHG	O9-C7-C8-C9
23	y	312	CLA	C4-C3-C5-C6
26	A	408	SQD	C13-C14-C15-C16
28	X	201	3PH	O21-C21-C22-C23
33	C	515	DGD	O2G-C1B-C2B-C3B
39	g	605	CHL	CAA-CBA-CGA-O2A
39	s	607	CHL	CAA-CBA-CGA-O2A

There are no ring outliers.

310 monomers are involved in 716 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	n	610	CLA	7	0
31	C	521	LNL	4	0
30	a	412	LHG	4	0
30	A	412	LHG	1	0
40	s	615	LUT	3	0
27	d	409	LMG	2	0
23	C	509	CLA	2	0
39	R	607	CHL	3	0
25	B	618	BCR	2	0
39	G	601	CHL	2	0
33	C	515	DGD	3	0
23	s	613	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	602	CLA	6	0
23	N	604	CLA	1	0
25	z	101	BCR	1	0
31	C	519	LNL	1	0
23	a	404	CLA	3	0
25	Z	101	BCR	3	0
28	L	102	3PH	2	0
23	D	406	CLA	1	0
41	s	617	NEX	2	0
23	c	507	CLA	1	0
31	A	413	LNL	1	0
23	r	611	CLA	1	0
40	n	616	LUT	5	0
33	d	411	DGD	3	0
23	G	610	CLA	6	0
23	g	602	CLA	3	0
40	G	616	LUT	5	0
42	n	617	XAT	3	0
23	s	610	CLA	2	0
23	N	612	CLA	4	0
30	Y	318	LHG	5	0
23	r	602	CLA	1	0
23	c	504	CLA	1	0
23	y	314	CLA	4	0
27	D	409	LMG	1	0
23	n	613	CLA	4	0
28	W	201	3PH	2	0
23	c	501	CLA	1	0
23	y	305	CLA	4	0
23	Y	303	CLA	5	0
41	S	617	NEX	2	0
31	b	625	LNL	1	0
39	g	608	CHL	3	0
31	C	522	LNL	2	0
23	c	505	CLA	4	0
26	a	409	SQD	3	0
28	C	524	3PH	4	0
31	A	414	LNL	2	0
30	L	103	LHG	2	0
23	Y	313	CLA	4	0
39	G	606	CHL	4	0
23	Y	311	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	r	610	CLA	1	0
39	r	605	CHL	3	0
39	S	606	CHL	4	0
23	b	608	CLA	1	0
39	s	606	CHL	2	0
39	n	608	CHL	2	0
23	a	407	CLA	1	0
23	Y	312	CLA	1	0
23	s	608	CLA	1	0
23	c	512	CLA	3	0
25	k	101	BCR	1	0
23	g	603	CLA	3	0
23	c	513	CLA	3	0
23	g	611	CLA	1	0
41	g	617	NEX	4	0
35	C	523	VIV	5	0
41	n	618	NEX	4	0
23	G	604	CLA	2	0
23	a	403	CLA	2	0
23	B	616	CLA	6	0
23	n	604	CLA	1	0
39	G	609	CHL	8	0
23	s	604	CLA	2	0
40	R	613	LUT	2	0
23	N	613	CLA	3	0
30	N	618	LHG	3	0
31	b	624	LNL	1	0
23	c	503	CLA	2	0
23	R	610	CLA	2	0
23	B	615	CLA	7	0
23	b	615	CLA	3	0
23	Y	304	CLA	3	0
39	R	605	CHL	2	0
32	B	621	PAM	1	0
23	y	311	CLA	2	0
39	R	606	CHL	3	0
36	D	401	BCT	5	0
40	Y	315	LUT	4	0
30	d	408	LHG	4	0
23	C	513	CLA	1	0
23	G	613	CLA	2	0
27	b	628	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	r	603	CLA	2	0
23	B	610	CLA	5	0
23	b	610	CLA	5	0
24	A	405	PHO	3	0
25	C	514	BCR	6	0
23	c	506	CLA	4	0
23	y	312	CLA	2	0
23	C	508	CLA	3	0
40	y	317	LUT	2	0
26	L	101	SQD	4	0
39	N	608	CHL	2	0
40	g	616	LUT	6	0
27	A	409	LMG	5	0
42	R	615	XAT	2	0
25	b	618	BCR	2	0
23	n	603	CLA	5	0
27	b	620	LMG	8	0
23	R	604	CLA	2	0
24	d	402	PHO	2	0
23	A	402	CLA	2	0
25	A	407	BCR	4	0
23	s	602	CLA	5	0
23	C	506	CLA	1	0
23	B	609	CLA	2	0
25	b	617	BCR	1	0
25	D	411	BCR	2	0
42	N	619	XAT	6	0
26	M	101	SQD	2	0
39	S	607	CHL	4	0
31	C	517	LNL	1	0
40	S	614	LUT	3	0
39	g	606	CHL	2	0
23	c	511	CLA	3	0
42	Y	301	XAT	4	0
35	y	301	VIV	4	0
25	B	617	BCR	7	0
23	n	614	CLA	1	0
28	w	202	3PH	4	0
40	g	615	LUT	8	0
40	G	615	LUT	7	0
23	S	608	CLA	2	0
23	A	403	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	G	612	CLA	2	0
23	S	609	CLA	9	0
23	B	612	CLA	1	0
28	x	201	3PH	3	0
23	B	604	CLA	2	0
27	R	617	LMG	3	0
25	d	410	BCR	3	0
36	d	401	BCT	5	0
30	D	408	LHG	5	0
29	a	411	PL9	7	0
23	b	609	CLA	4	0
23	A	406	CLA	1	0
30	n	619	LHG	2	0
28	a	410	3PH	9	0
23	b	616	CLA	3	0
40	S	615	LUT	3	0
23	B	605	CLA	1	0
40	n	615	LUT	6	0
23	S	610	CLA	2	0
31	a	401	LNL	1	0
30	b	627	LHG	1	0
23	C	511	CLA	3	0
39	Y	302	CHL	3	0
25	B	619	BCR	5	0
30	g	618	LHG	3	0
23	B	607	CLA	7	0
40	N	616	LUT	6	0
23	B	611	CLA	1	0
23	N	603	CLA	5	0
23	S	612	CLA	1	0
23	b	605	CLA	2	0
23	s	612	CLA	3	0
28	A	410	3PH	4	0
31	c	520	LNL	1	0
23	b	604	CLA	2	0
26	A	408	SQD	2	0
25	c	514	BCR	3	0
37	b	626	DGA	4	0
23	y	313	CLA	3	0
39	r	606	CHL	4	0
40	r	613	LUT	3	0
39	Y	306	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	G	602	CLA	4	0
23	N	614	CLA	2	0
42	r	615	XAT	3	0
23	C	504	CLA	1	0
23	S	602	CLA	1	0
24	D	402	PHO	4	0
39	G	620	CHL	2	0
23	C	512	CLA	2	0
40	Y	316	LUT	5	0
39	N	605	CHL	1	0
31	c	517	LNL	3	0
23	d	405	CLA	4	0
41	N	617	NEX	2	0
23	B	614	CLA	6	0
33	H	502	DGD	1	0
23	b	613	CLA	1	0
23	c	510	CLA	3	0
39	n	606	CHL	3	0
39	g	607	CHL	1	0
23	n	612	CLA	3	0
23	b	607	CLA	4	0
30	s	616	LHG	2	0
40	N	615	LUT	4	0
41	R	618	NEX	2	0
42	y	302	XAT	2	0
23	b	611	CLA	2	0
31	a	413	LNL	1	0
23	B	606	CLA	3	0
23	C	501	CLA	1	0
39	s	607	CHL	1	0
23	y	306	CLA	3	0
31	i	101	LNL	2	0
23	B	603	CLA	1	0
39	Y	309	CHL	3	0
23	g	610	CLA	4	0
39	n	609	CHL	4	0
23	b	601	CLA	1	0
39	N	609	CHL	3	0
42	G	619	XAT	4	0
28	s	618	3PH	1	0
23	C	507	CLA	4	0
23	B	613	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	Y	314	CLA	5	0
23	g	612	CLA	4	0
39	Y	307	CHL	4	0
27	r	617	LMG	3	0
39	r	607	CHL	3	0
25	H	501	BCR	2	0
23	S	611	CLA	3	0
31	B	623	LNL	4	0
23	s	611	CLA	3	0
39	N	601	CHL	8	0
23	b	606	CLA	4	0
31	B	622	LNL	2	0
23	D	405	CLA	5	0
27	C	525	LMG	3	0
37	D	410	DGA	3	0
42	n	620	XAT	5	0
23	r	608	CLA	1	0
23	N	611	CLA	4	0
23	r	609	CLA	2	0
31	b	623	LNL	1	0
30	d	404	LHG	1	0
39	G	607	CHL	2	0
23	b	612	CLA	1	0
30	S	616	LHG	3	0
41	r	614	NEX	2	0
23	b	614	CLA	3	0
38	f	501	HEM	2	0
41	Y	317	NEX	1	0
39	y	310	CHL	1	0
23	R	609	CLA	1	0
40	y	316	LUT	3	0
39	N	606	CHL	3	0
23	n	602	CLA	2	0
39	g	609	CHL	1	0
25	a	408	BCR	4	0
39	n	605	CHL	3	0
24	a	406	PHO	3	0
23	g	604	CLA	2	0
39	n	607	CHL	4	0
31	B	625	LNL	3	0
30	G	618	LHG	3	0
39	s	605	CHL	1	0

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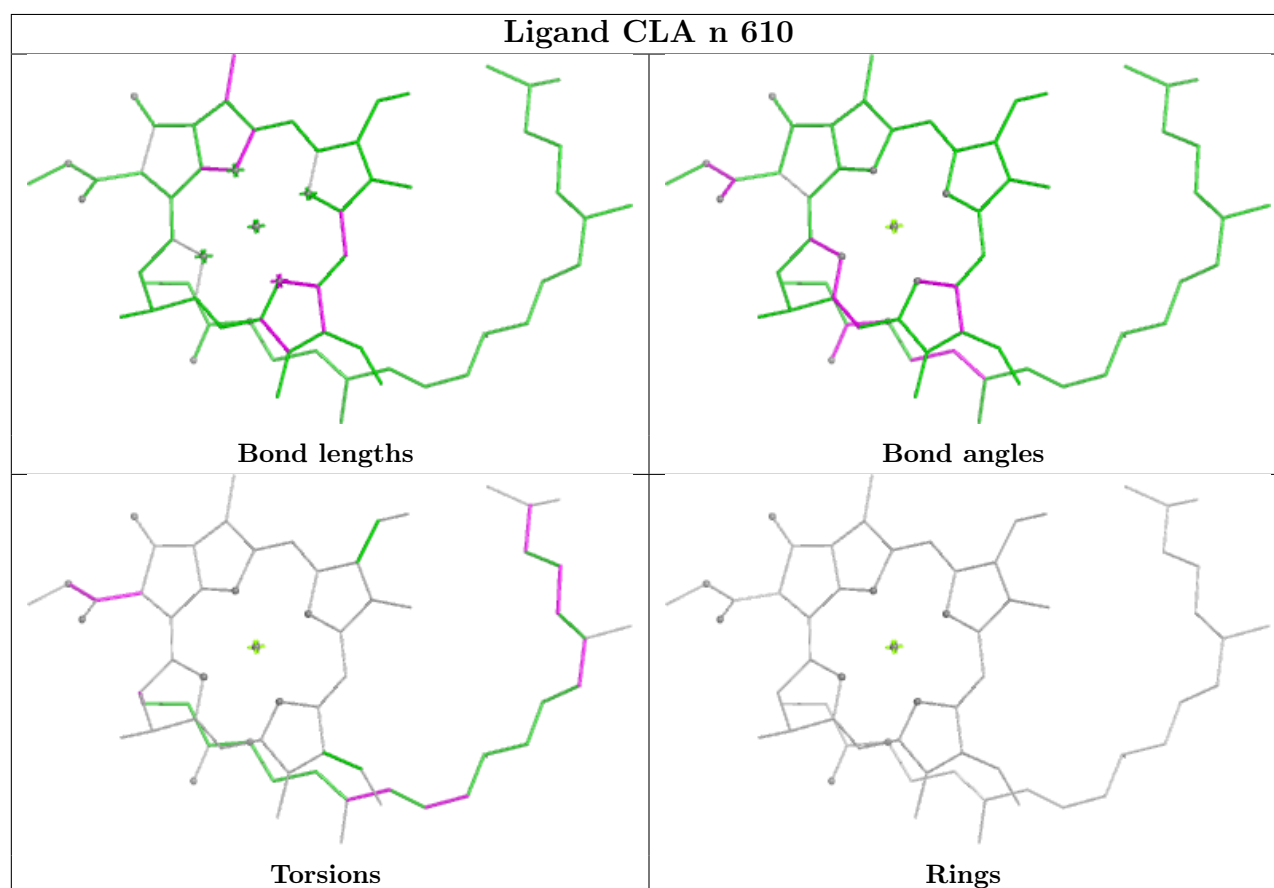
Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	Y	308	CHL	1	0
27	c	523	LMG	2	0
30	y	318	LHG	3	0
23	g	613	CLA	3	0
23	r	612	CLA	2	0
23	y	315	CLA	4	0
23	Y	310	CLA	2	0
39	S	601	CHL	1	0
23	C	505	CLA	3	0
23	R	608	CLA	2	0
23	N	610	CLA	5	0
23	B	608	CLA	3	0
23	S	604	CLA	3	0
23	Y	305	CLA	3	0
23	y	304	CLA	3	0
29	A	411	PL9	9	0
31	c	519	LNL	2	0
23	G	603	CLA	4	0
23	s	609	CLA	6	0
23	R	611	CLA	1	0
29	D	407	PL9	2	0
39	G	608	CHL	2	0
23	S	613	CLA	2	0
39	S	605	CHL	1	0
28	D	403	3PH	2	0
31	c	521	LNL	2	0
30	D	404	LHG	1	0
25	v	101	BCR	1	0
23	N	602	CLA	3	0
39	n	601	CHL	3	0
27	w	201	LMG	1	0
39	y	303	CHL	4	0
23	b	602	CLA	4	0
39	N	607	CHL	1	0
25	b	619	BCR	3	0
29	d	407	PL9	3	0
33	c	515	DGD	1	0
23	b	603	CLA	2	0
41	G	617	NEX	2	0
38	F	501	HEM	3	0
23	S	603	CLA	1	0
23	r	604	CLA	3	0

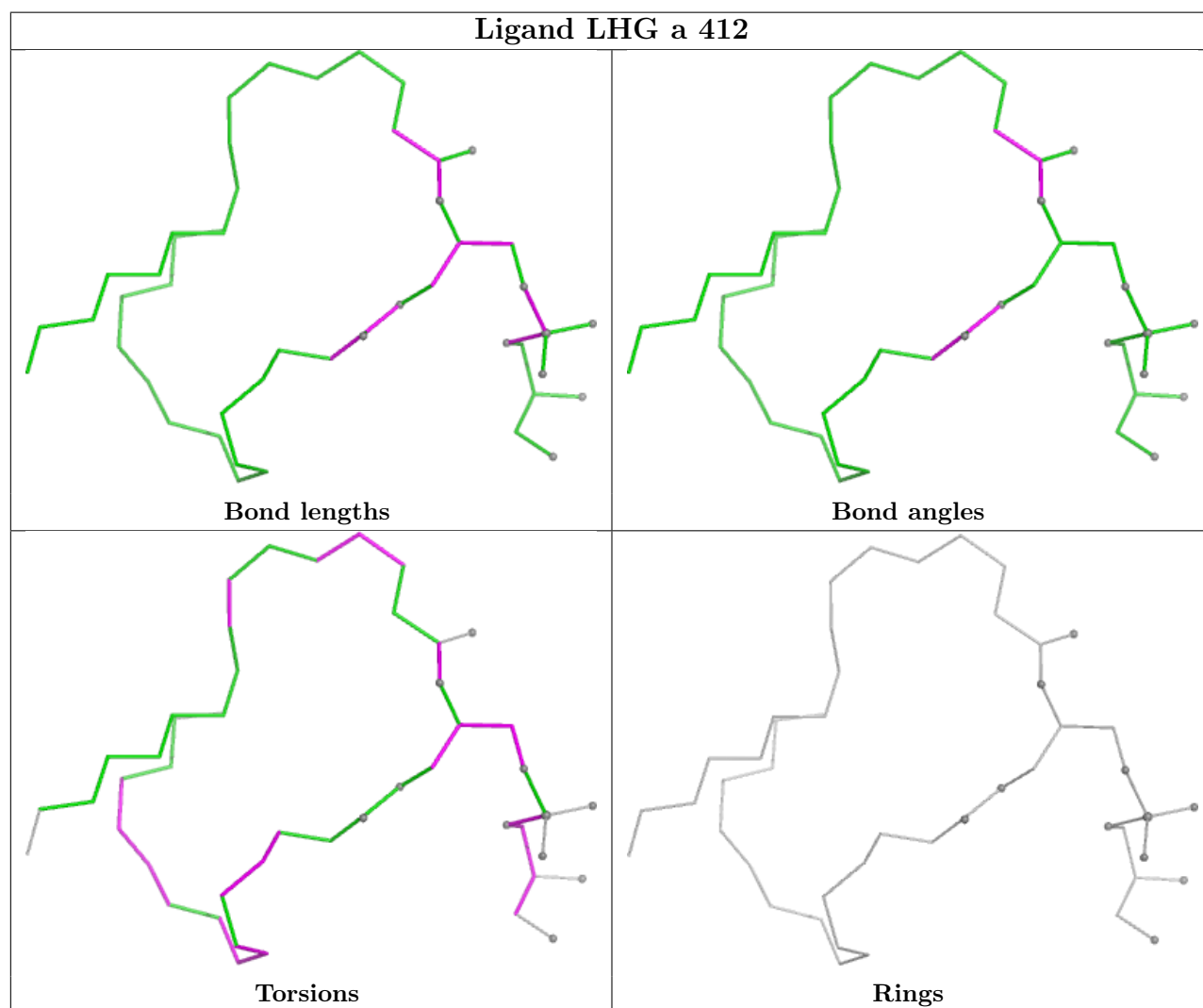
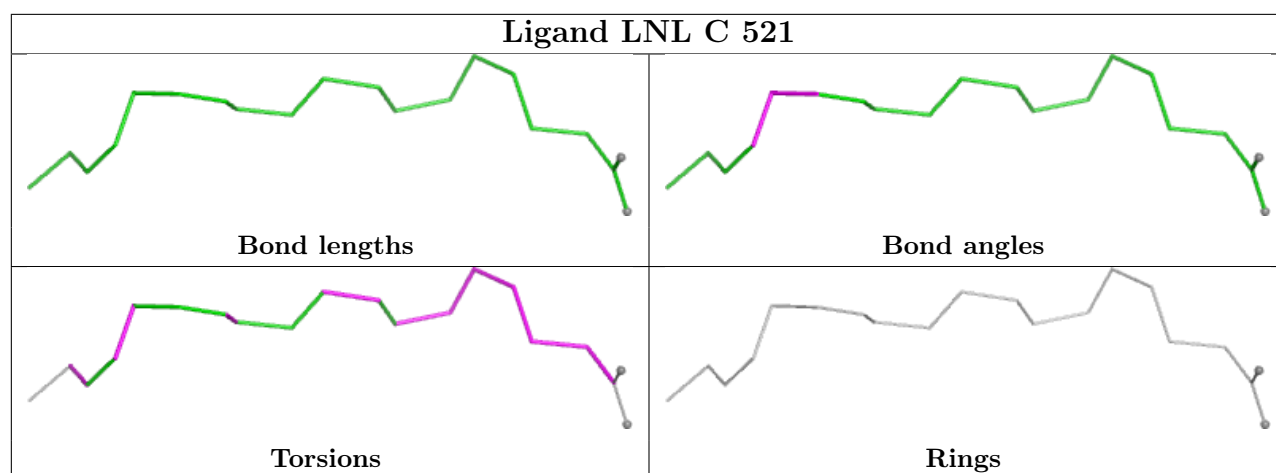
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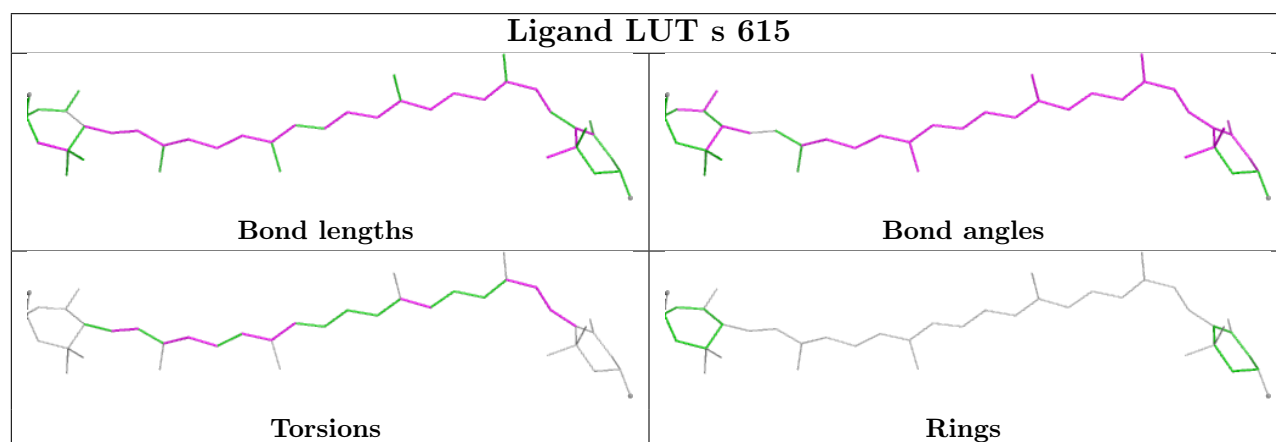
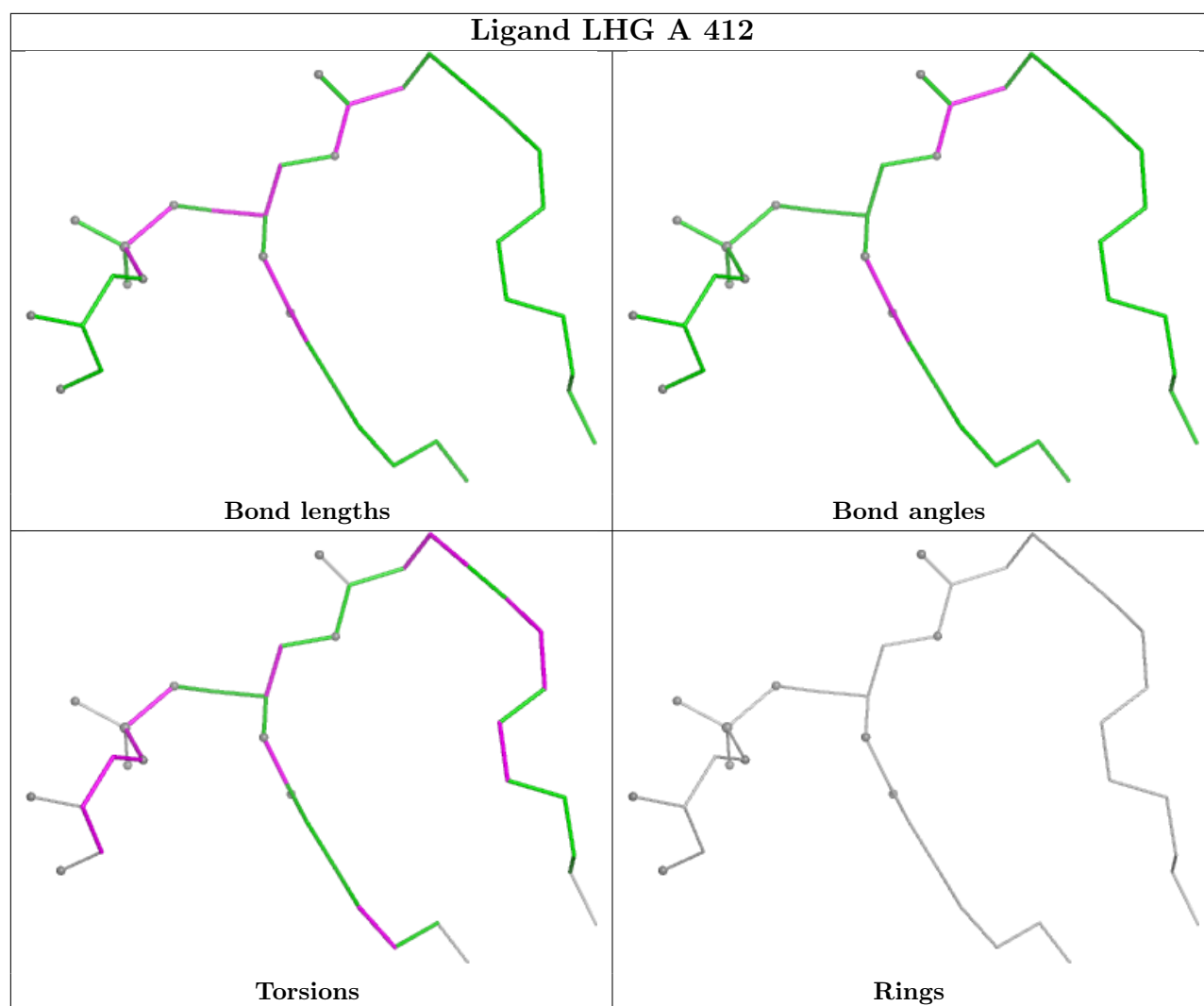
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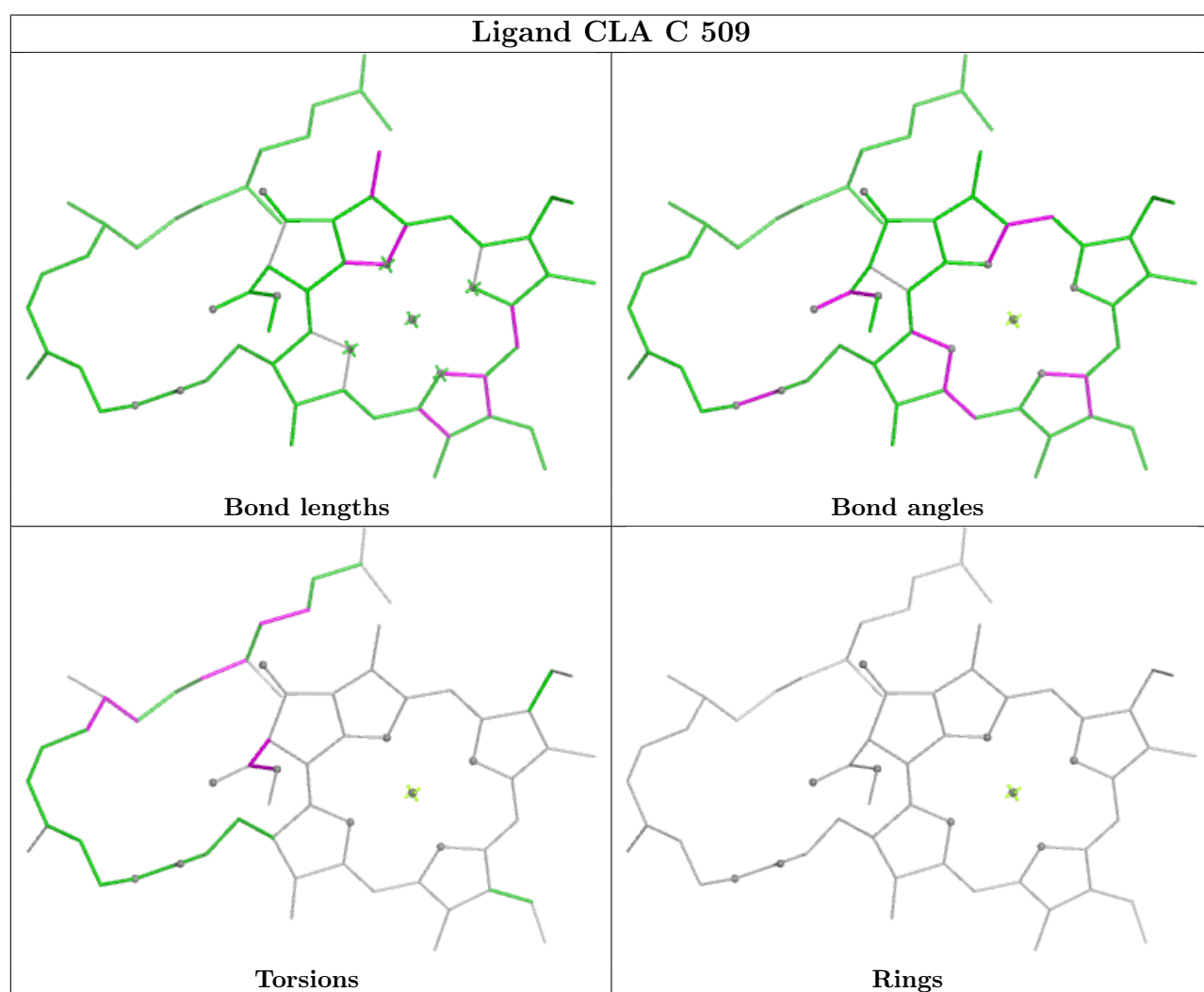
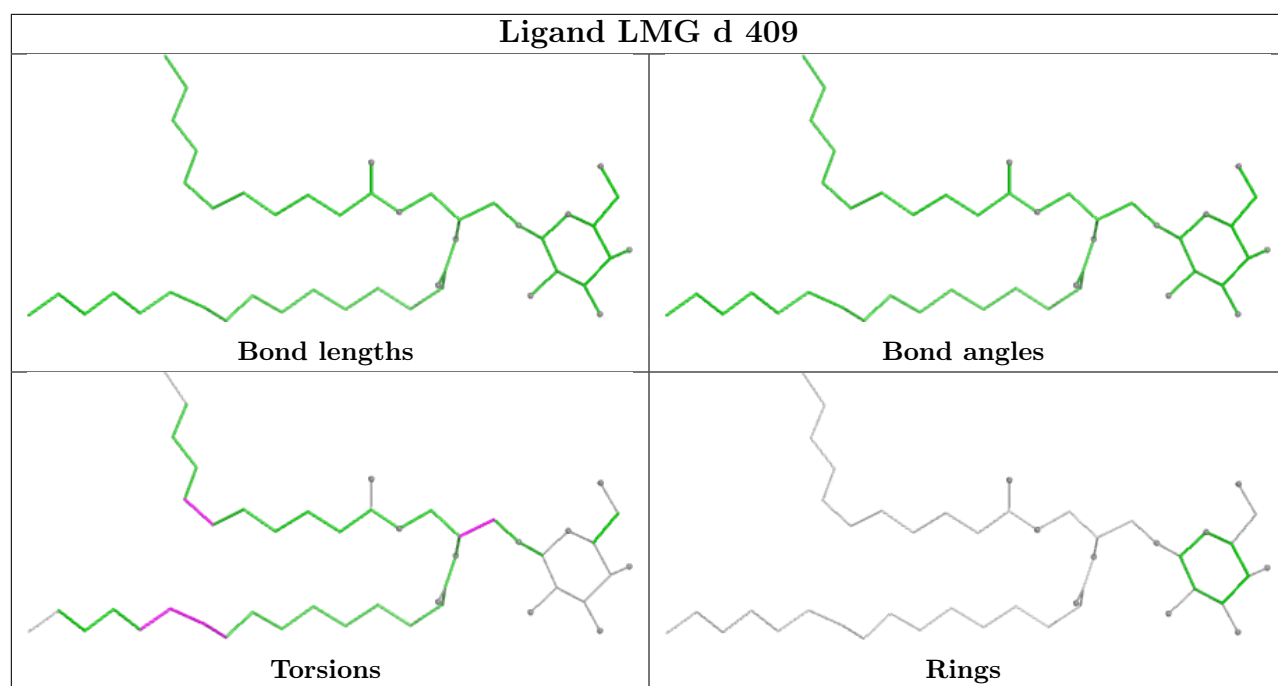
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	s	603	CLA	1	0
28	d	403	3PH	3	0
31	b	622	LNL	3	0
27	B	620	LMG	7	0

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.

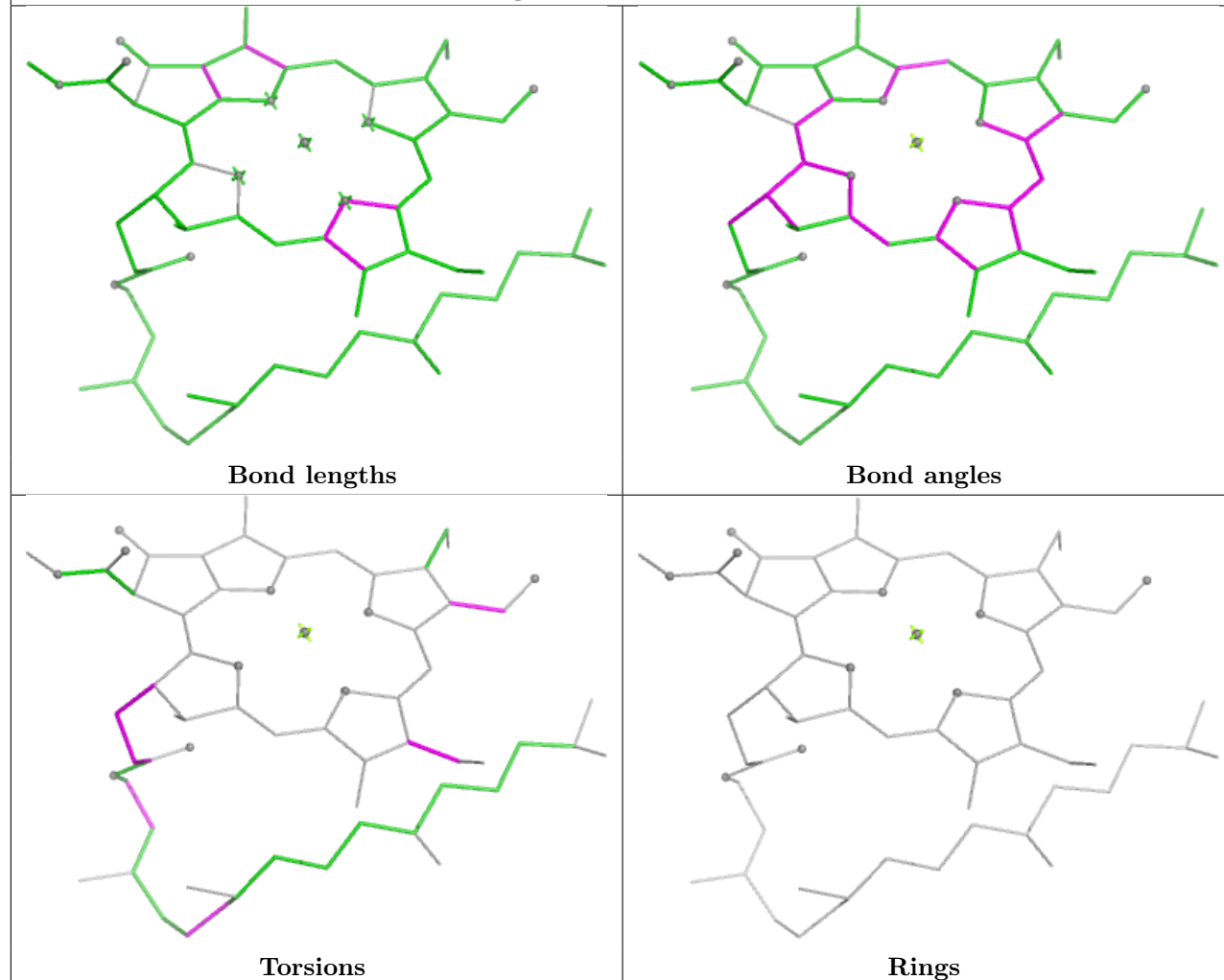




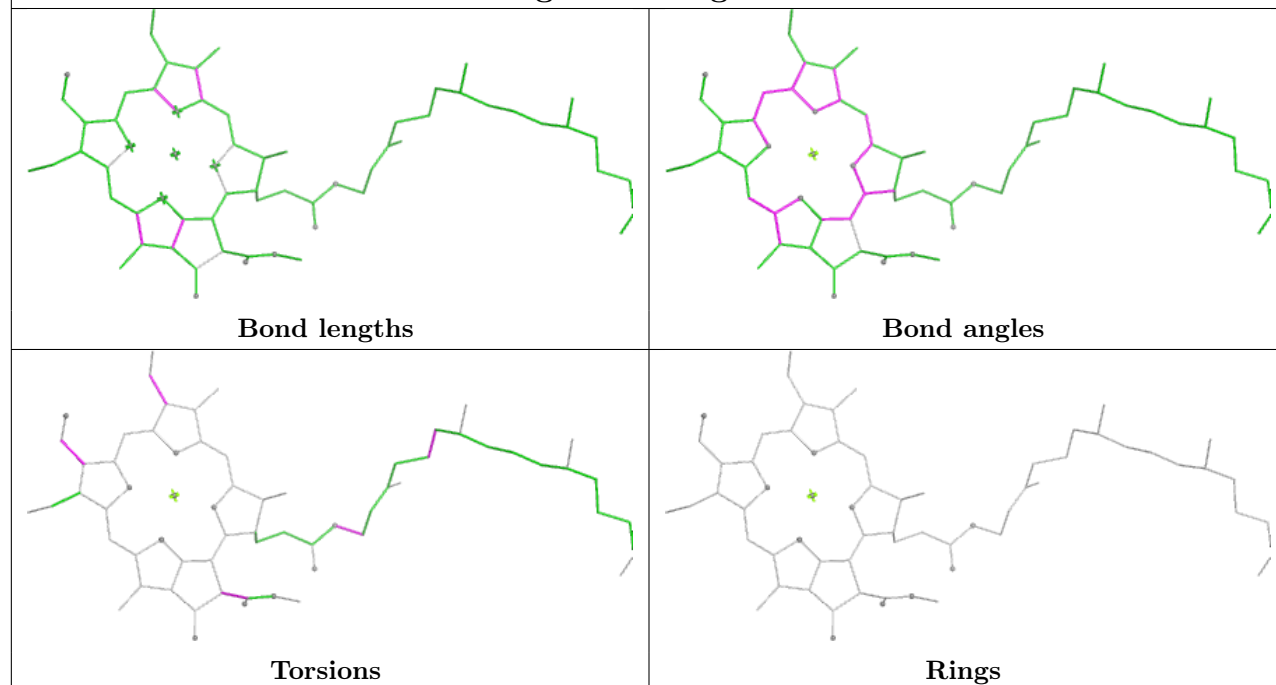


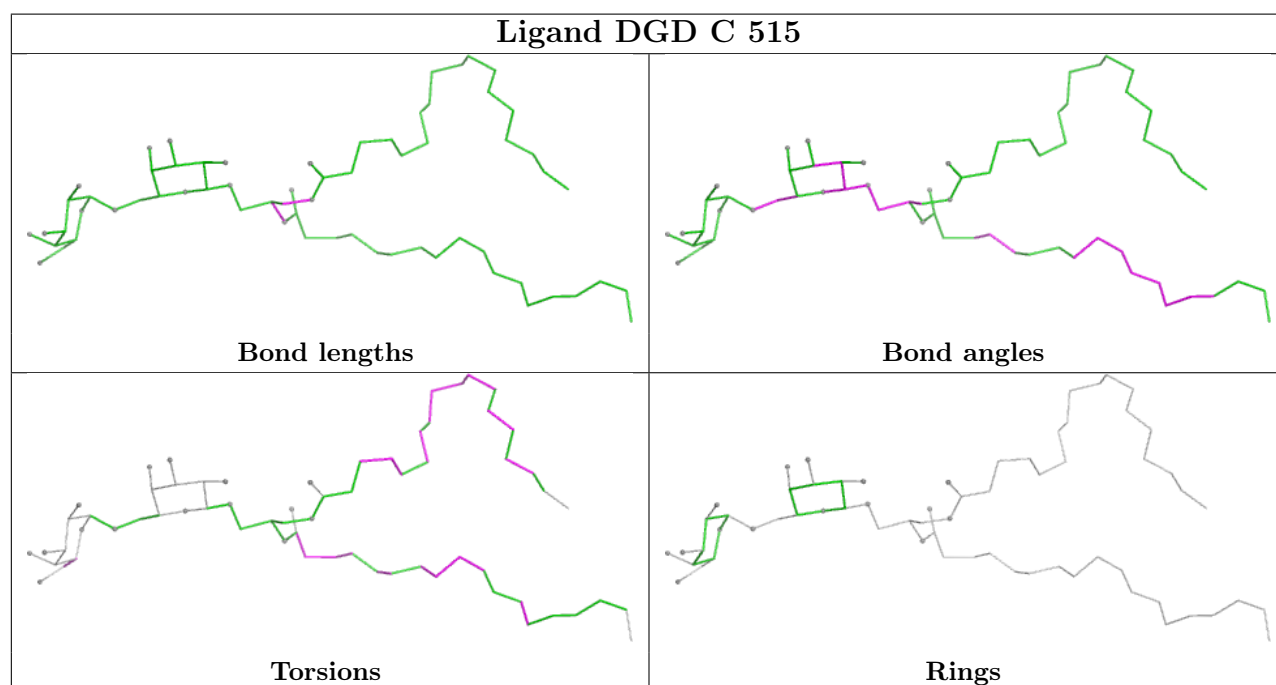
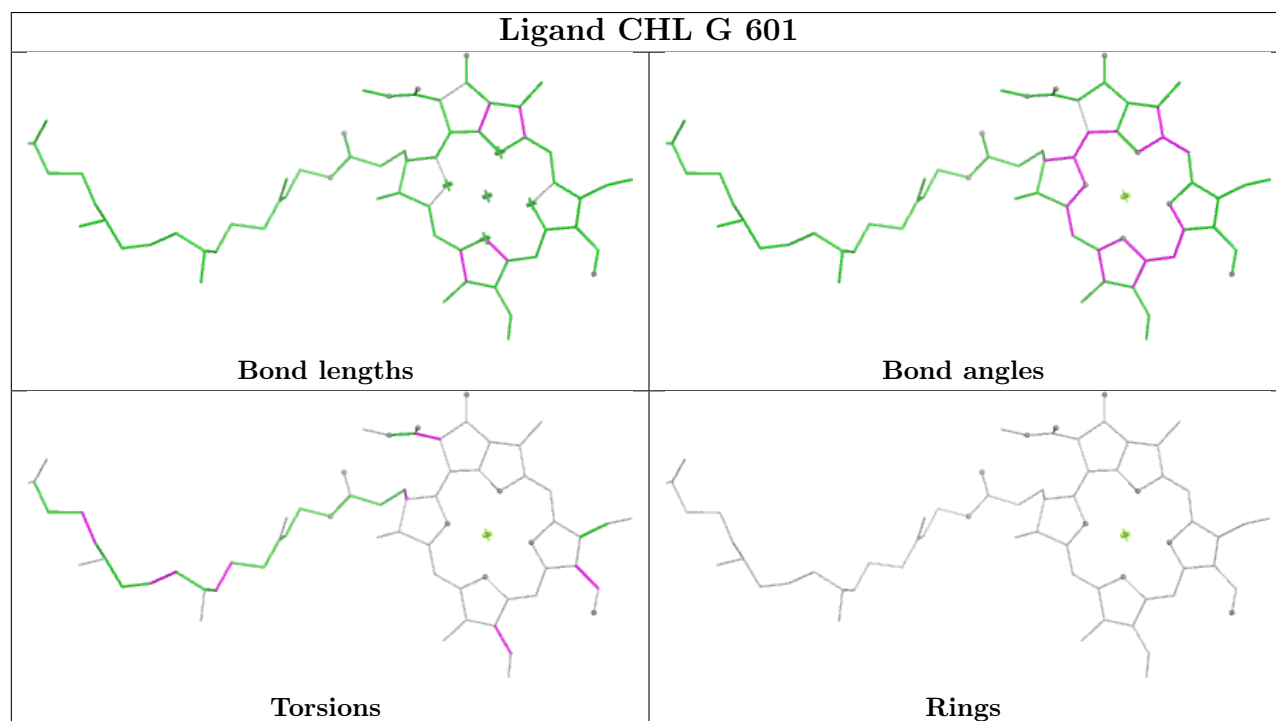
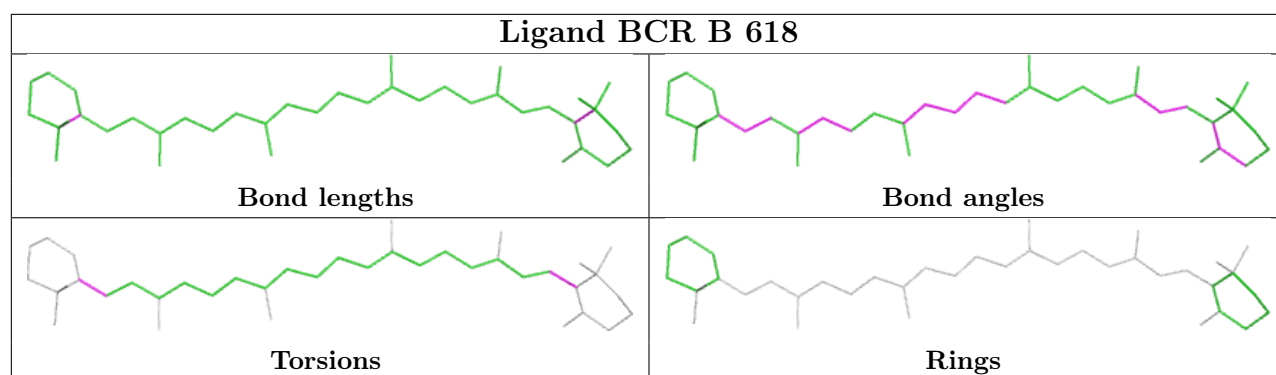


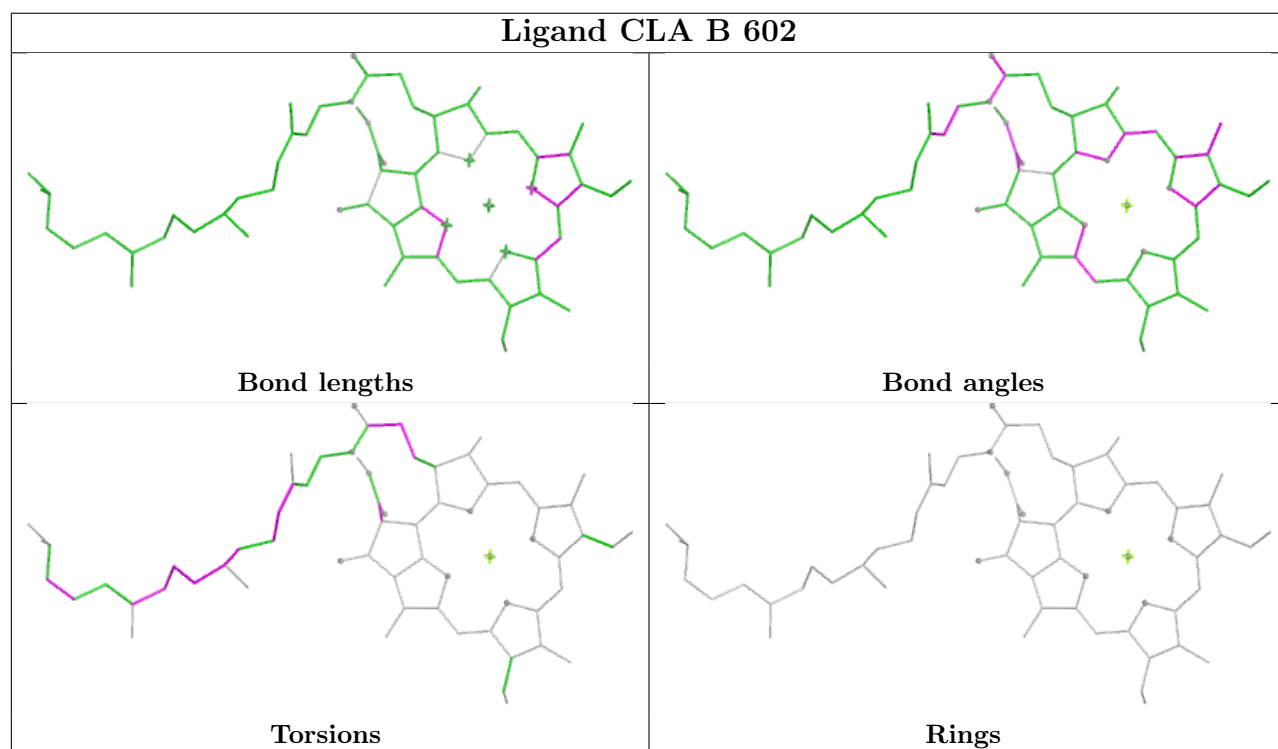
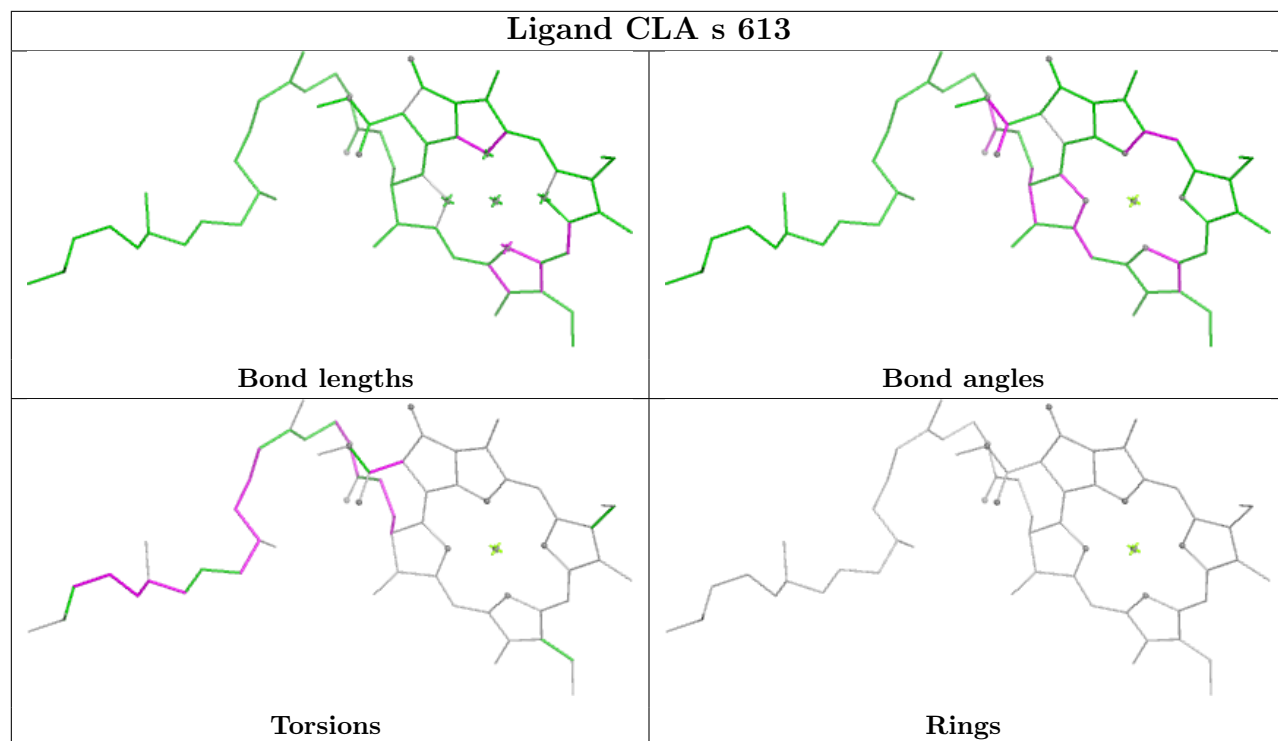
Ligand CHL R 607



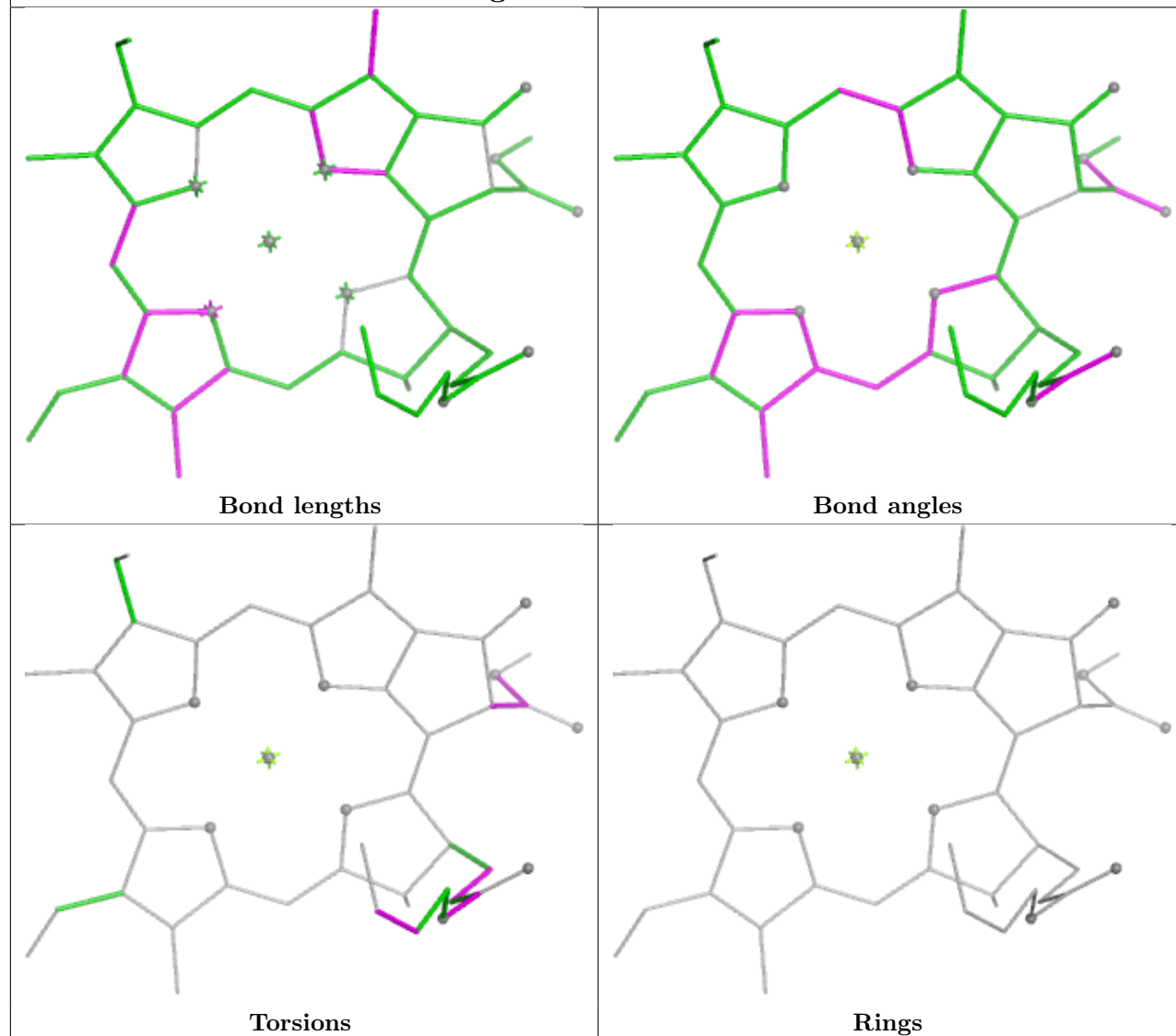
Ligand CHL g 601



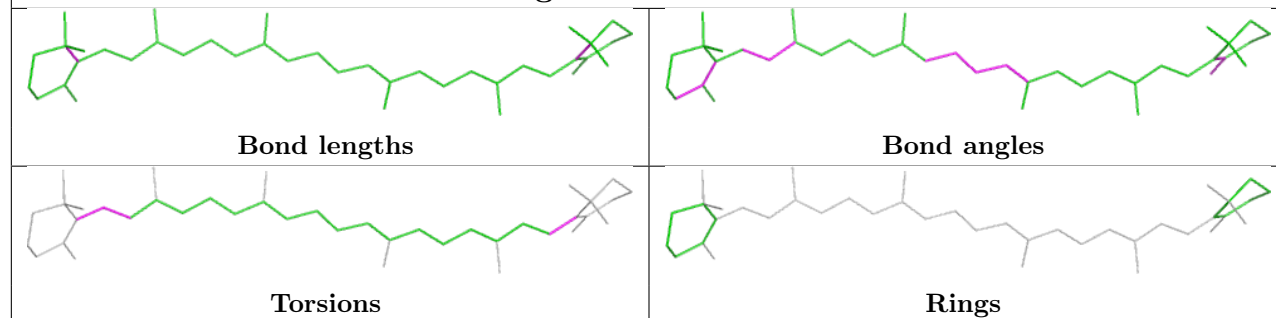


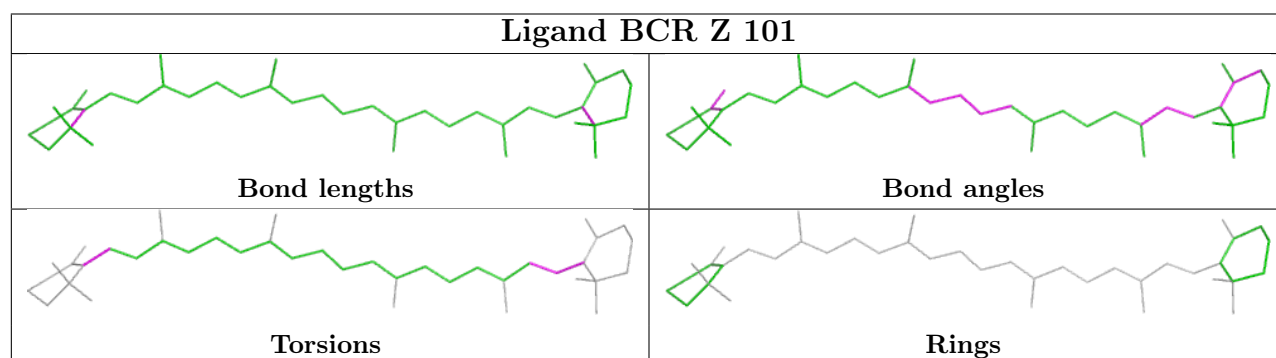
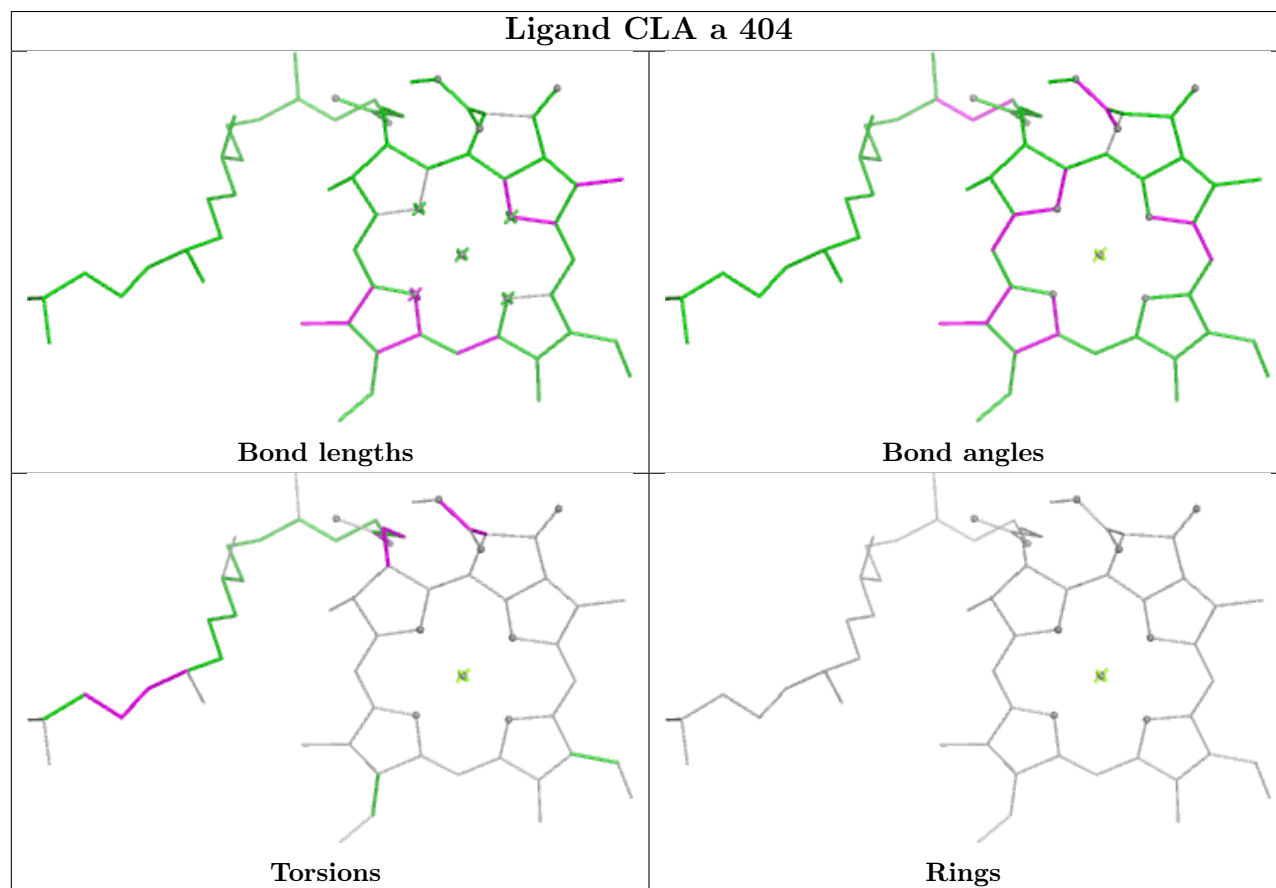
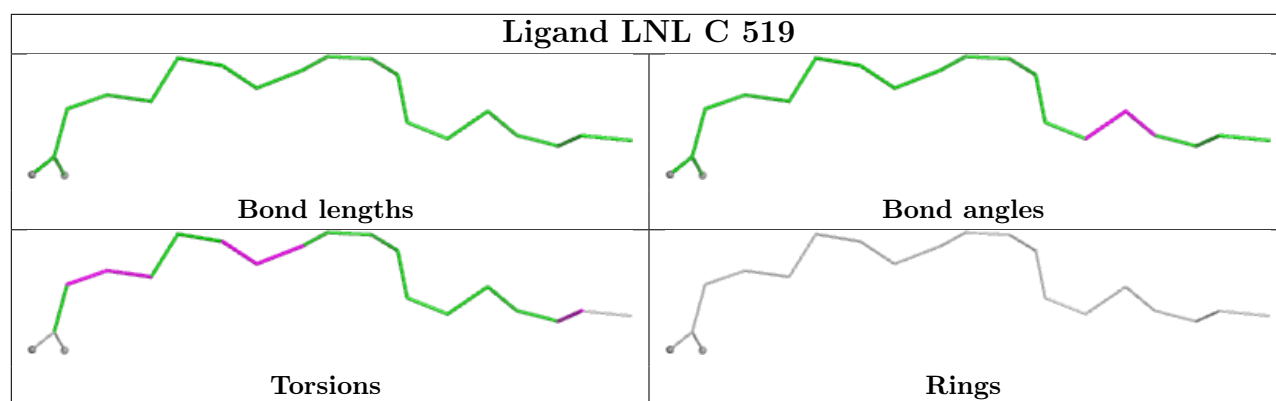


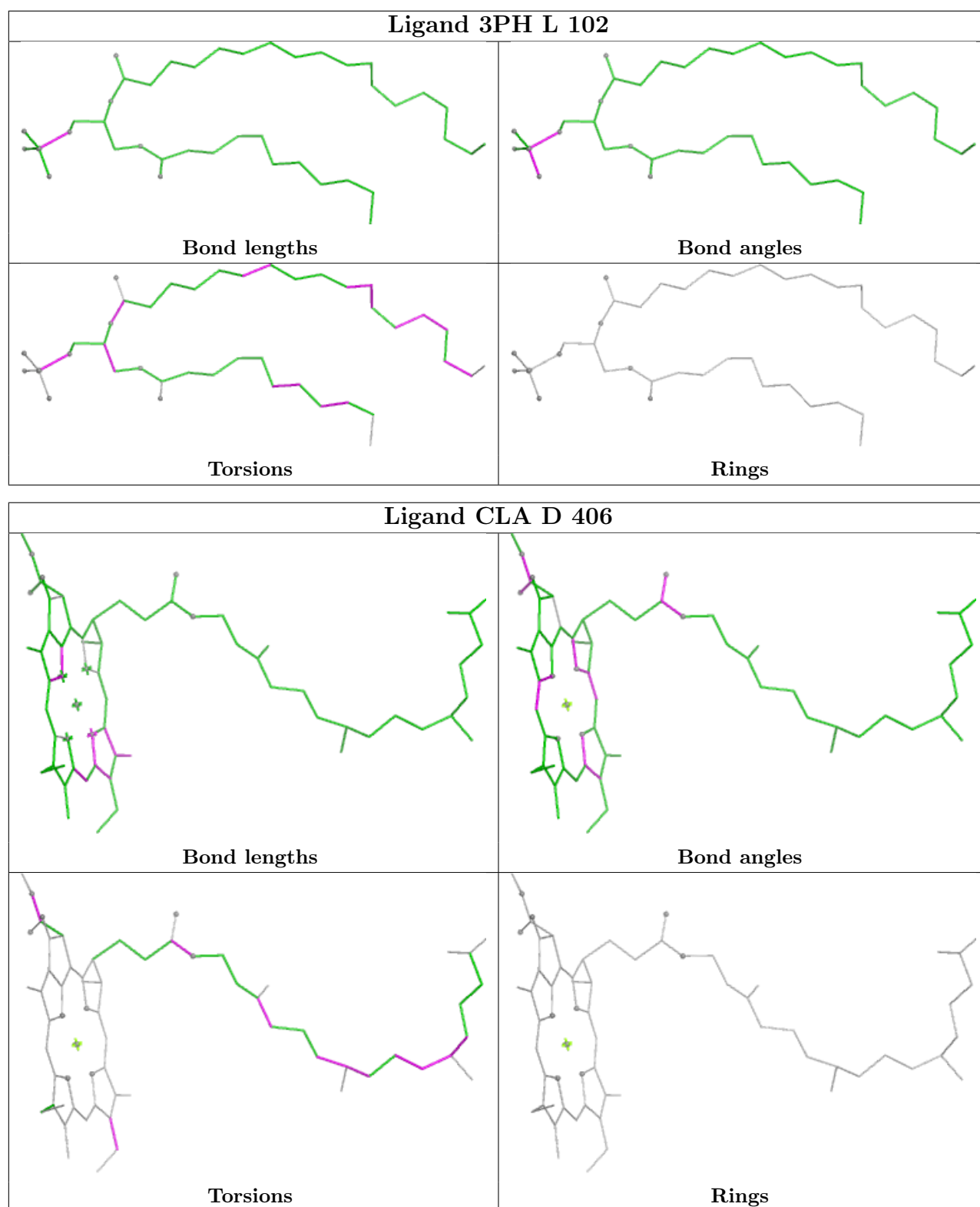
Ligand CLA N 604

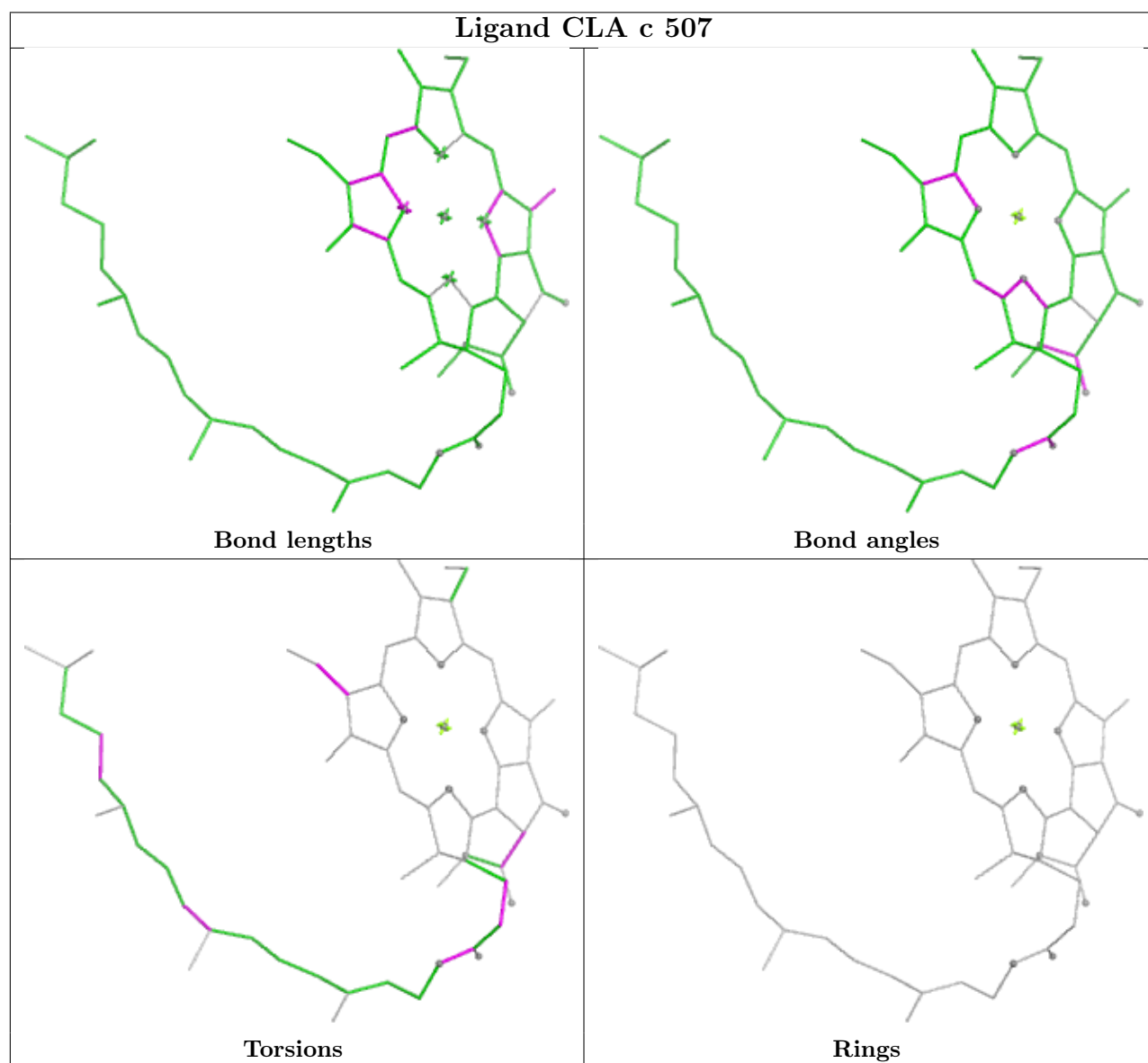
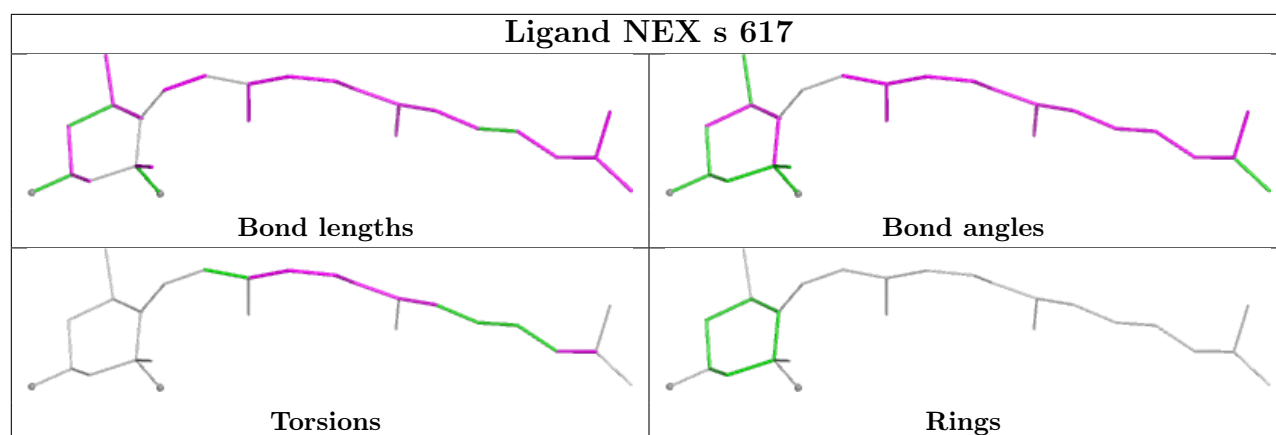


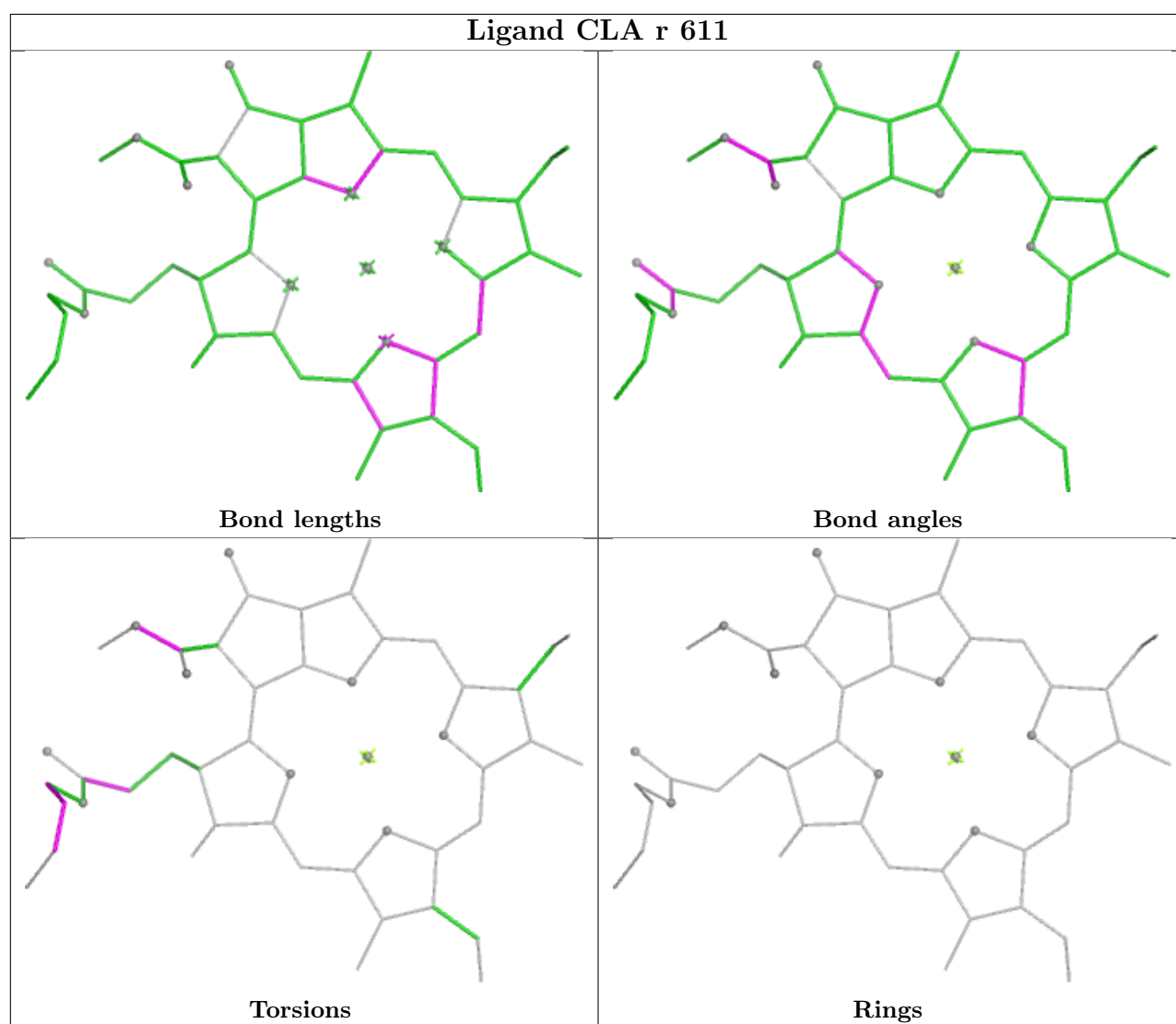
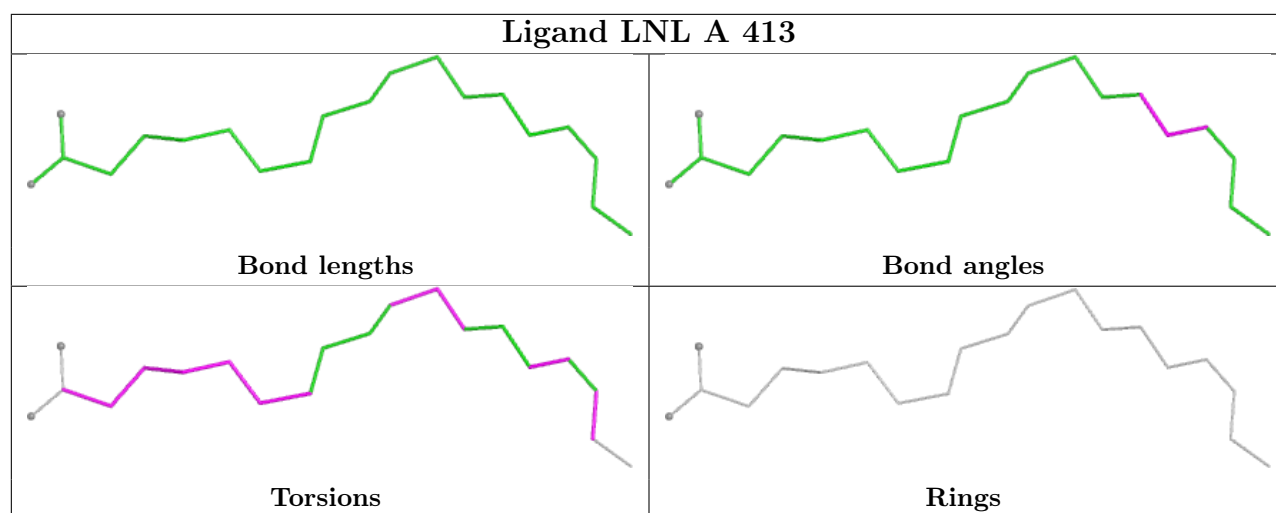
Ligand BCR z 101

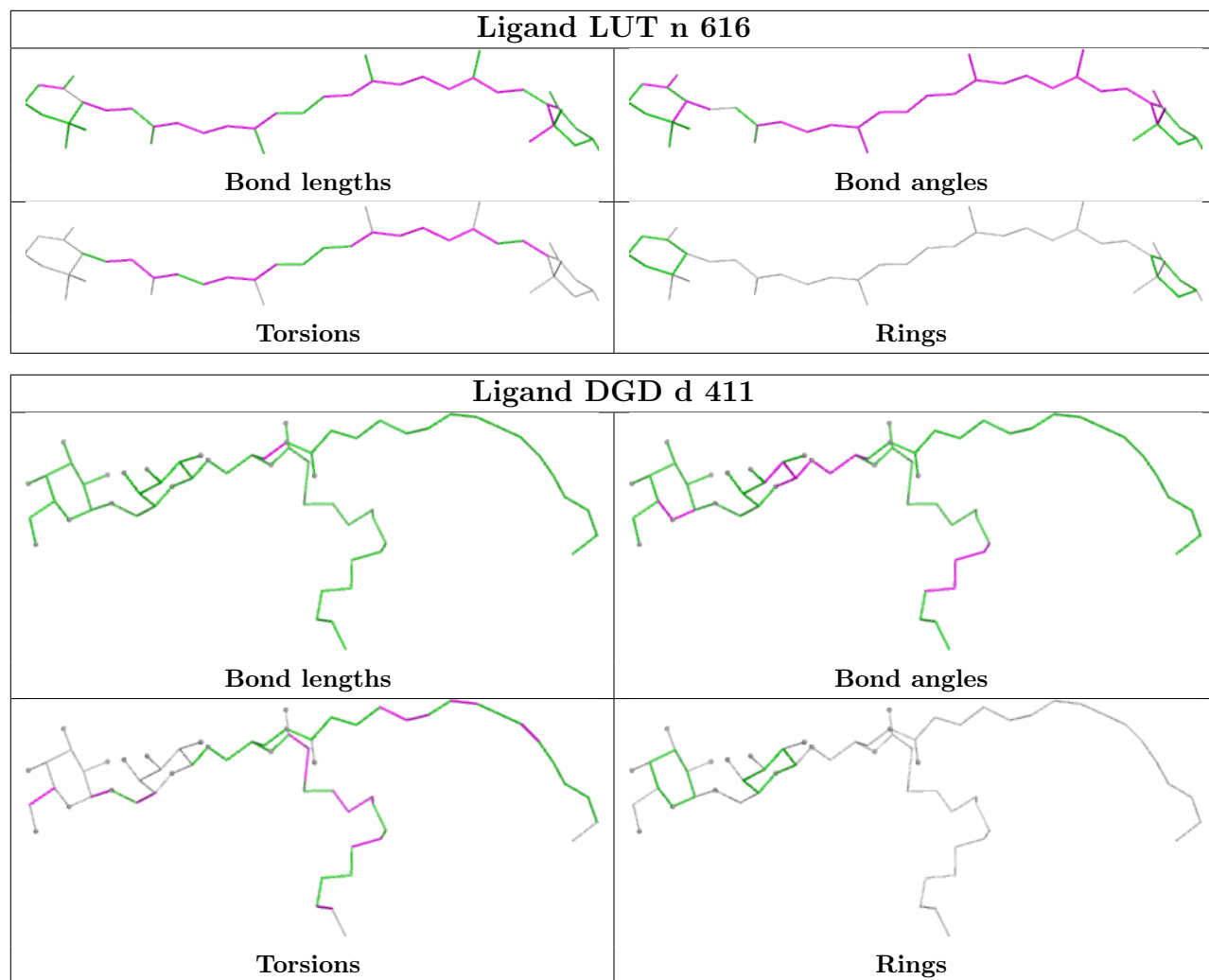


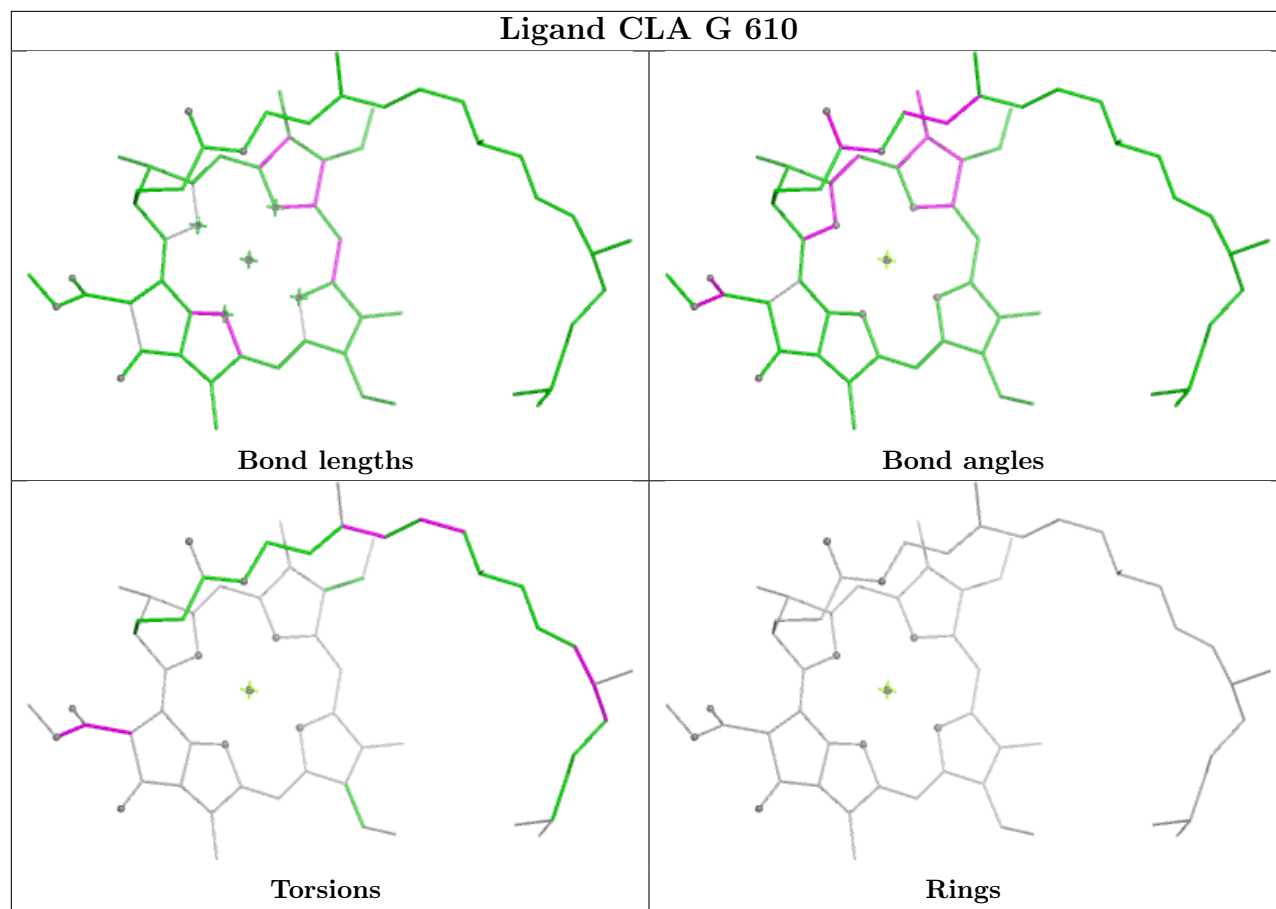


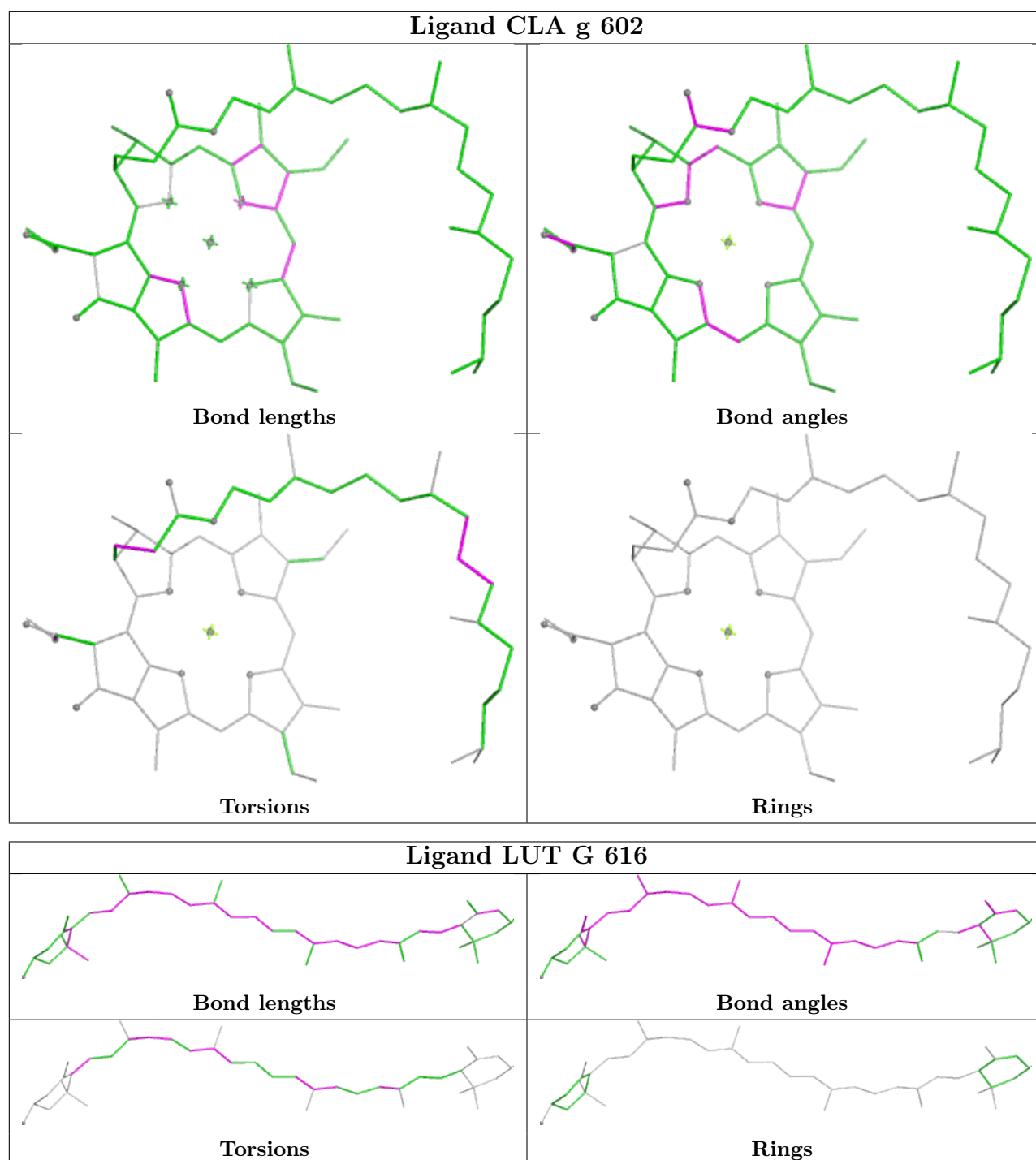


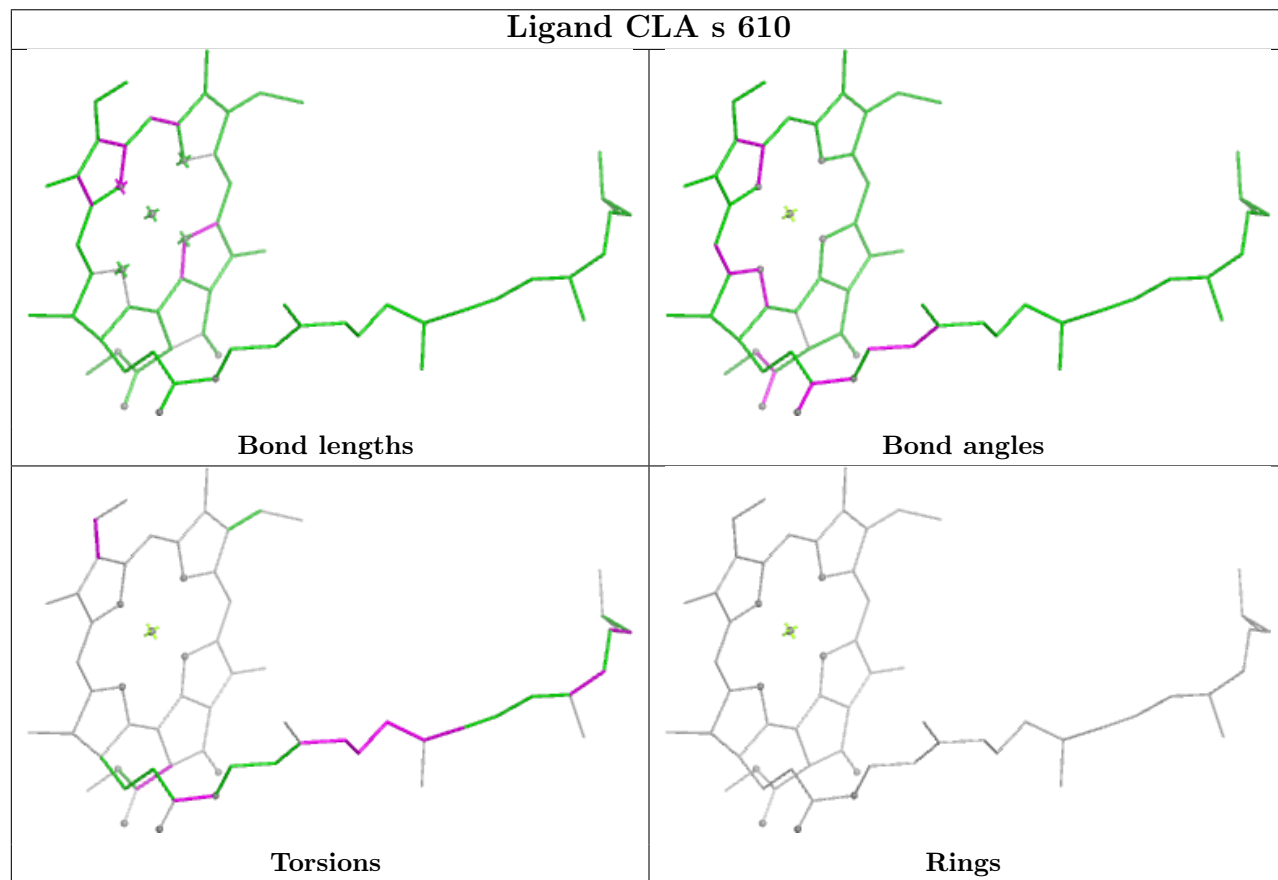
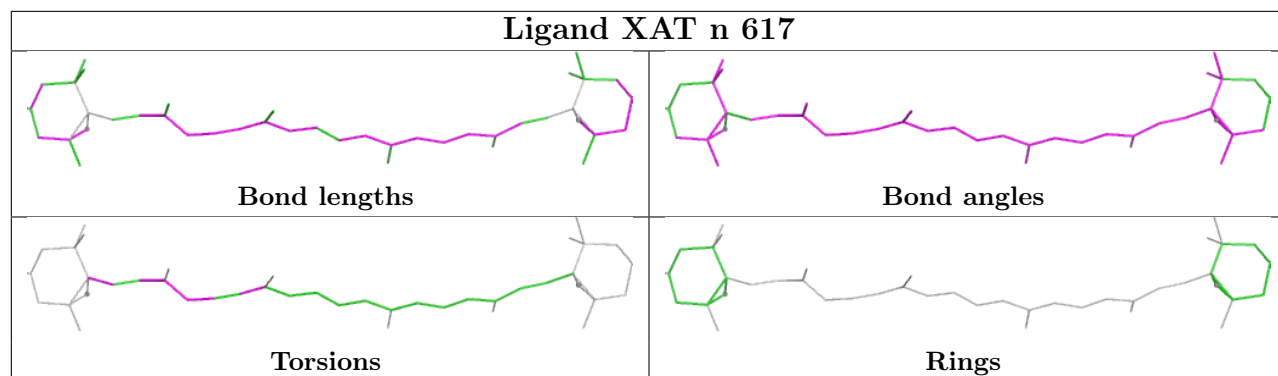


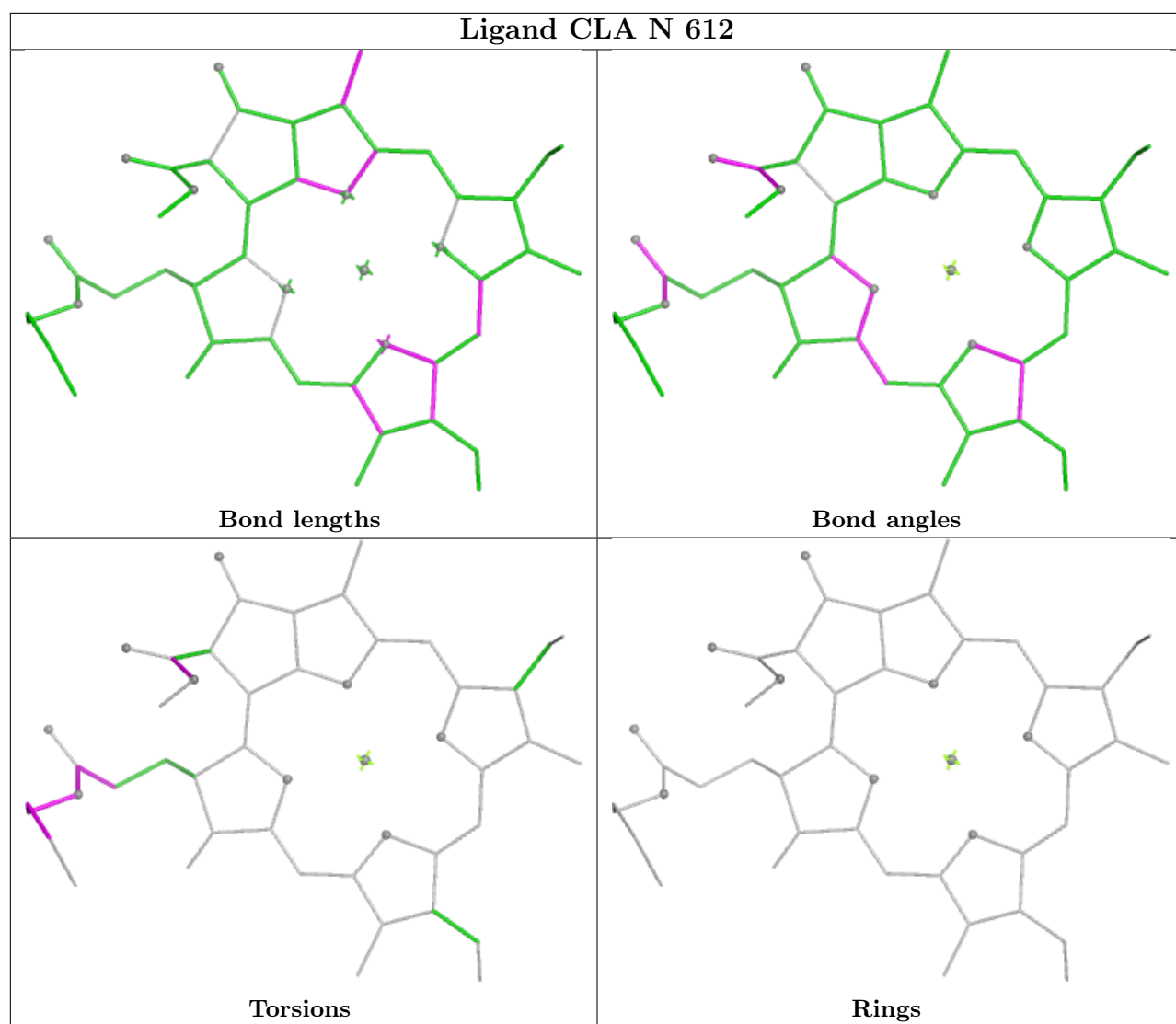


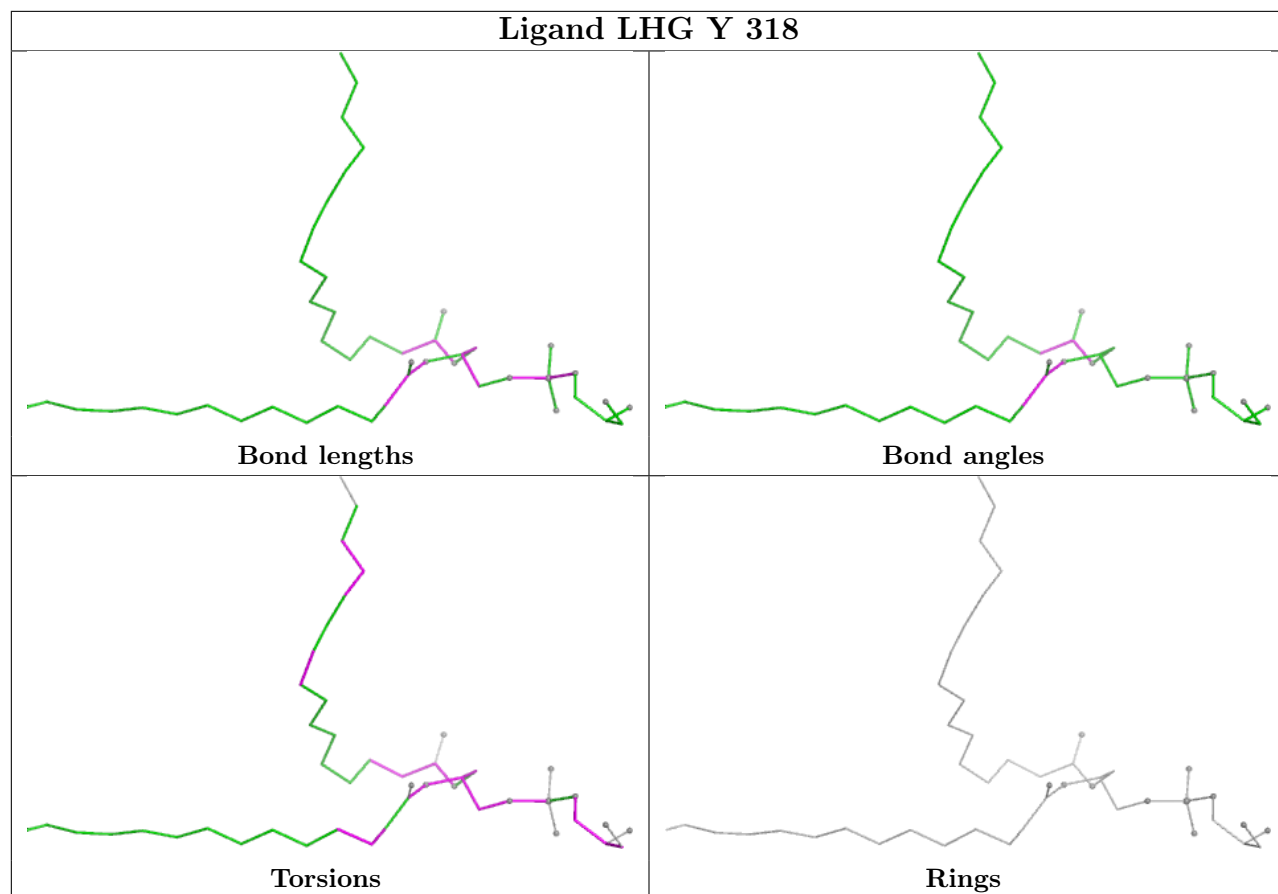


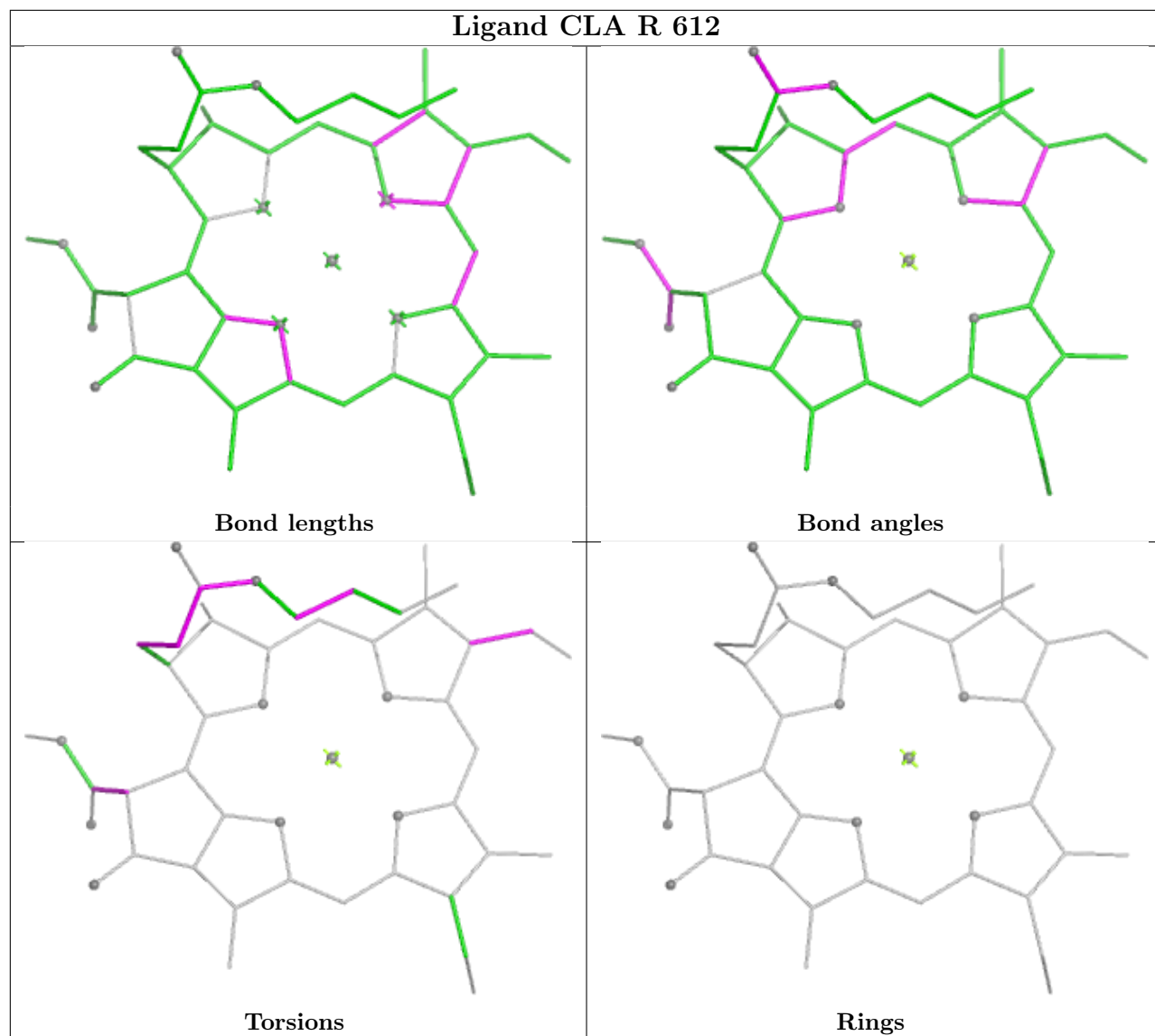


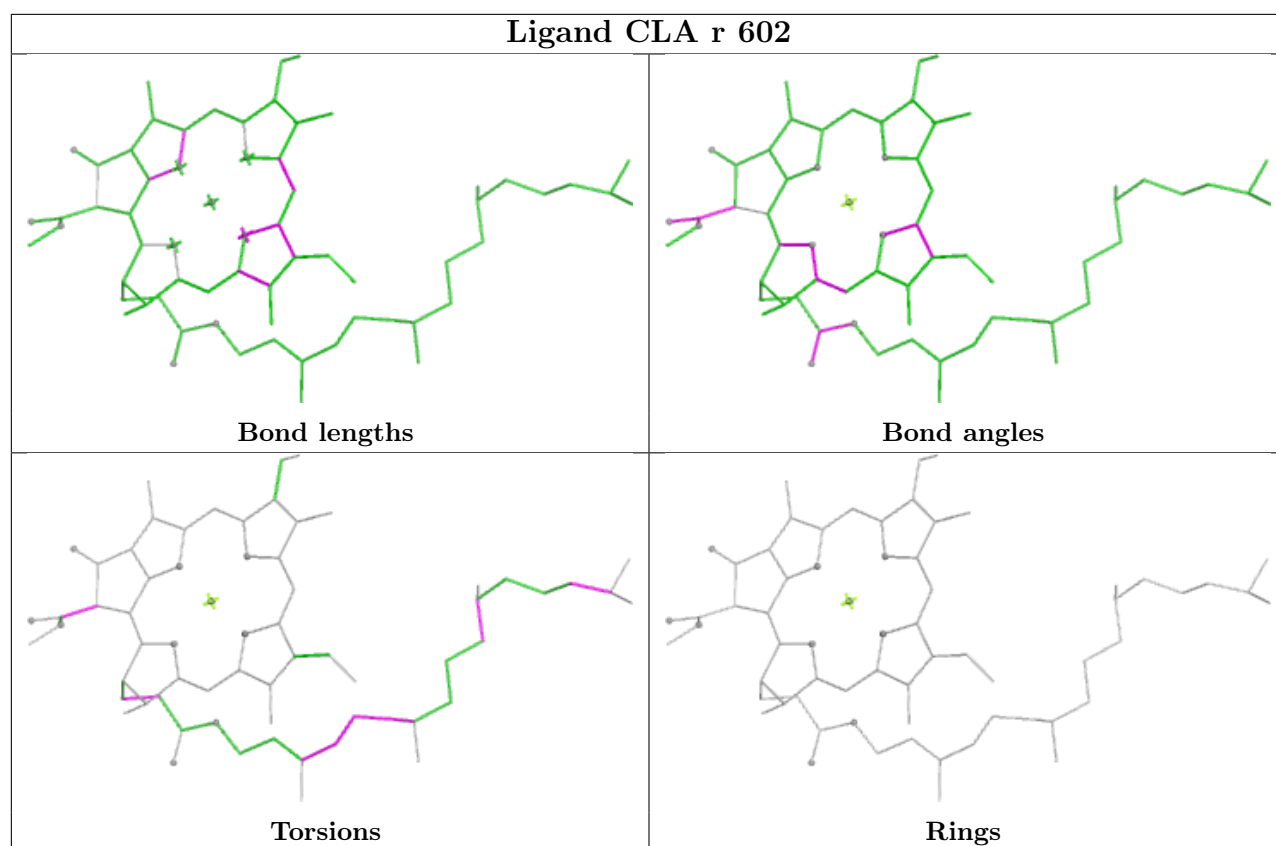




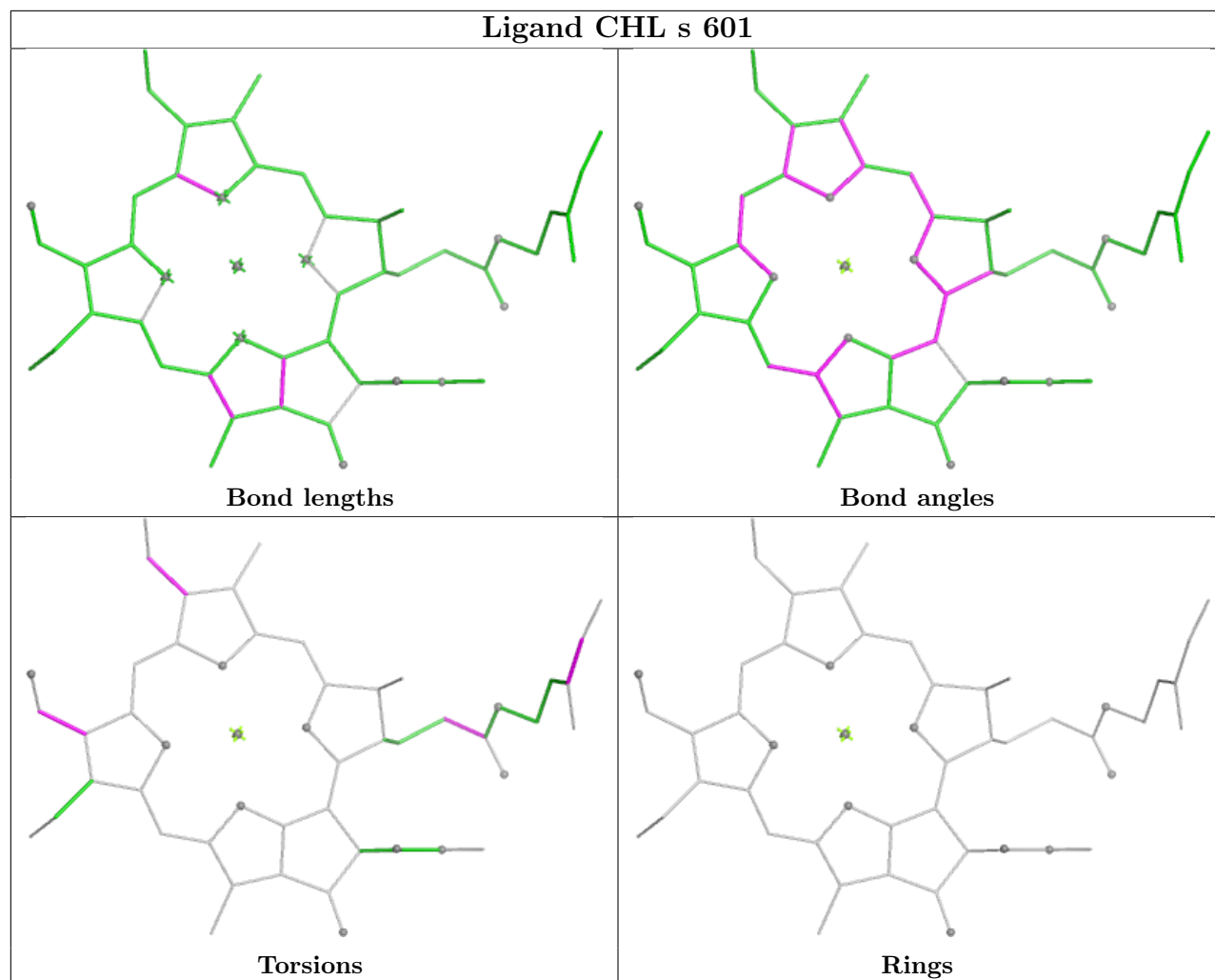




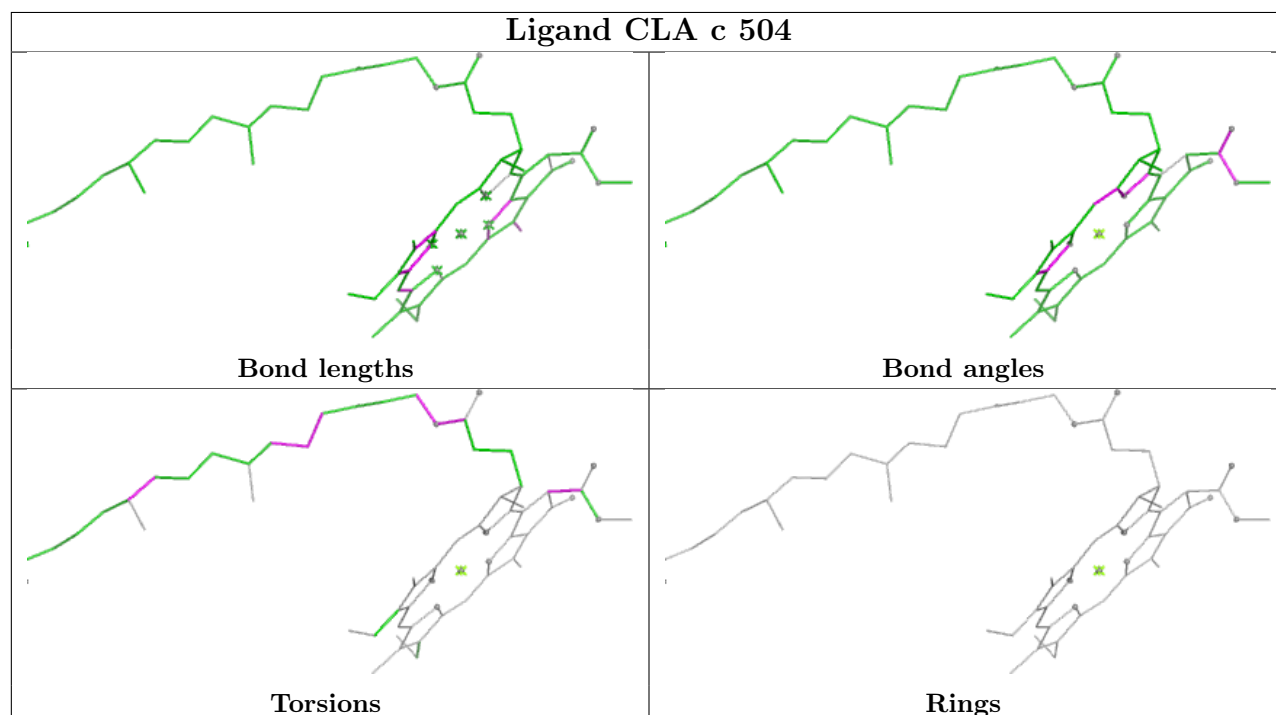


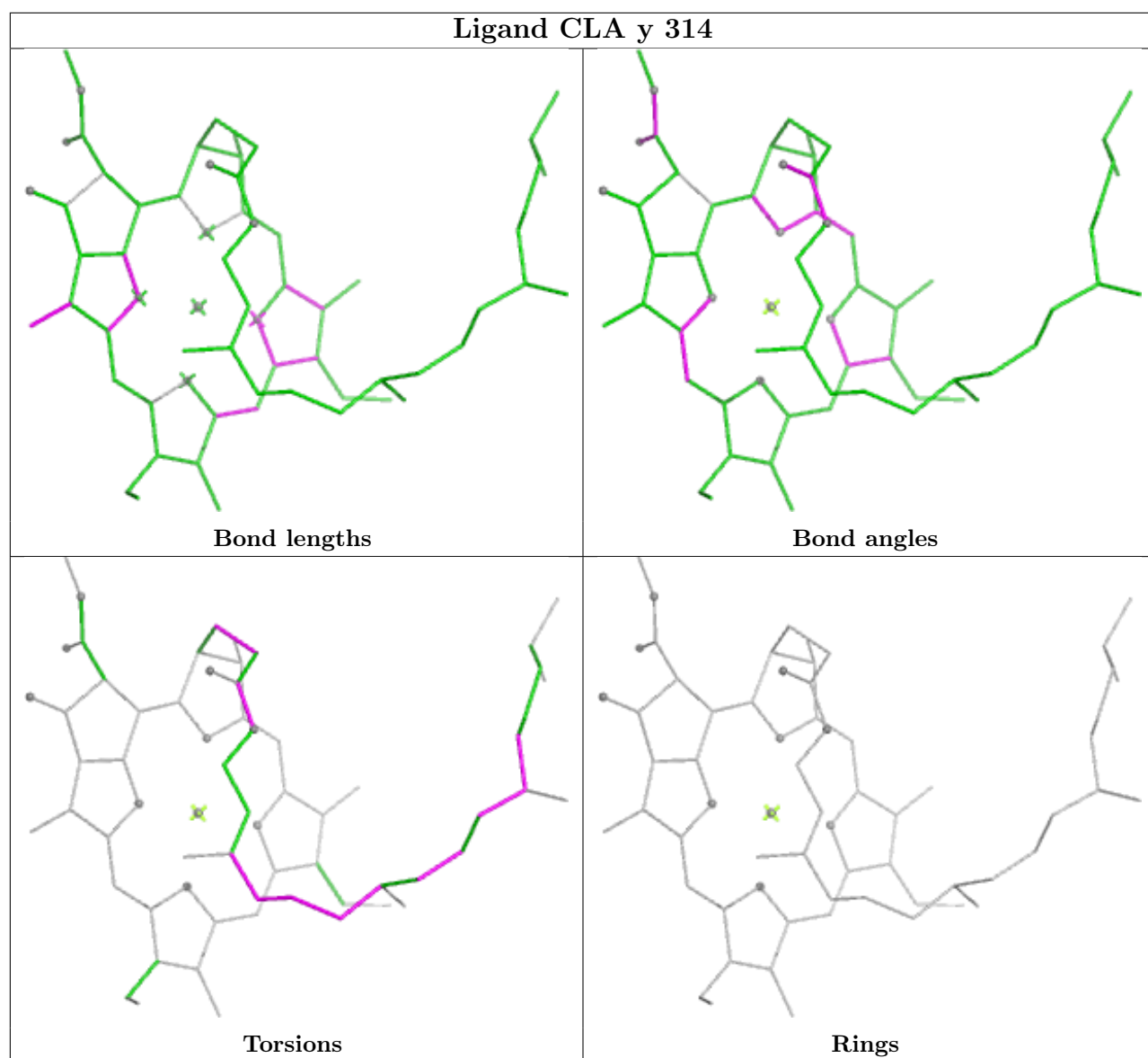


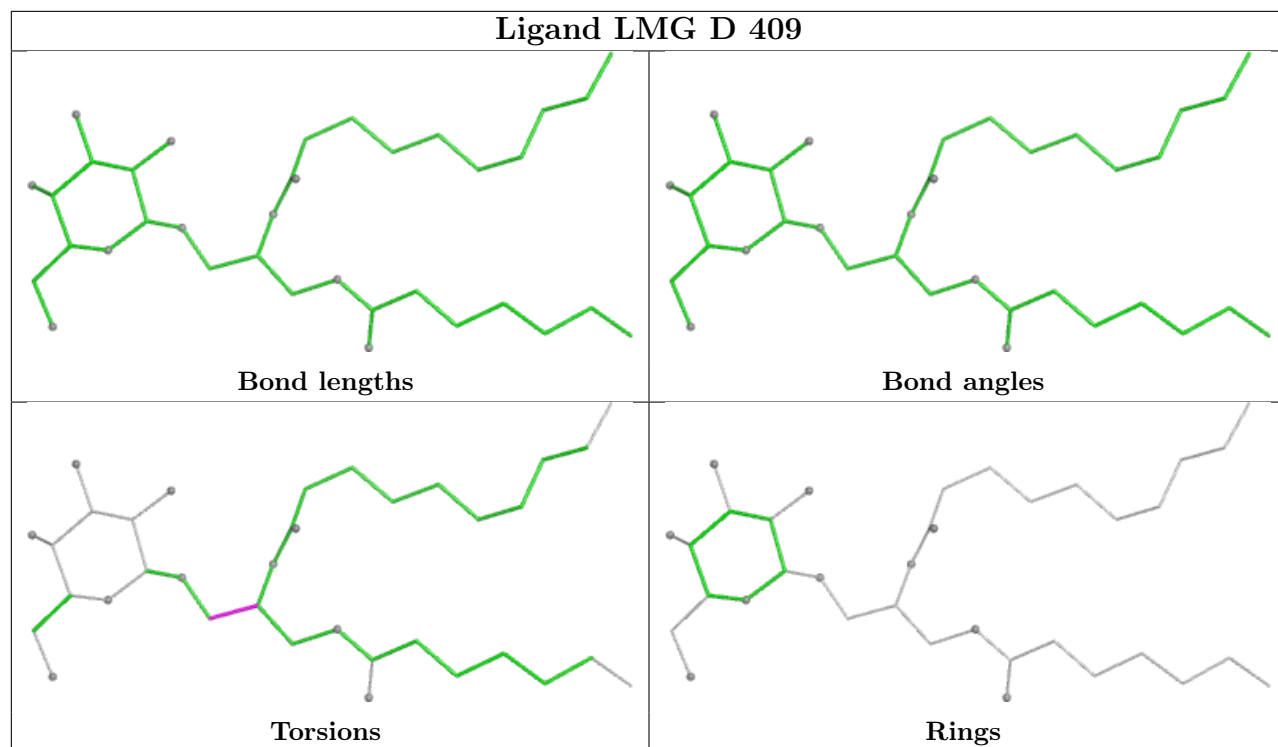
Ligand CHL s 601



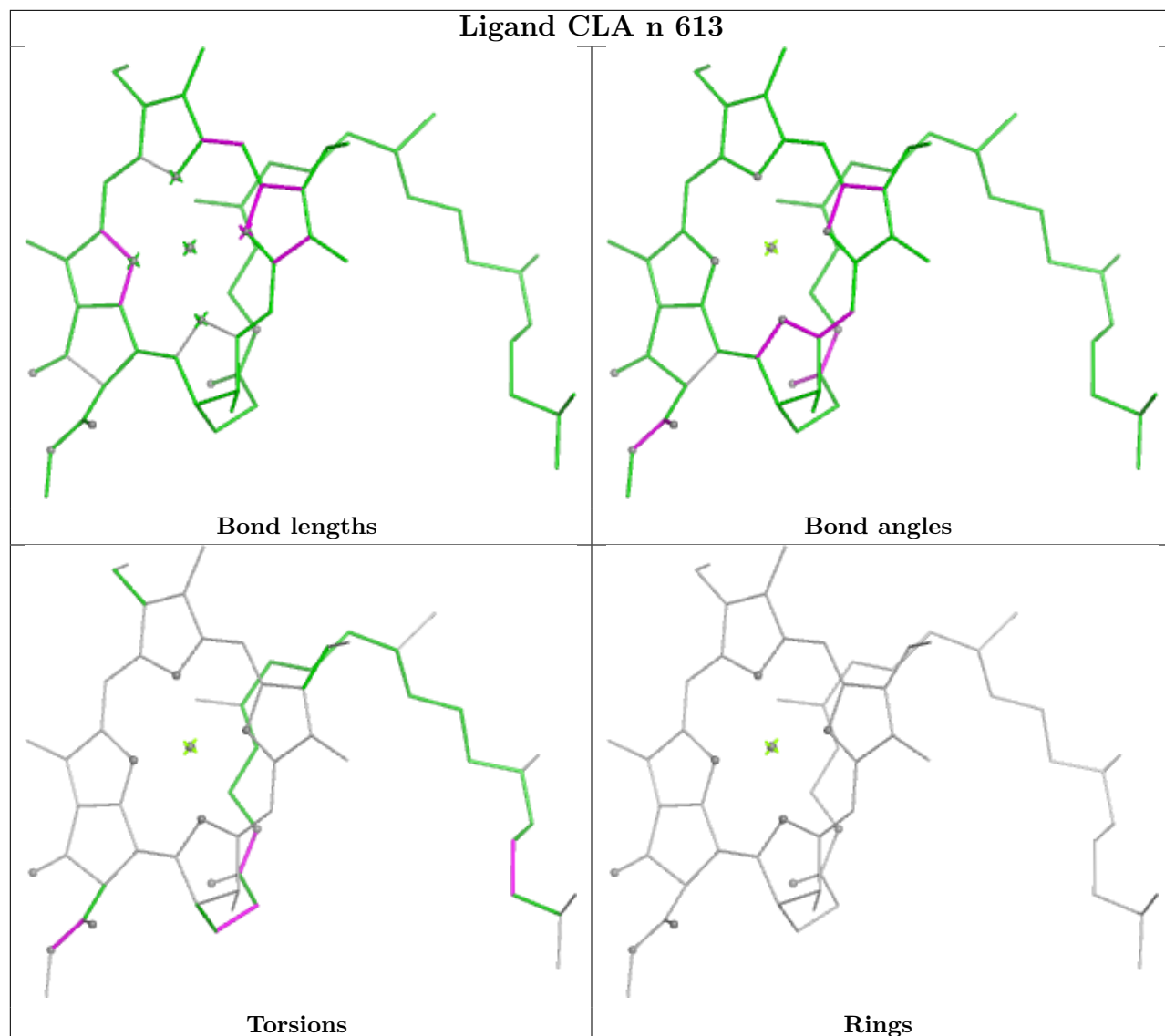
Ligand CLA c 504

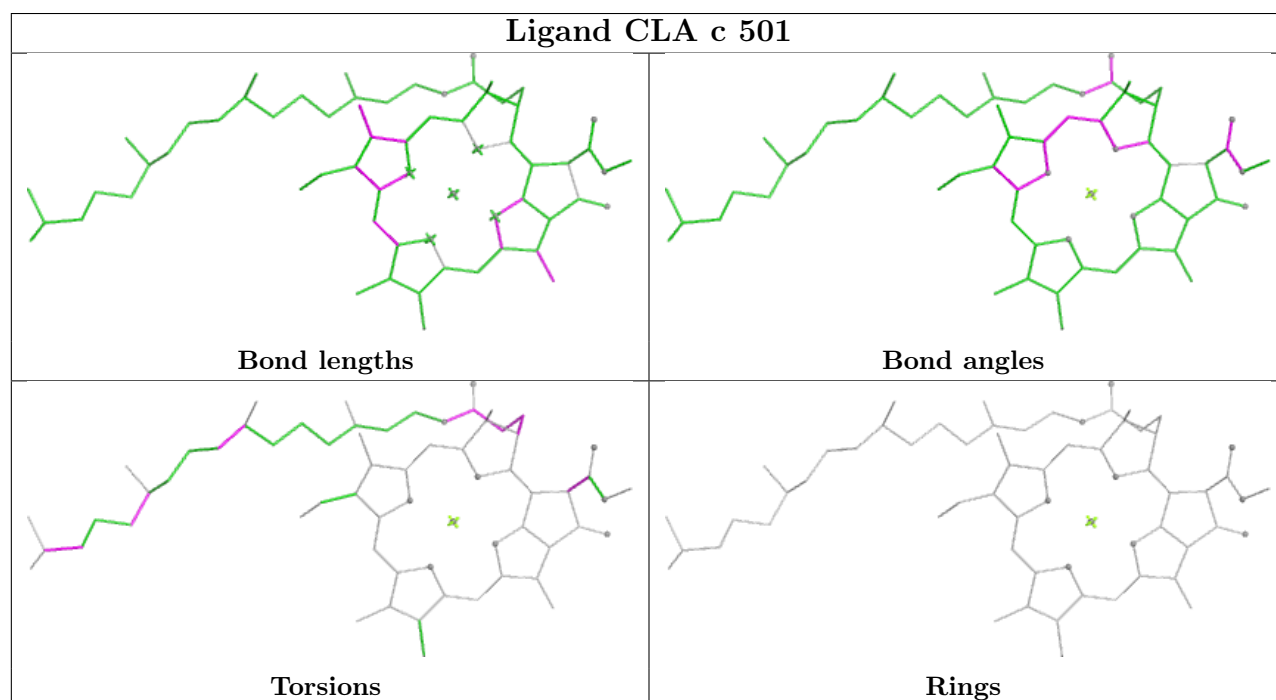
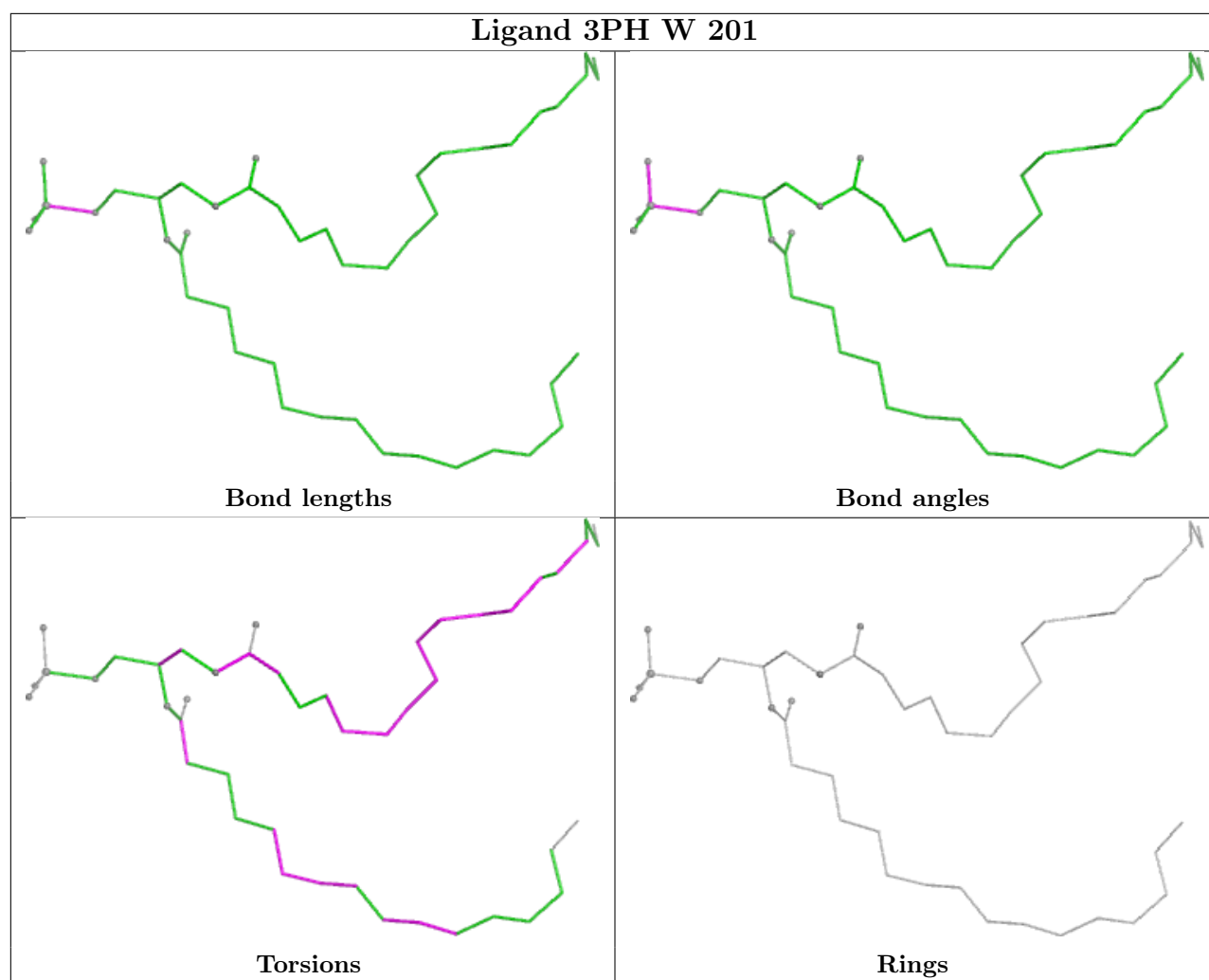


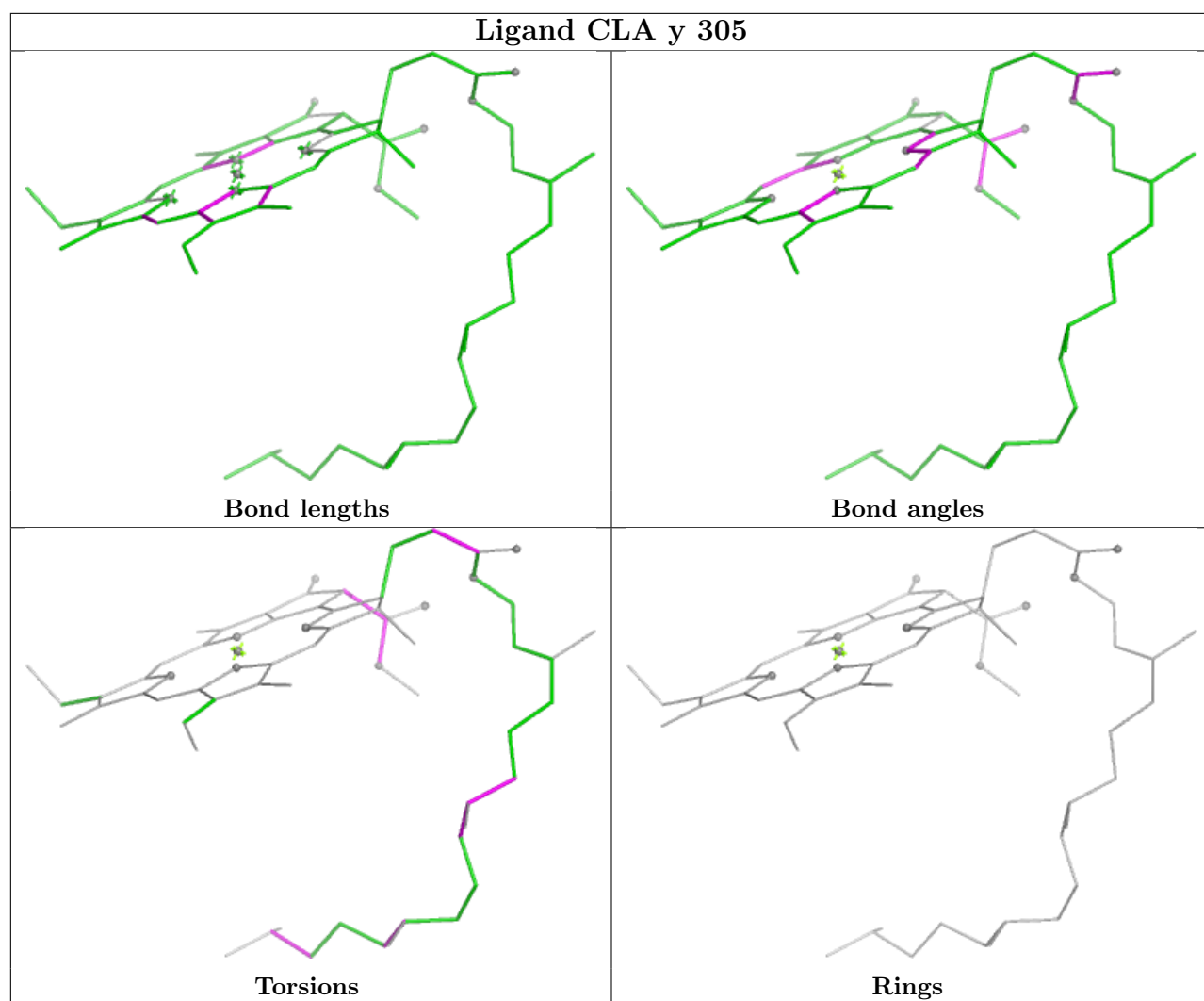




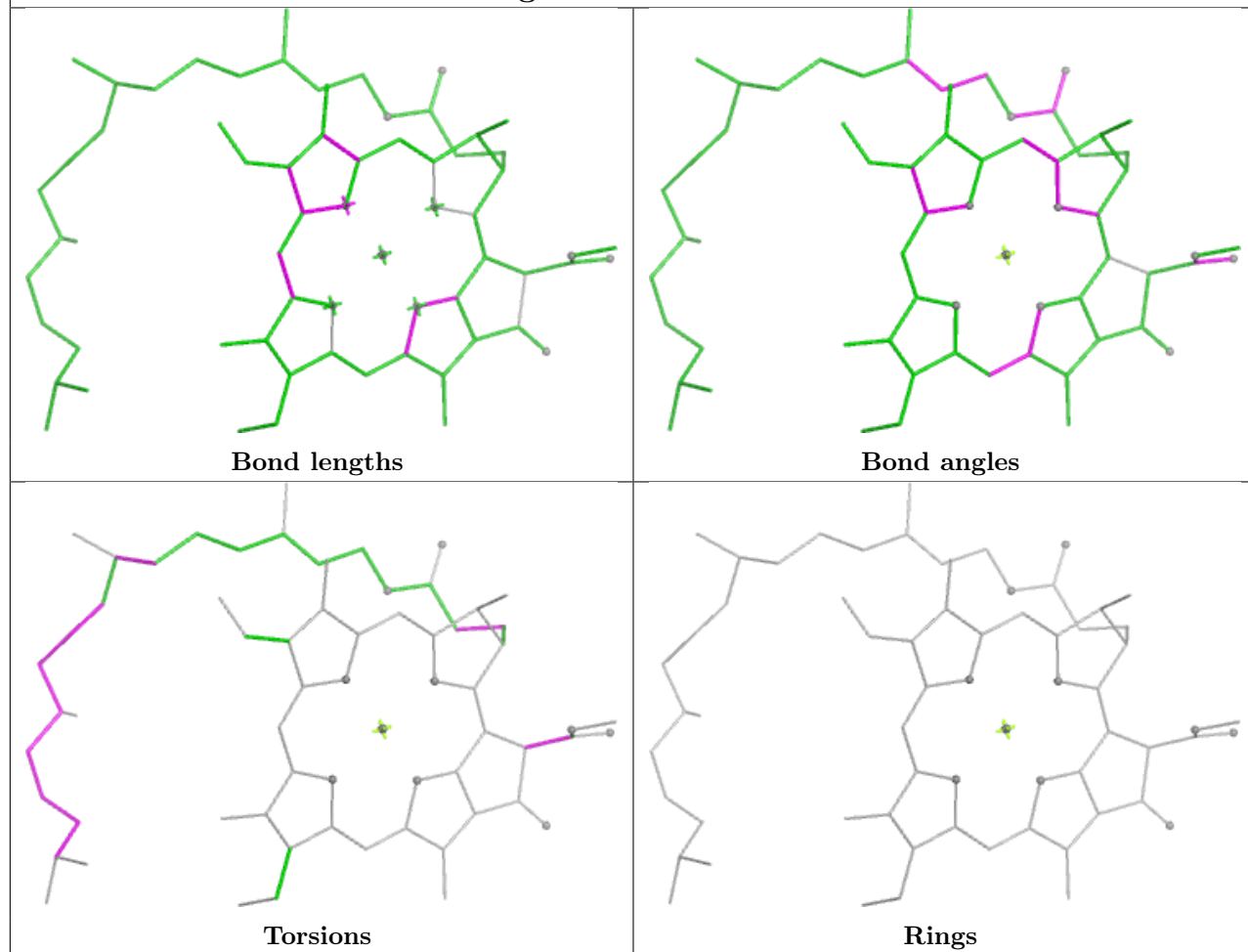
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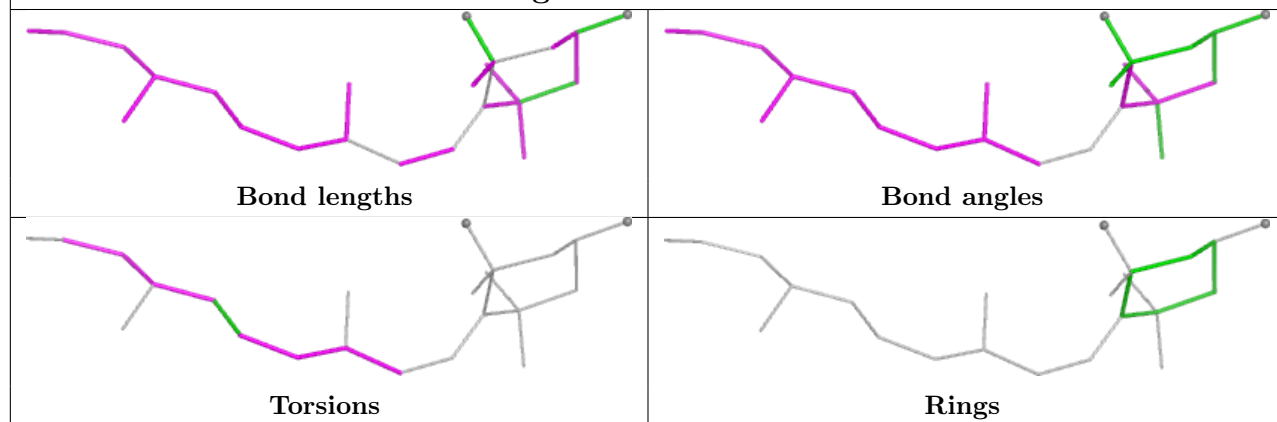


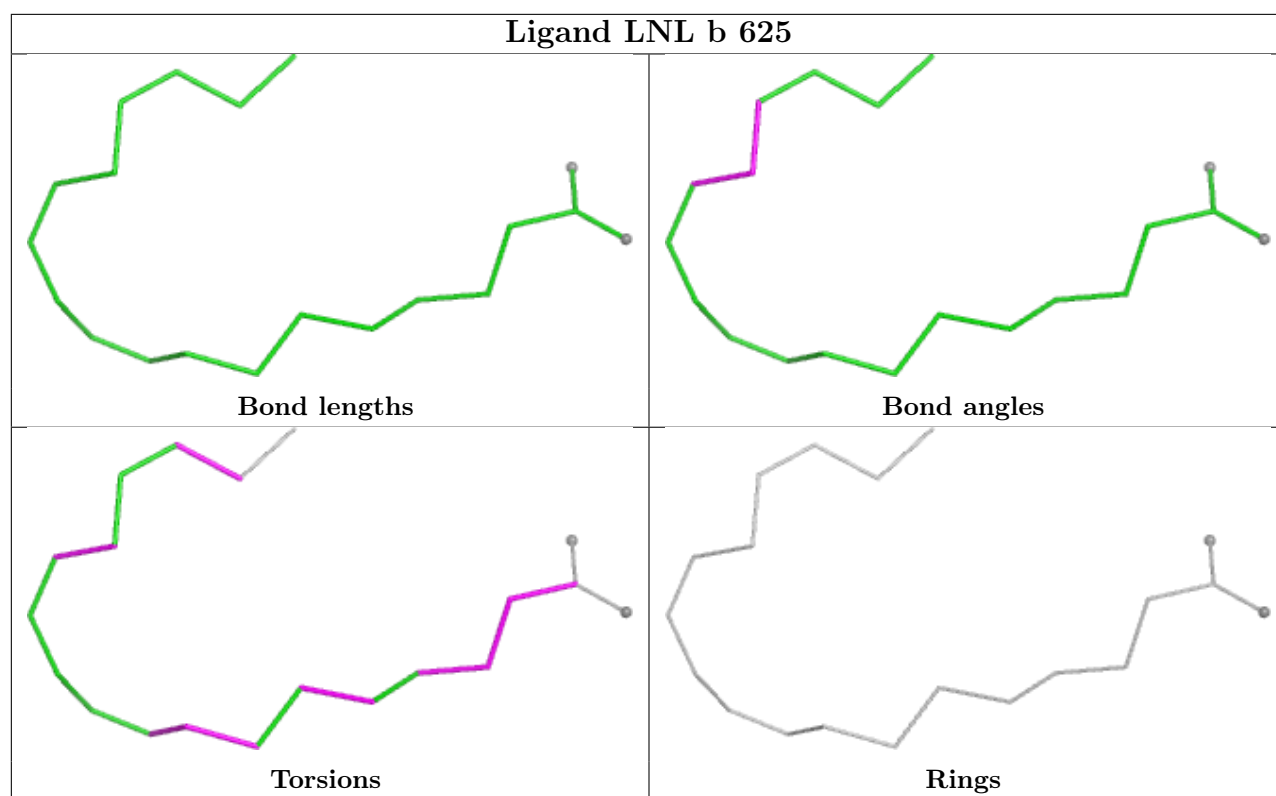


Ligand CLA Y 303

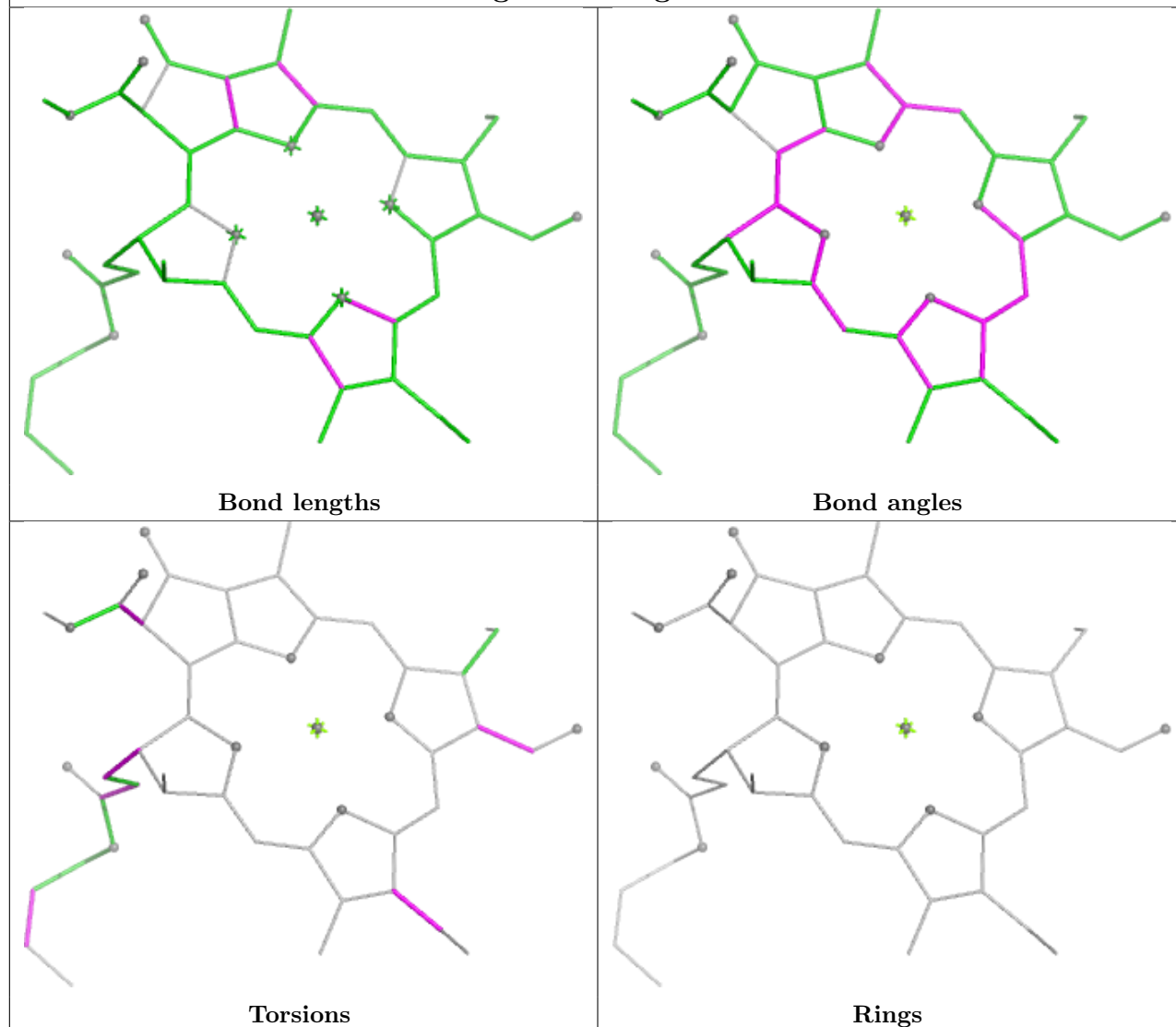


Ligand NEX S 617

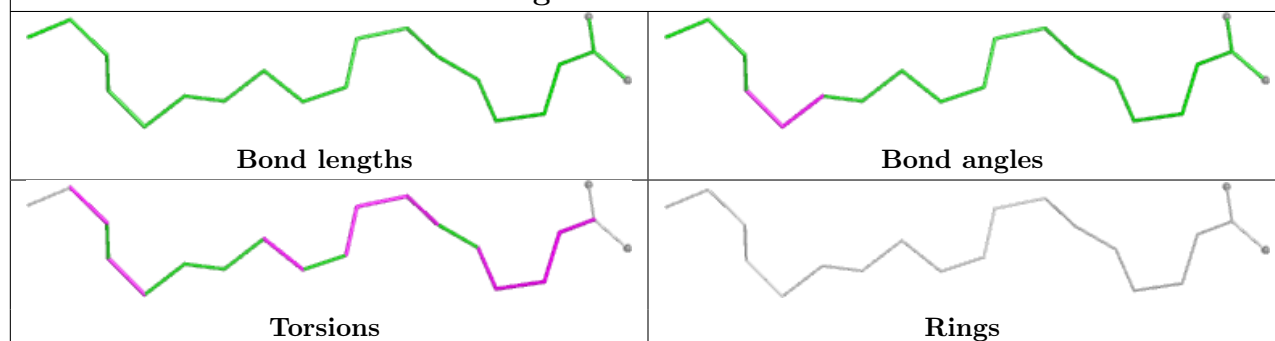


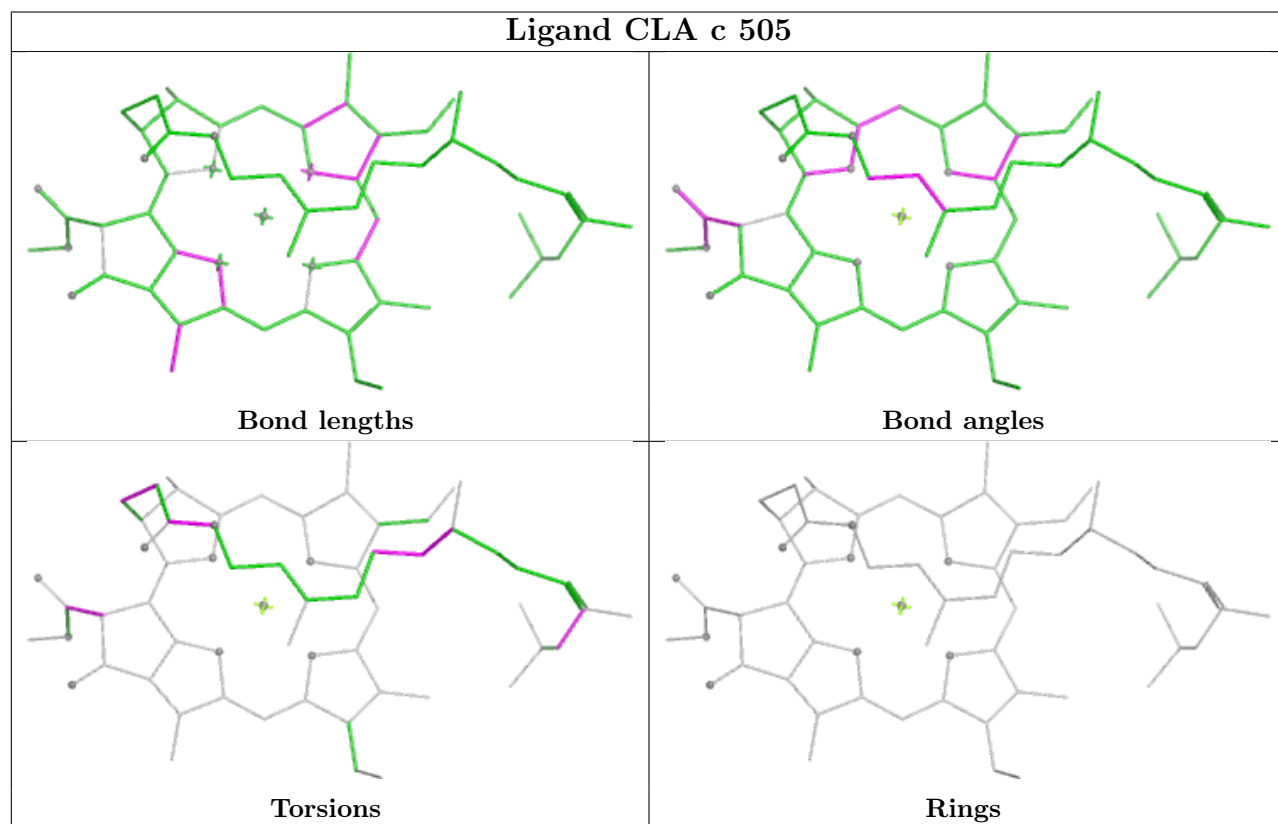
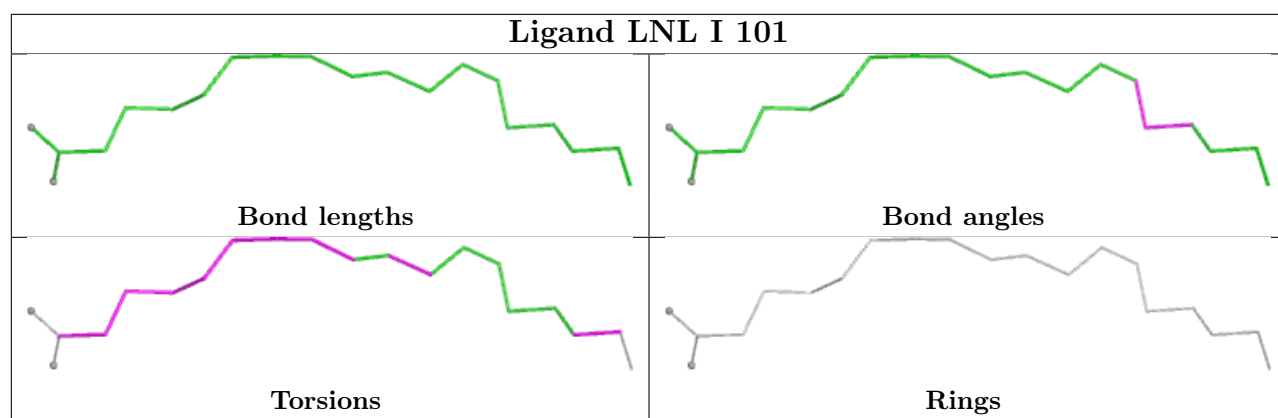


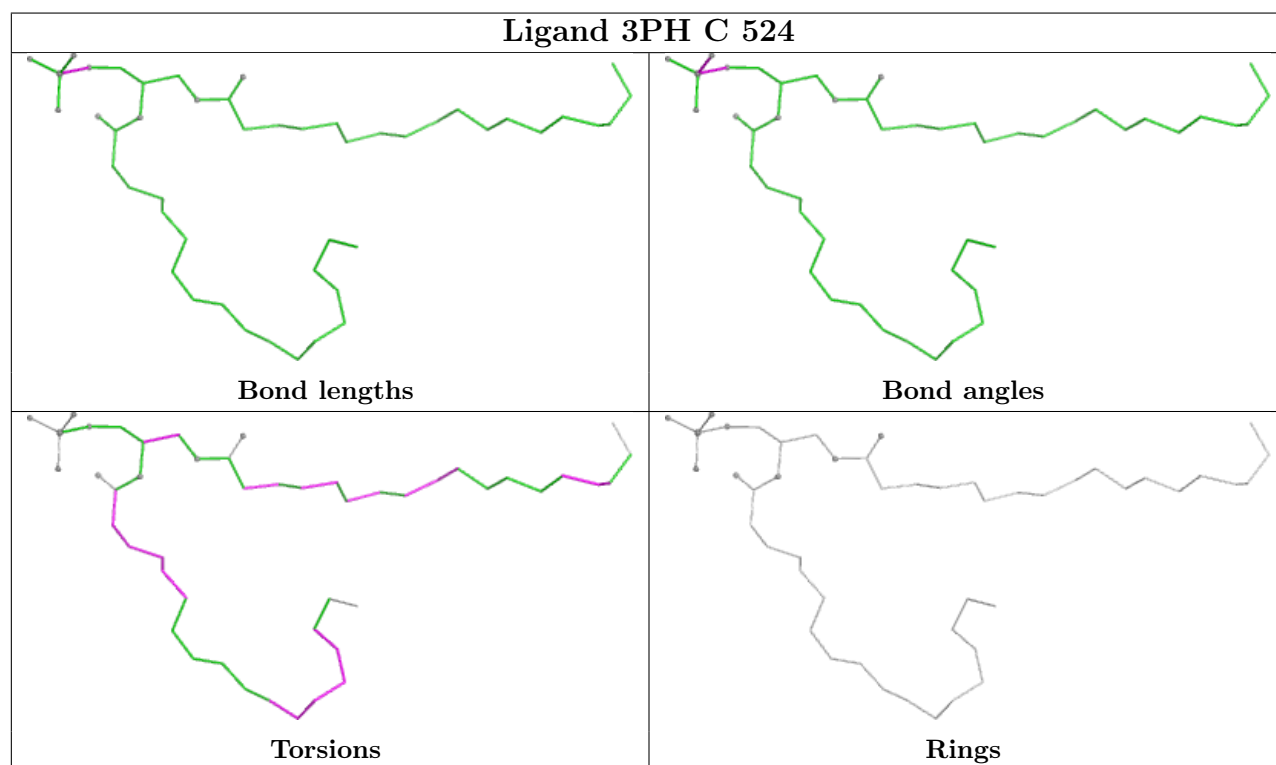
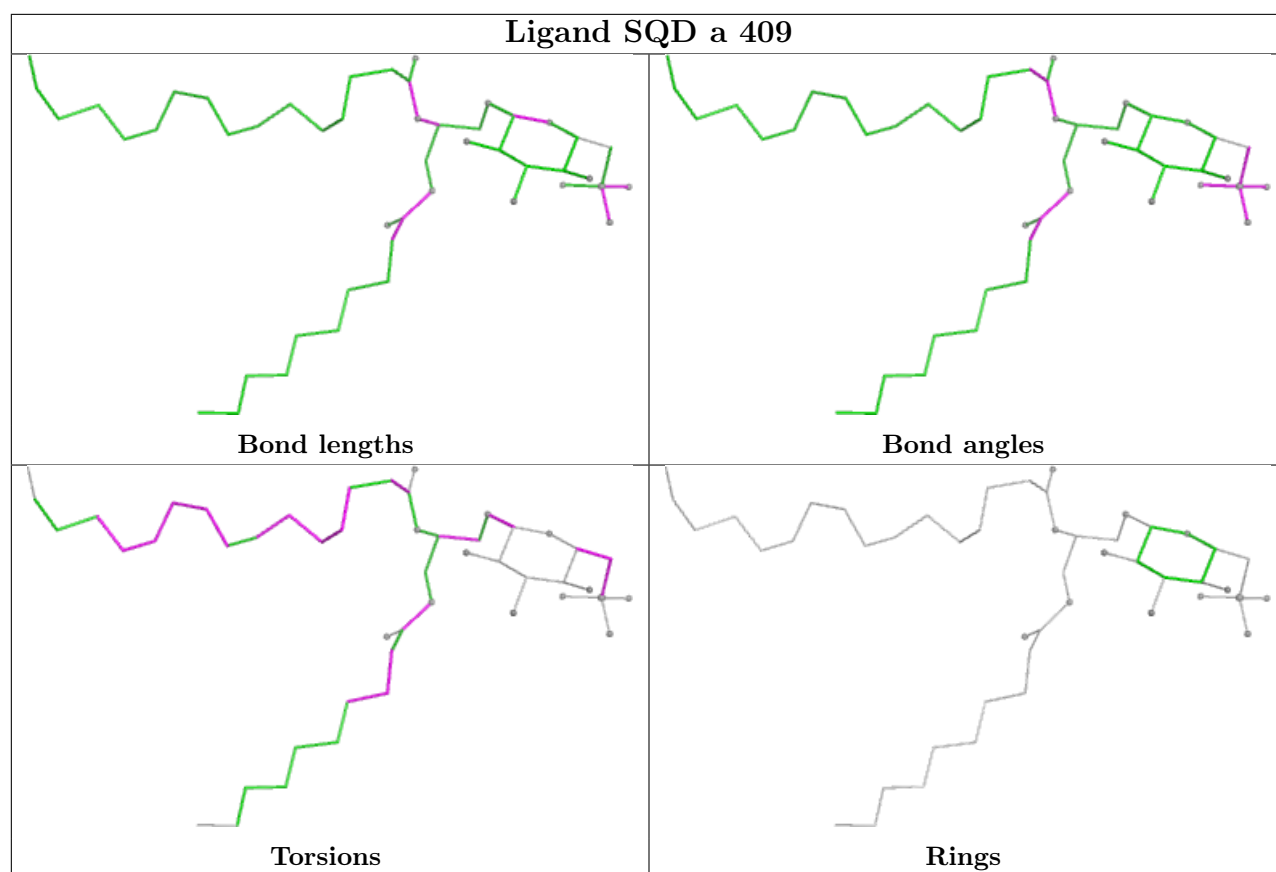
Ligand CHL g 608

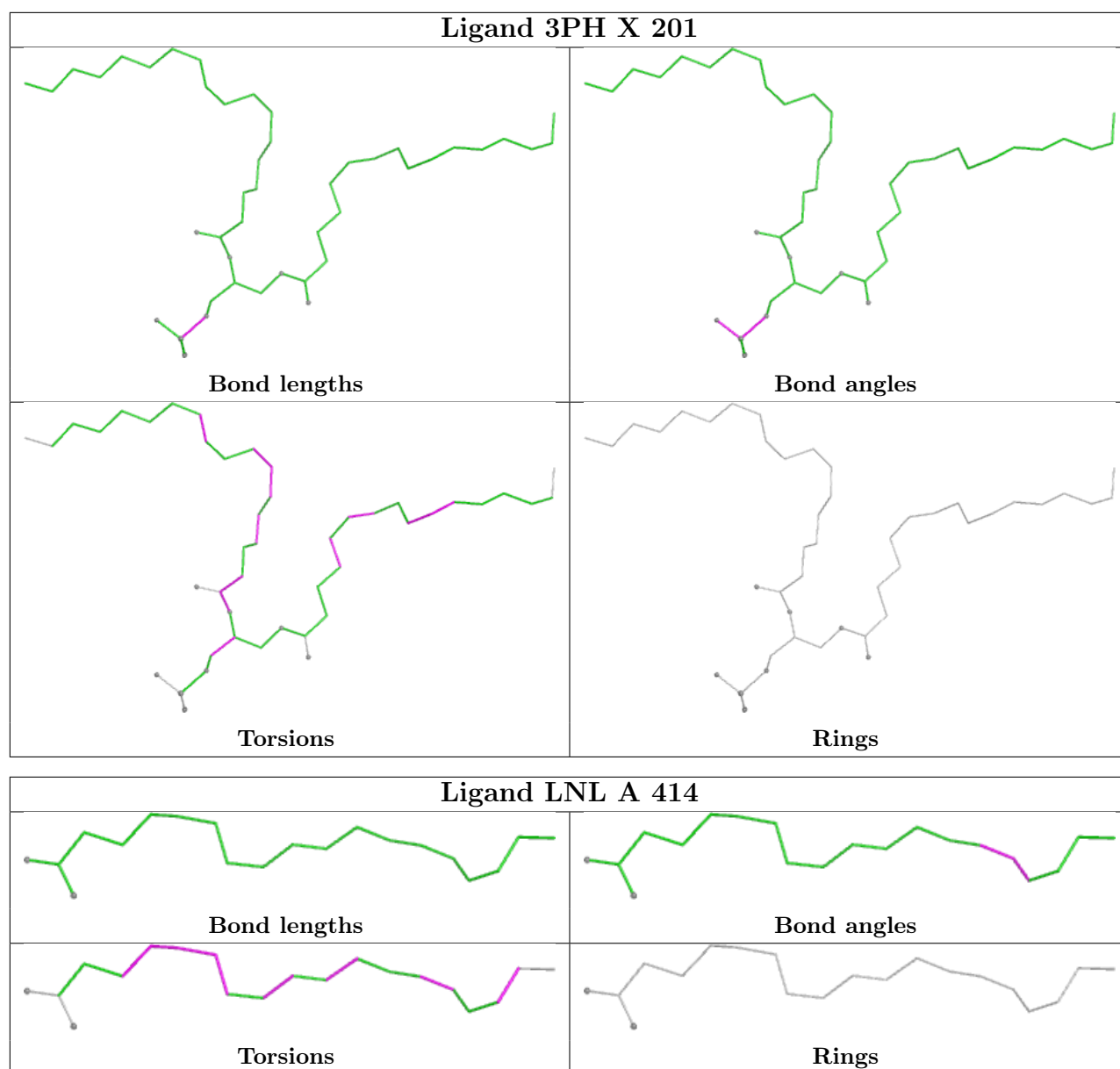


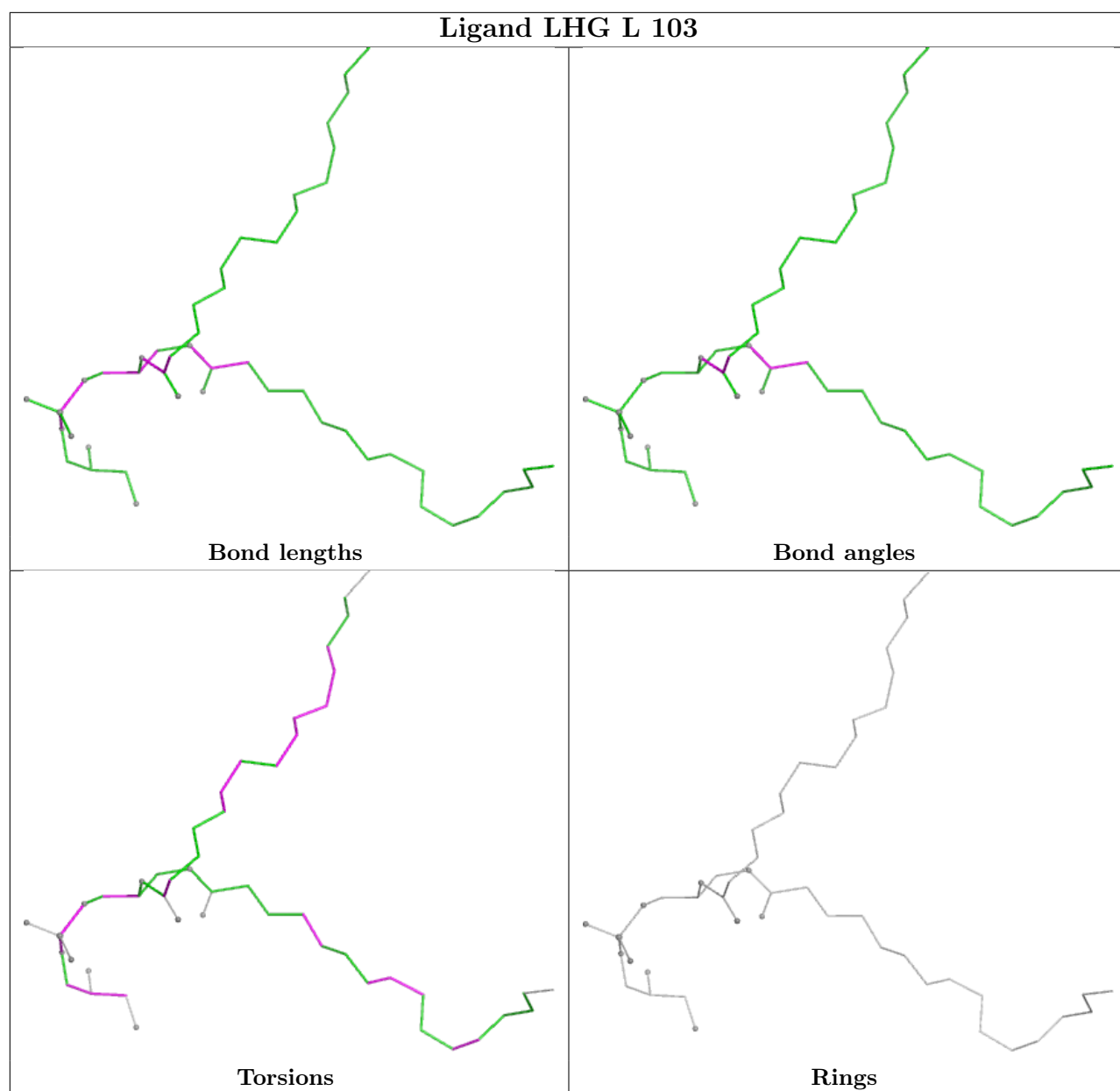
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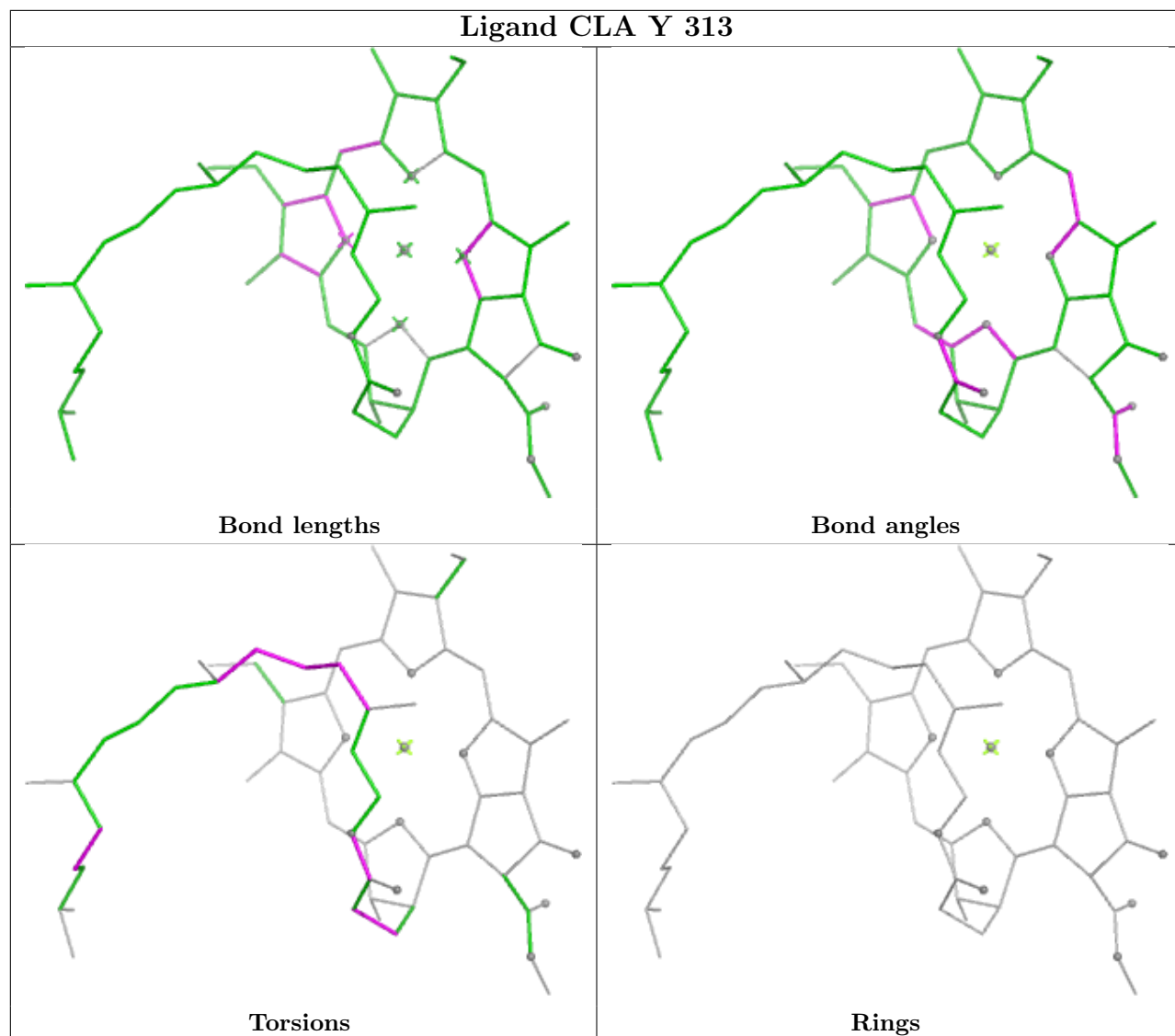




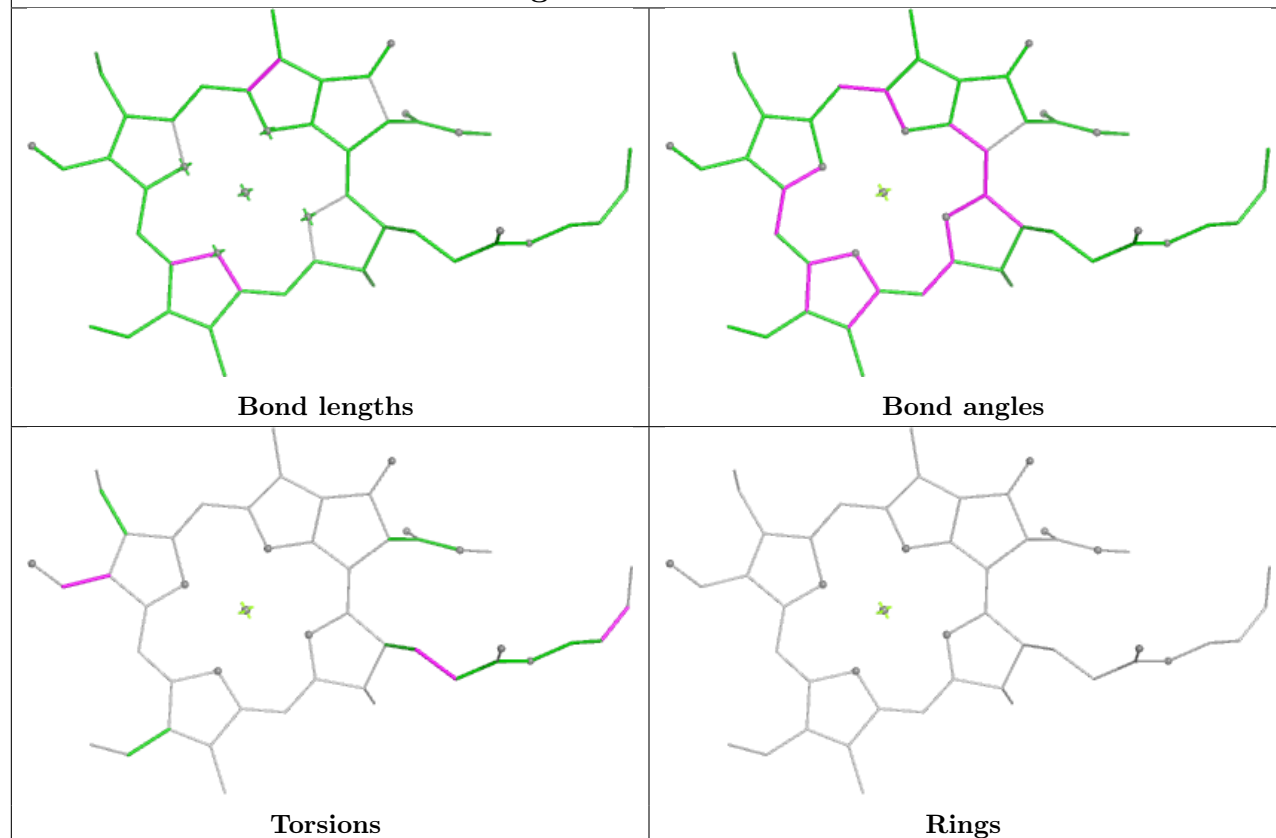




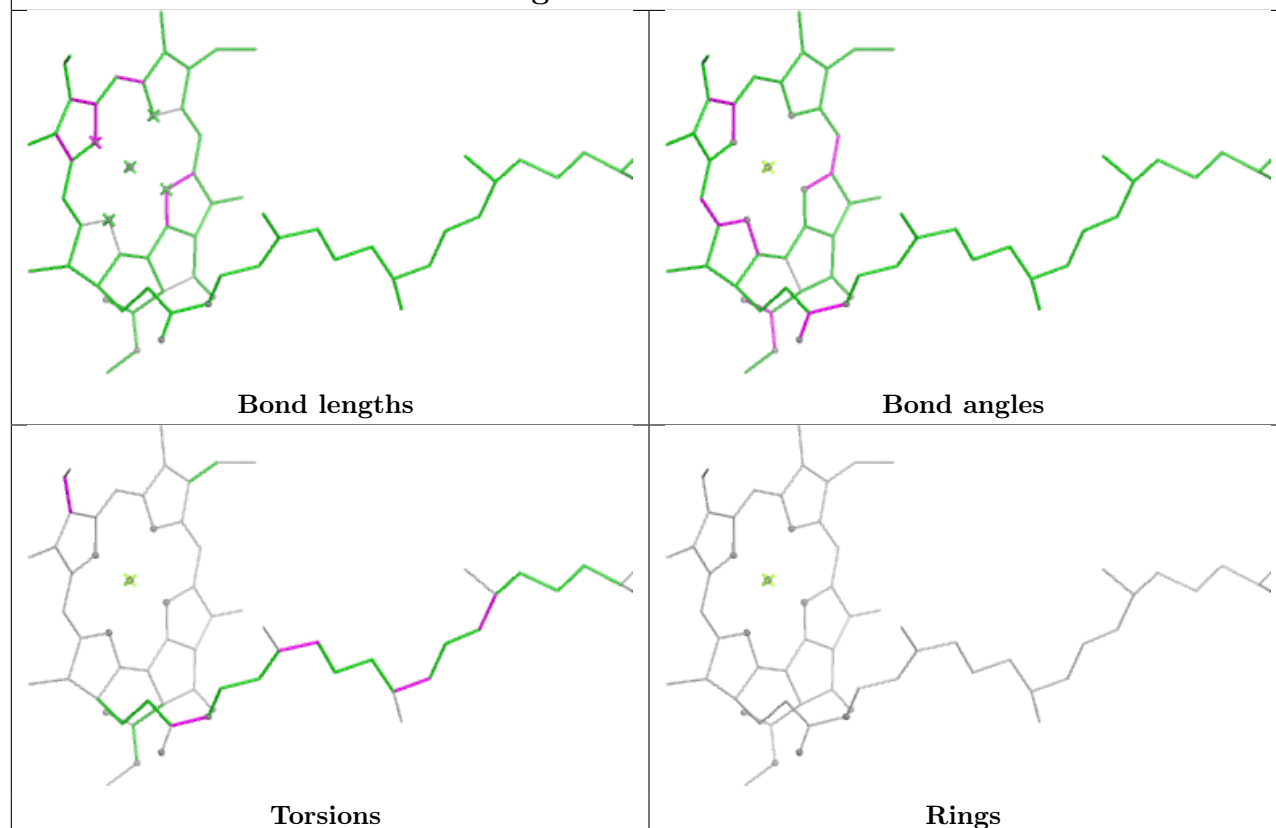


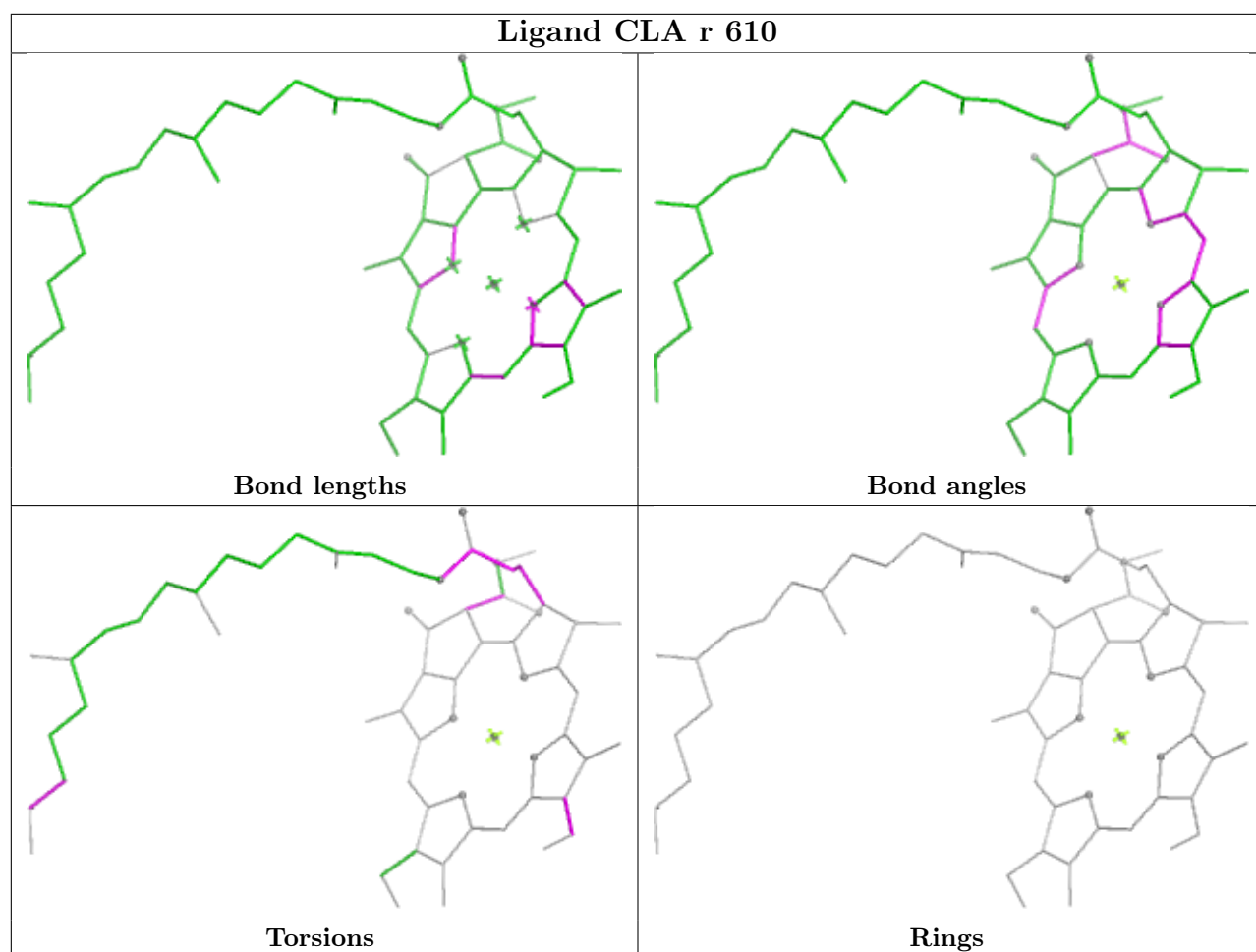


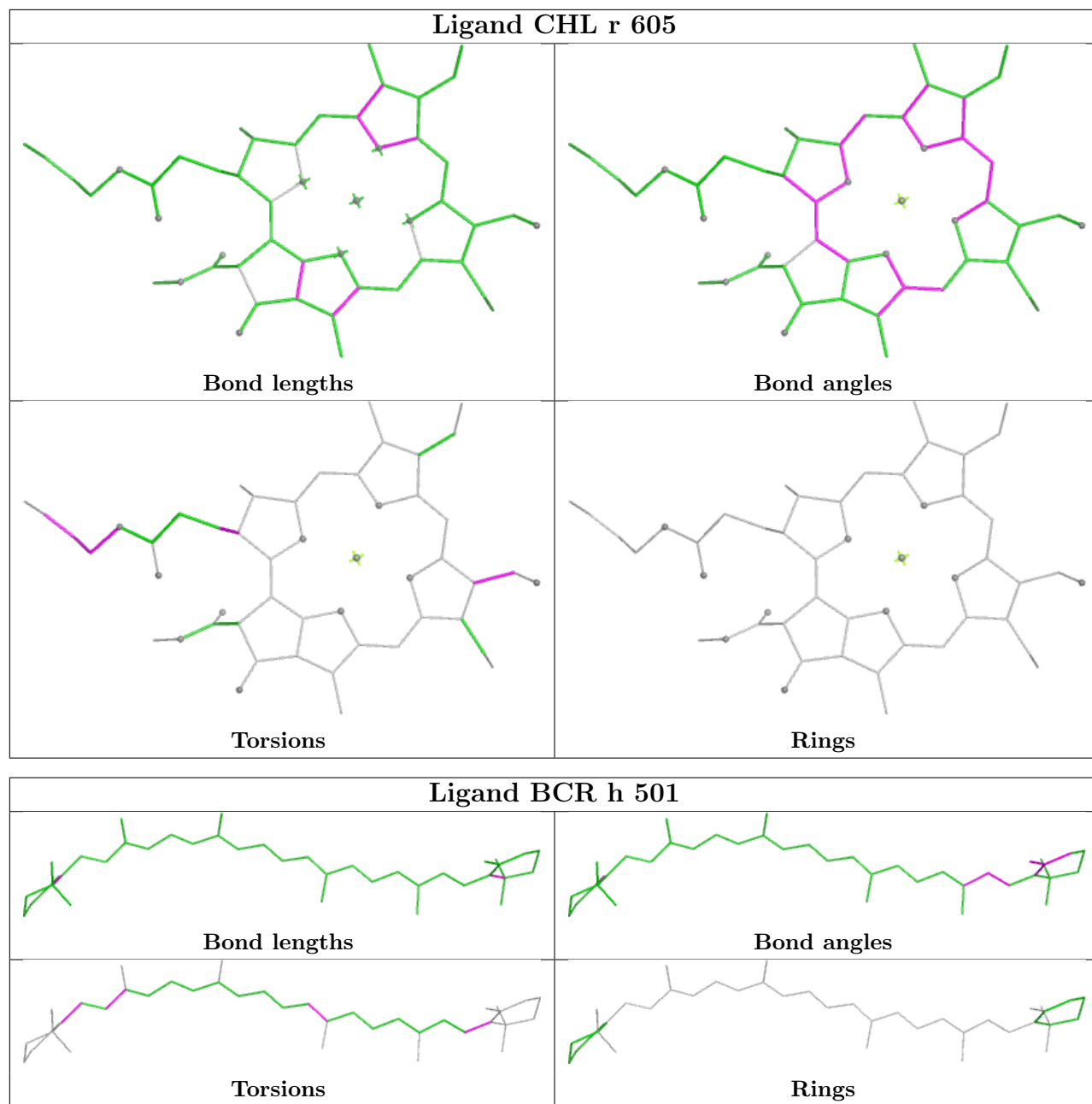
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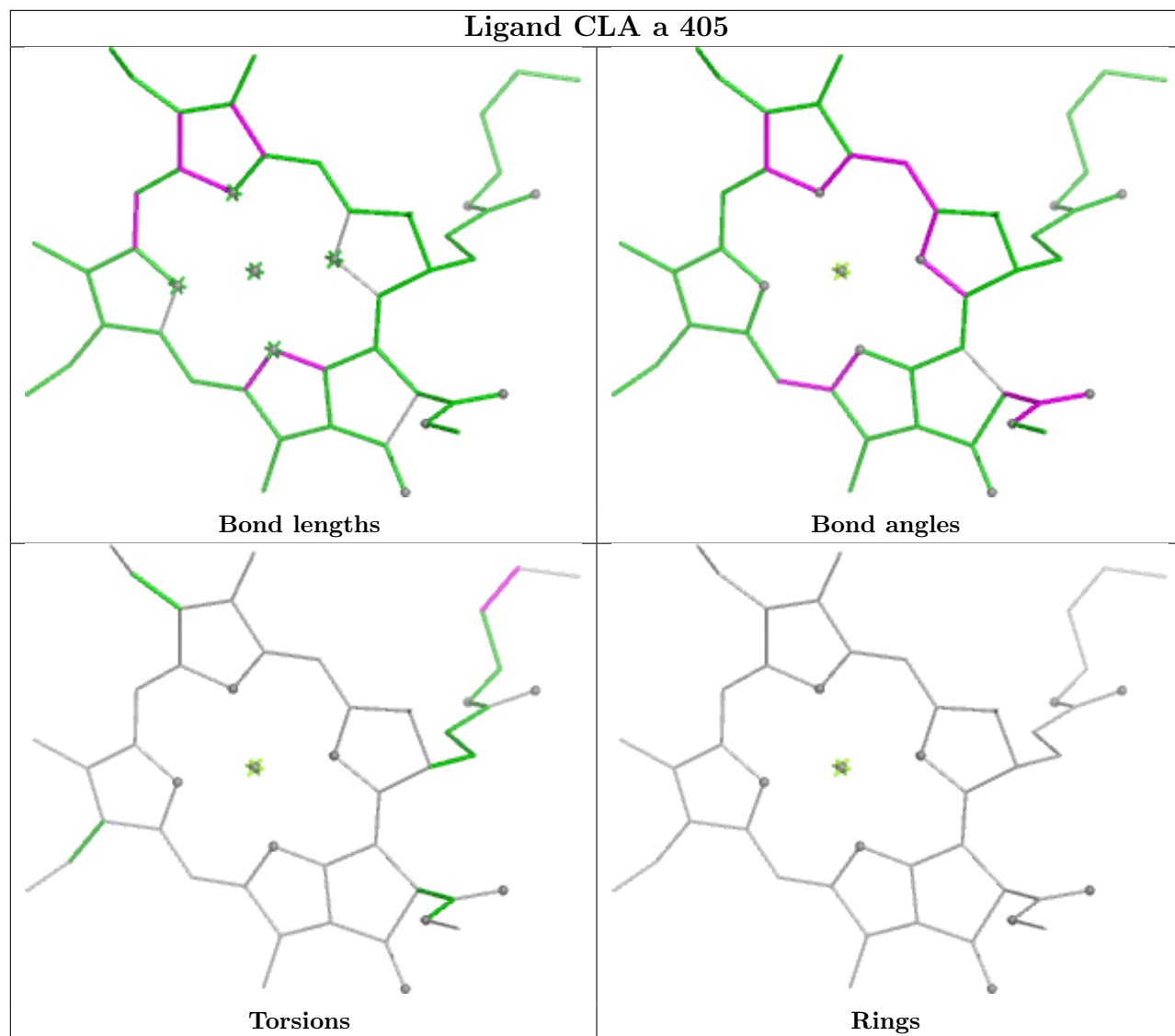


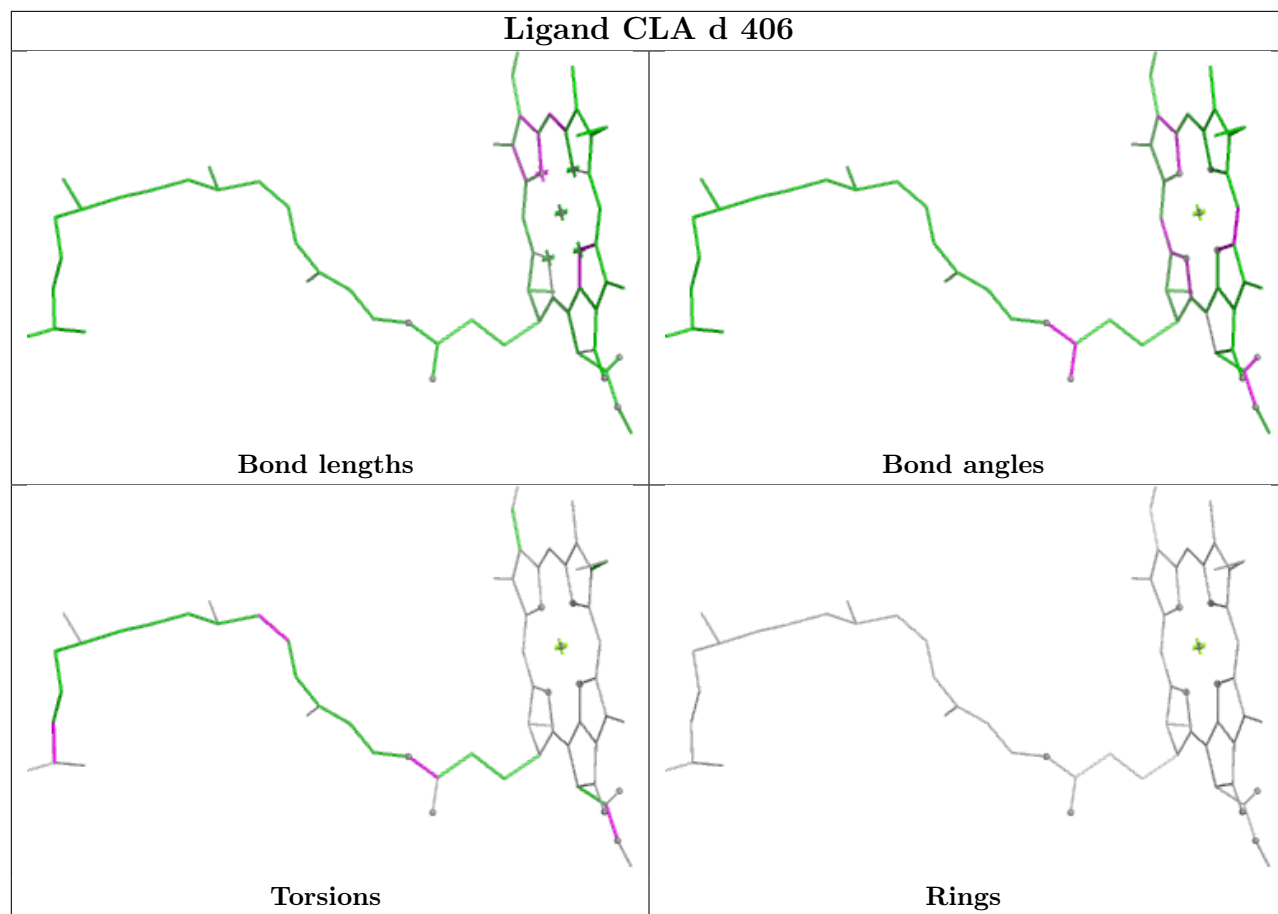
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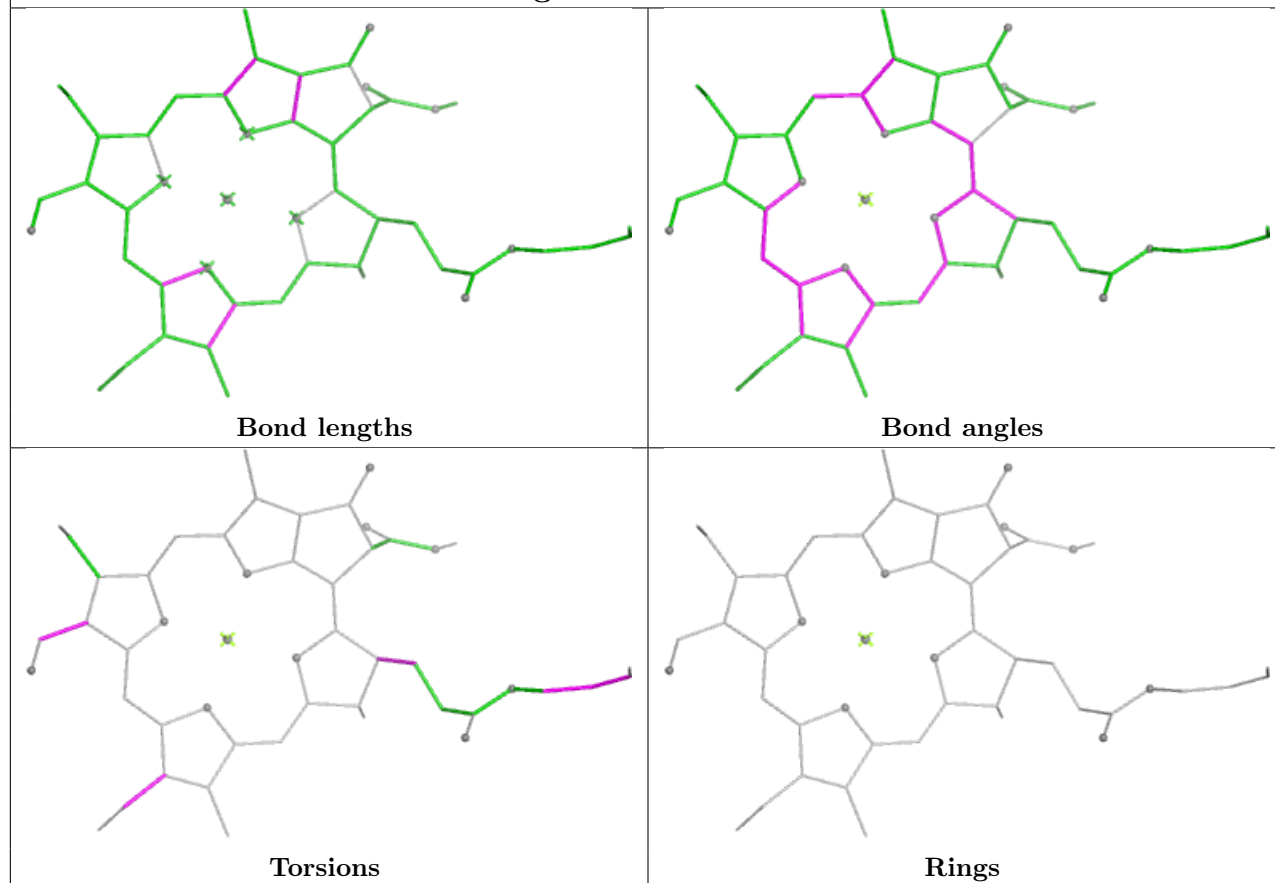




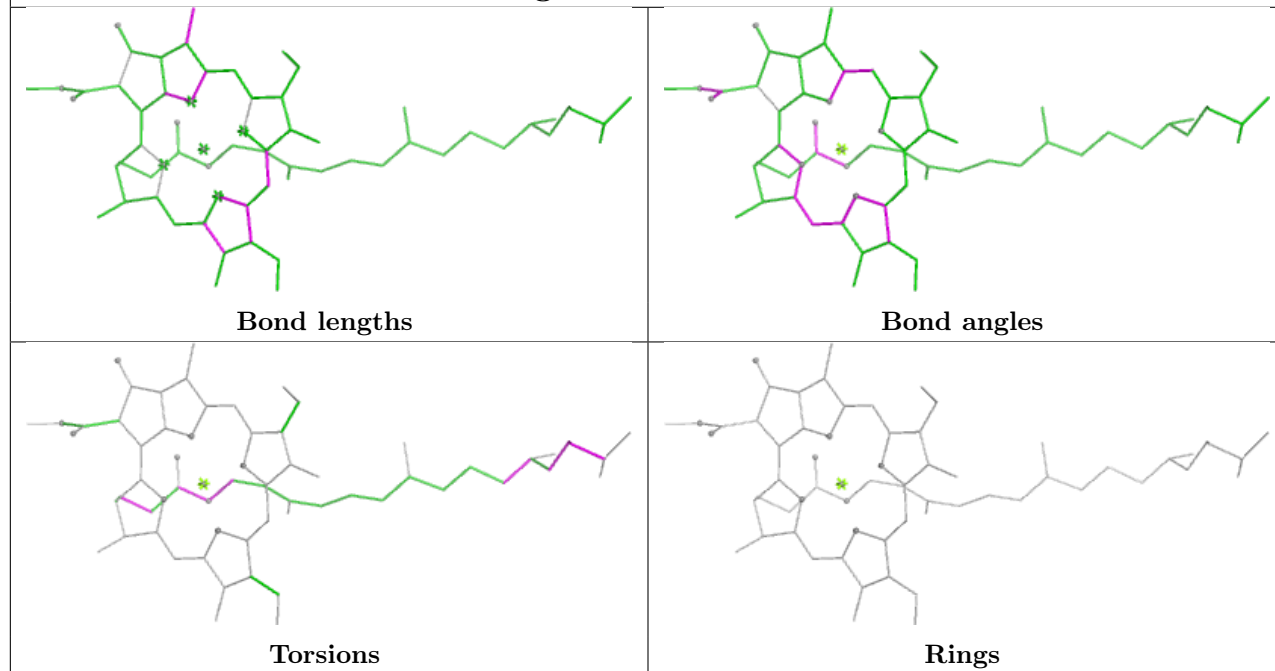


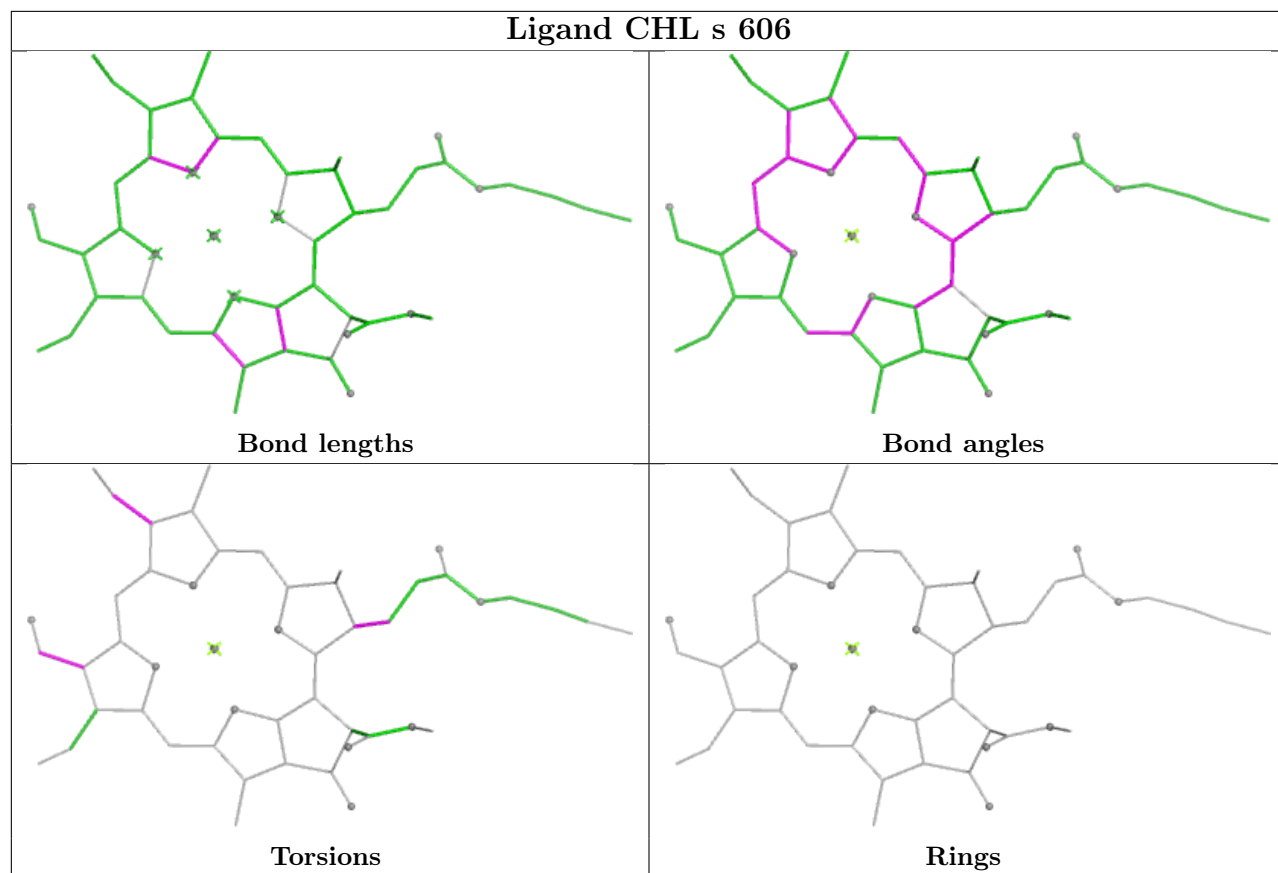


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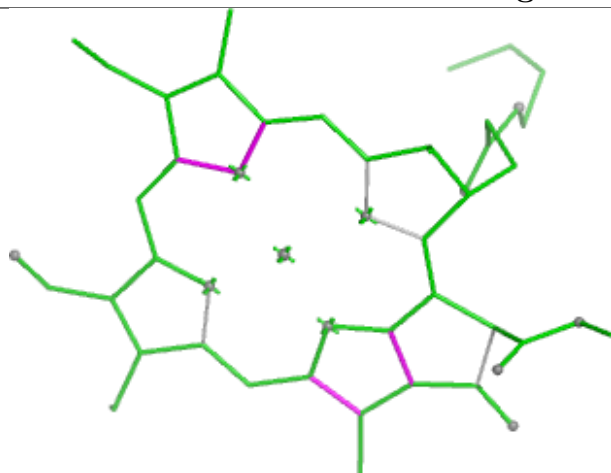


Ligand CLA b 608

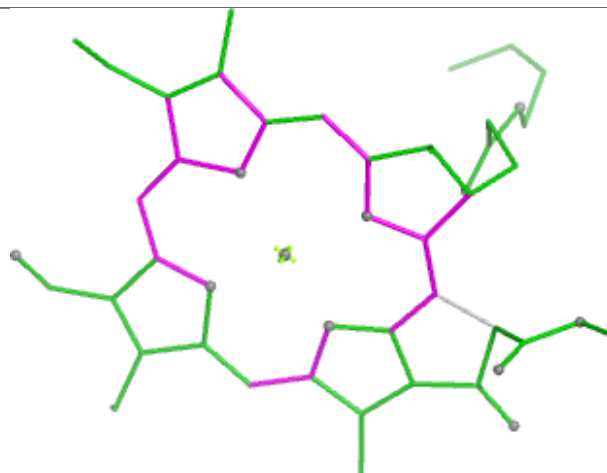




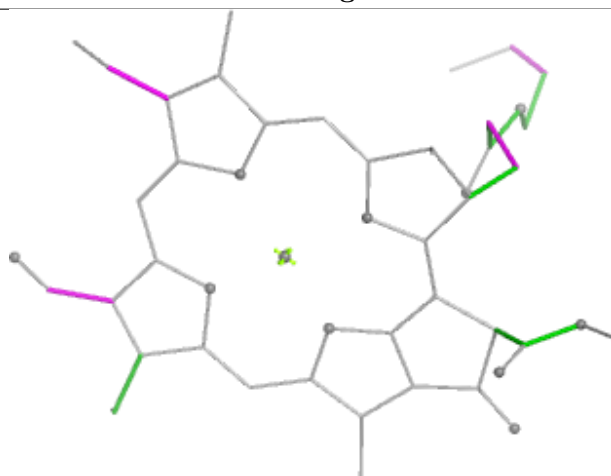
Ligand CHL n 608



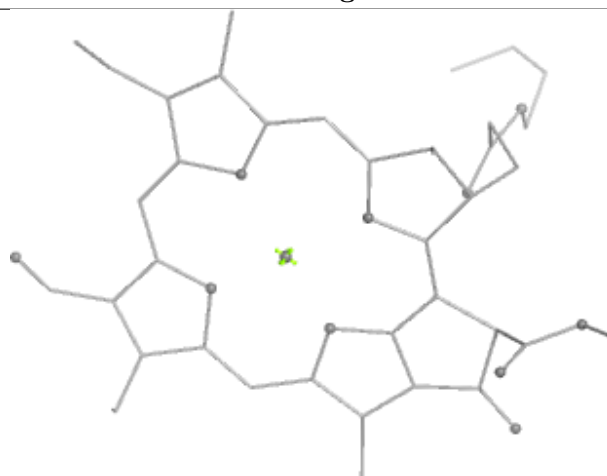
Bond lengths



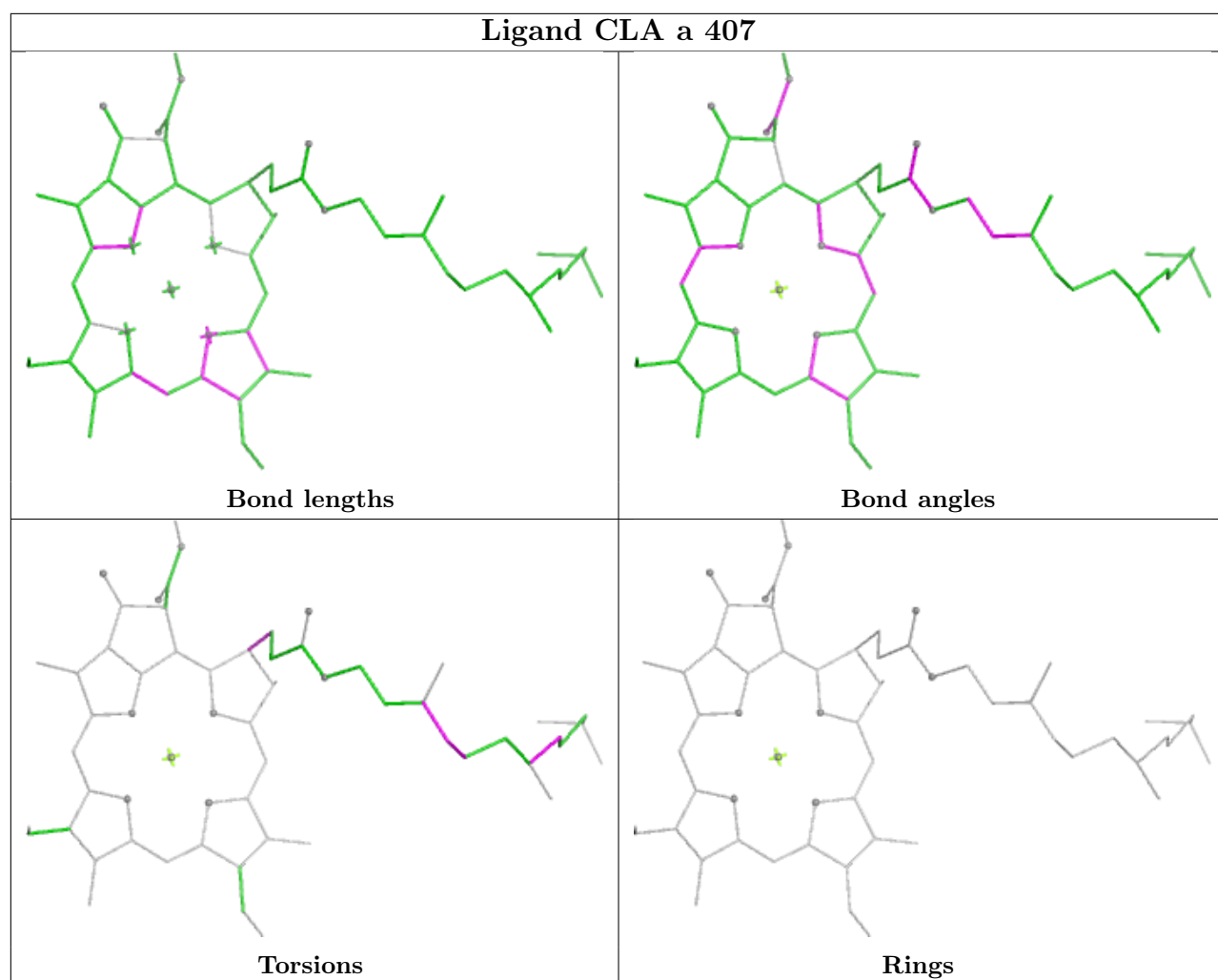
Bond angles

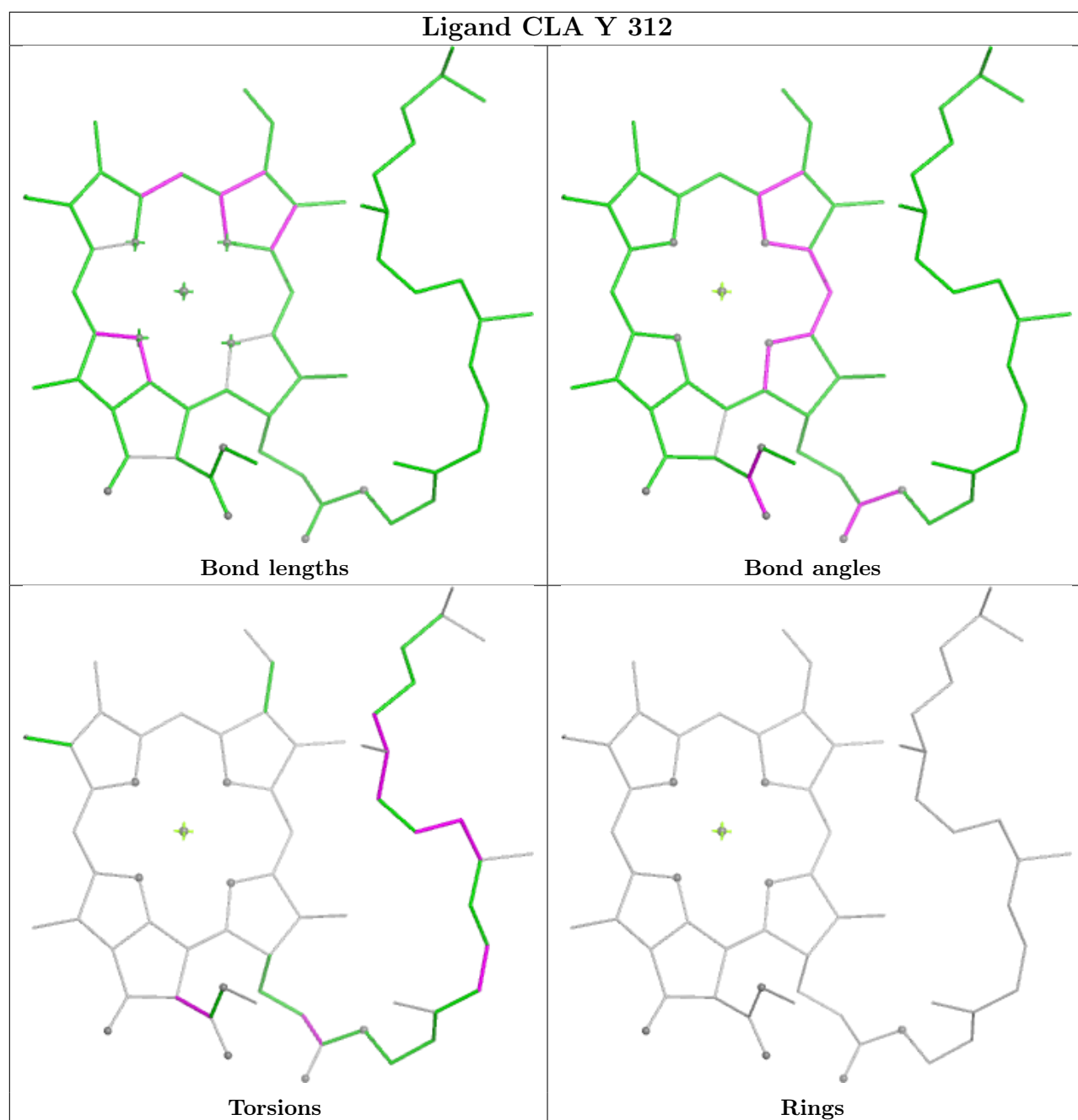


Torsions

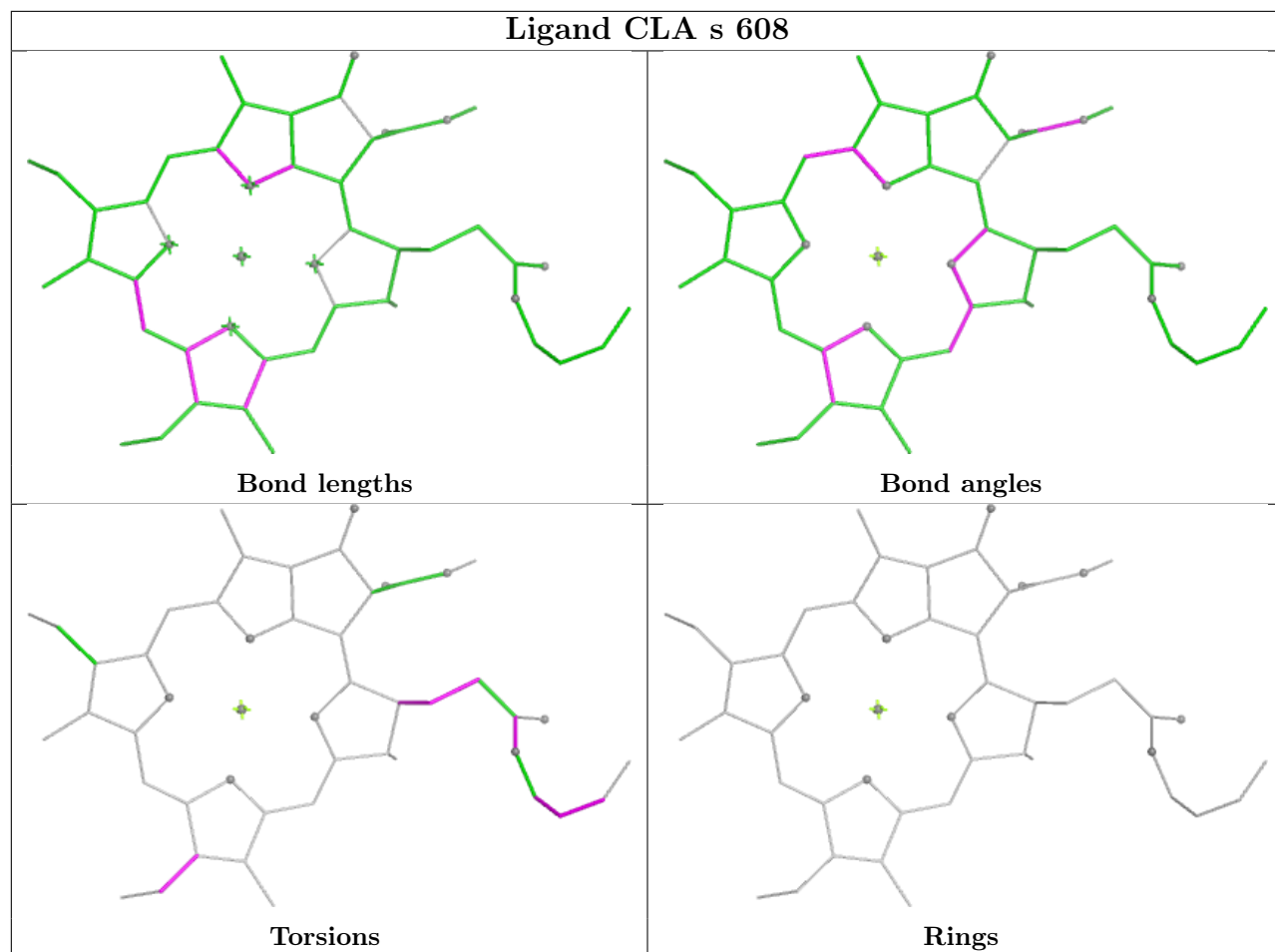


Rings

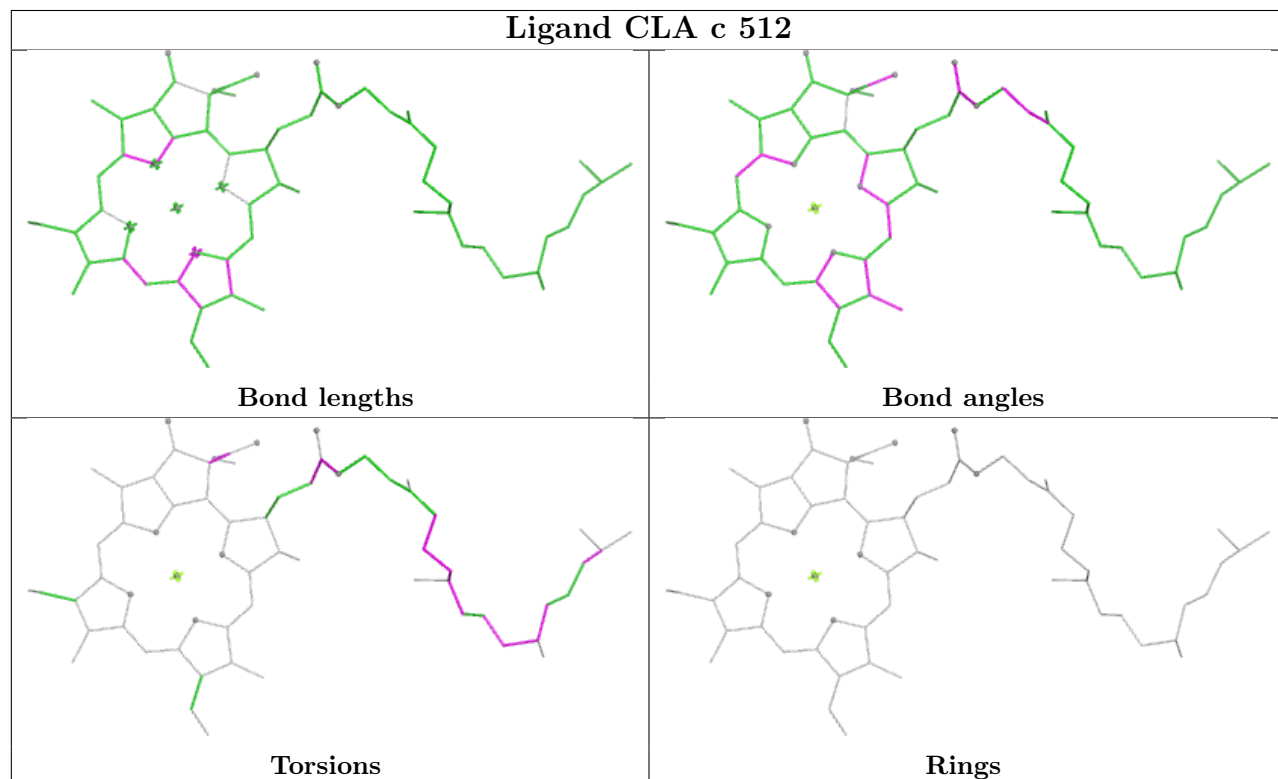


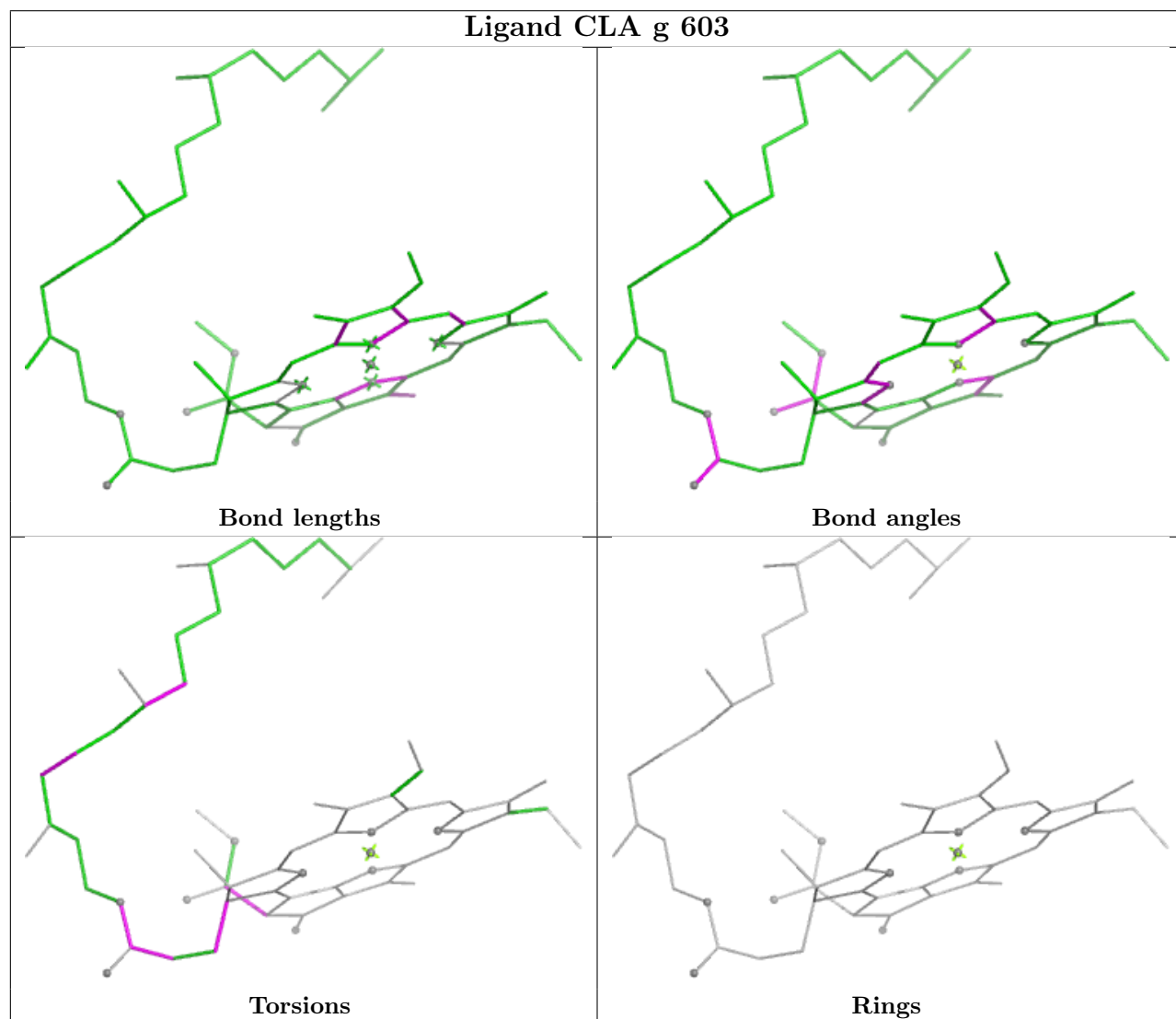
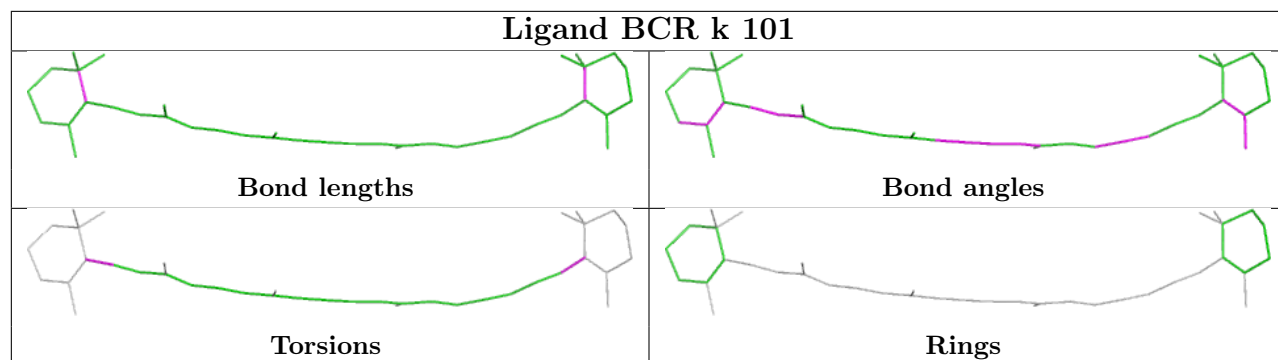


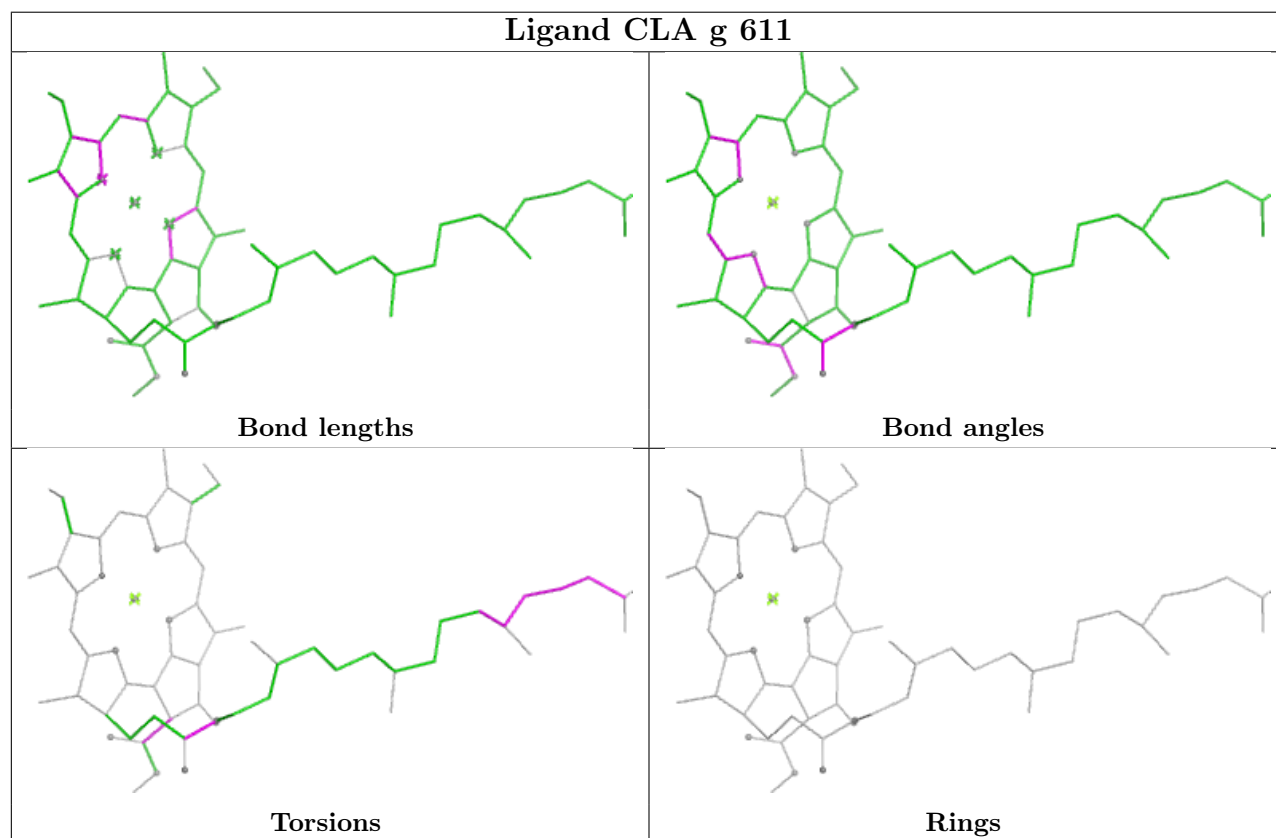
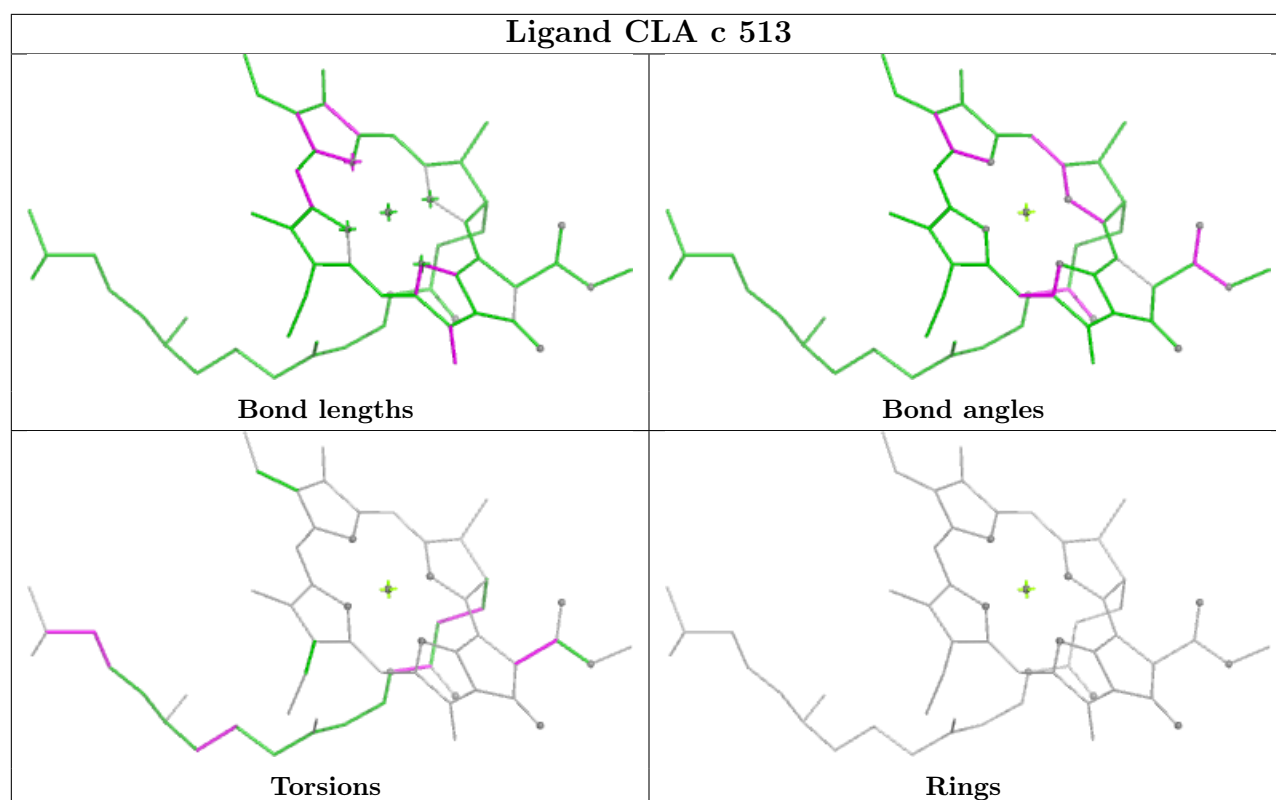
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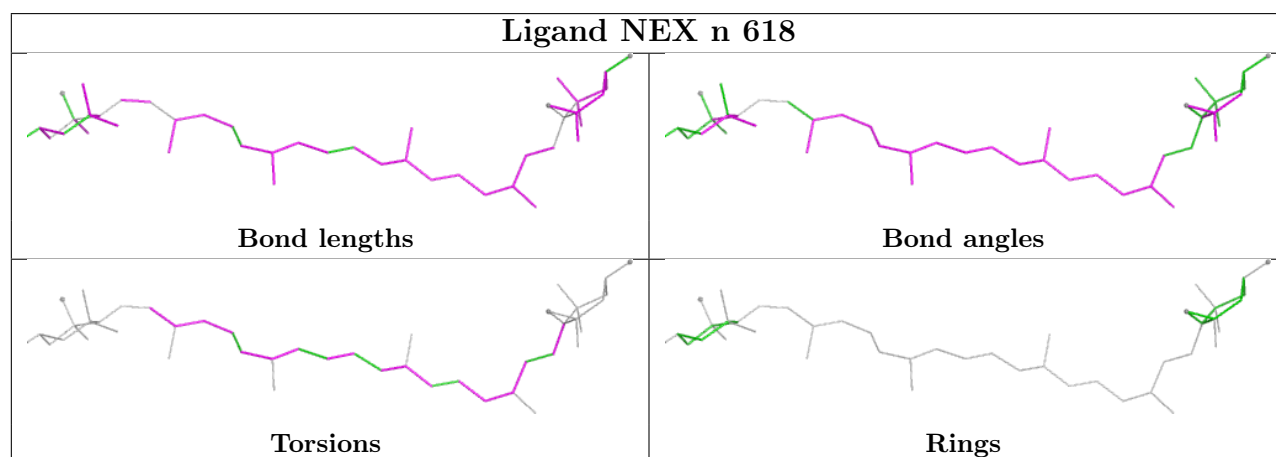
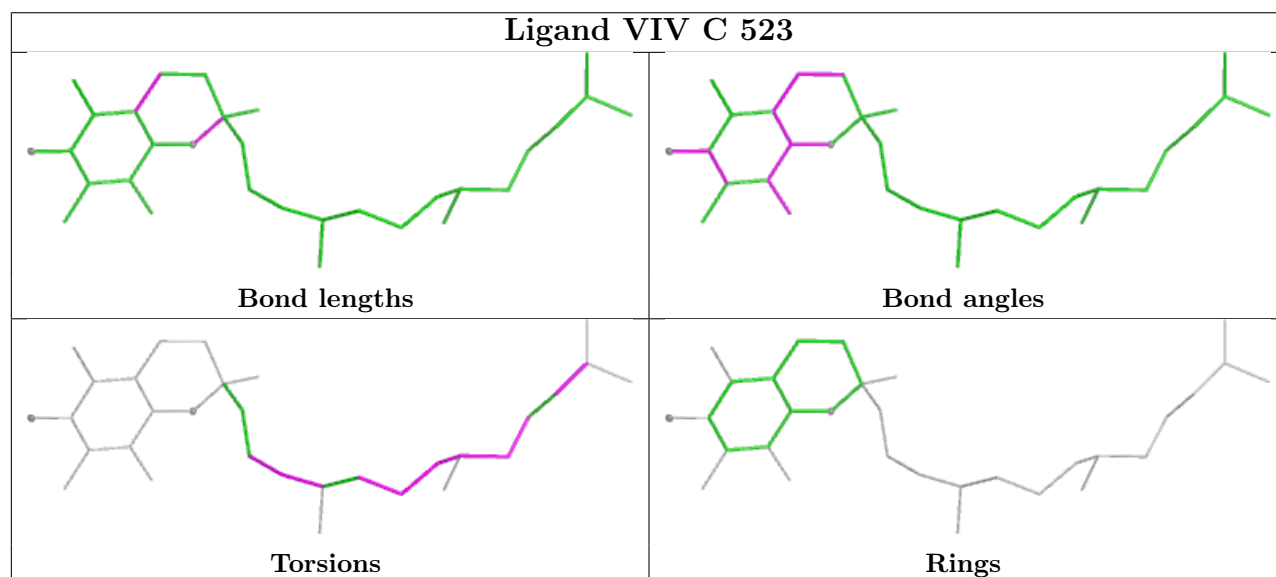
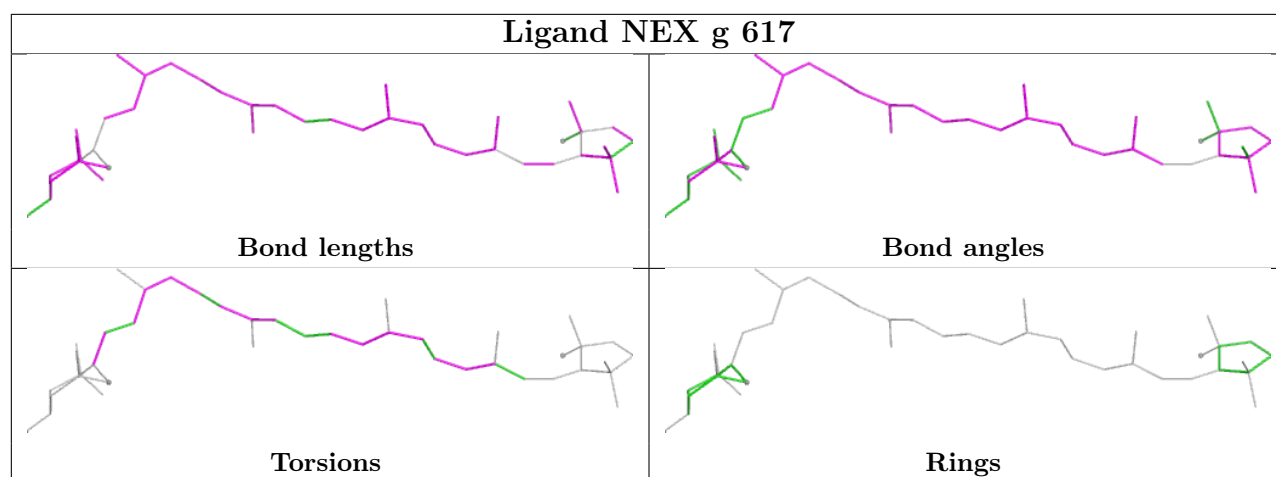


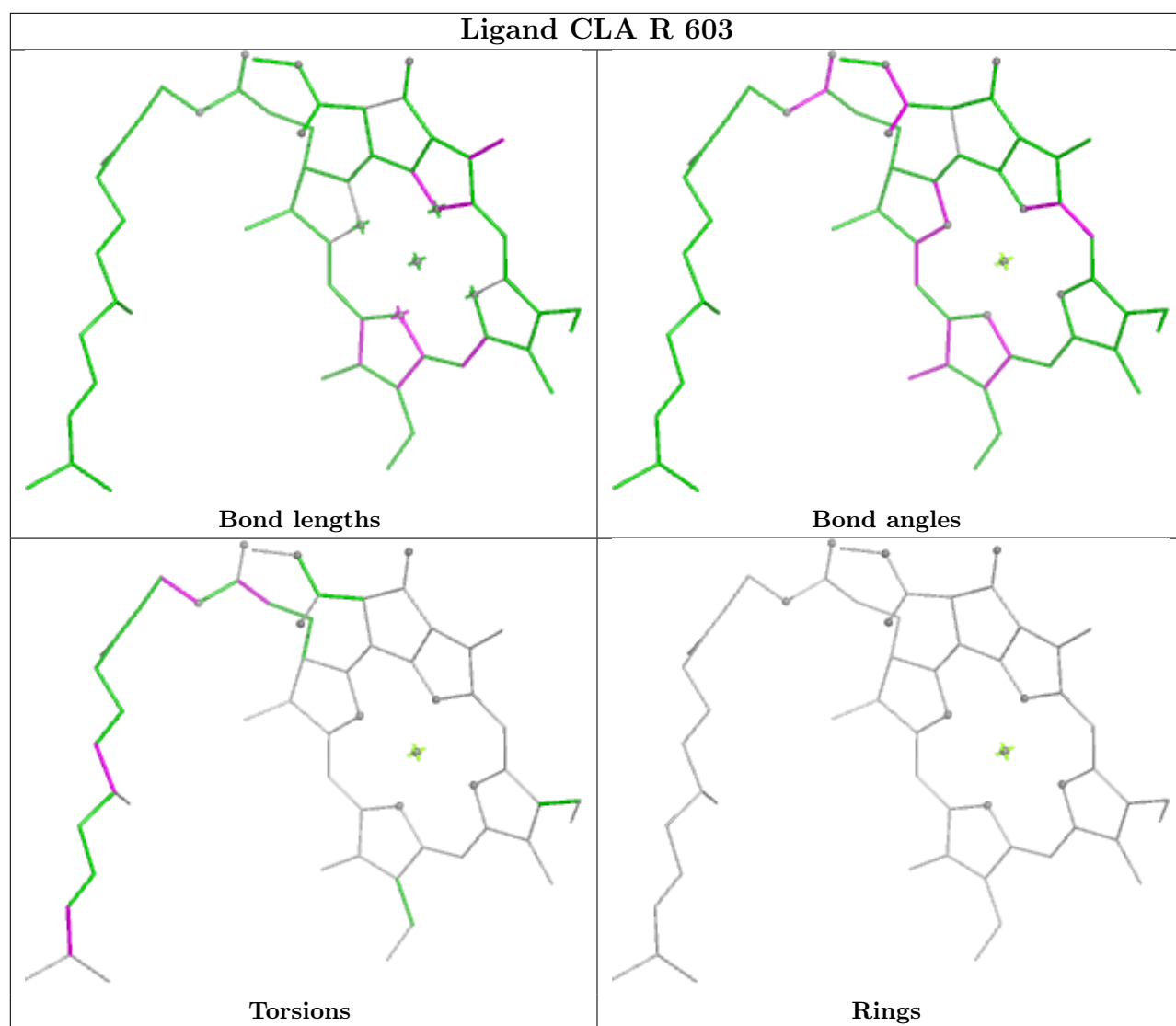
Ligand CLA c 512

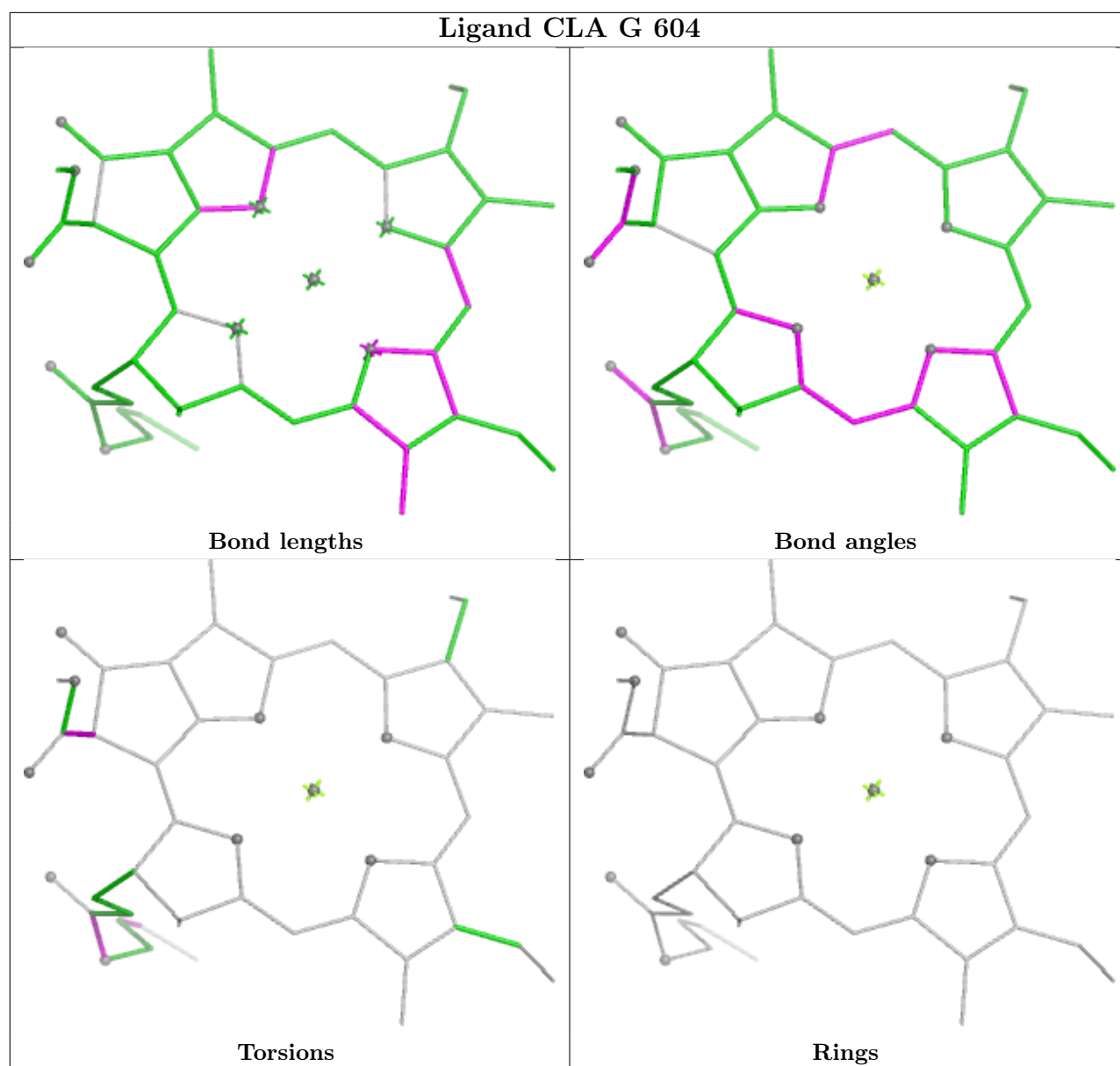


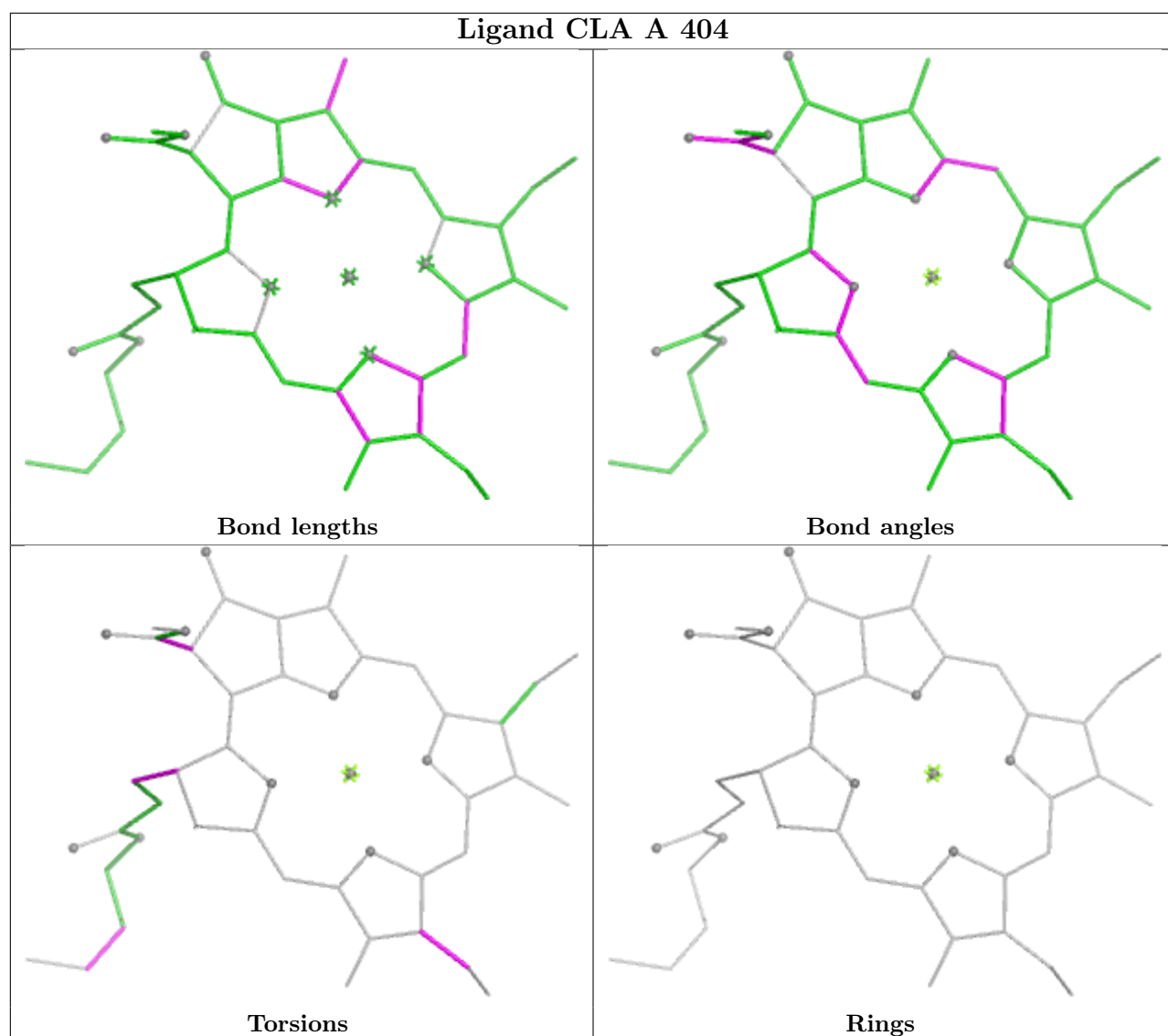




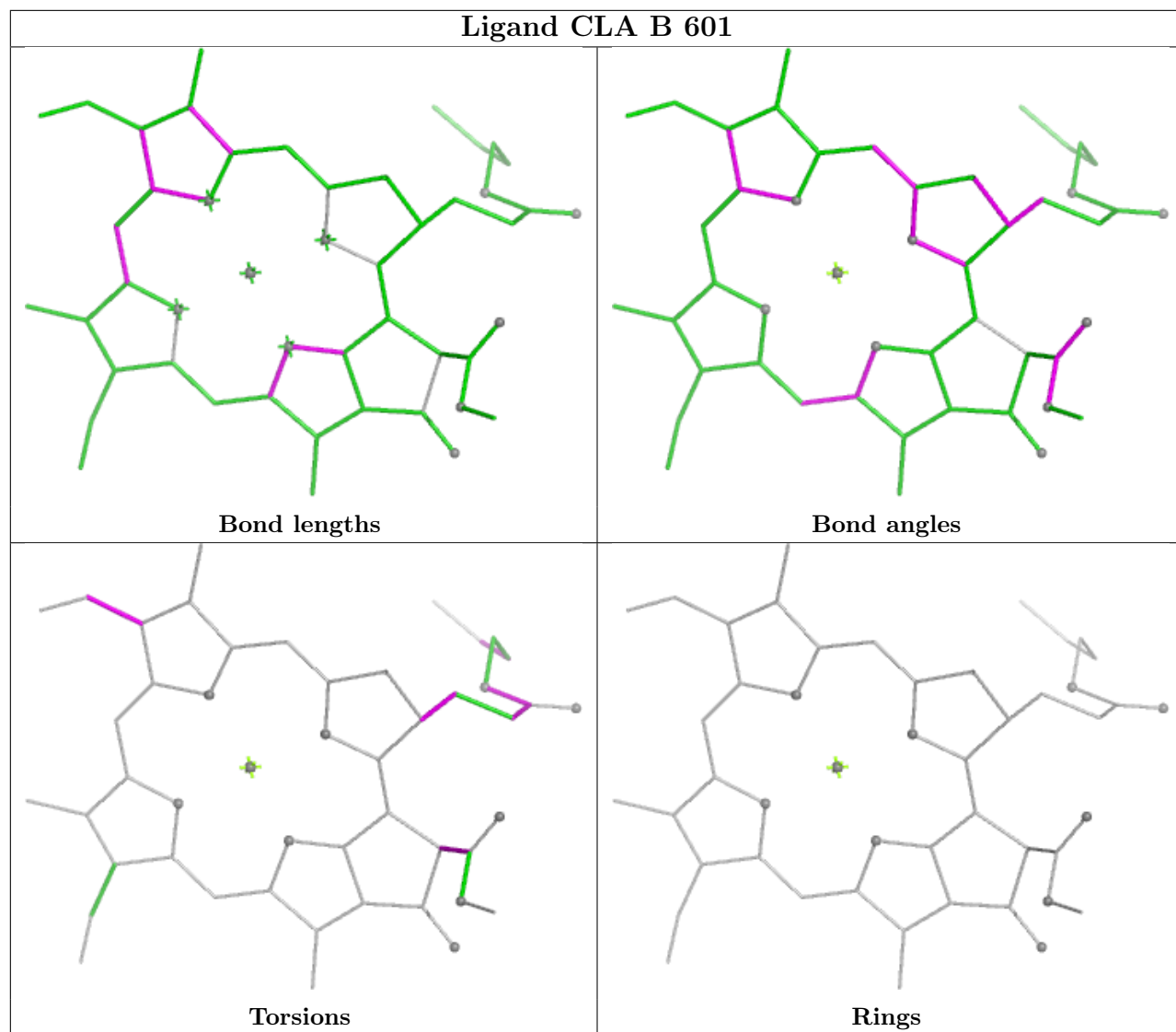


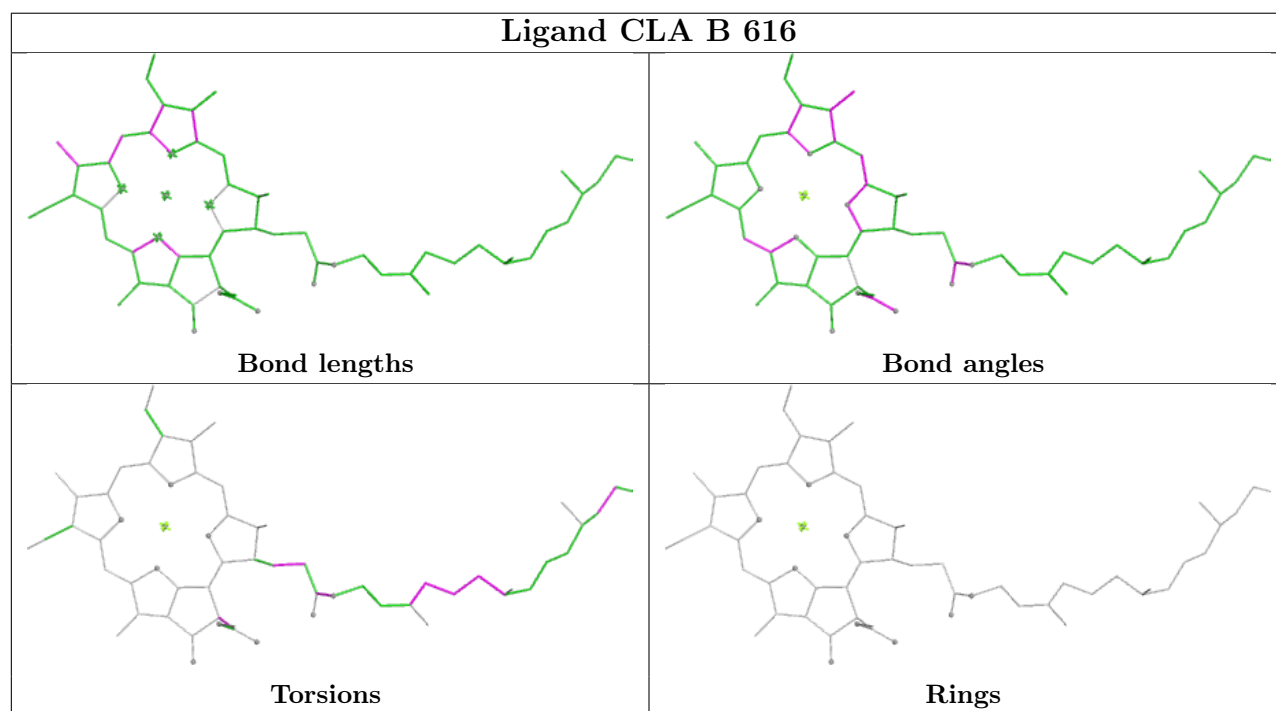
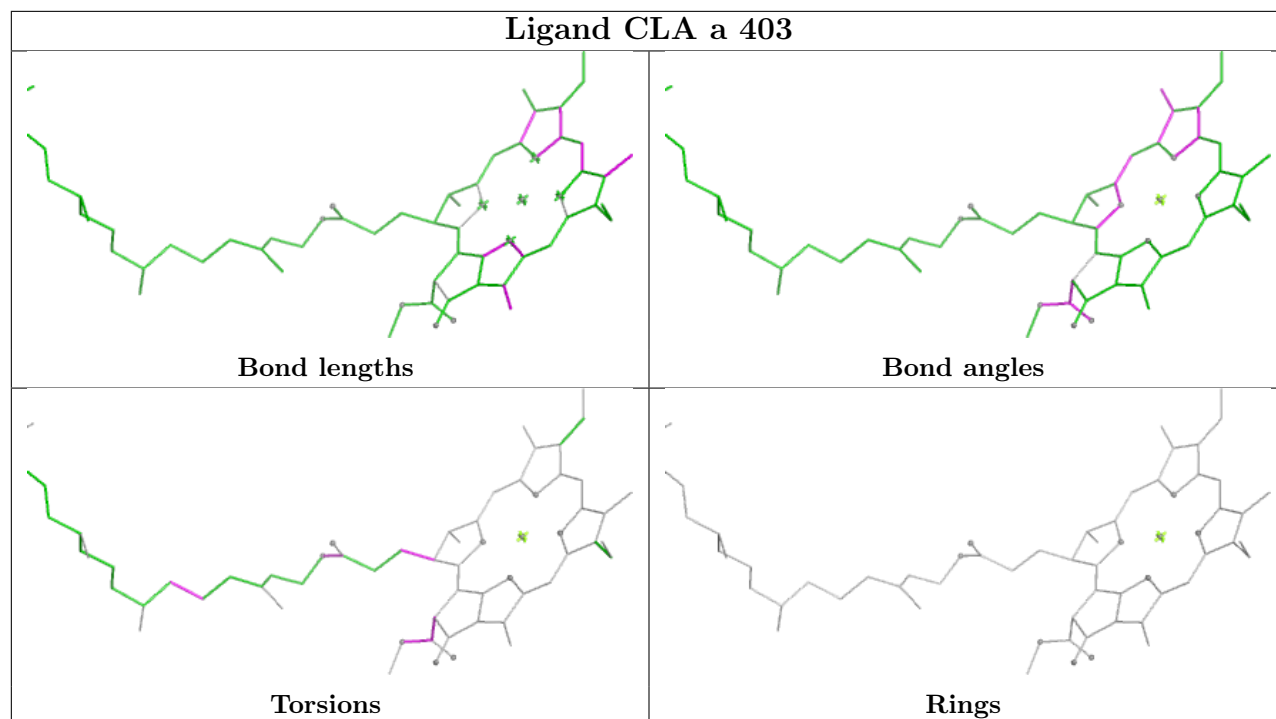




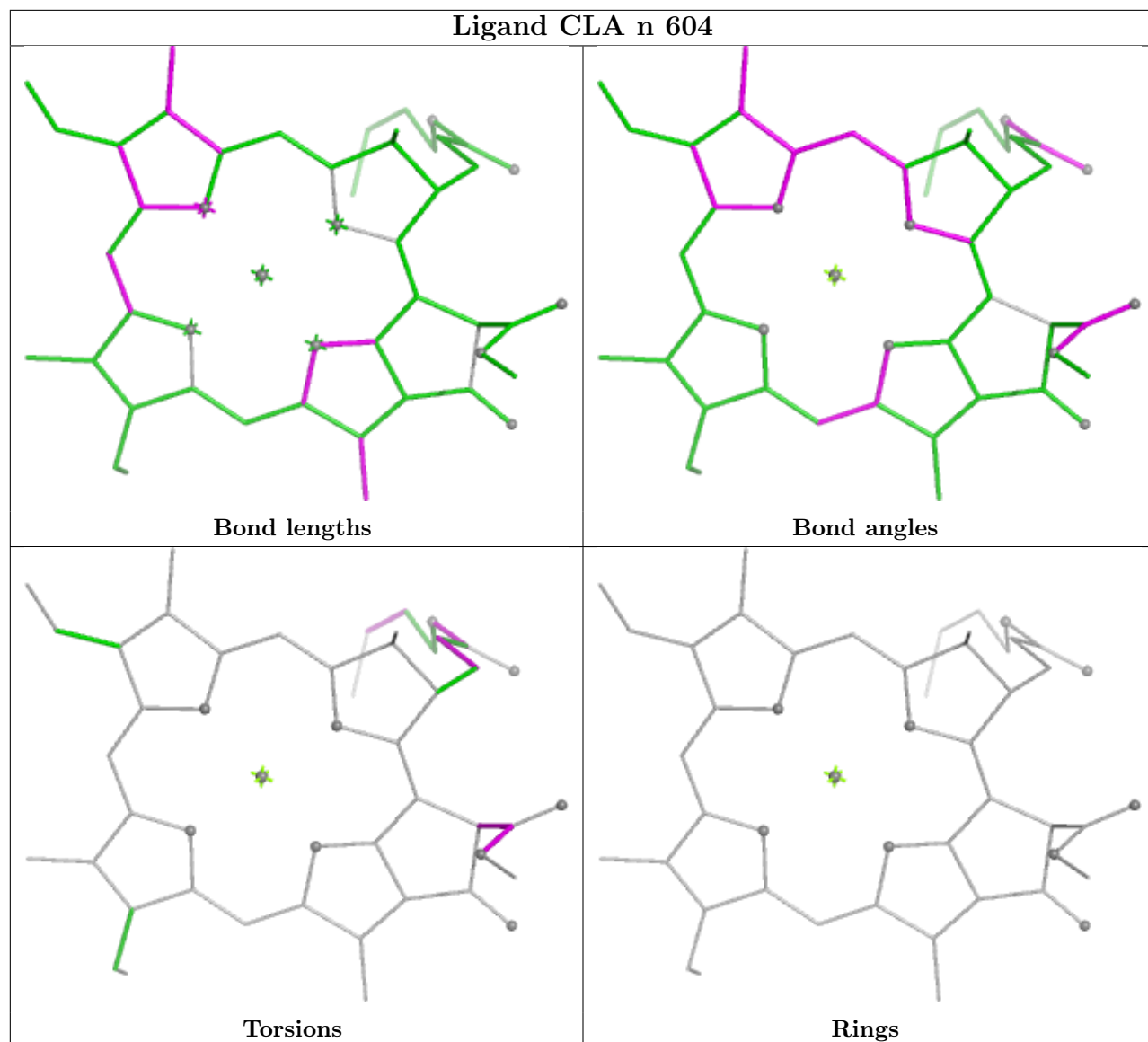


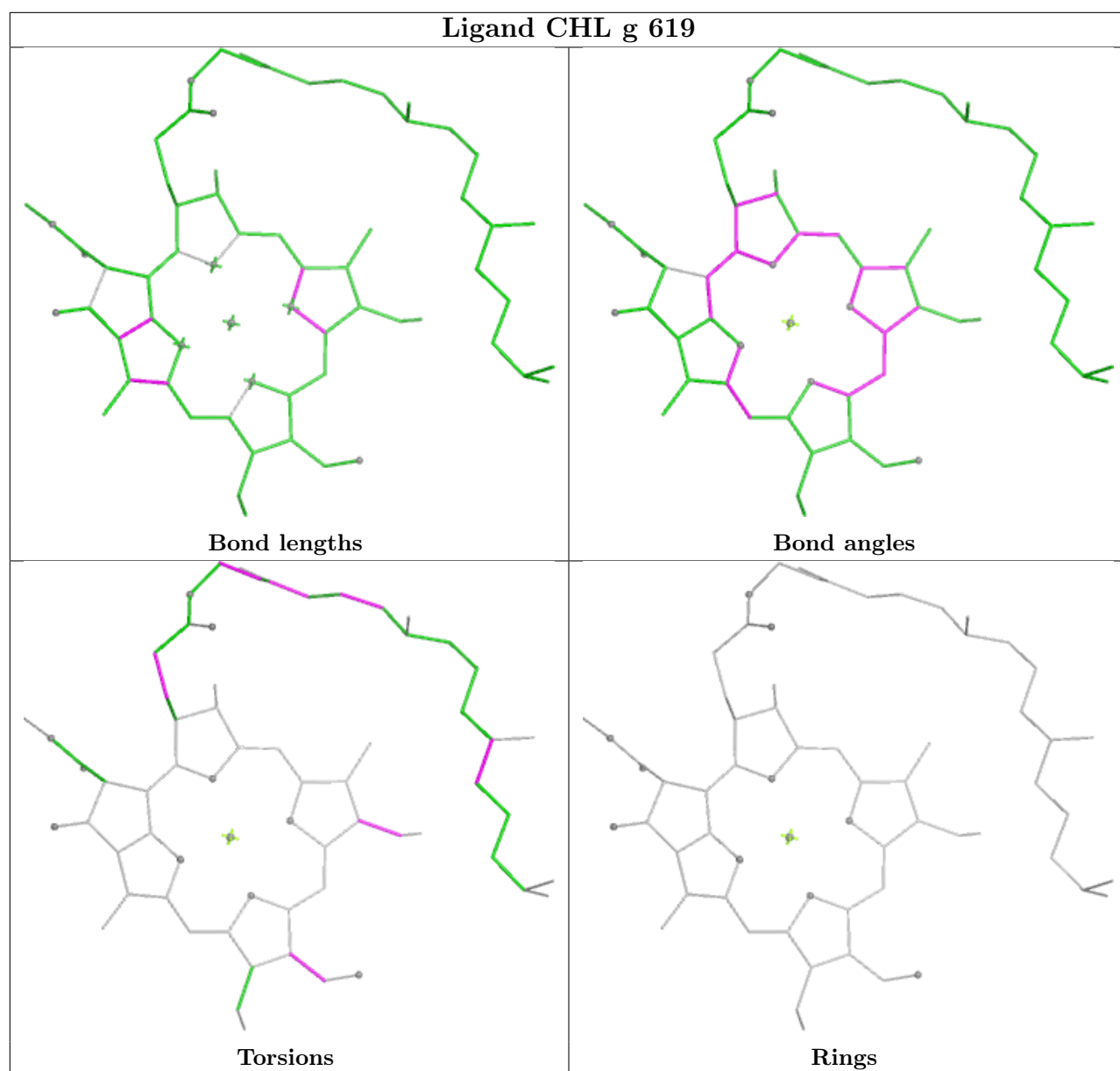
Ligand CLA B 601

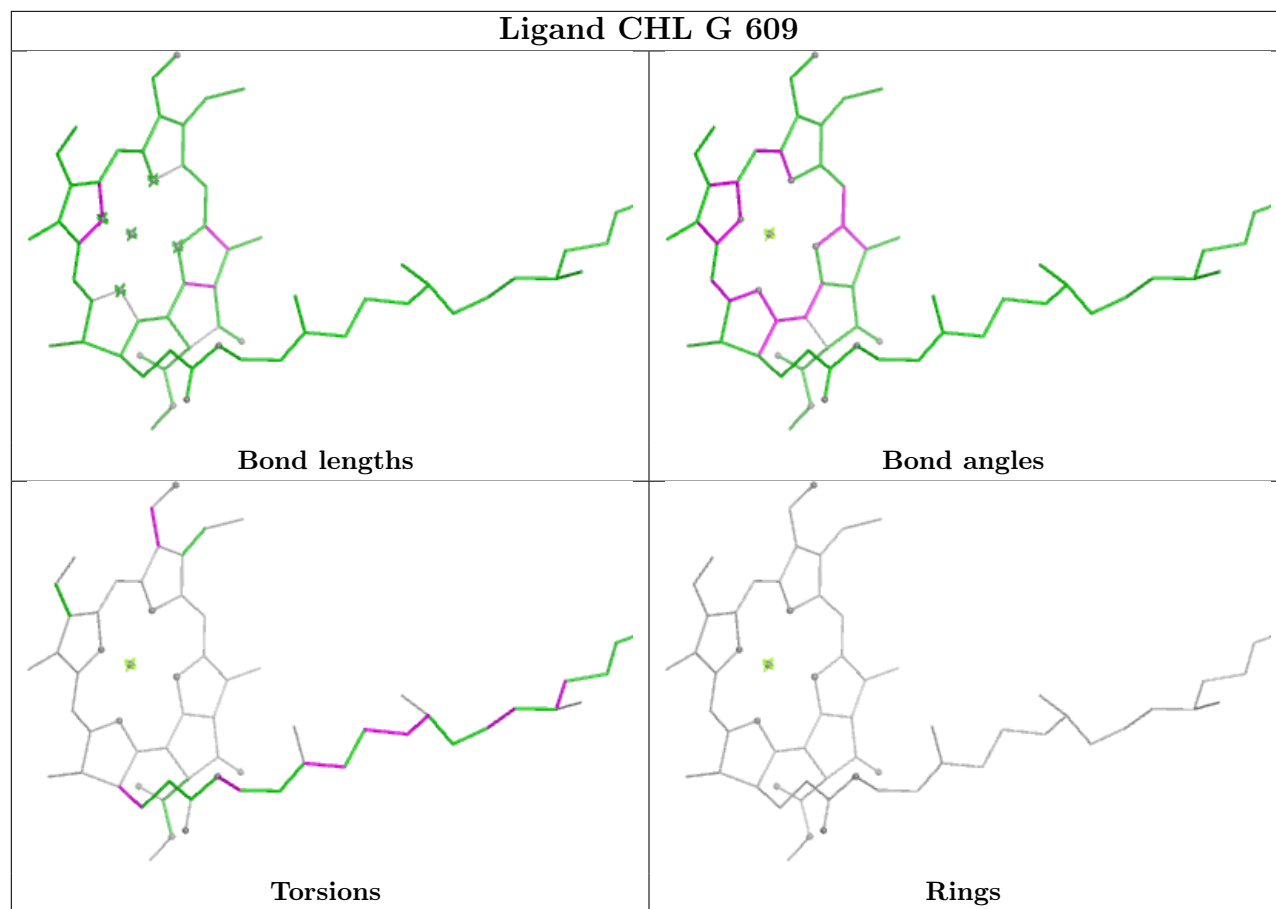




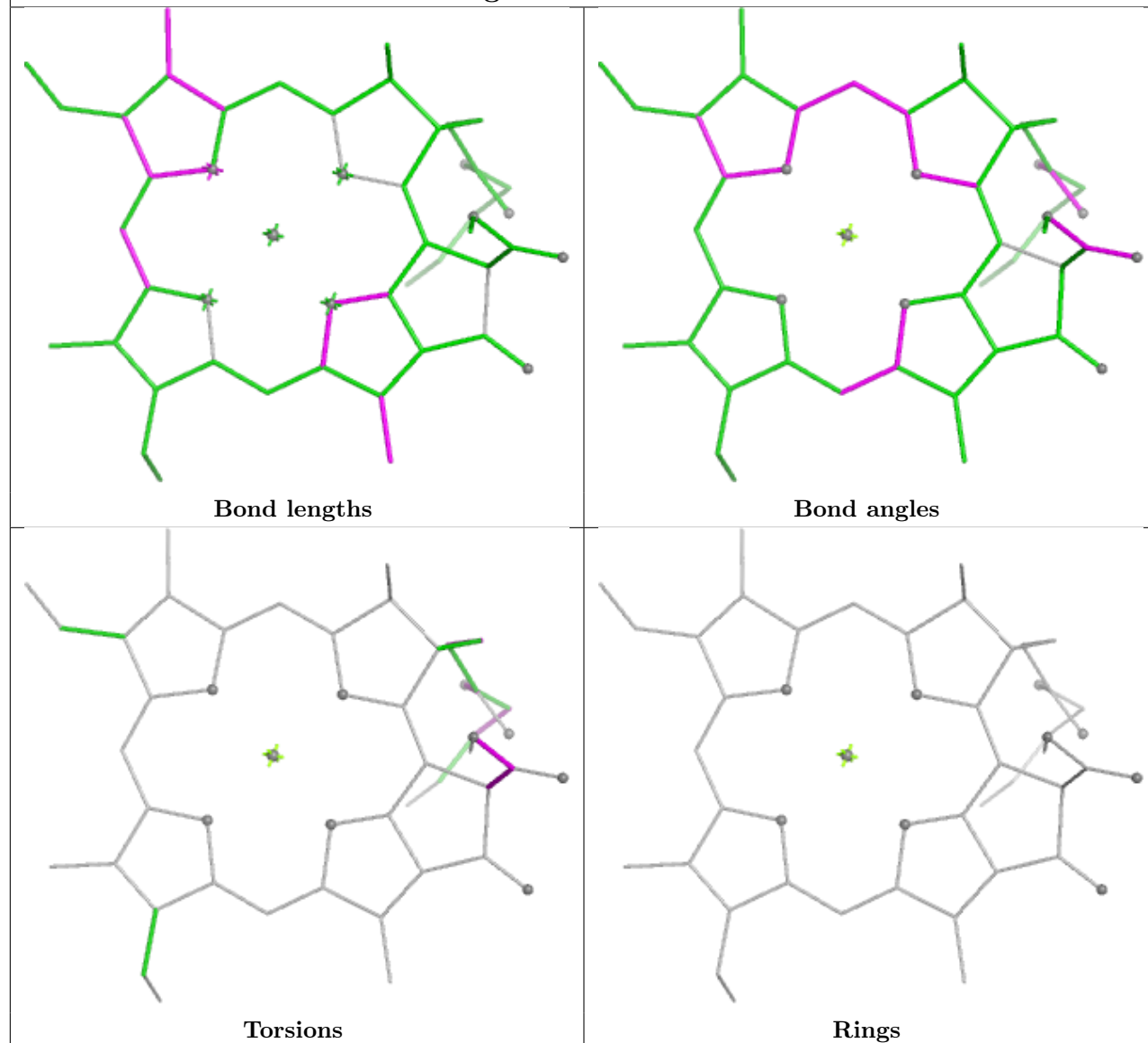
Ligand CLA n 604



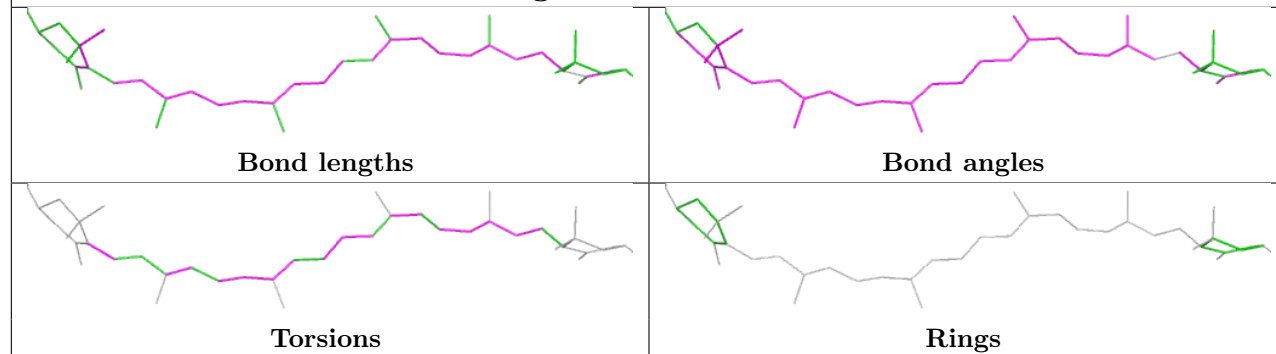




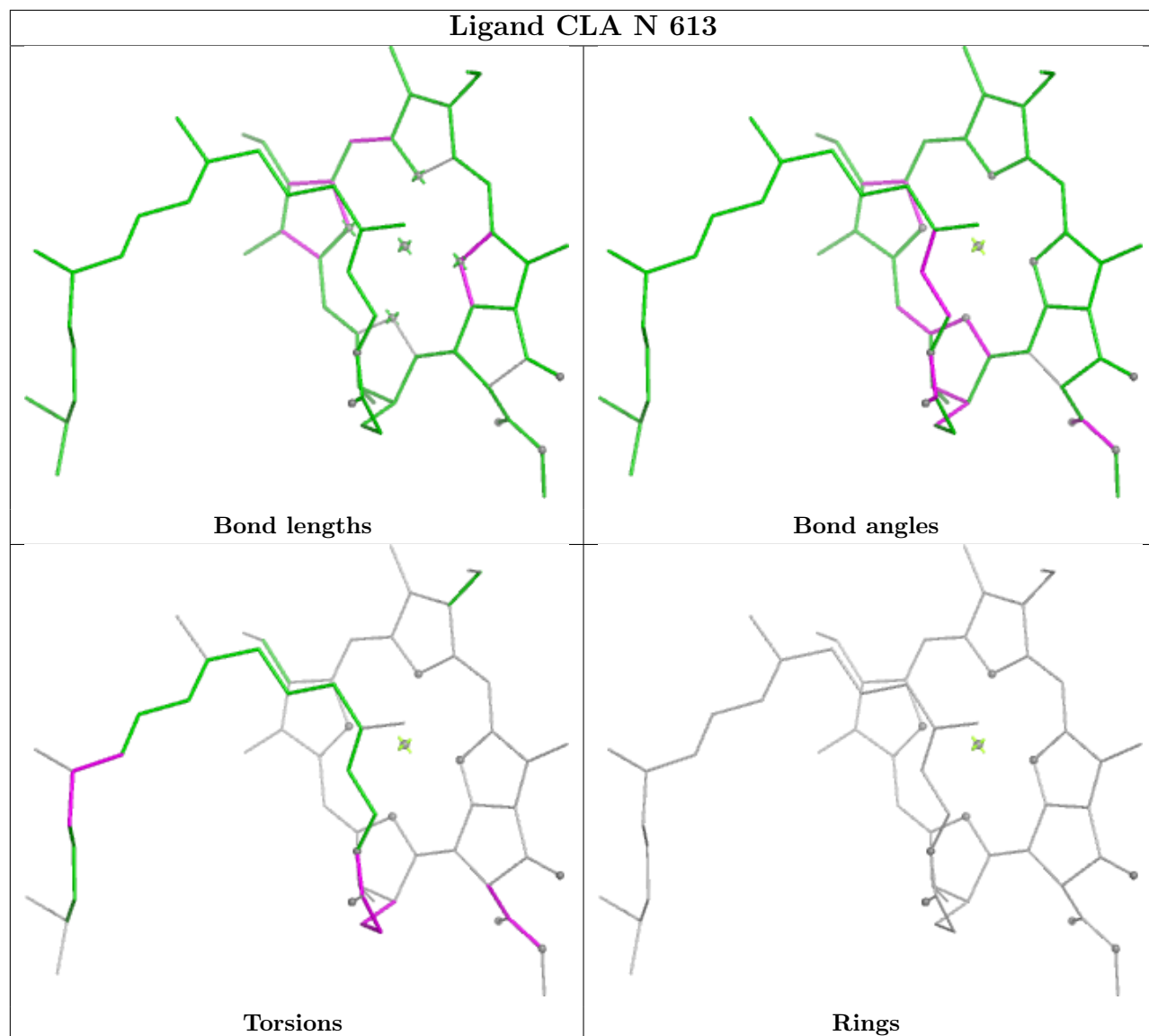
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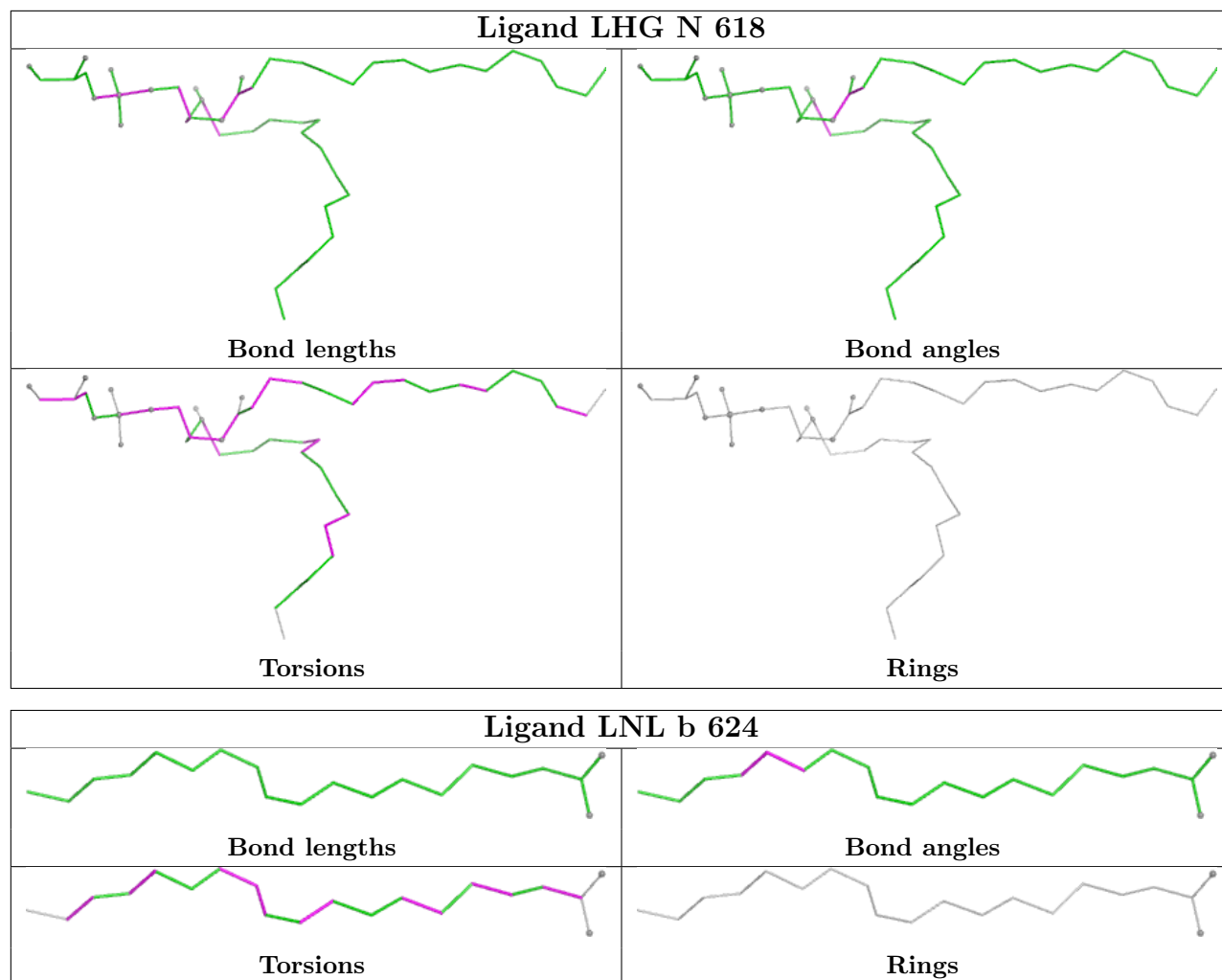


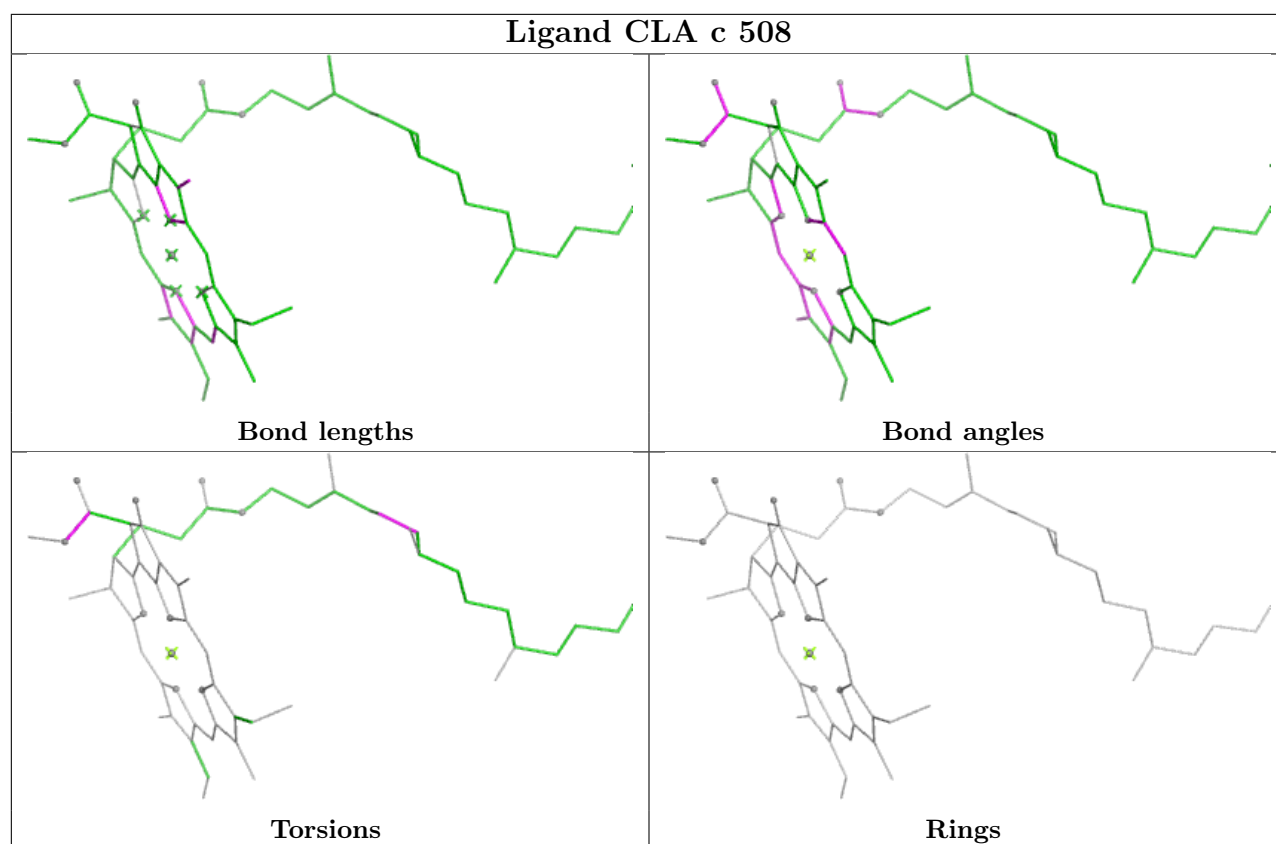
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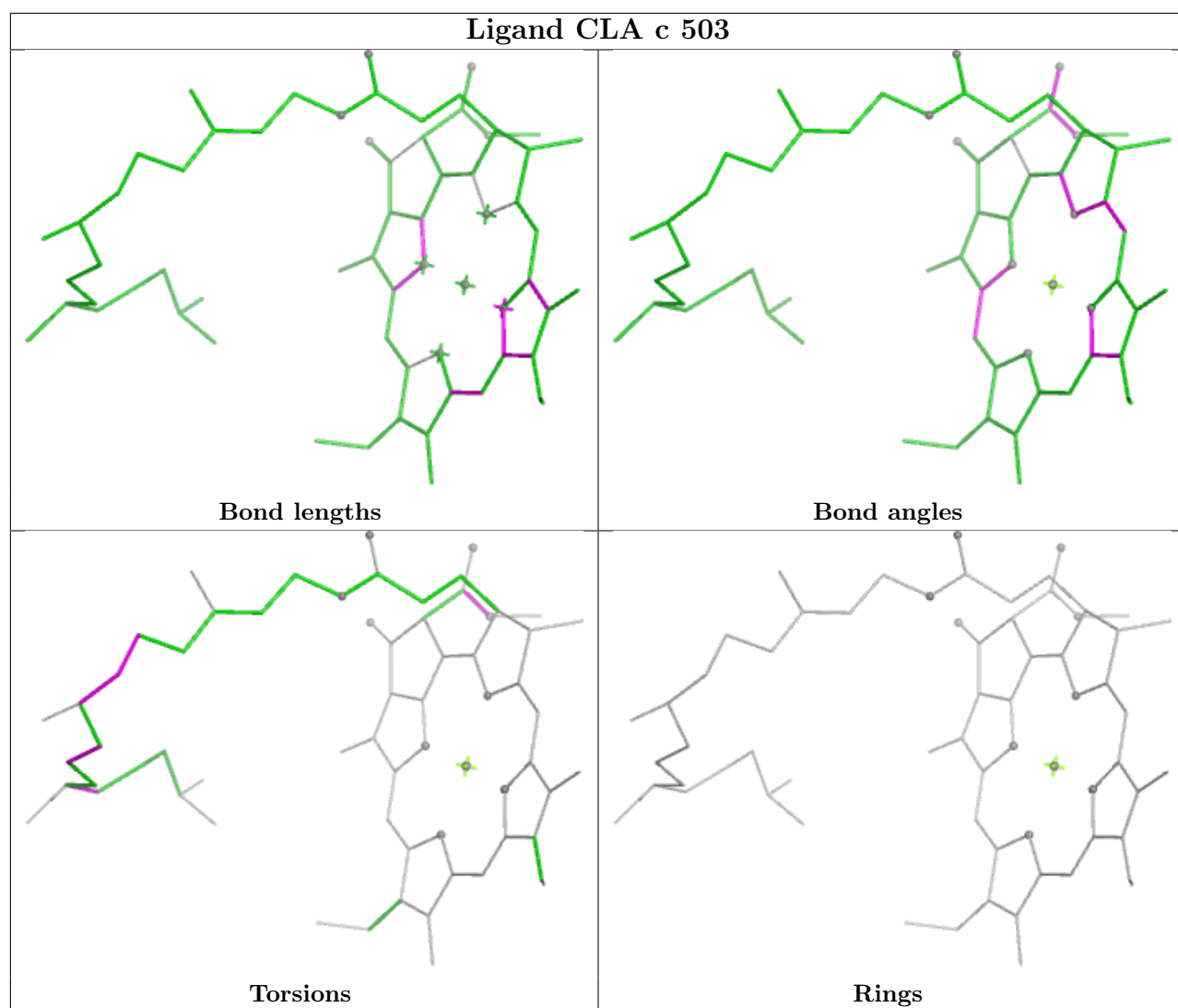


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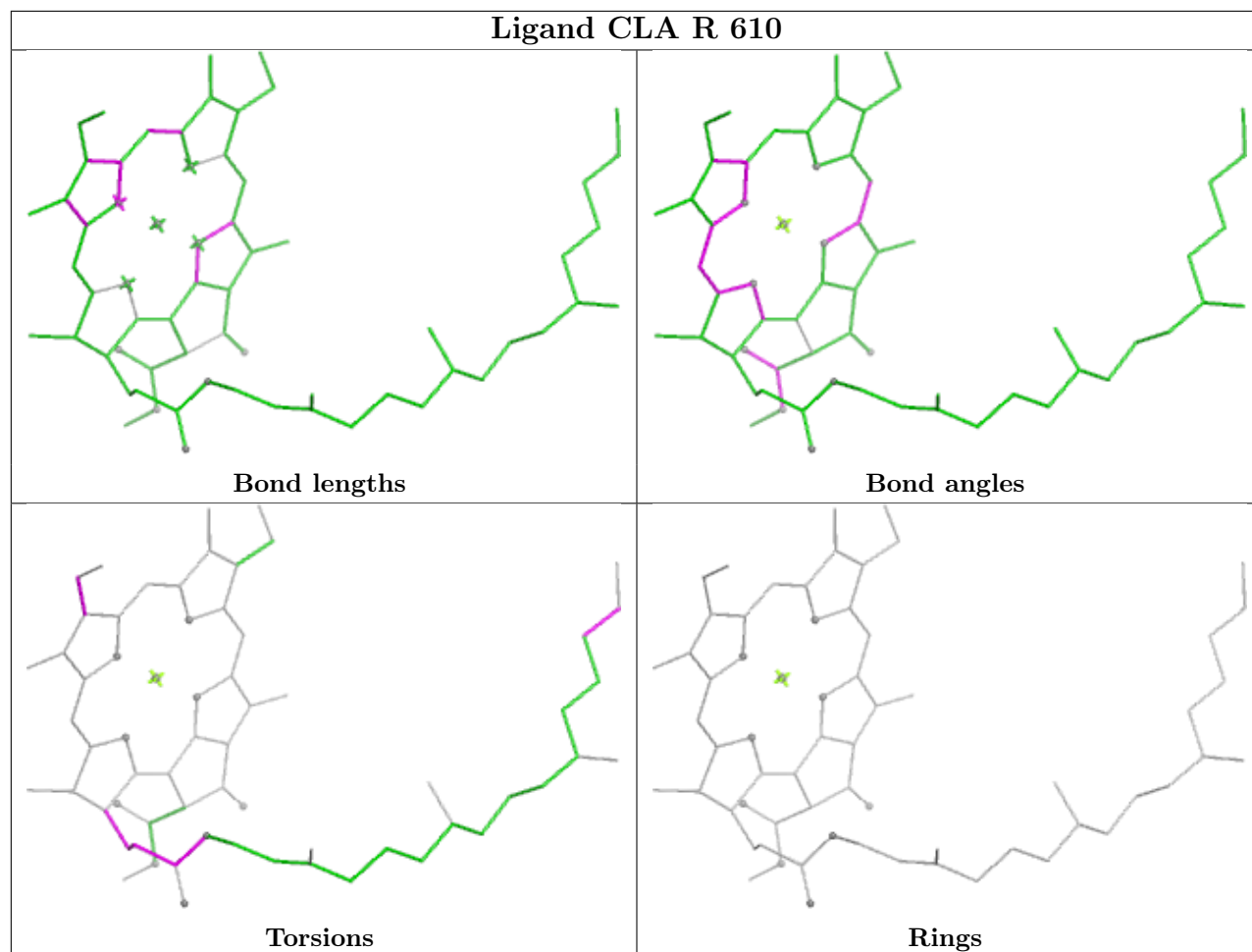




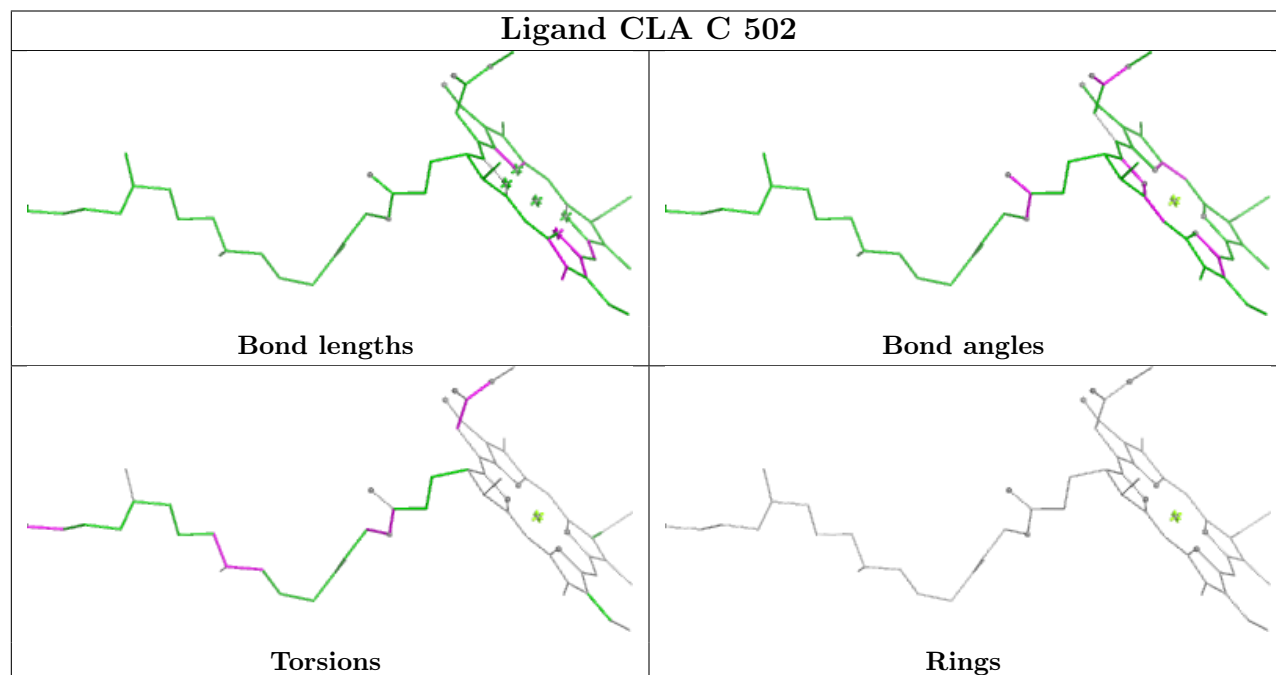


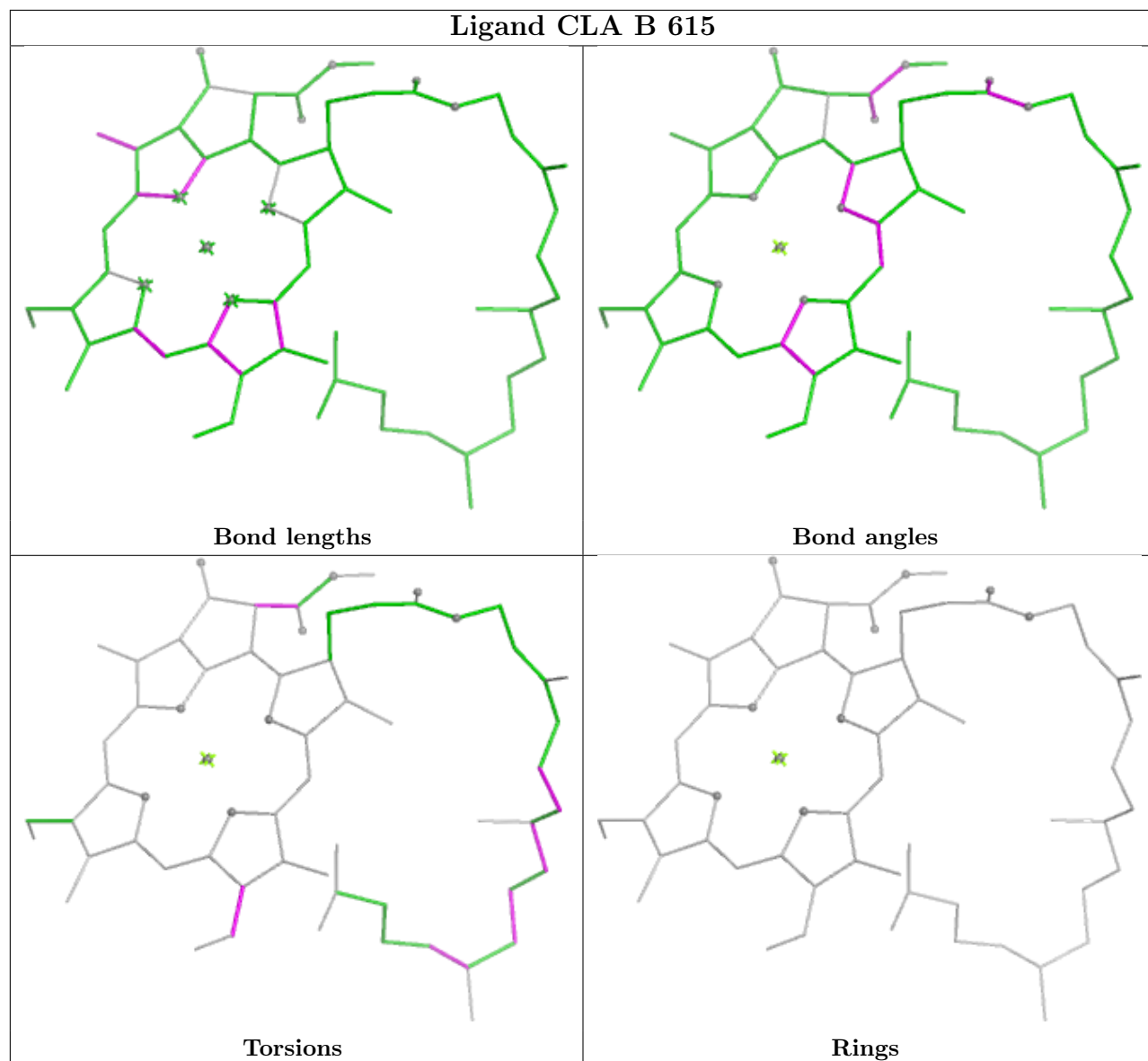


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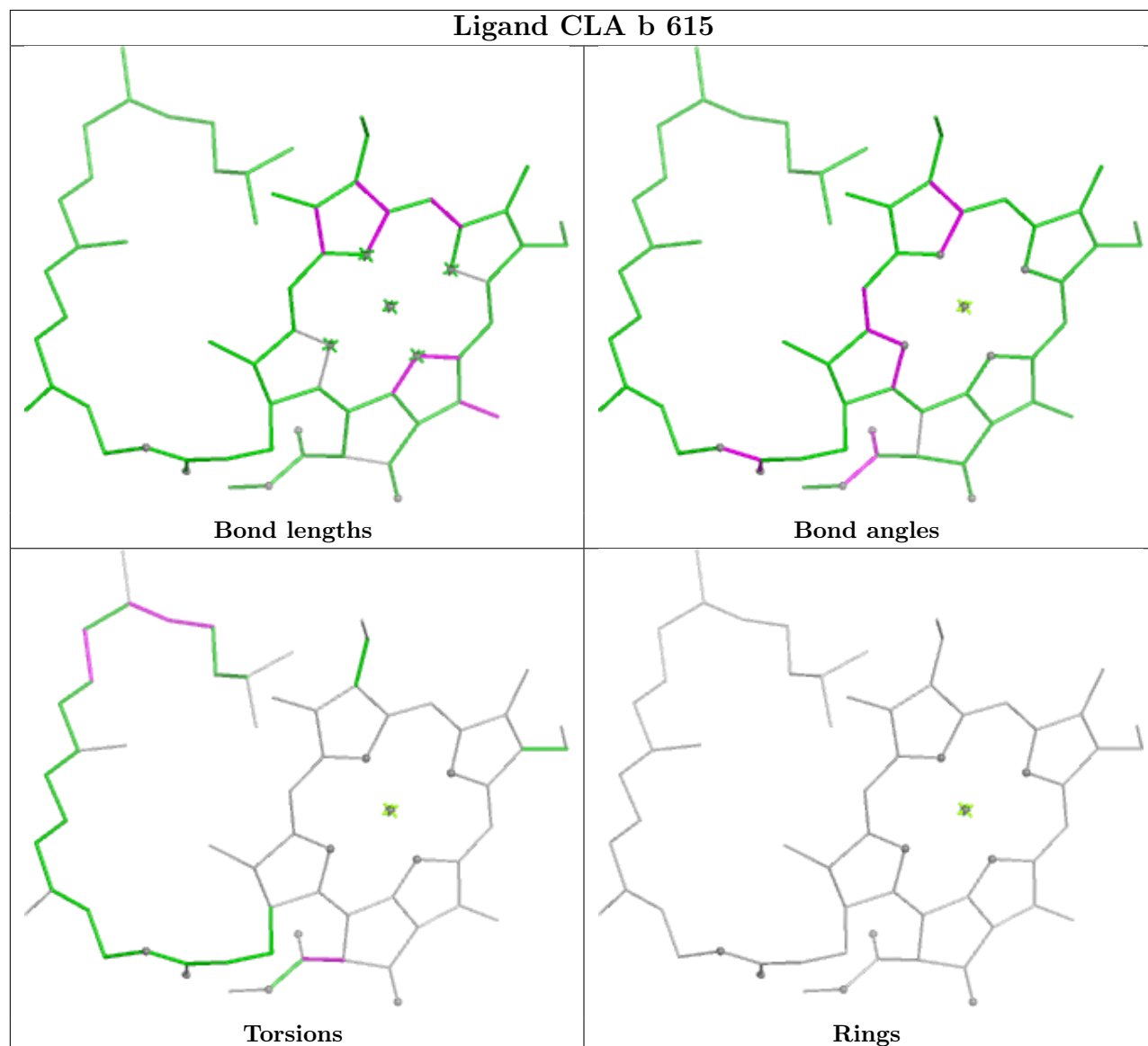


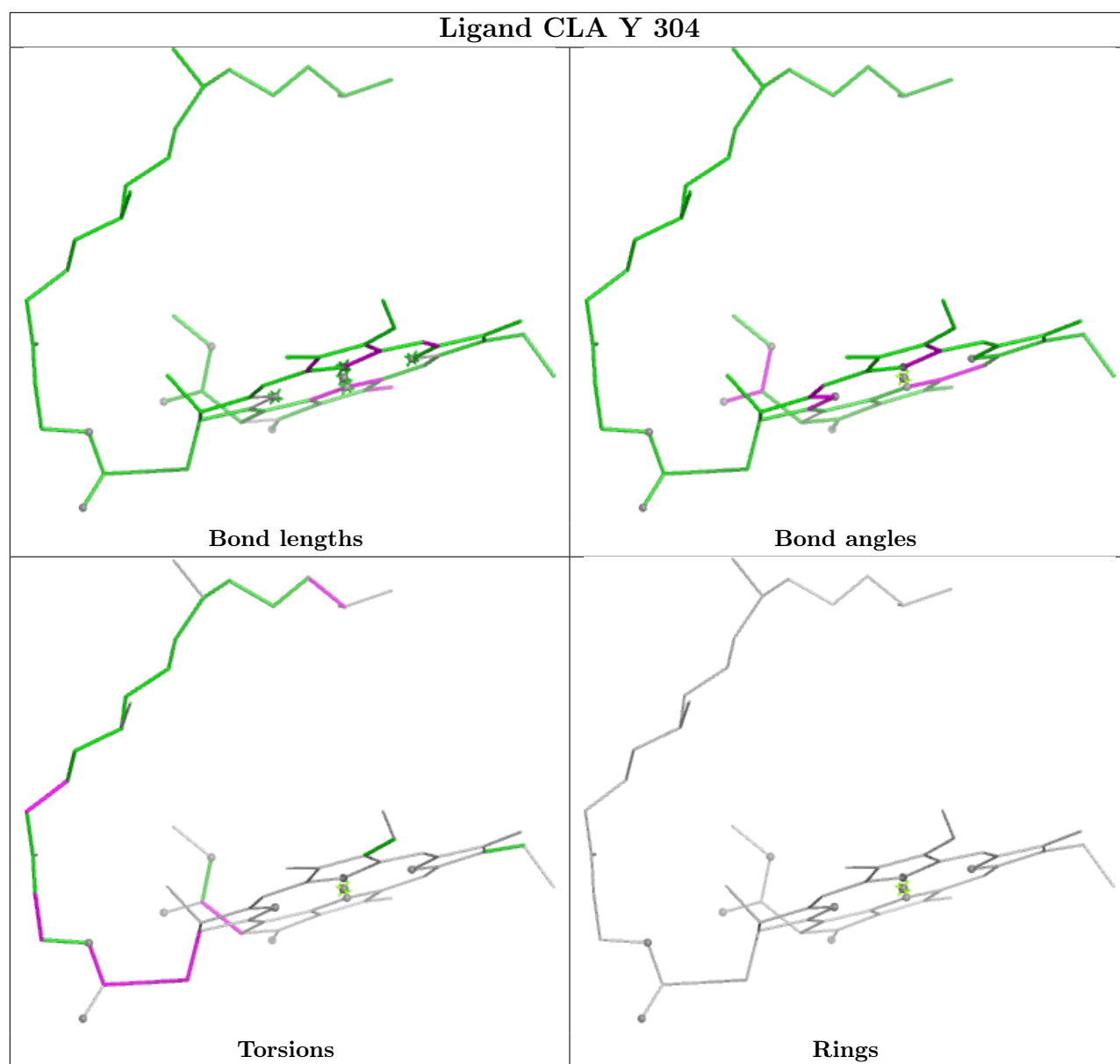
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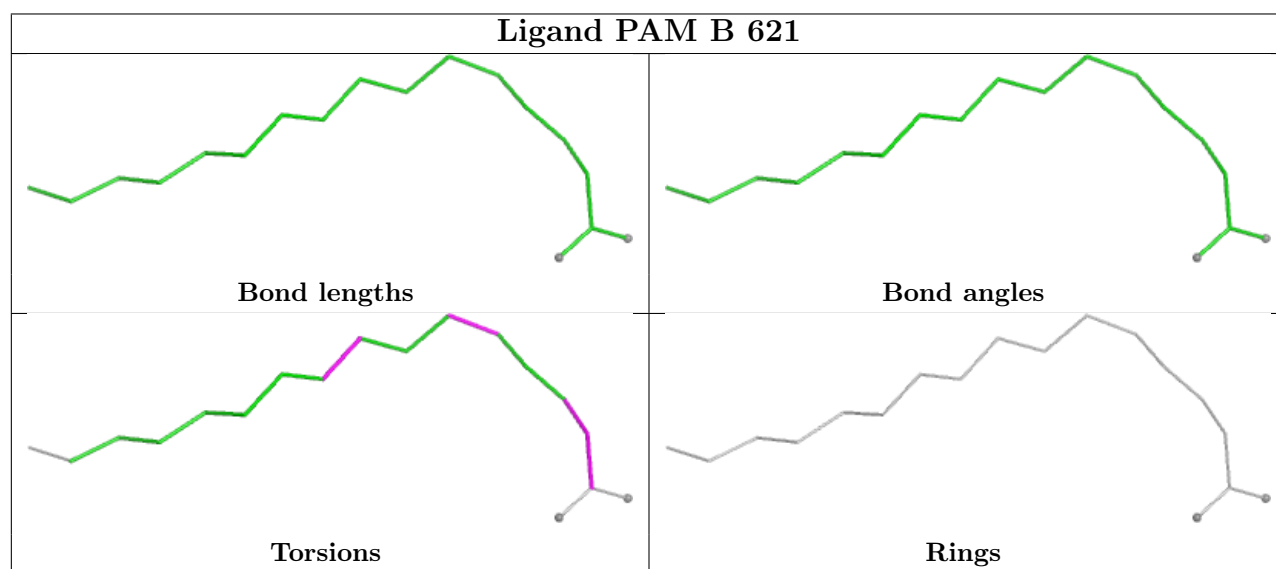
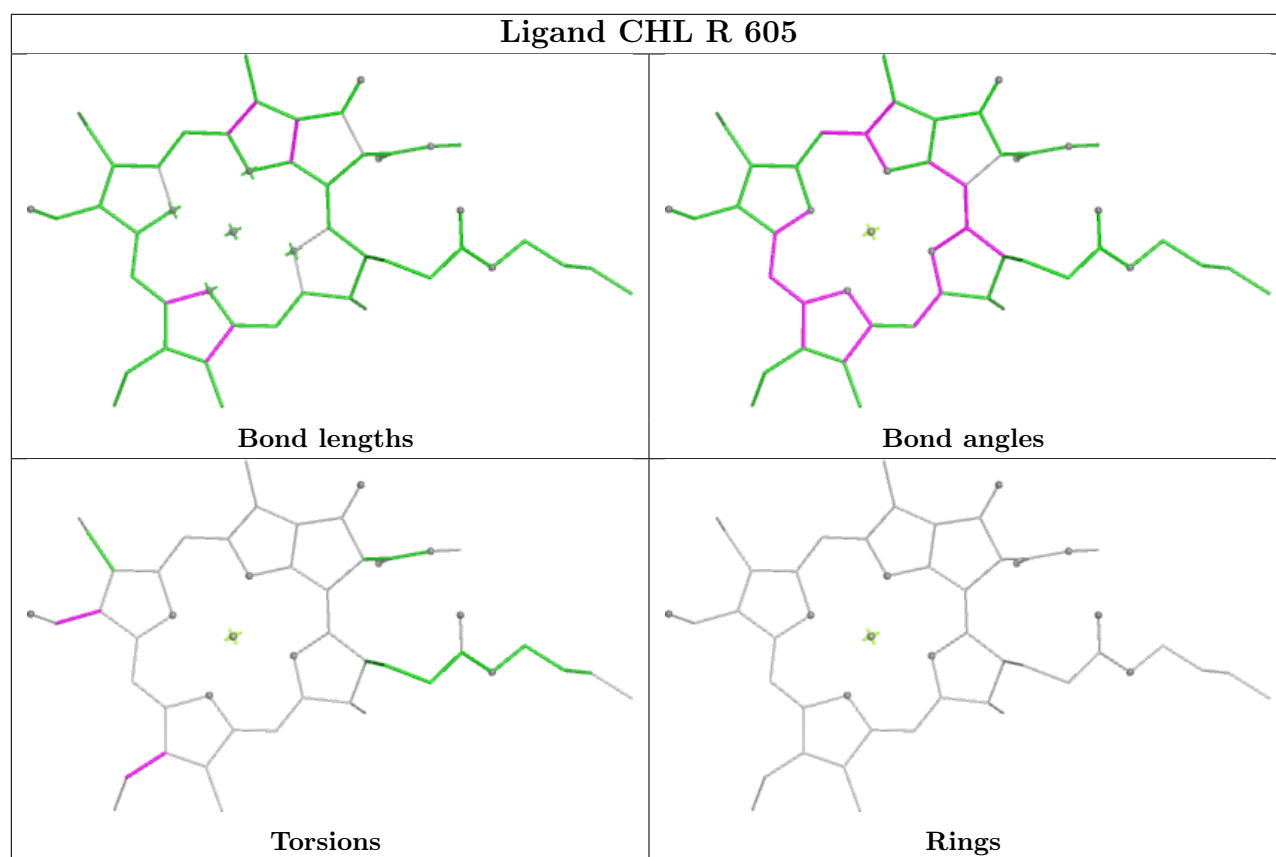


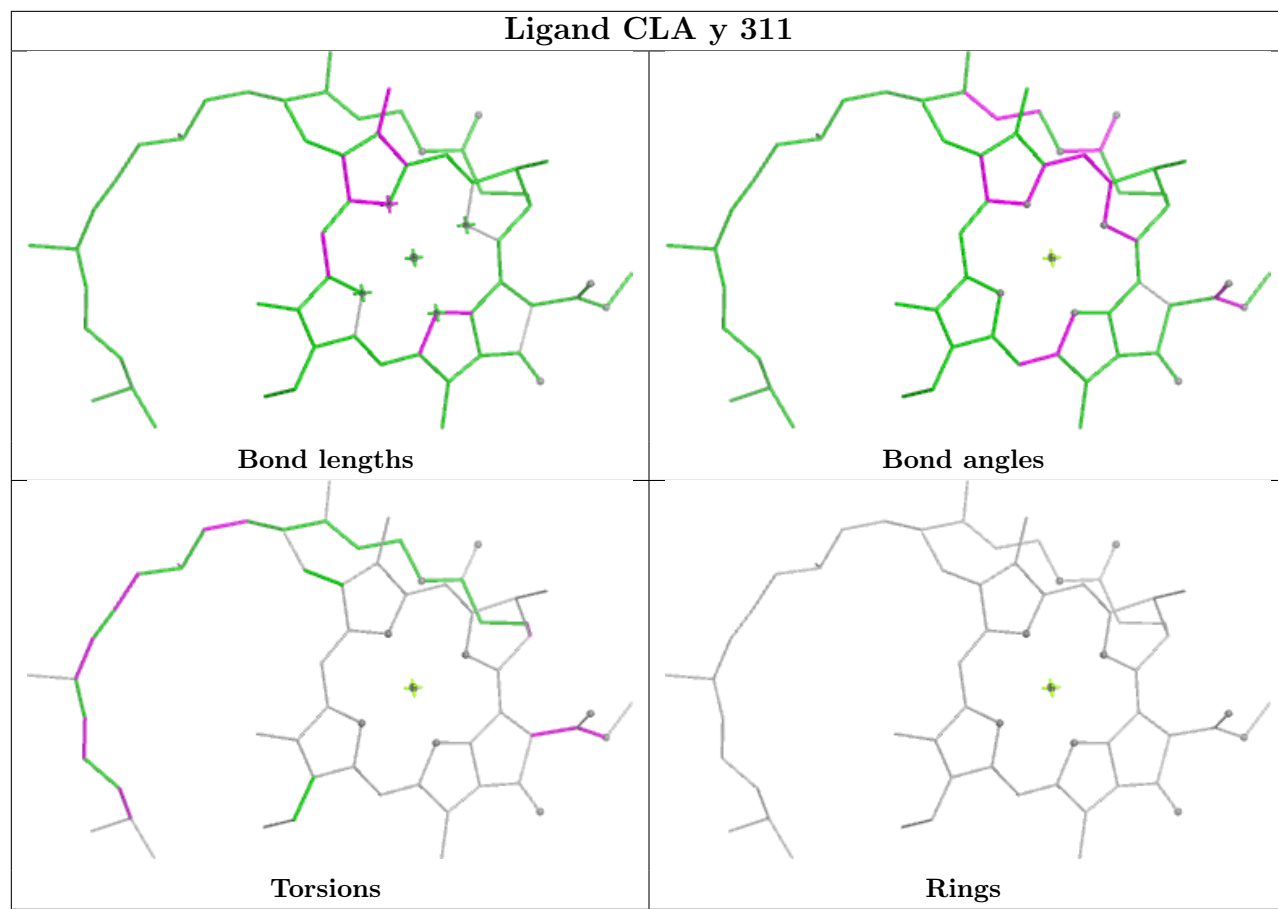


Ligand CLA b 615

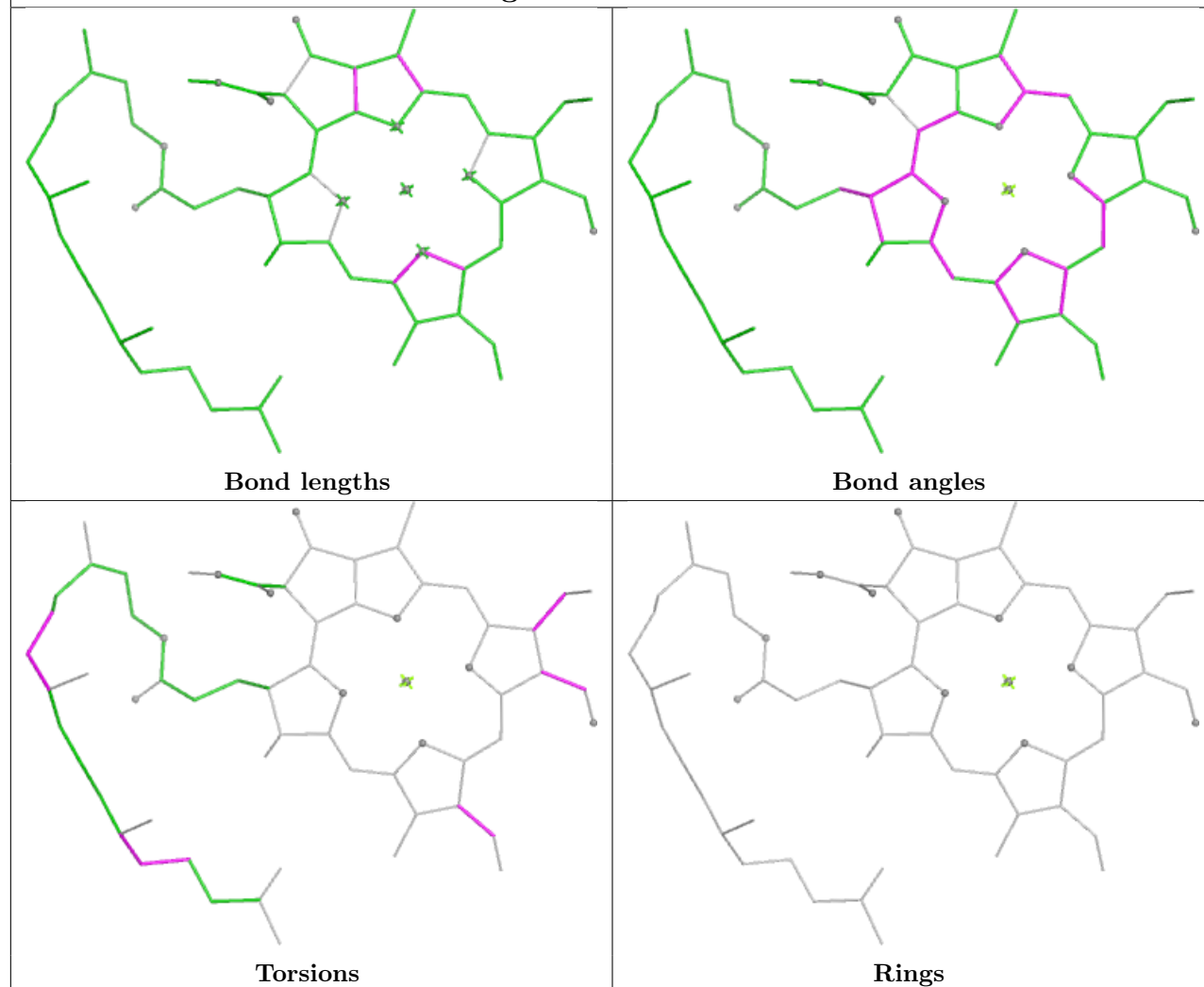




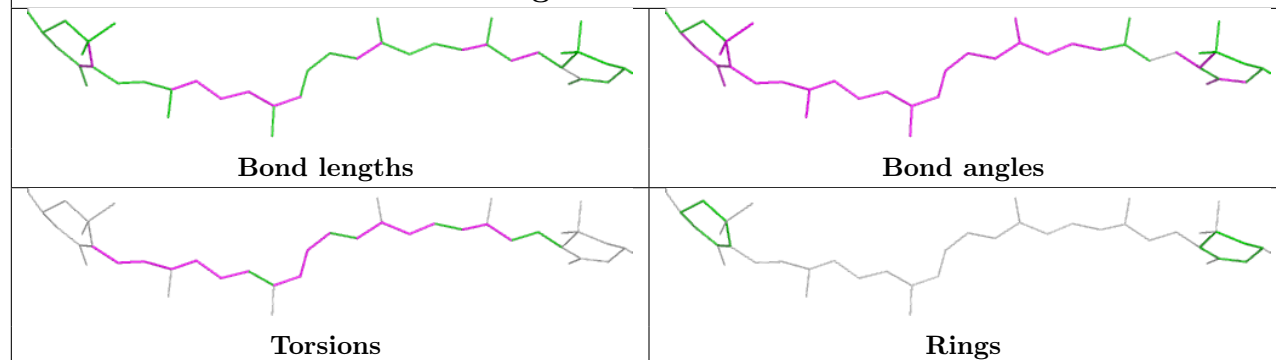


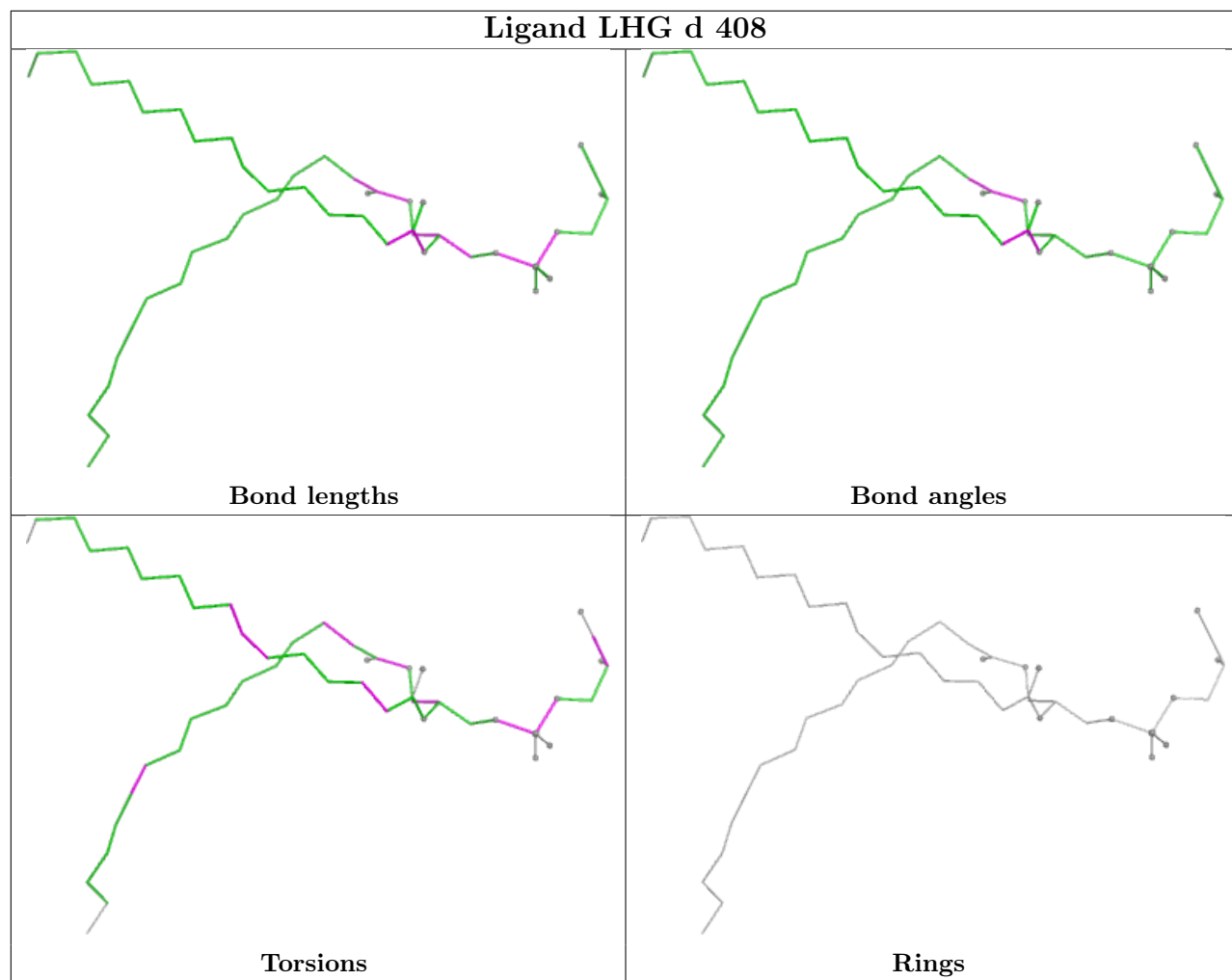


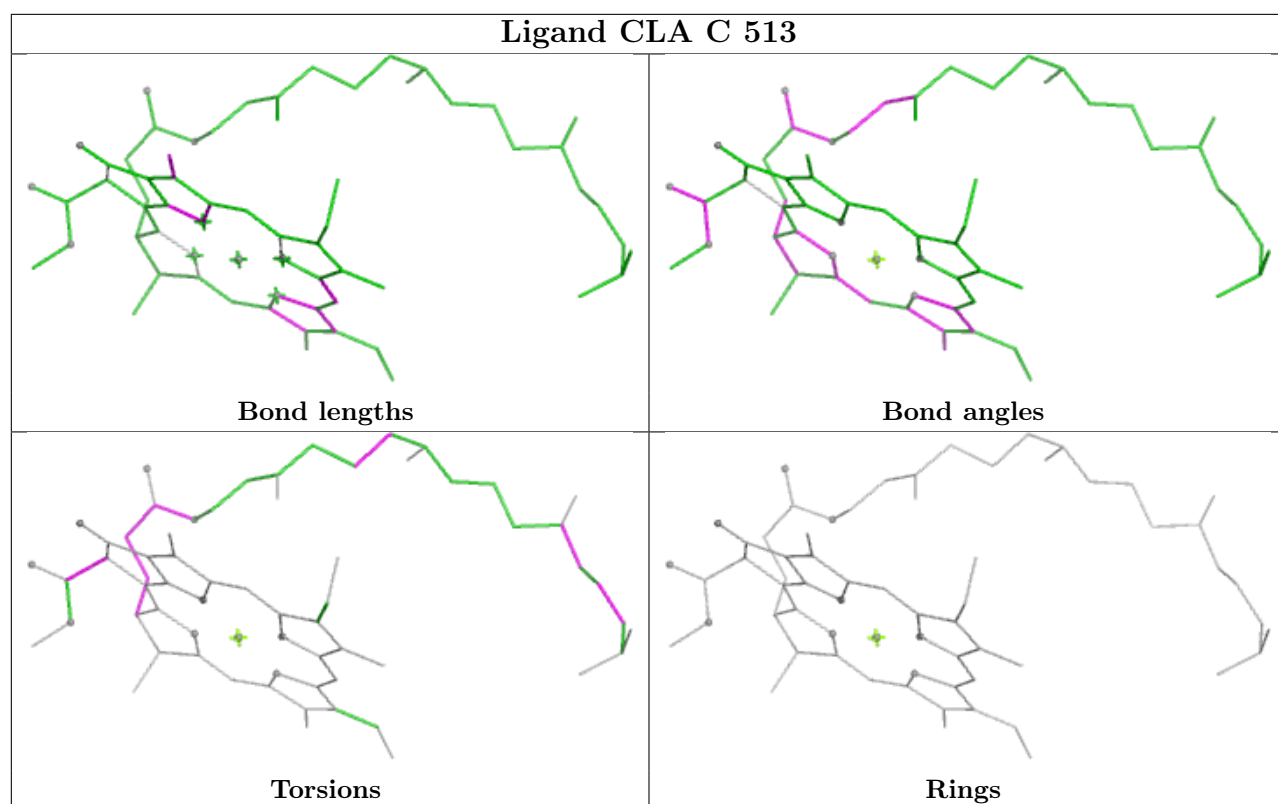
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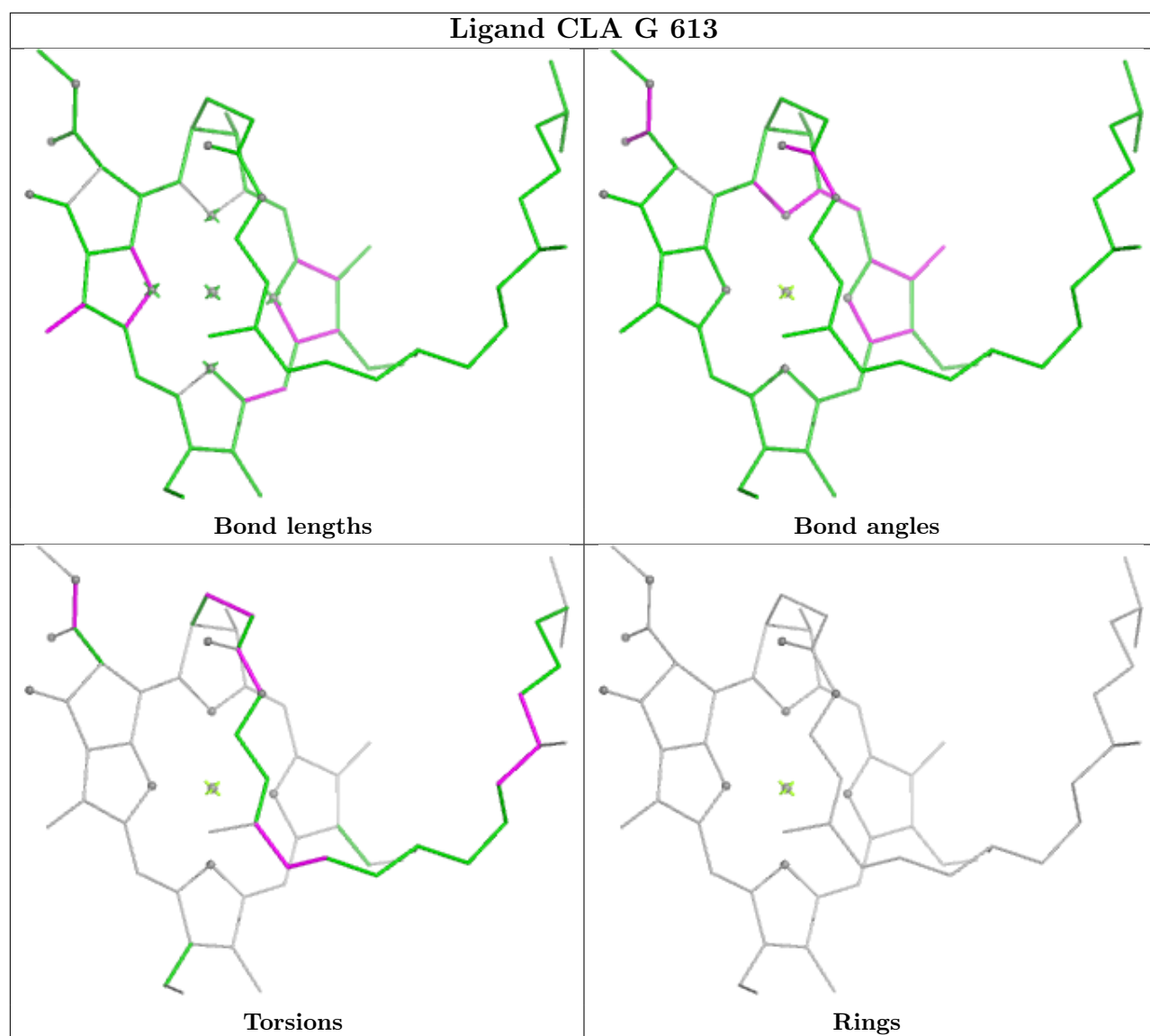


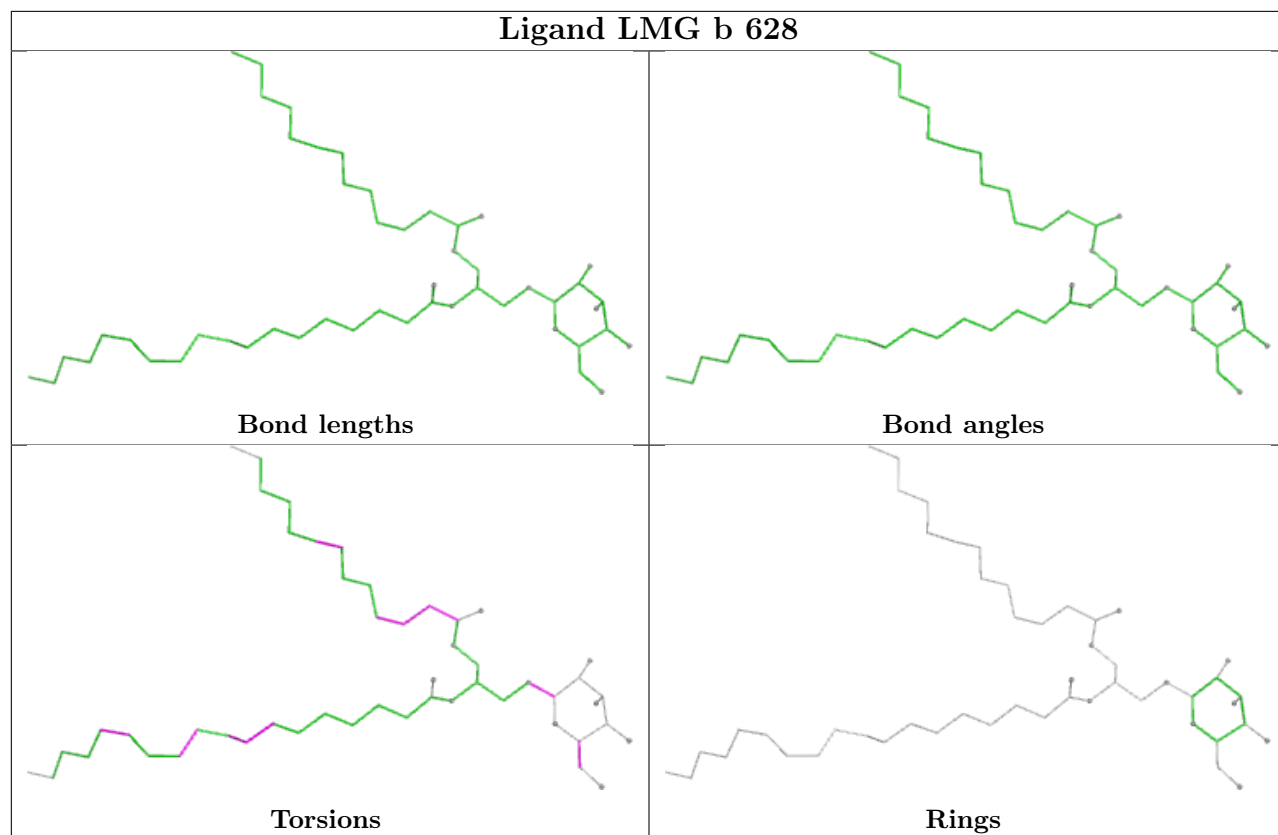
Ligand LUT Y 315



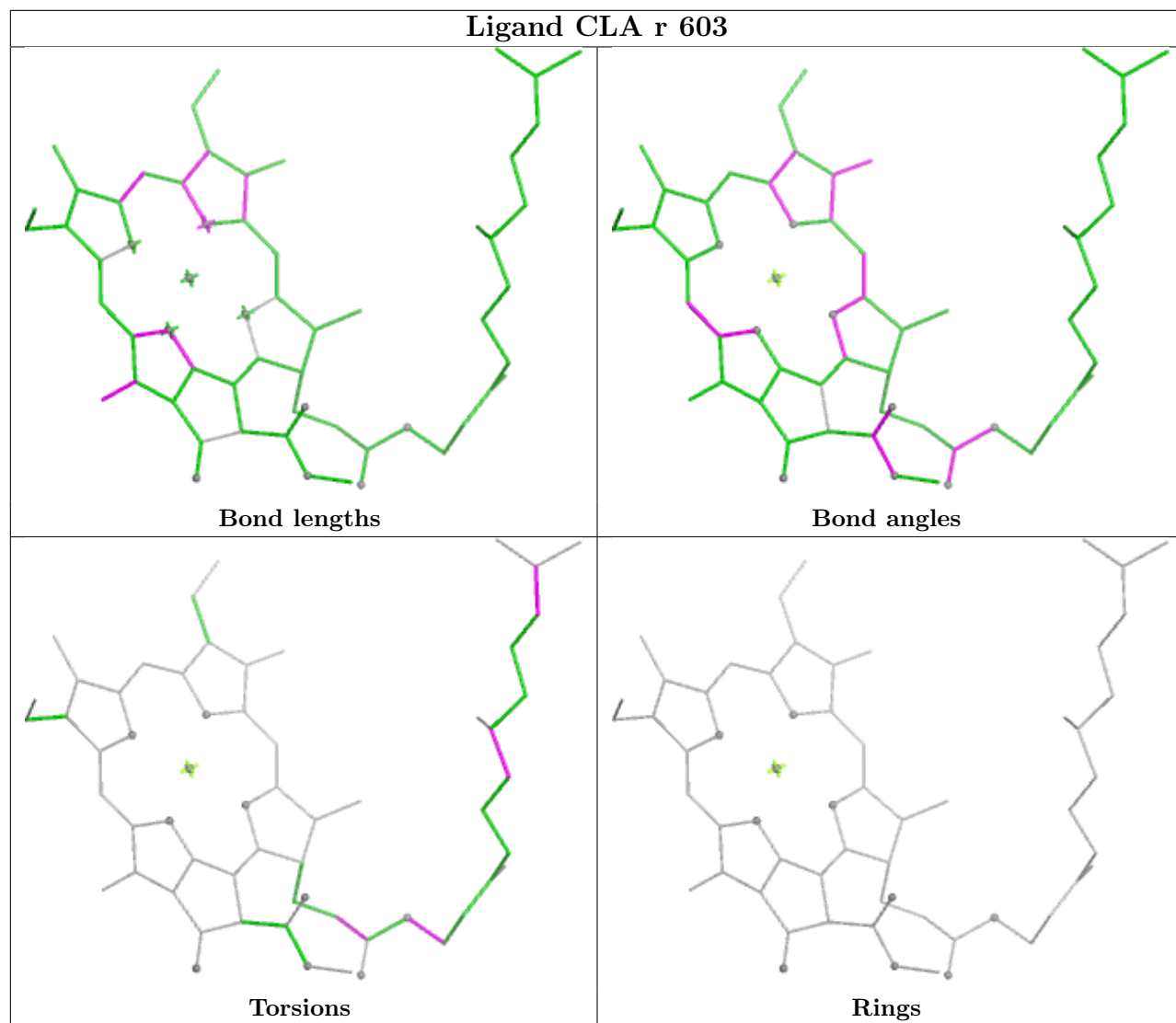


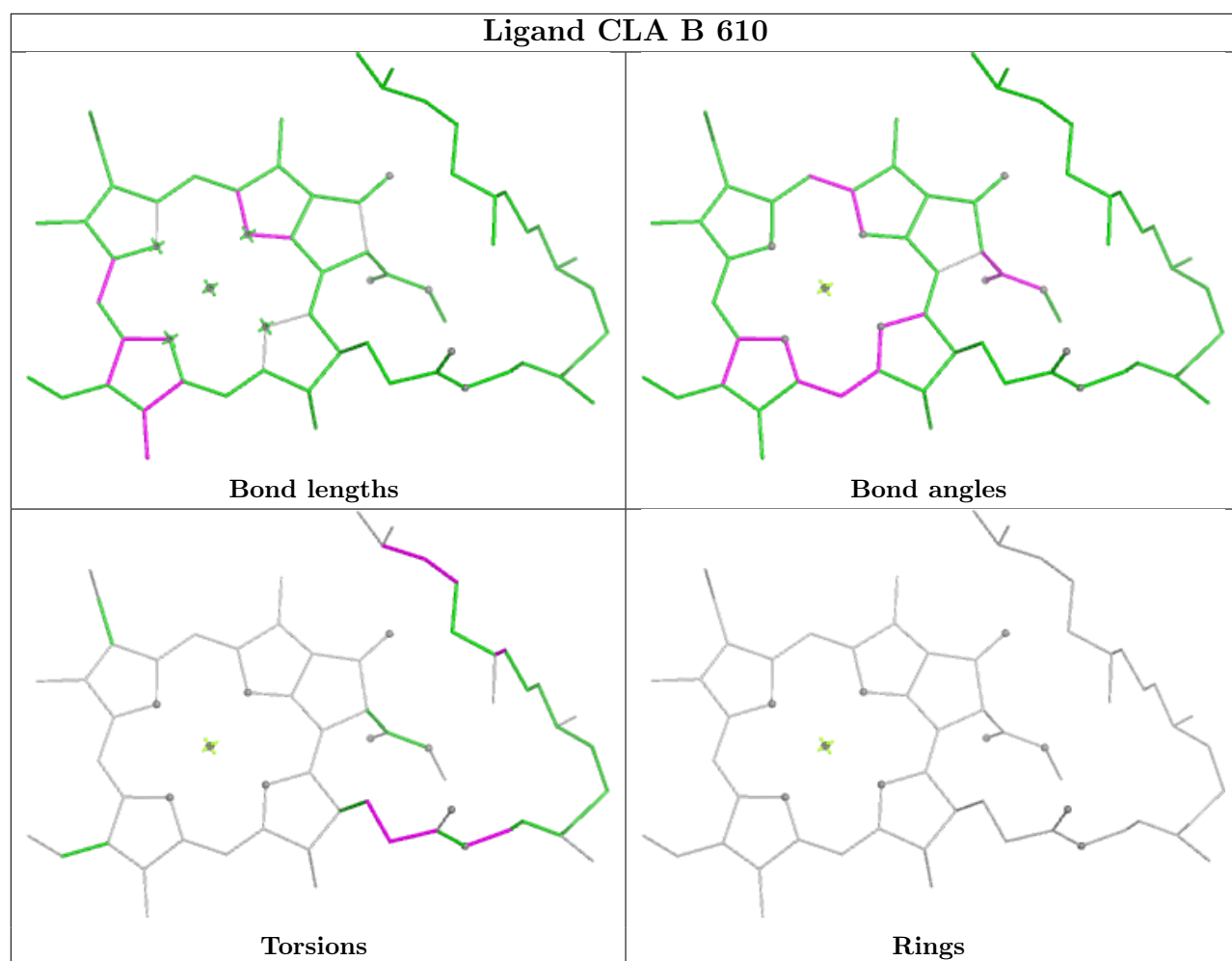


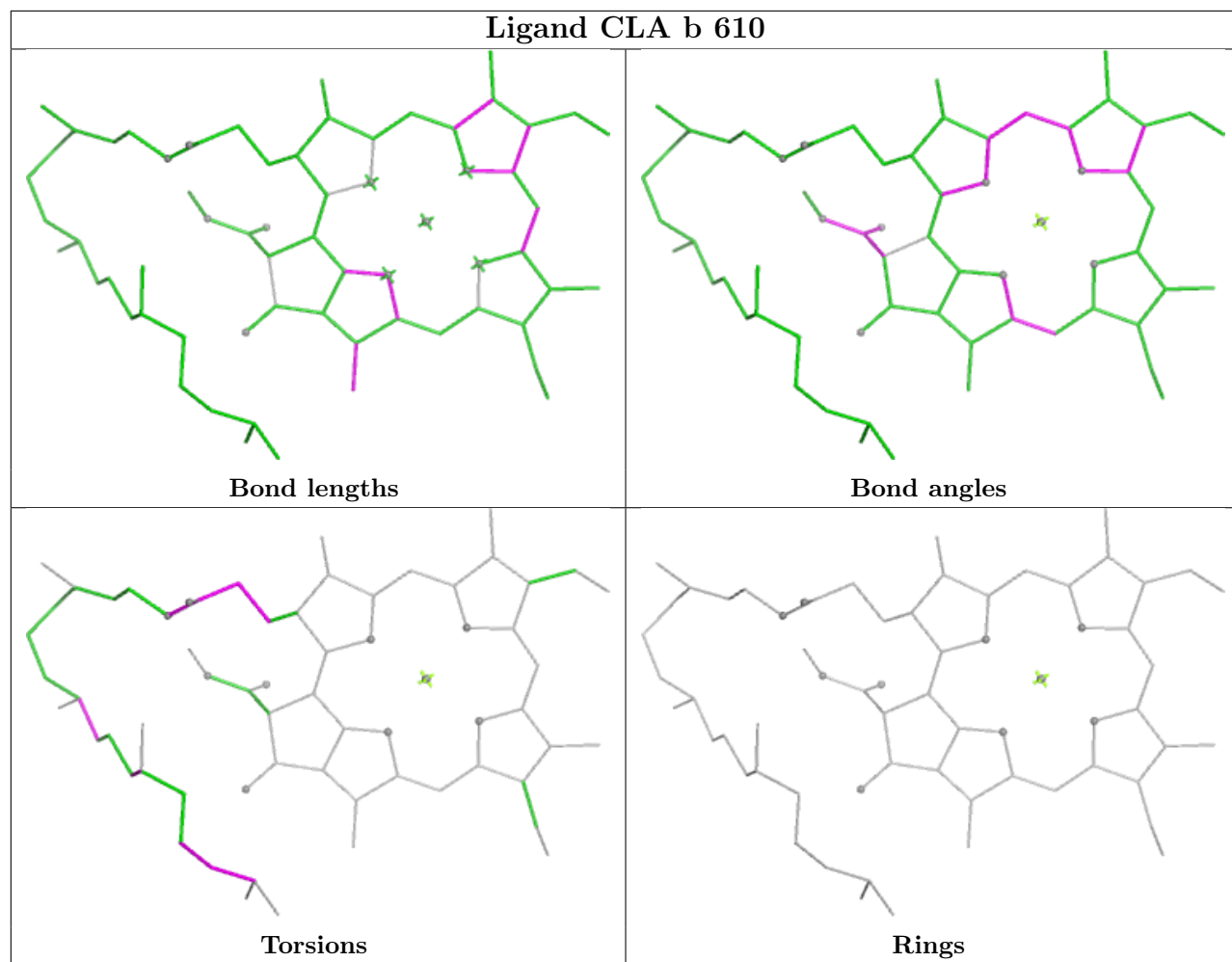


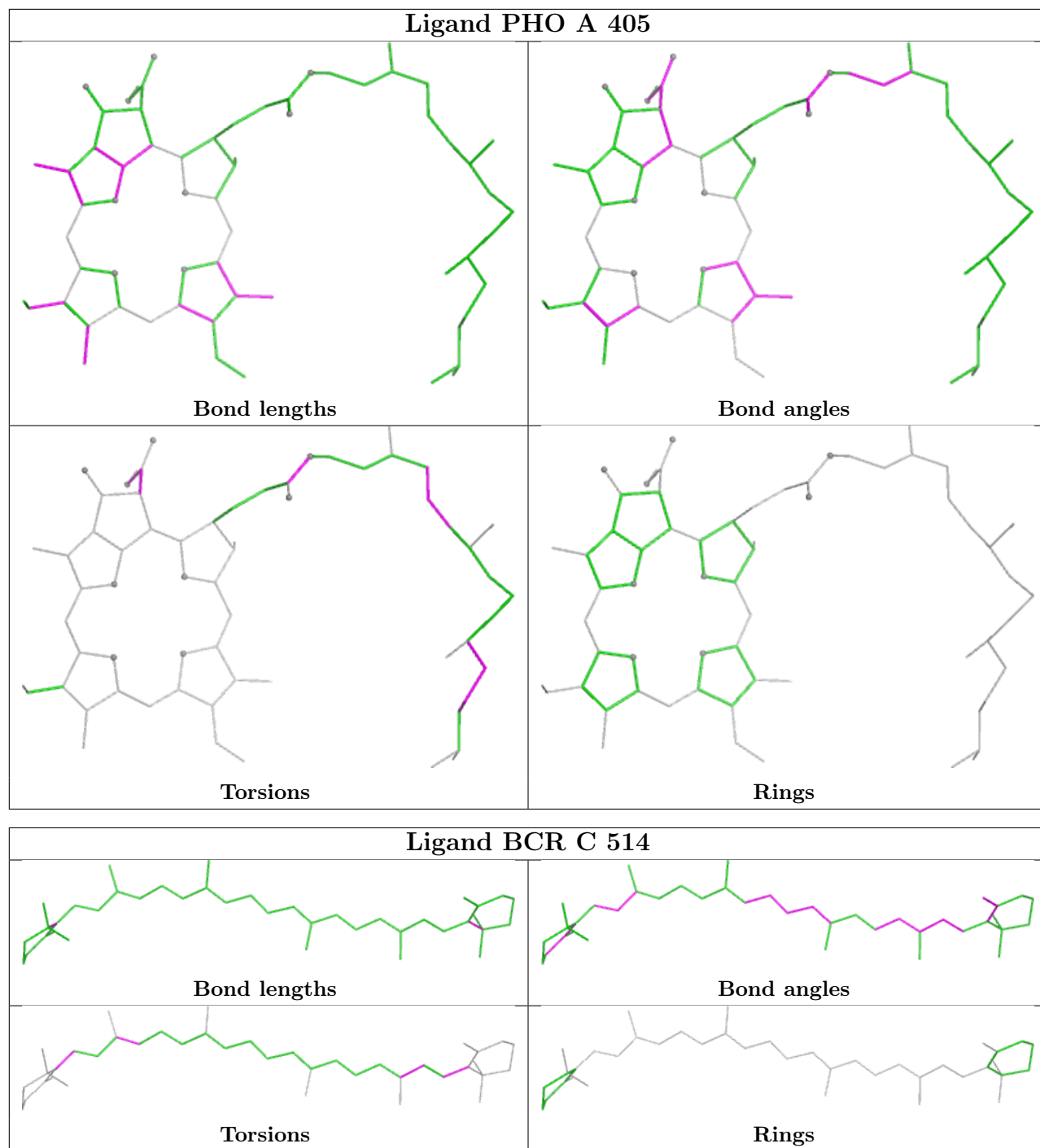


Ligand CLA r 603

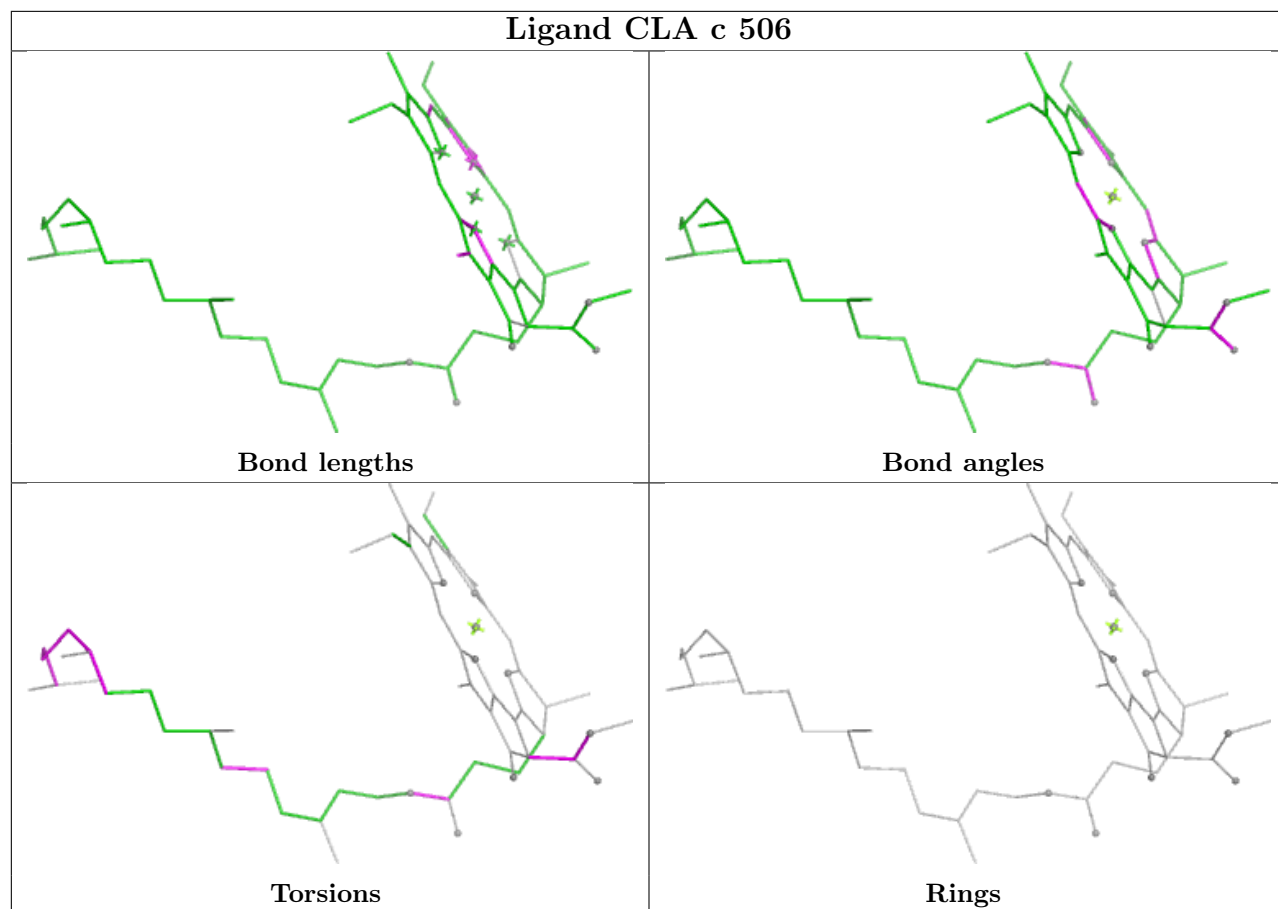




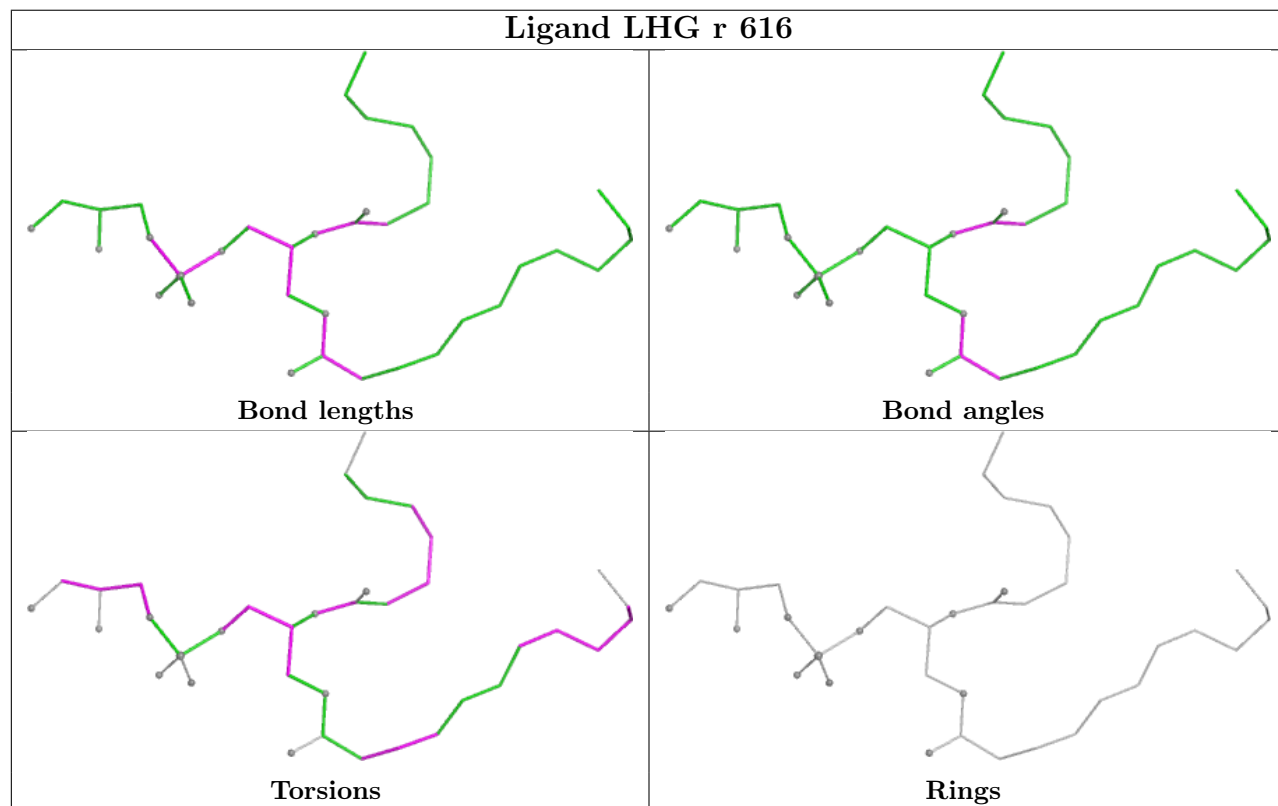


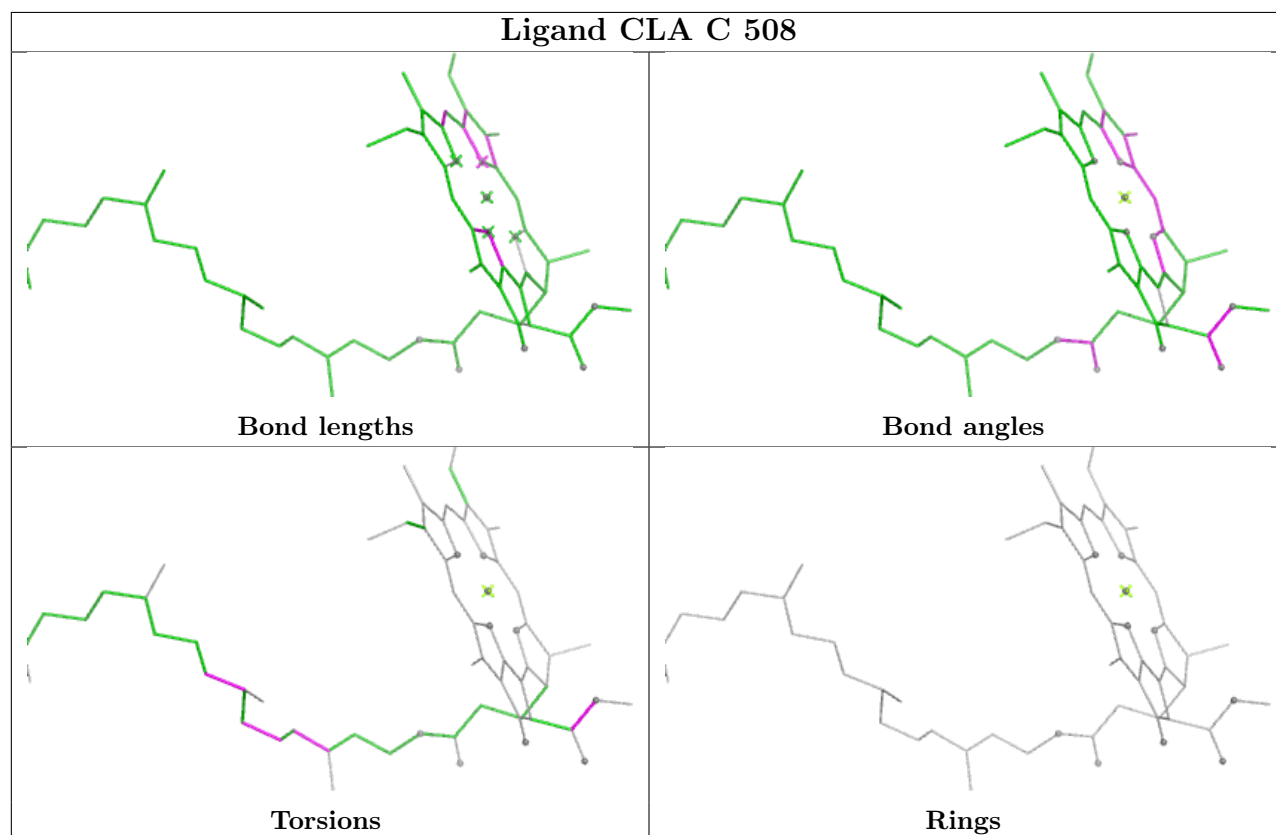
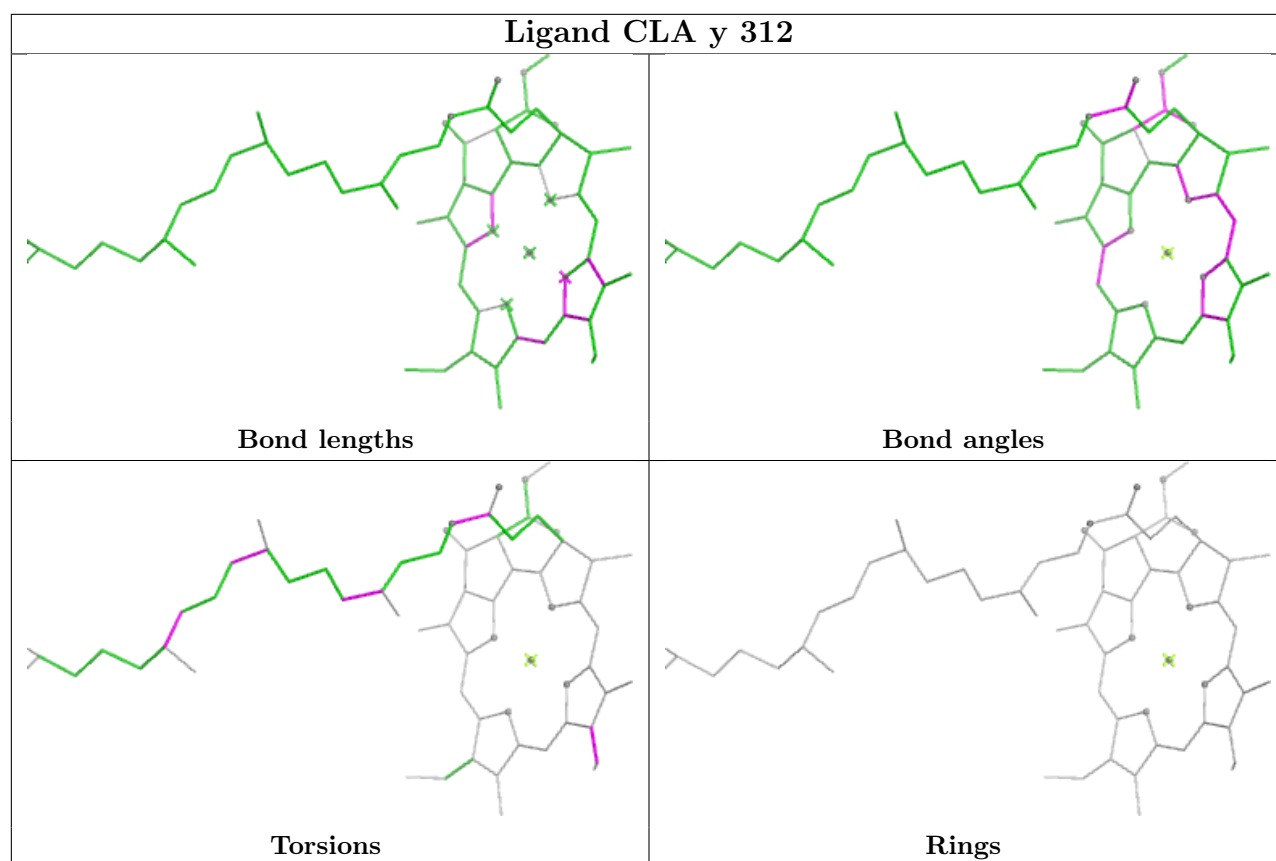


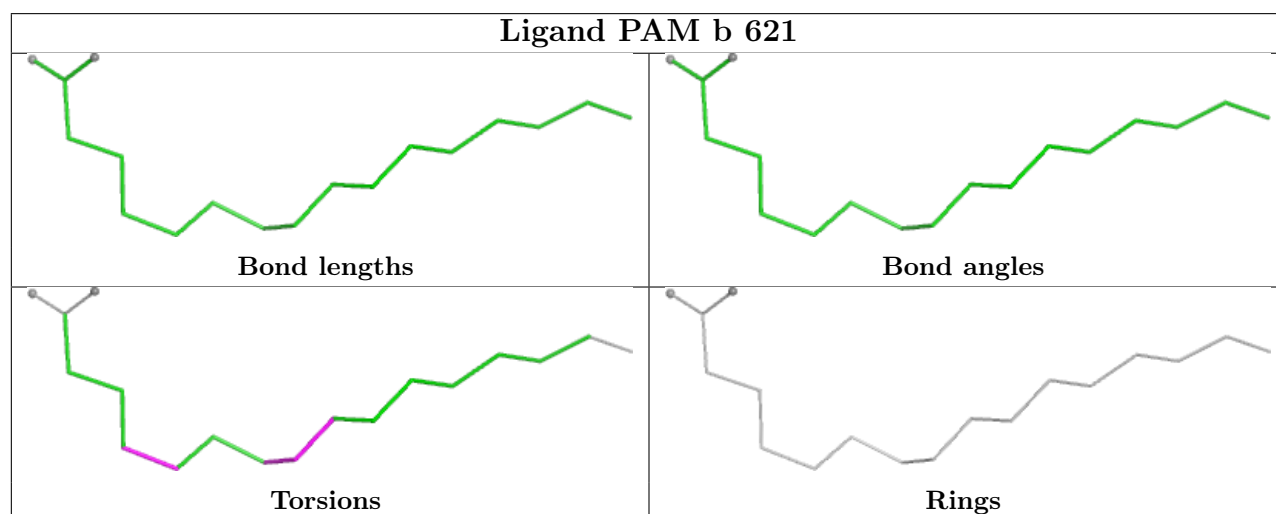
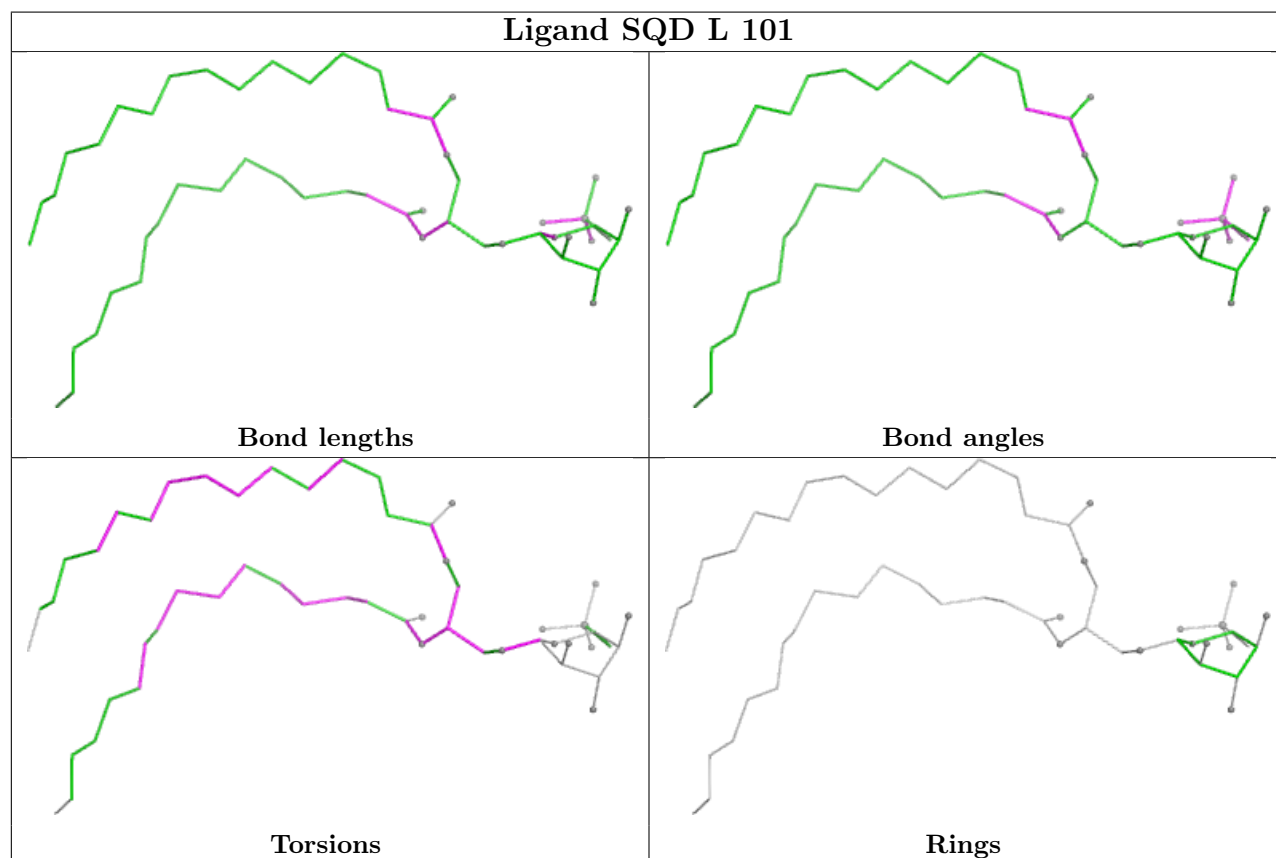
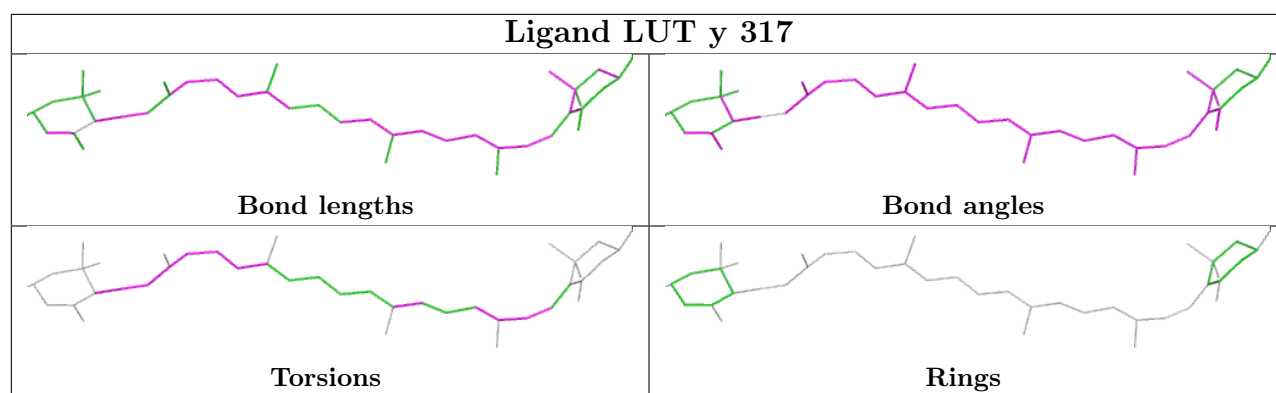
Ligand CLA c 506

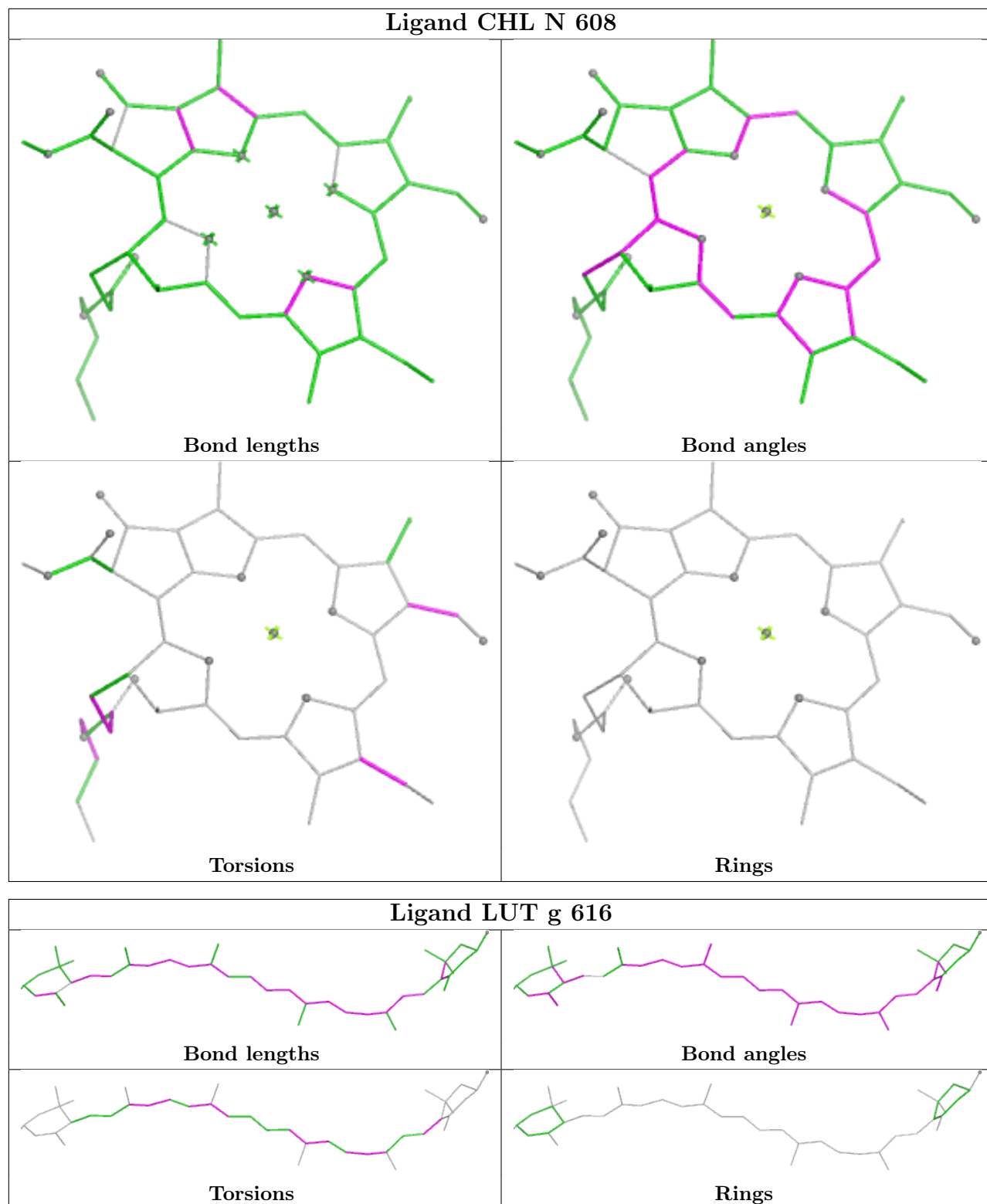


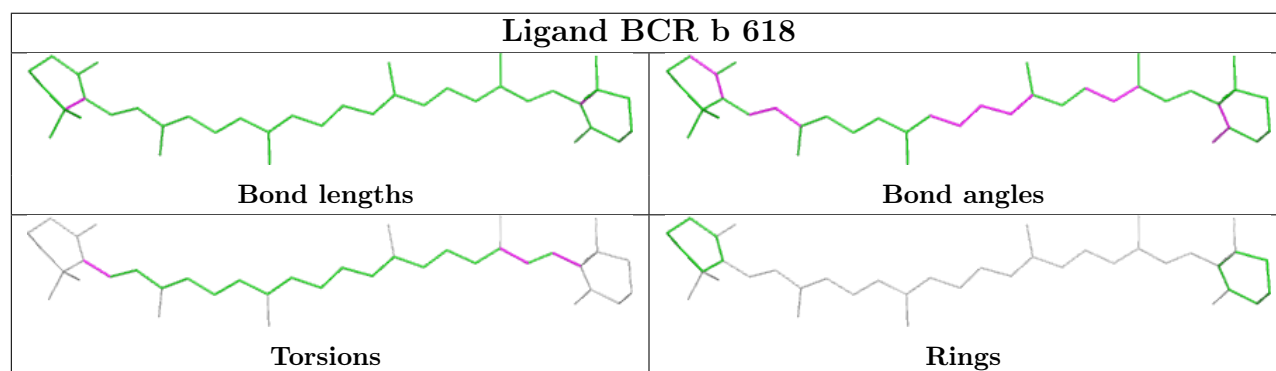
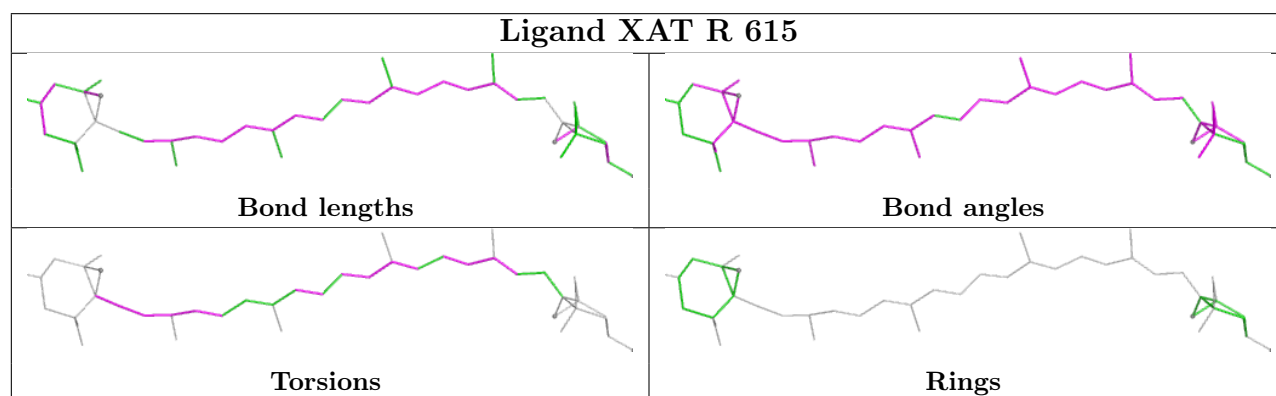
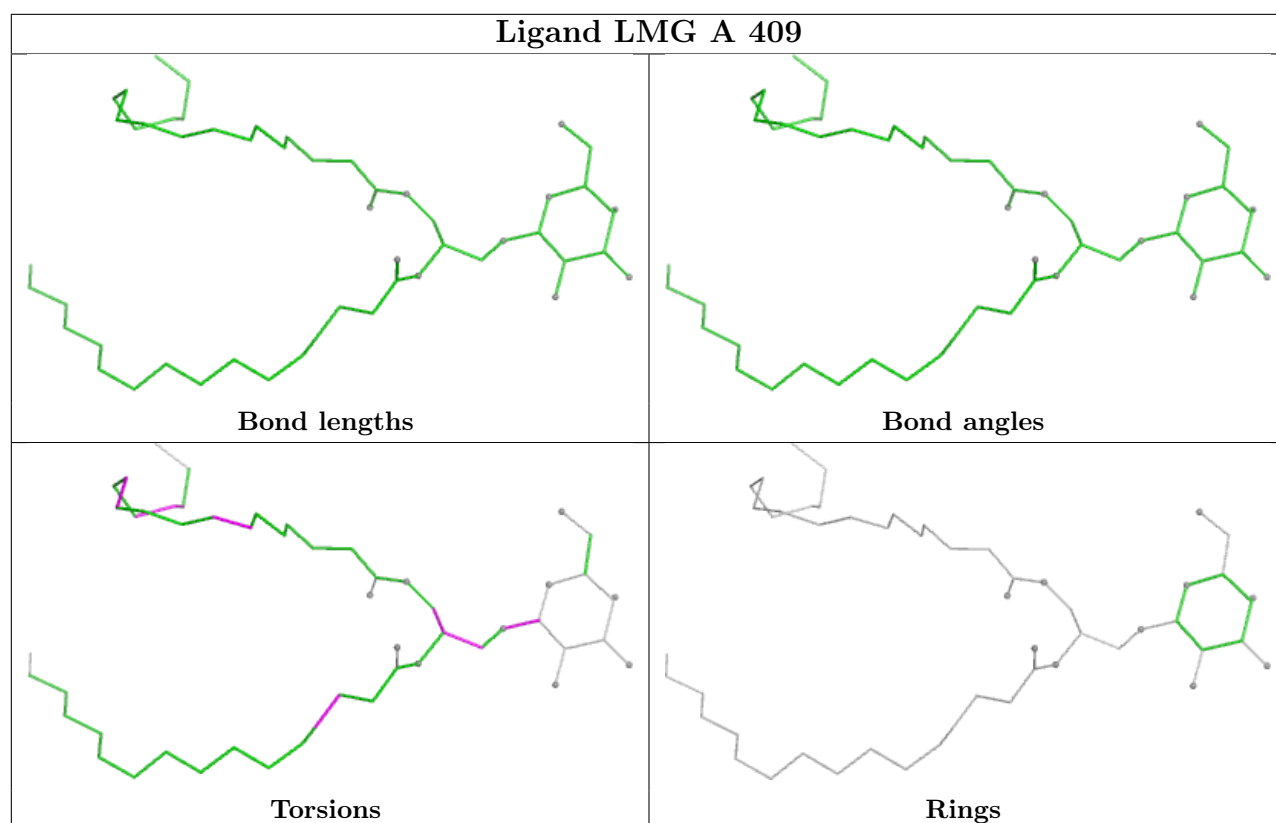
Ligand LHG r 616

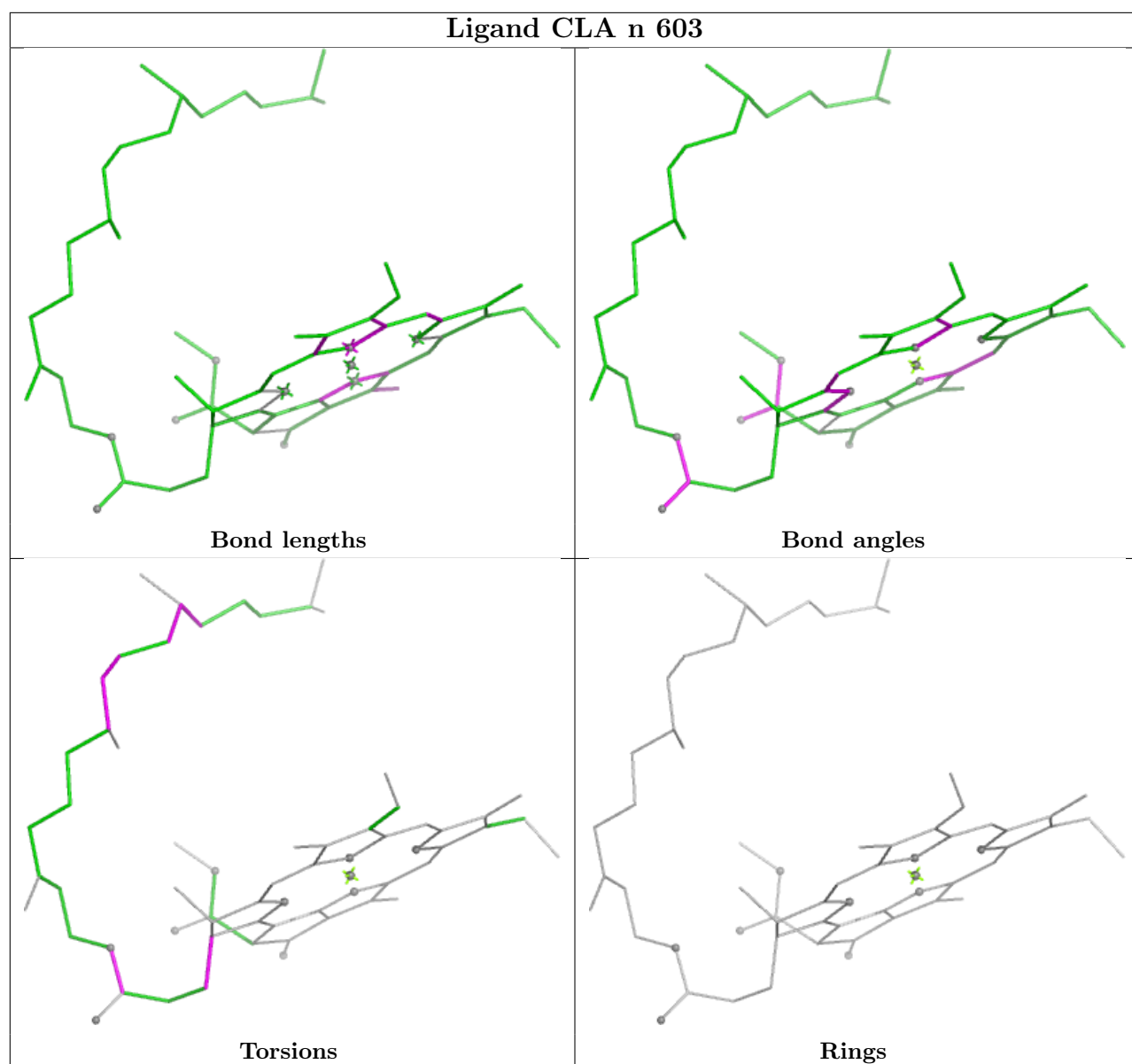


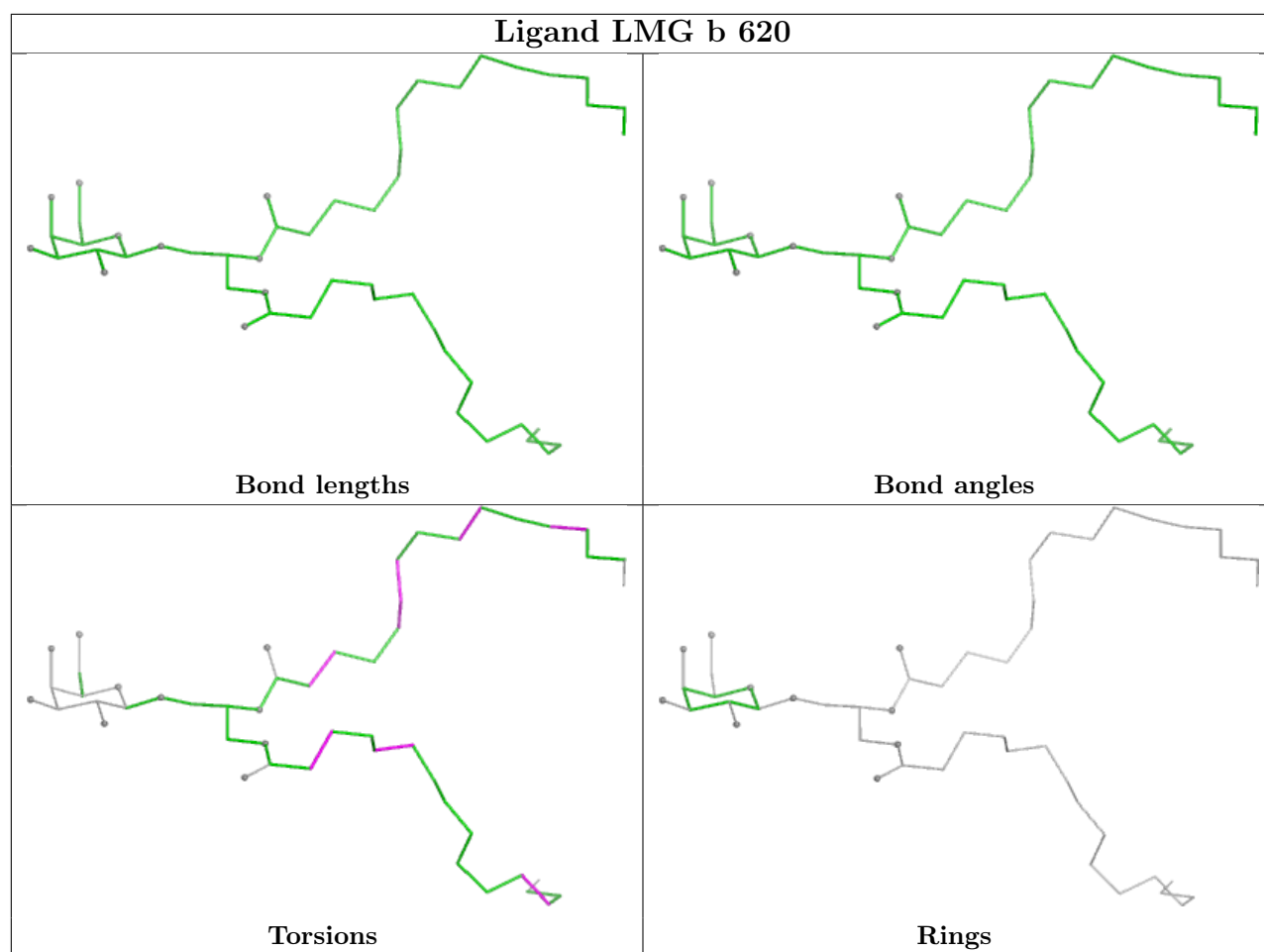


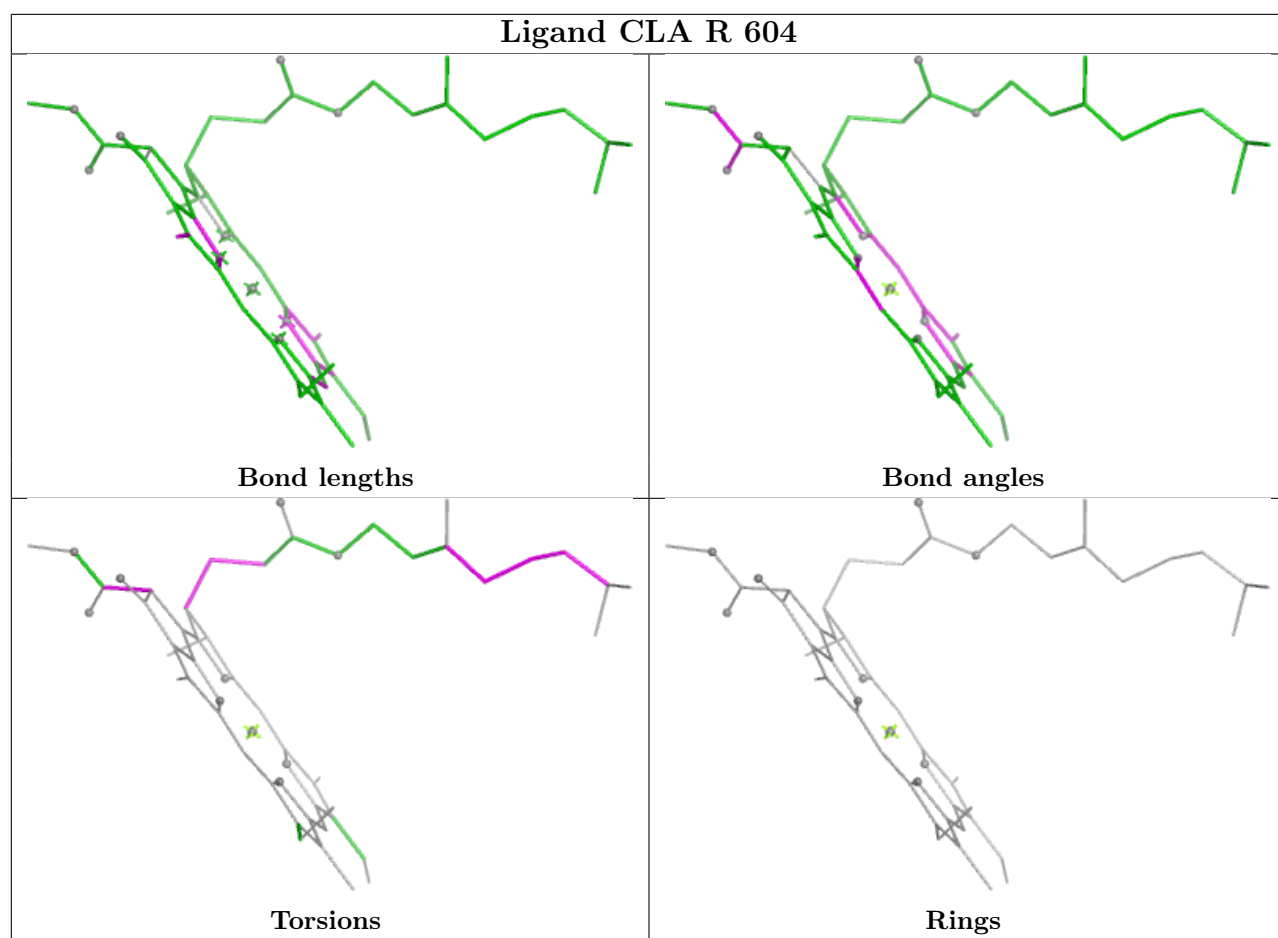


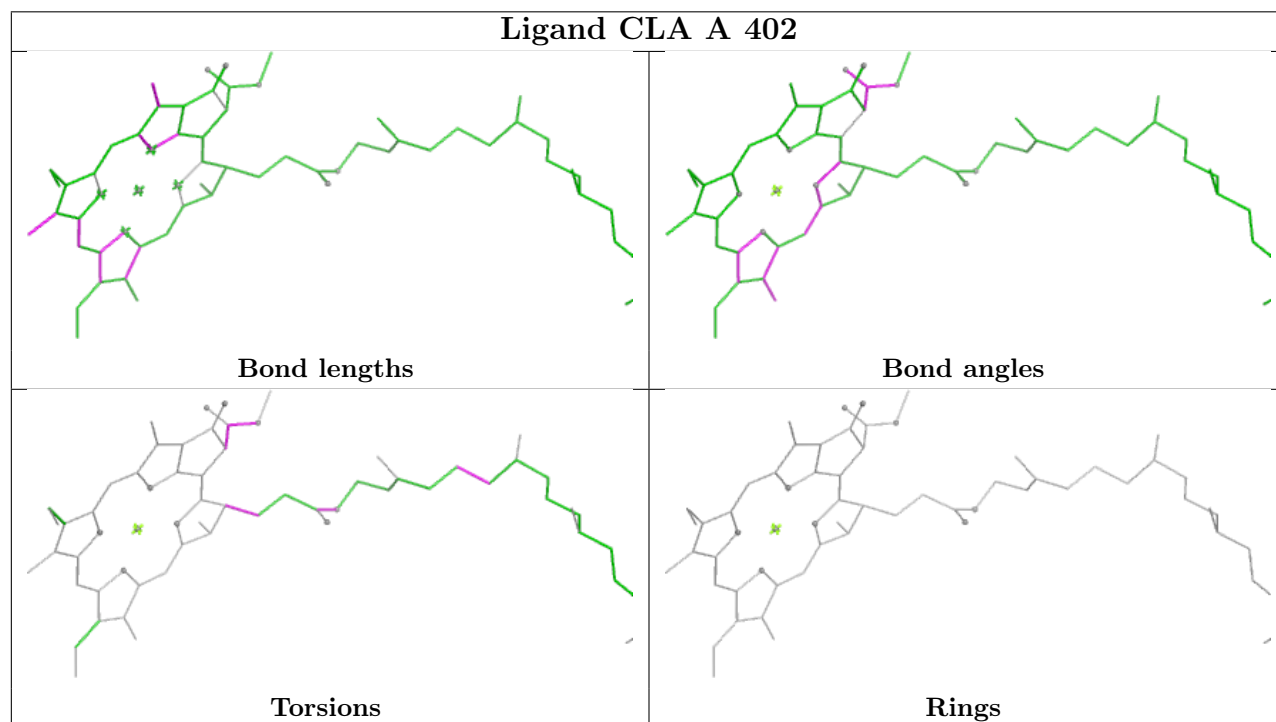
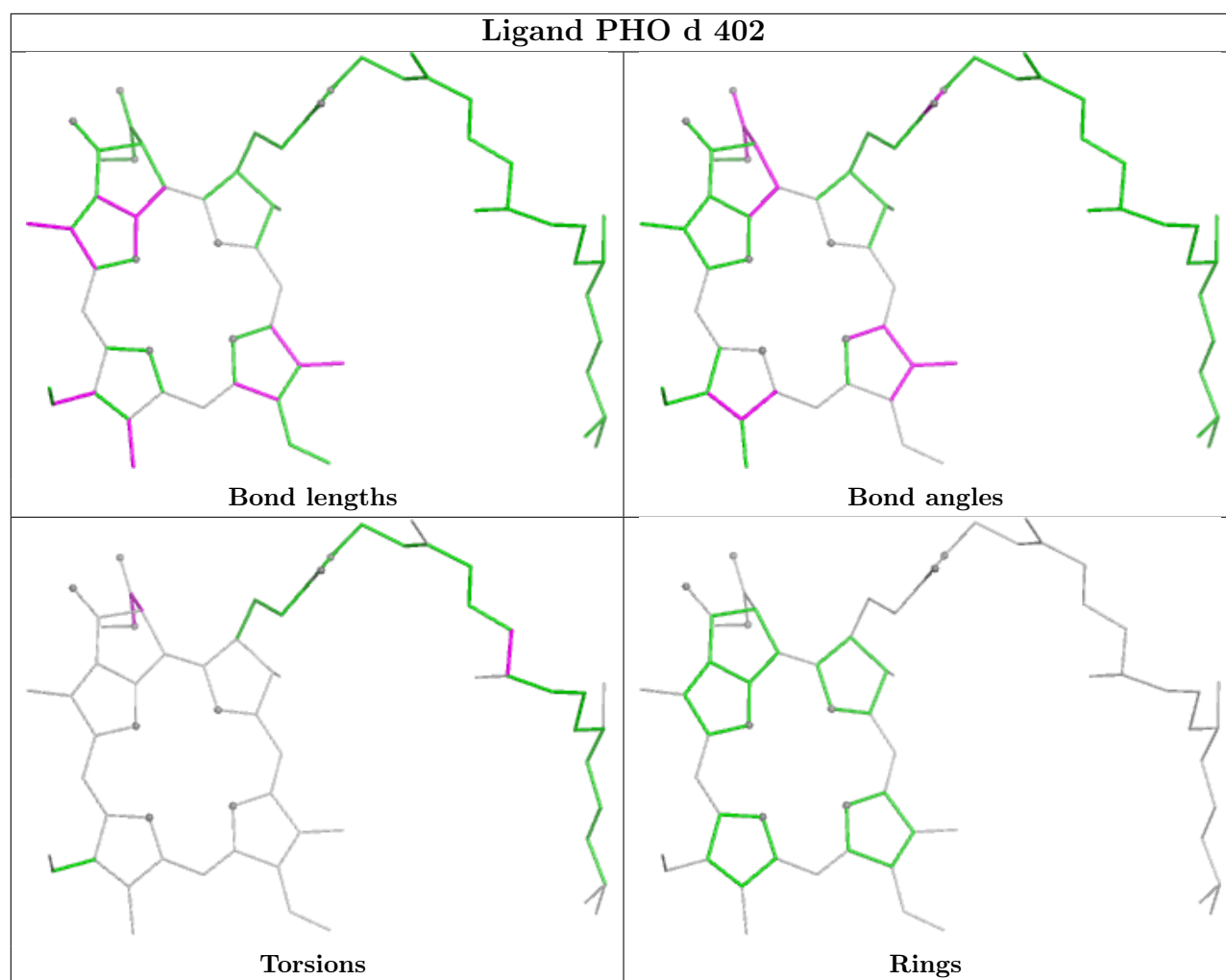


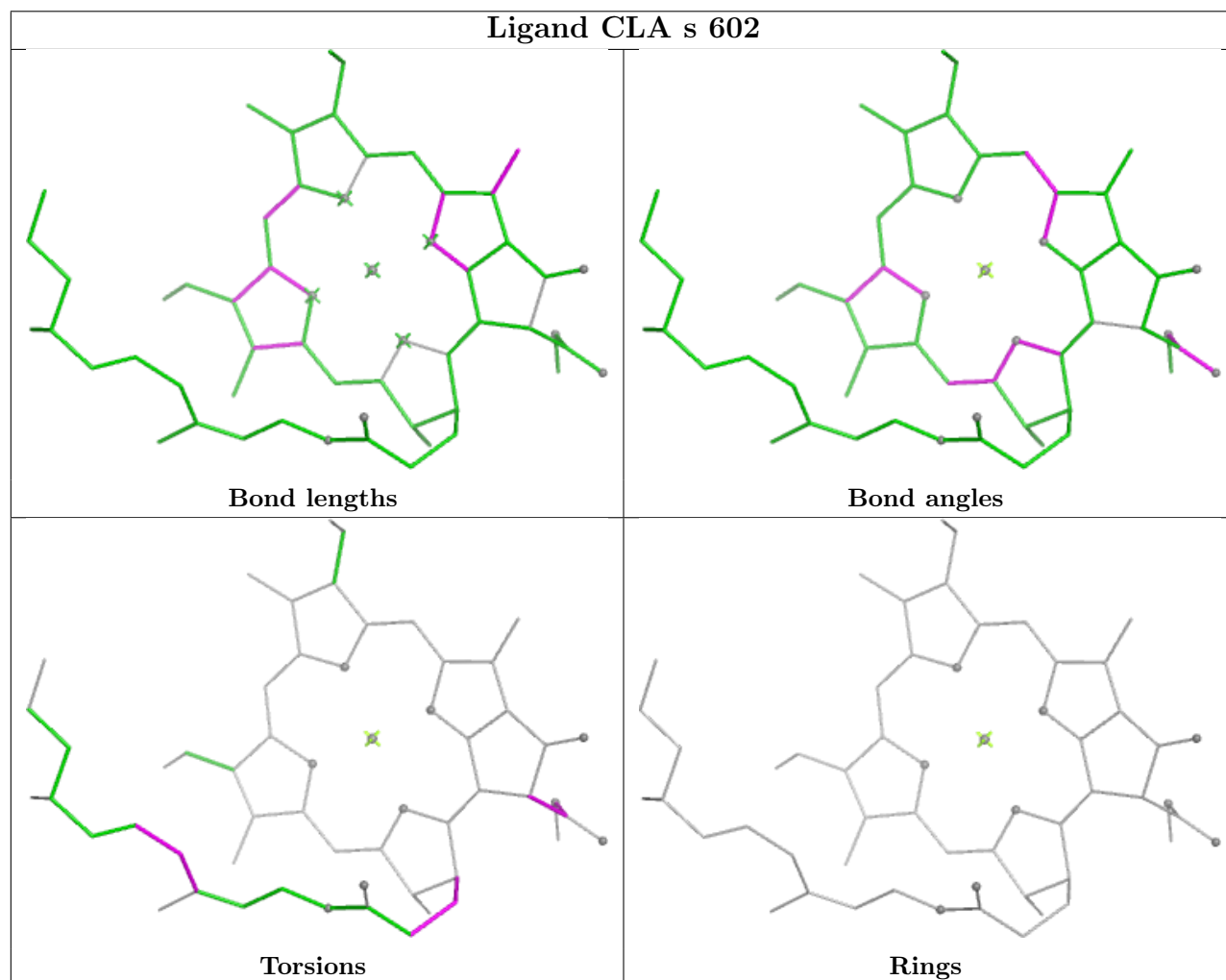
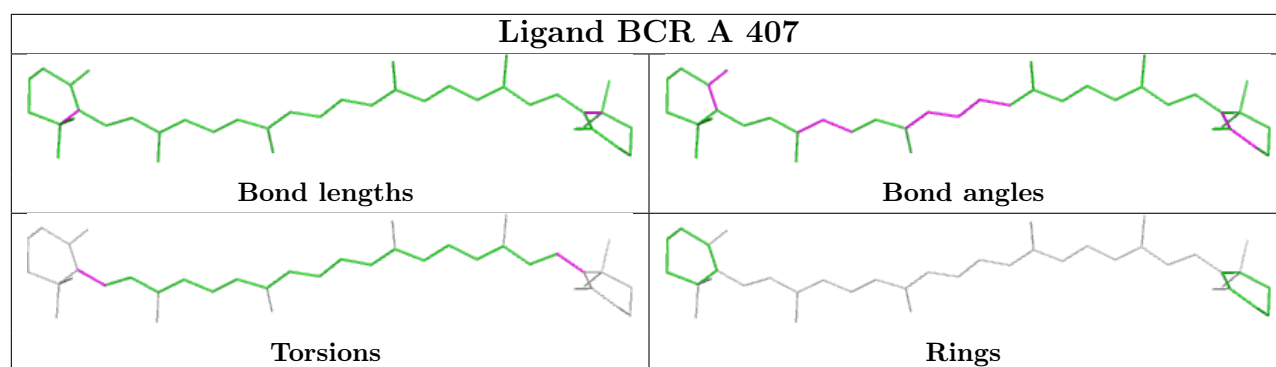


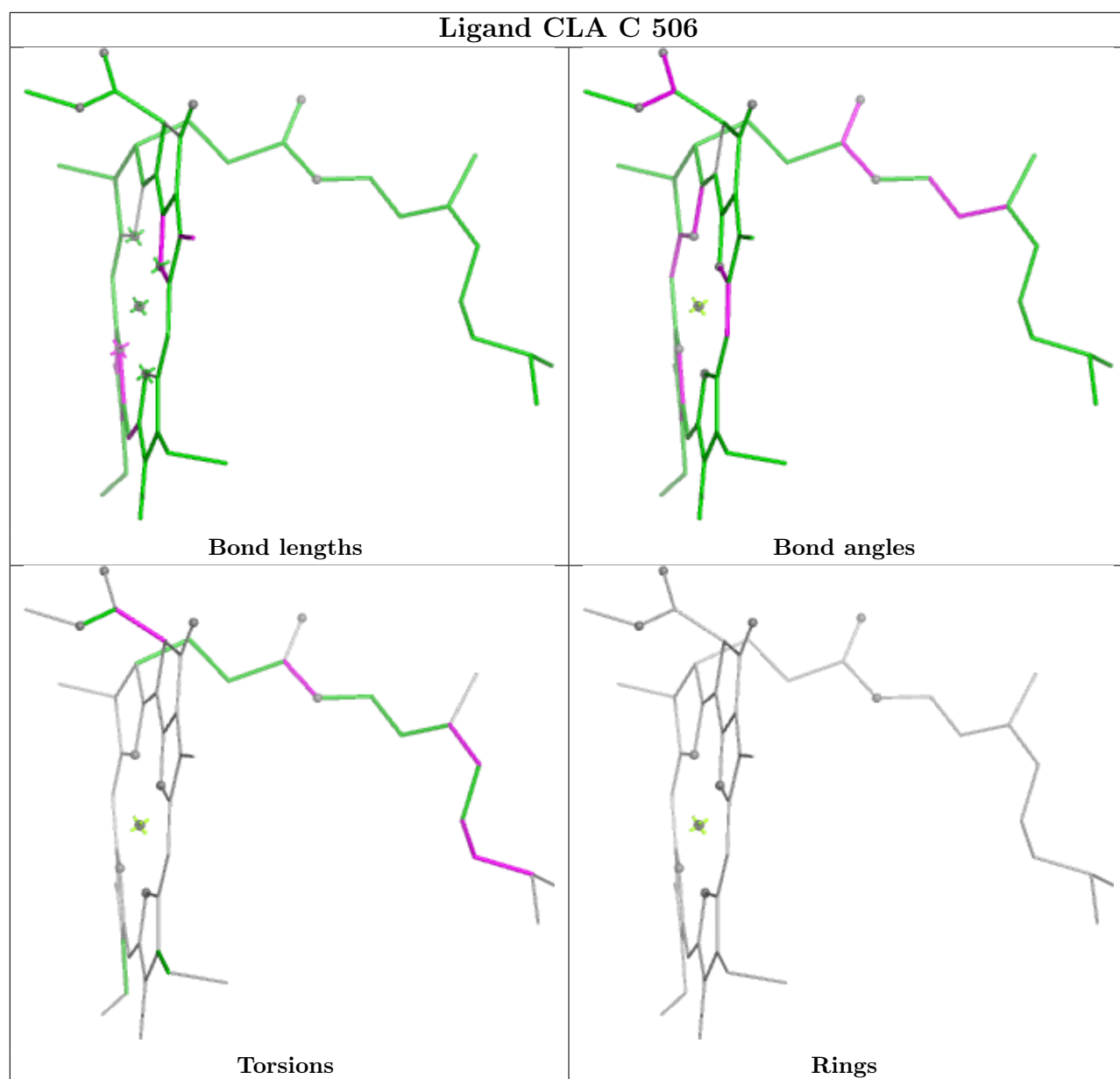


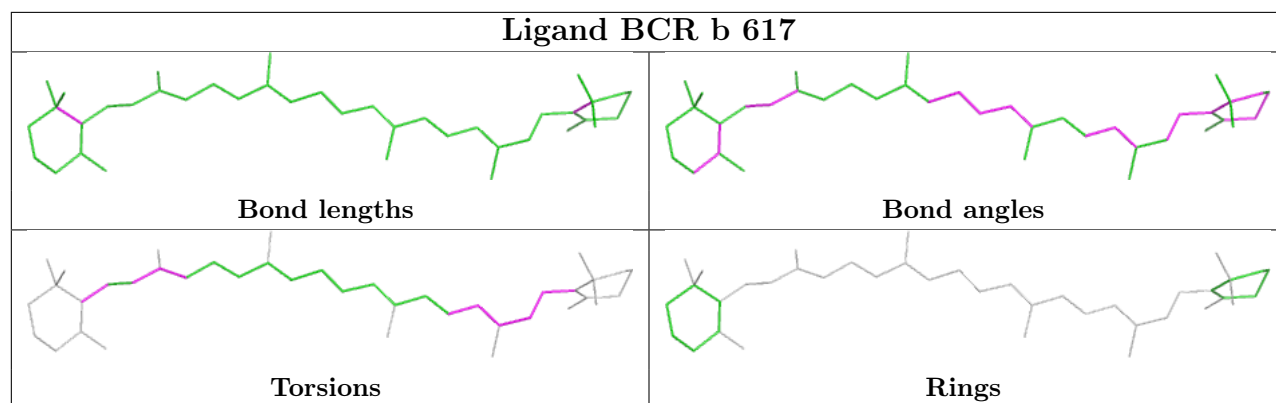
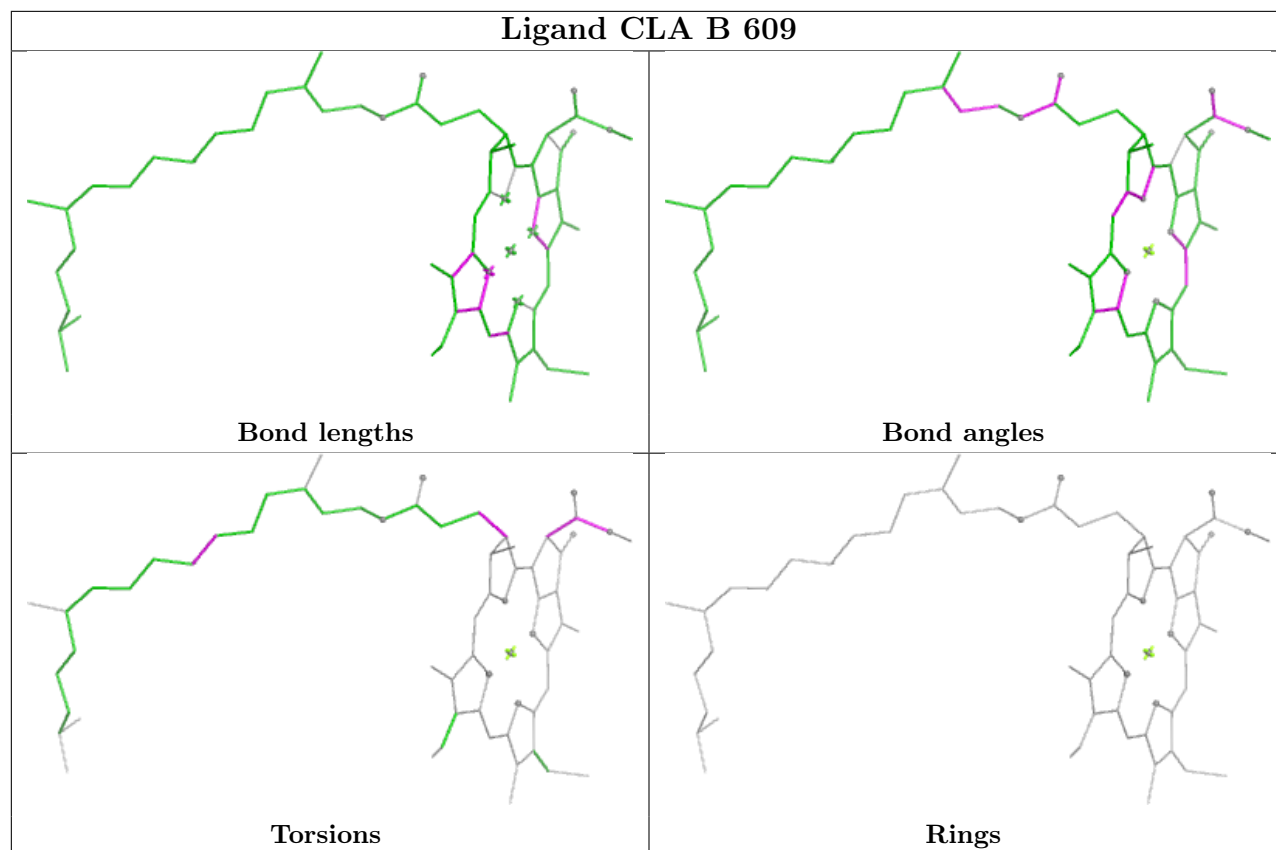




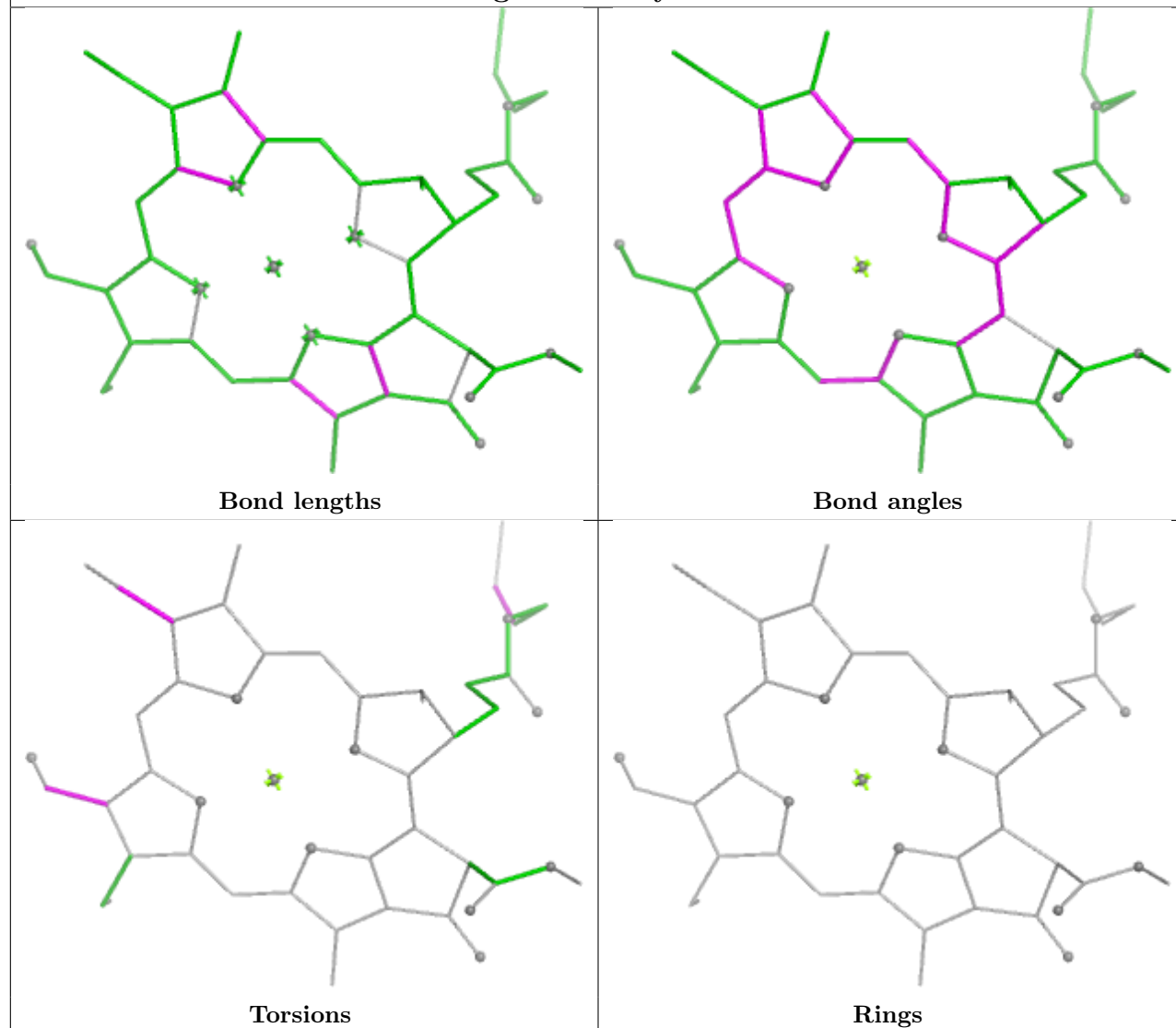




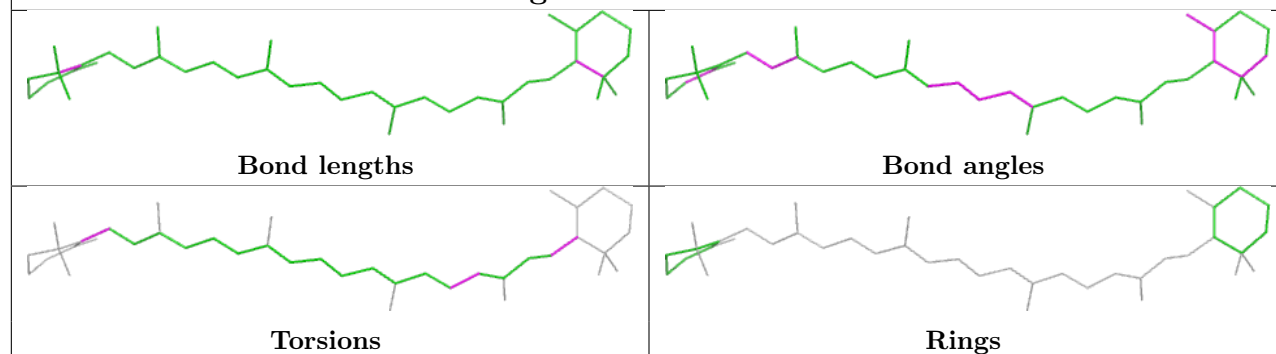




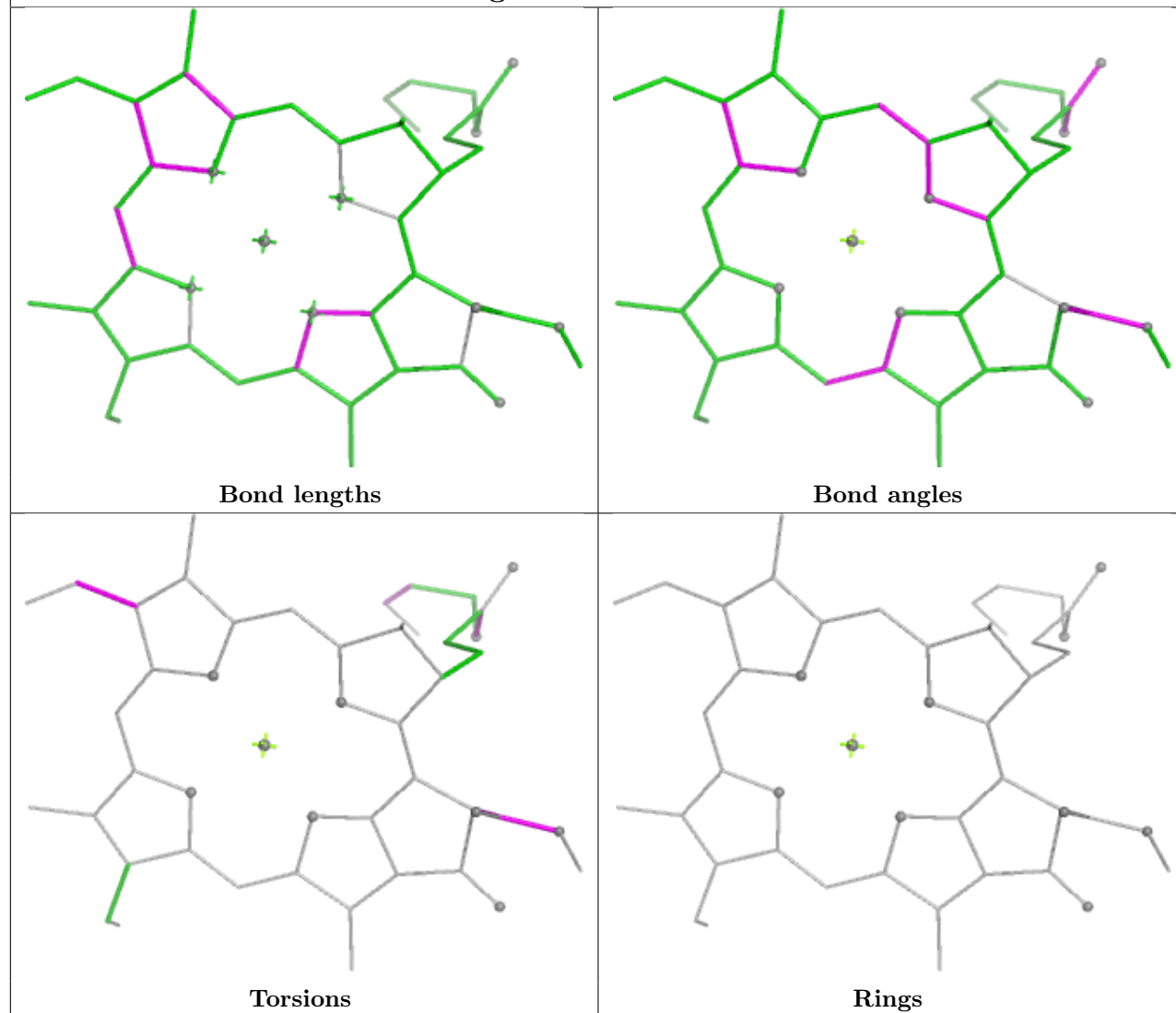
Ligand CHL y 309



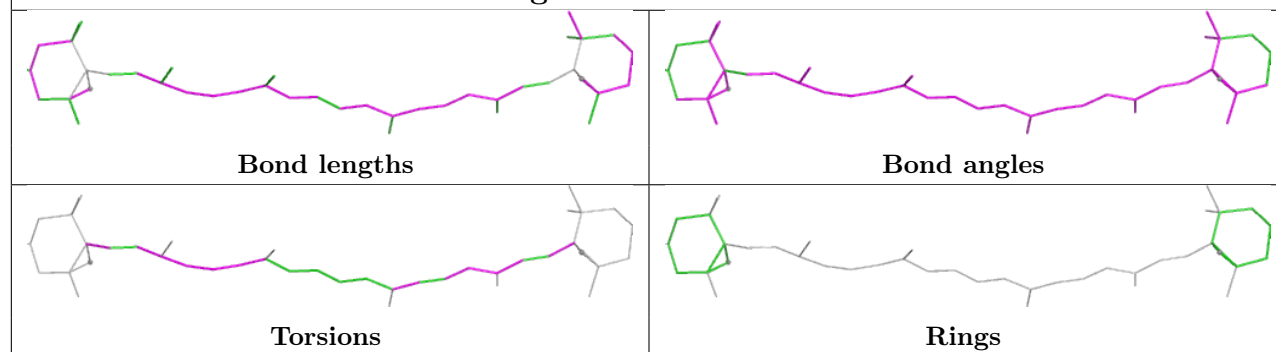
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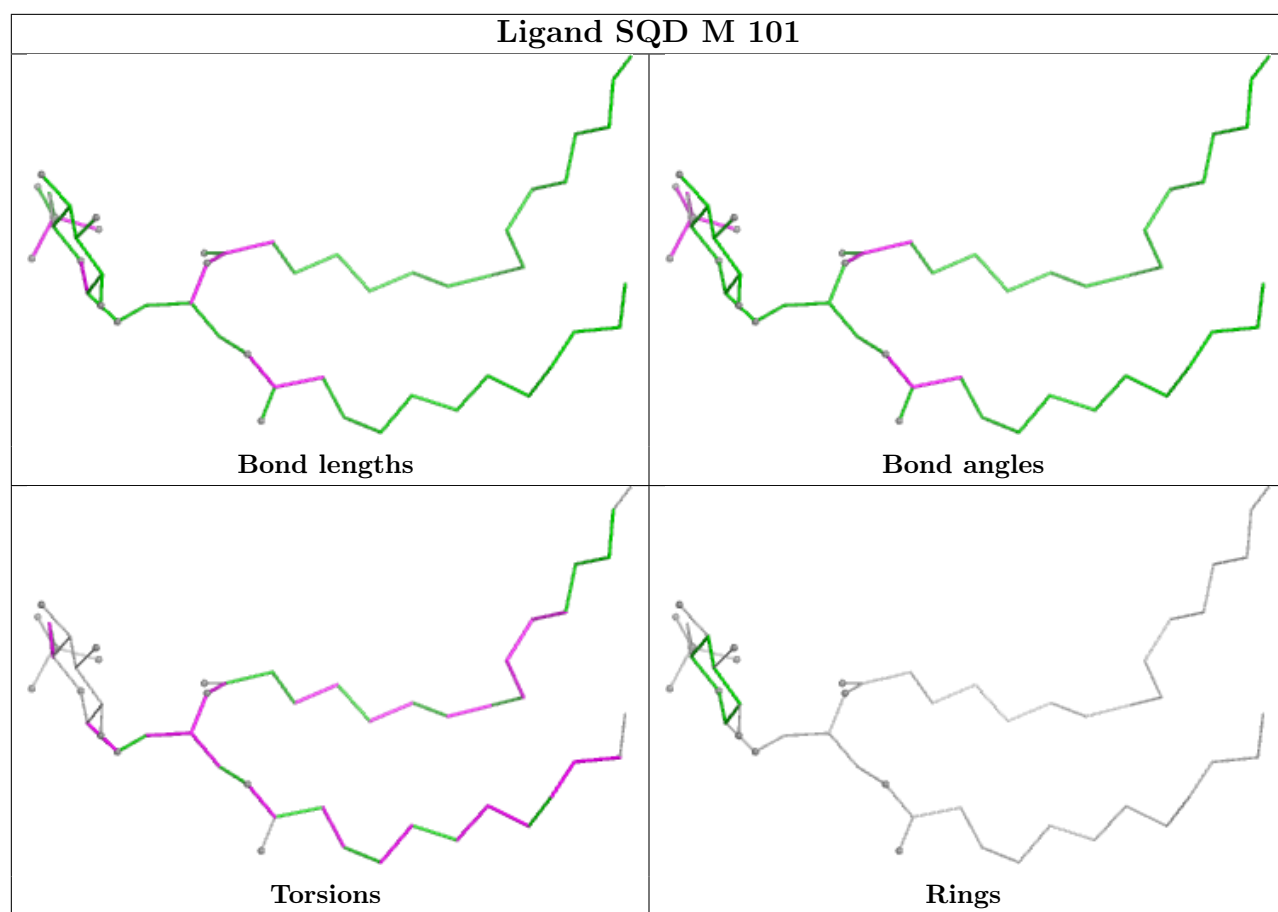


Ligand CLA G 614

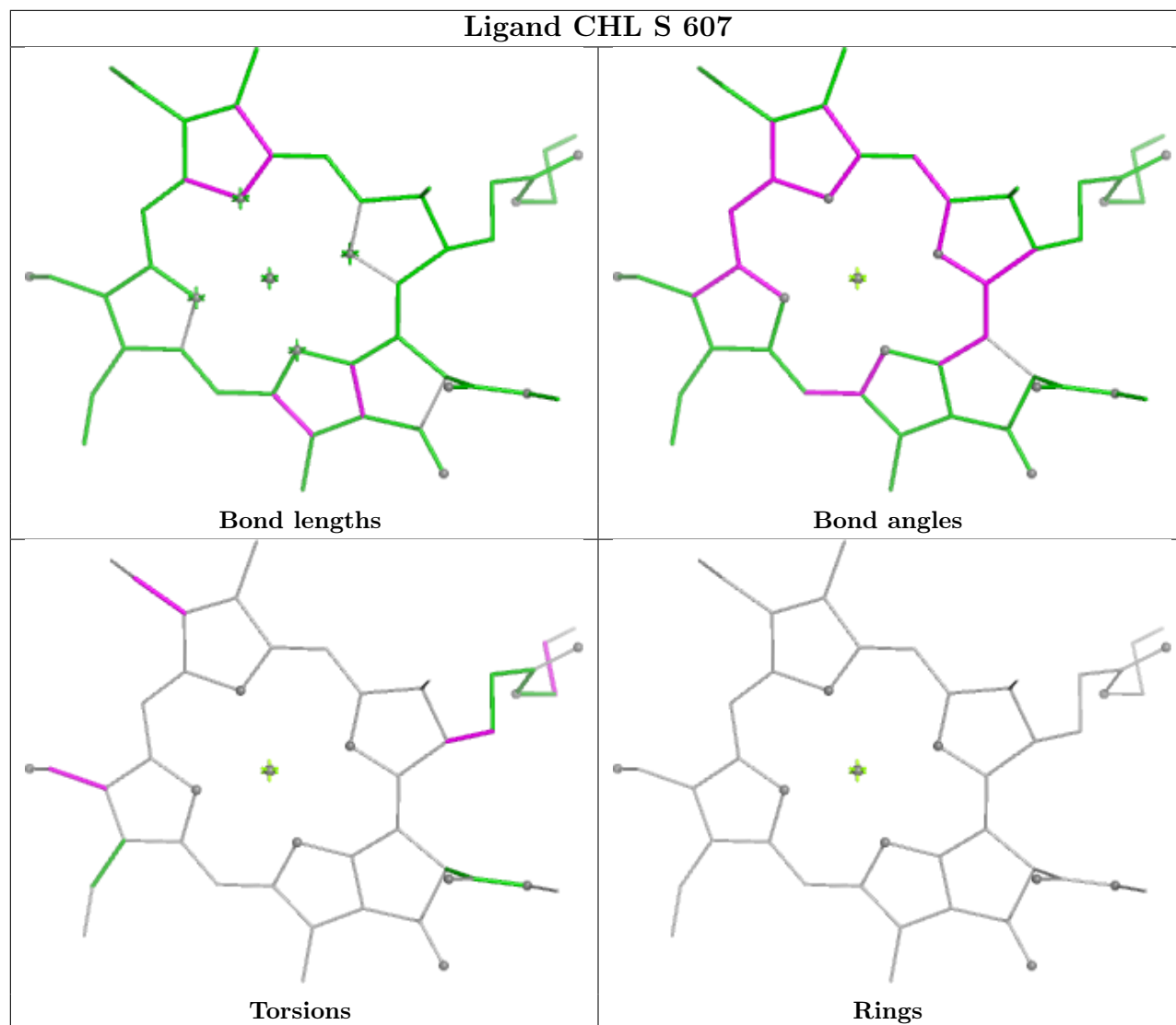


Ligand XAT N 619

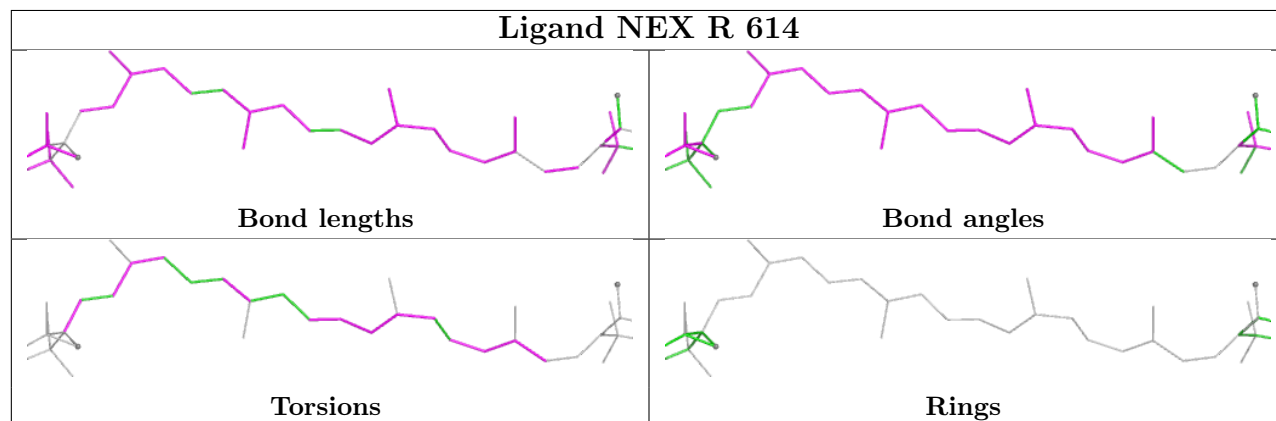


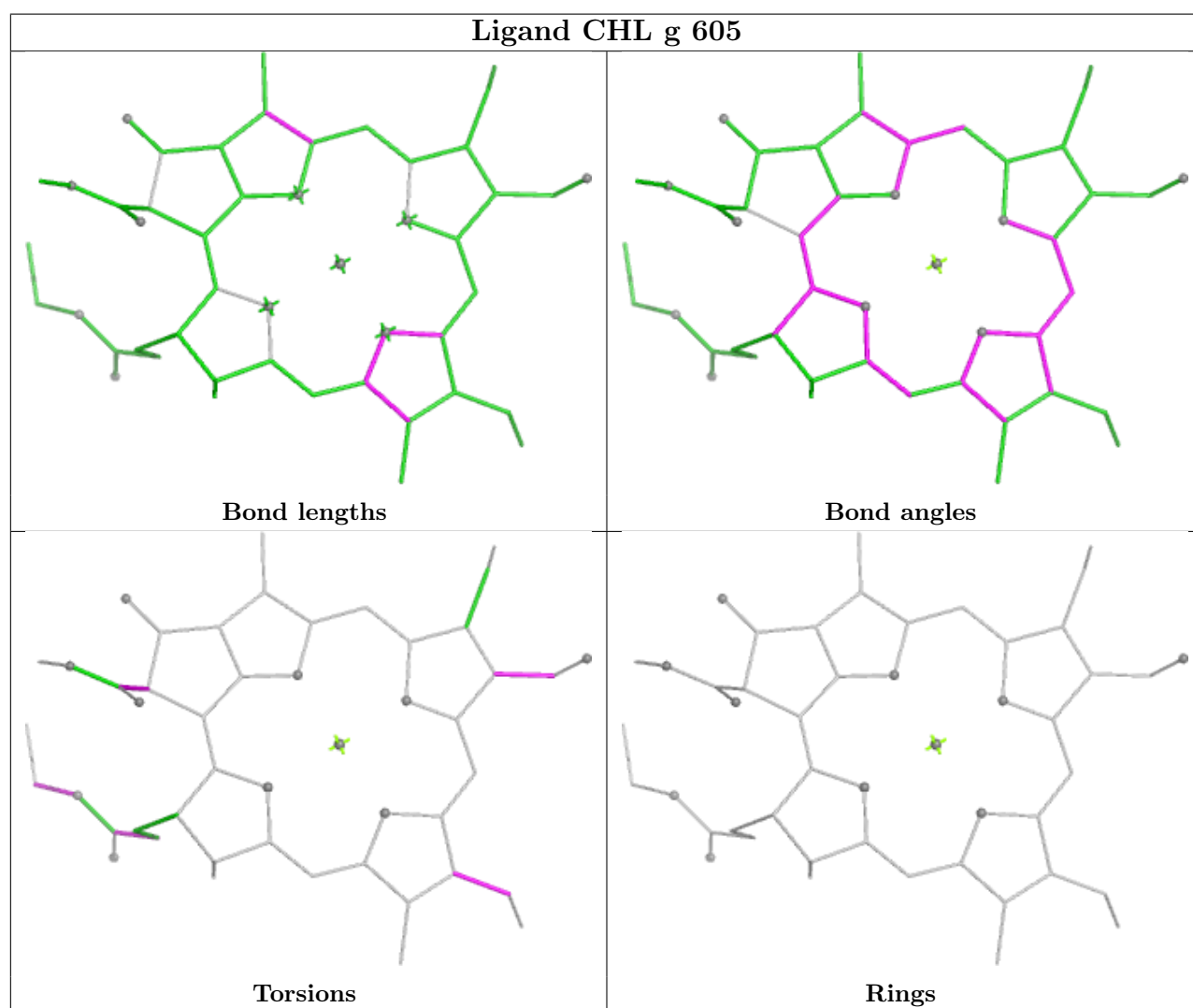
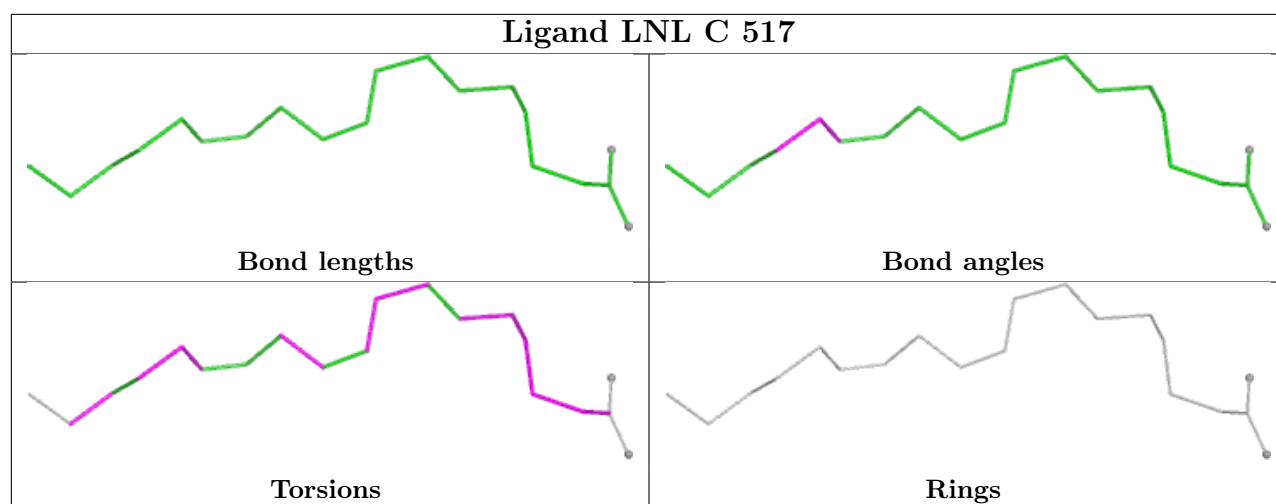


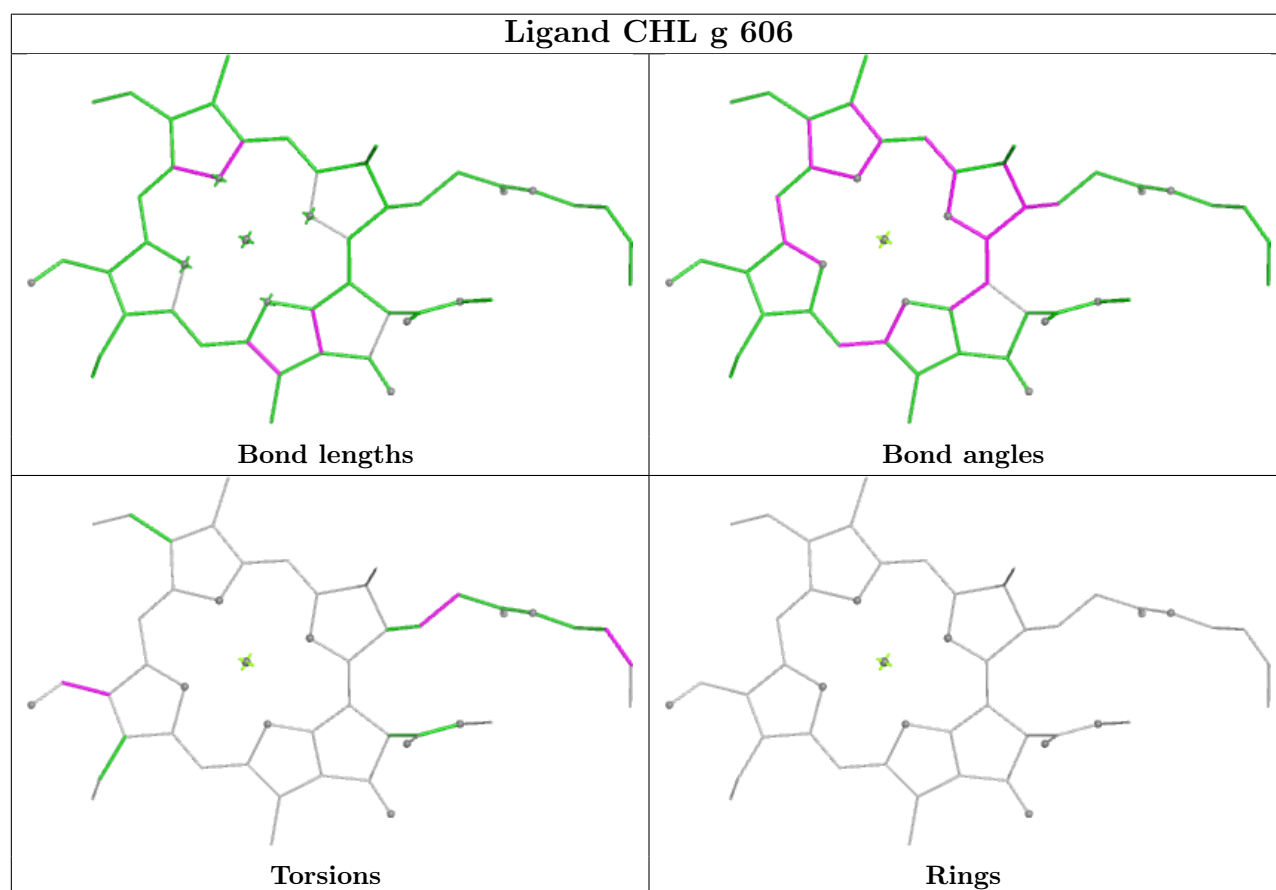
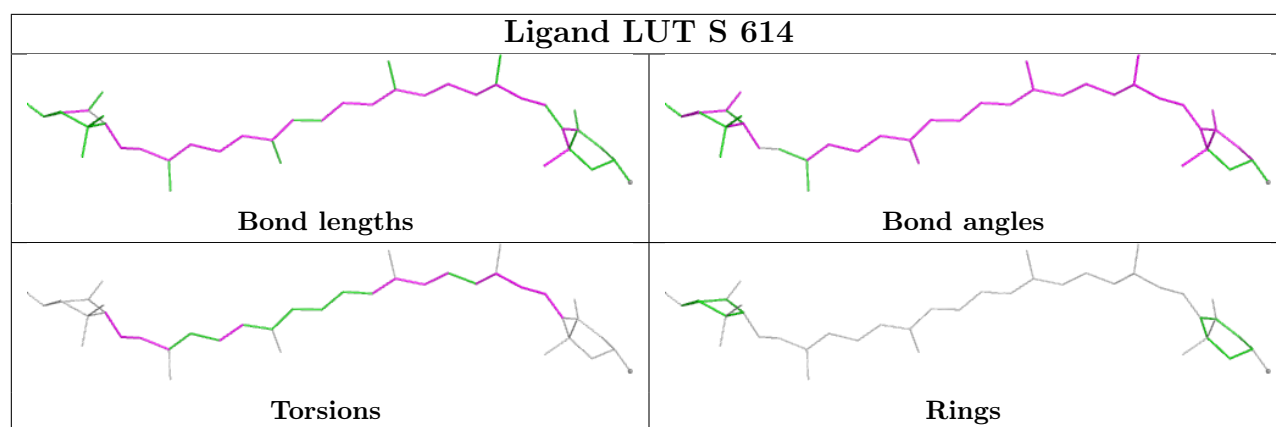
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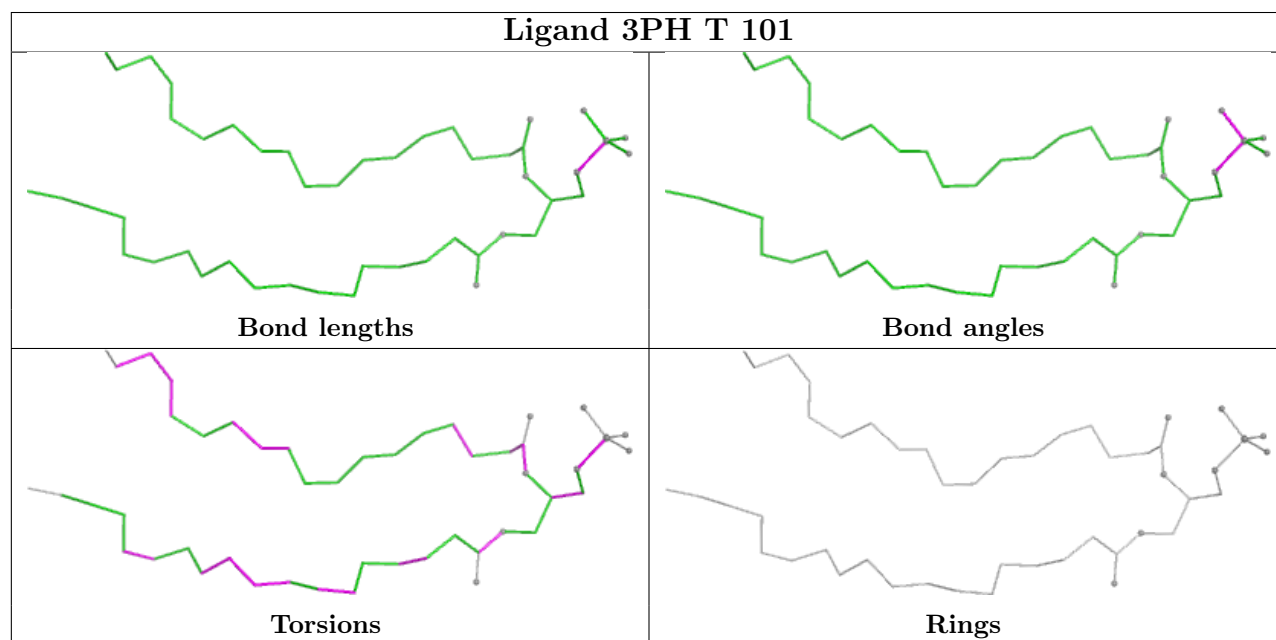
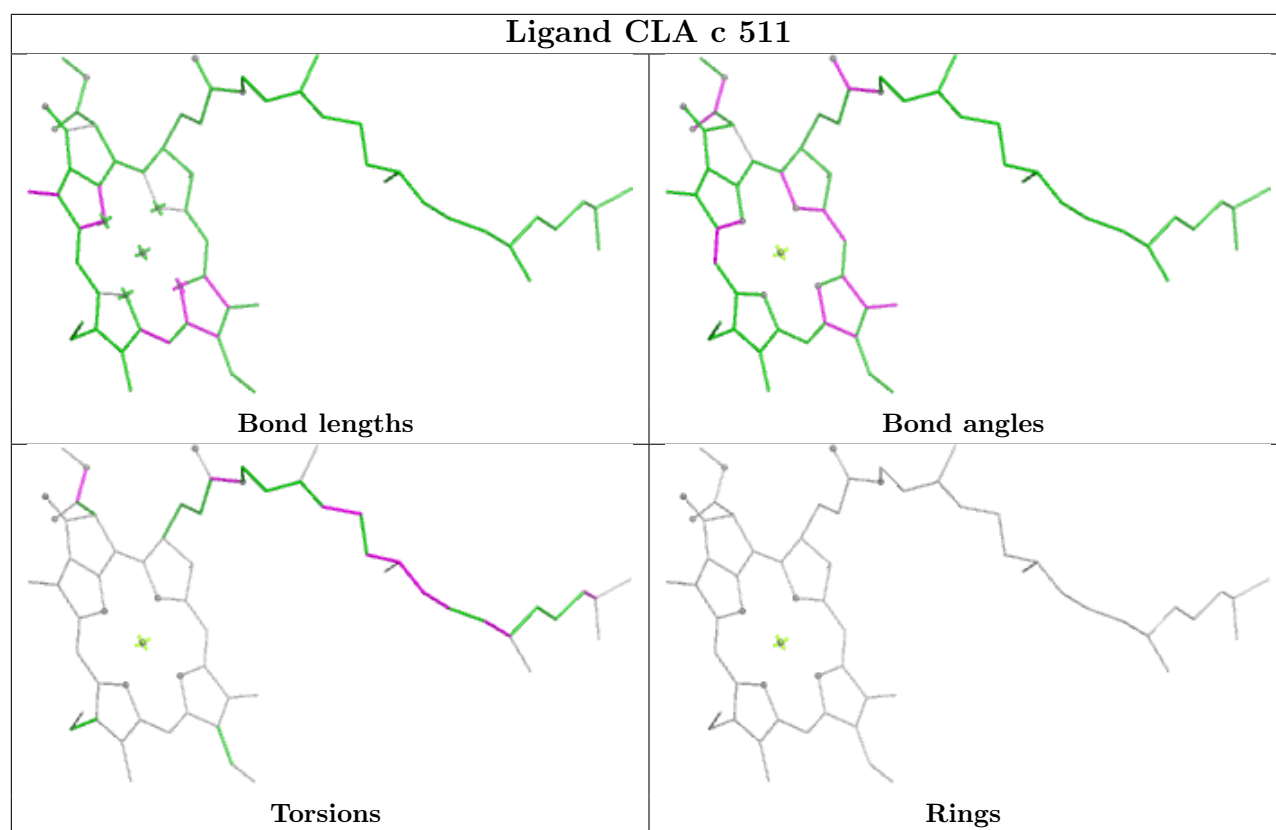


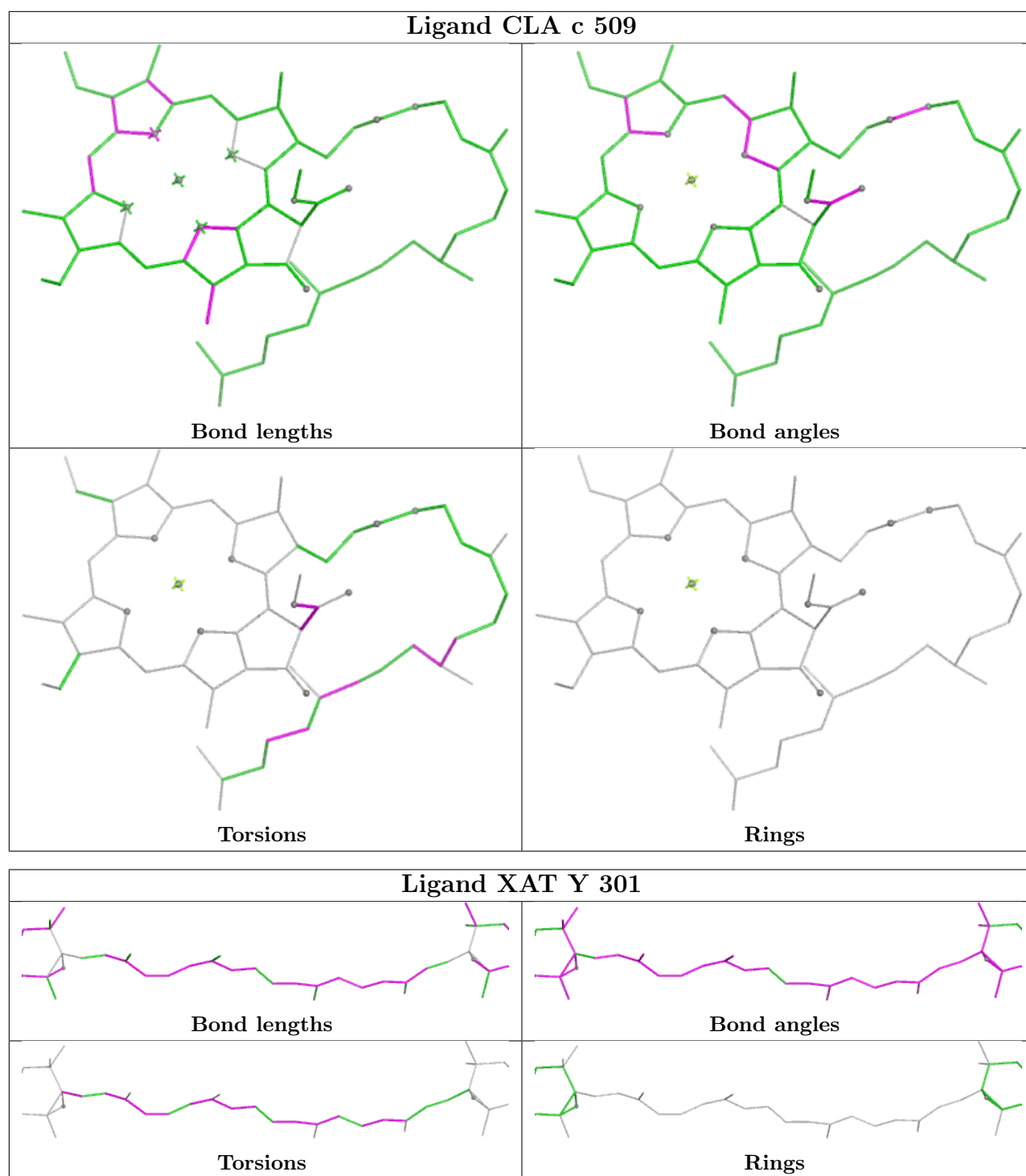
Ligand NEX R 614

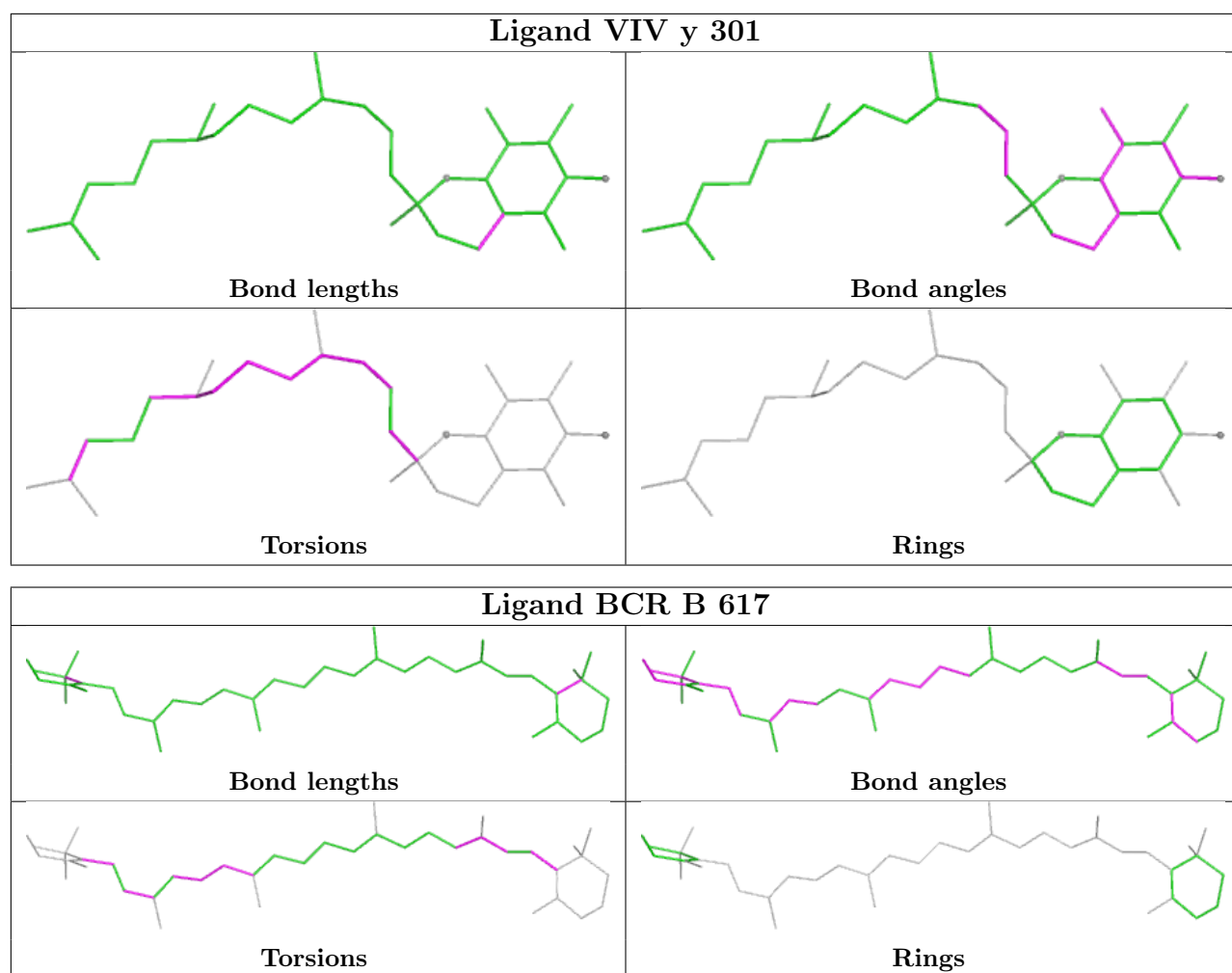


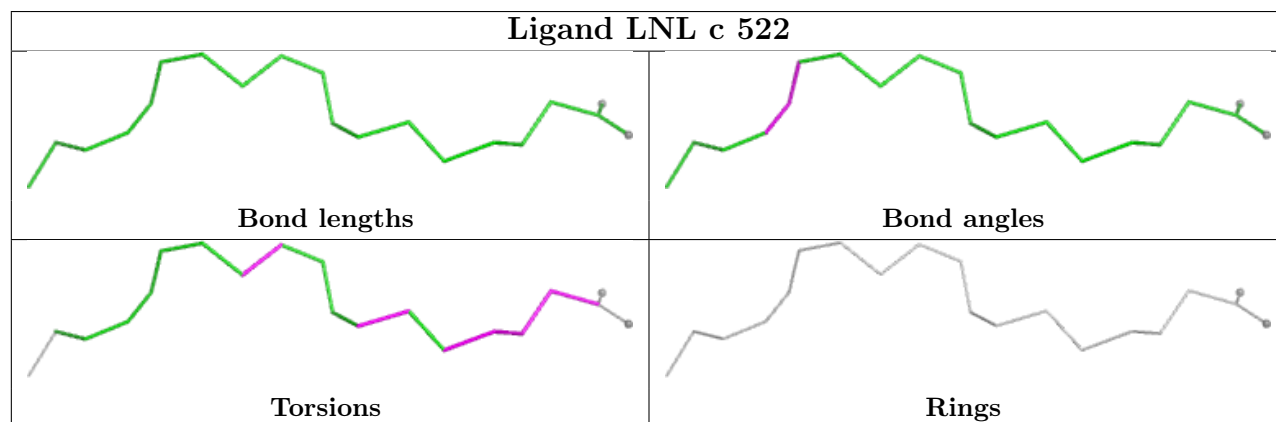
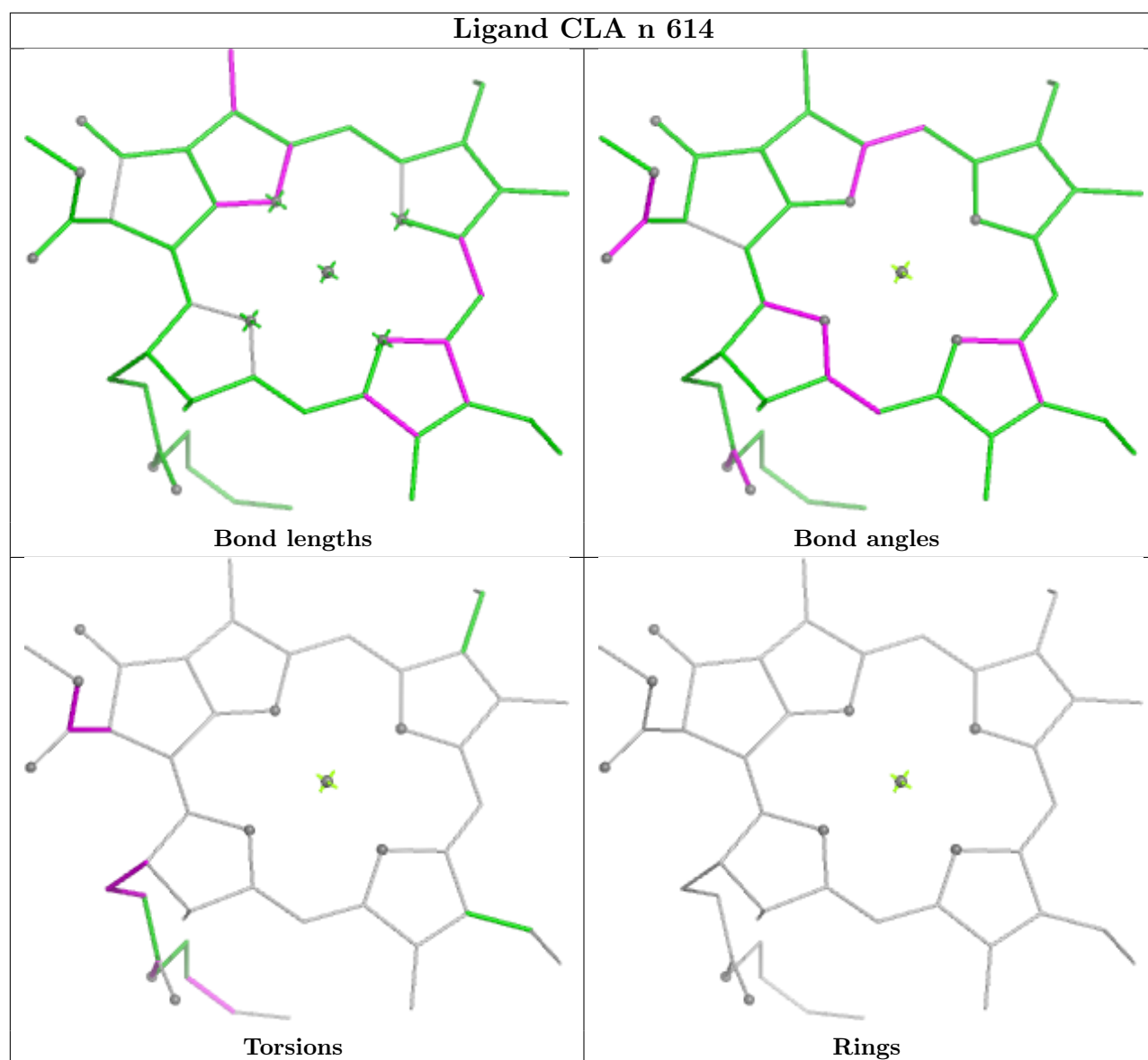


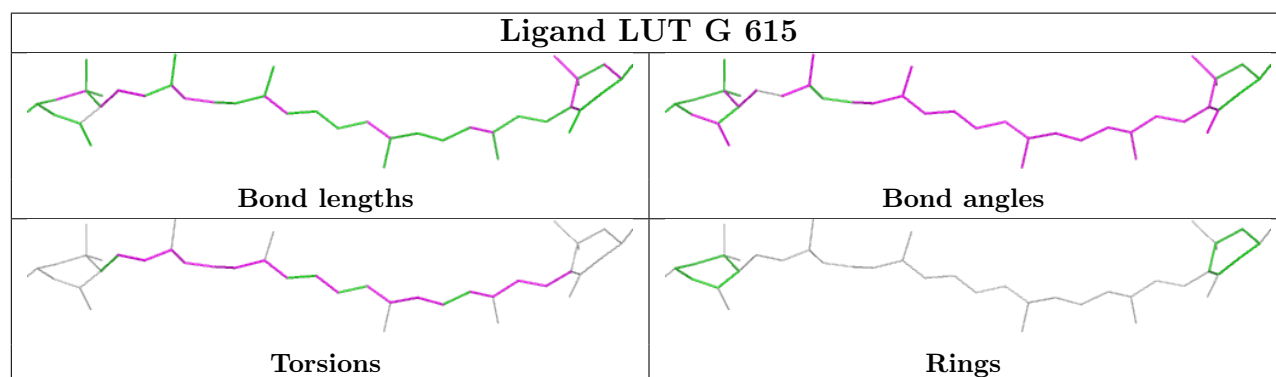
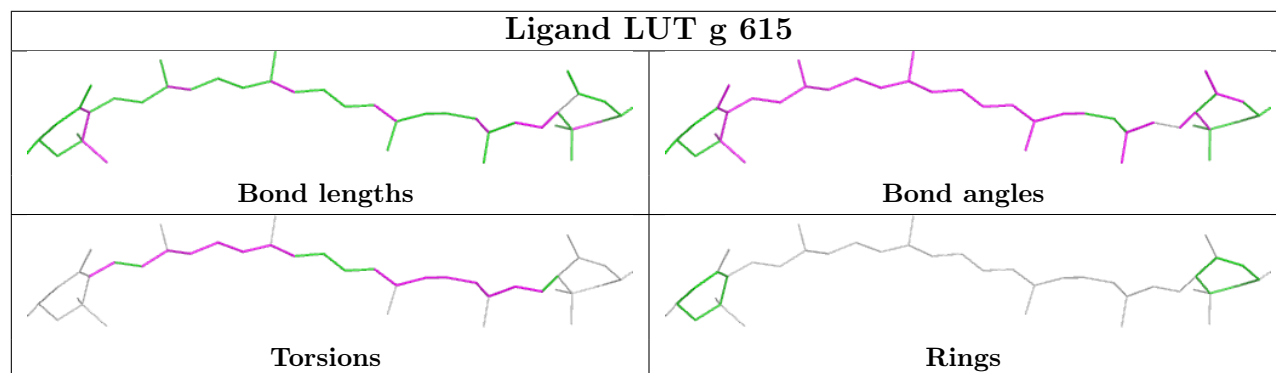
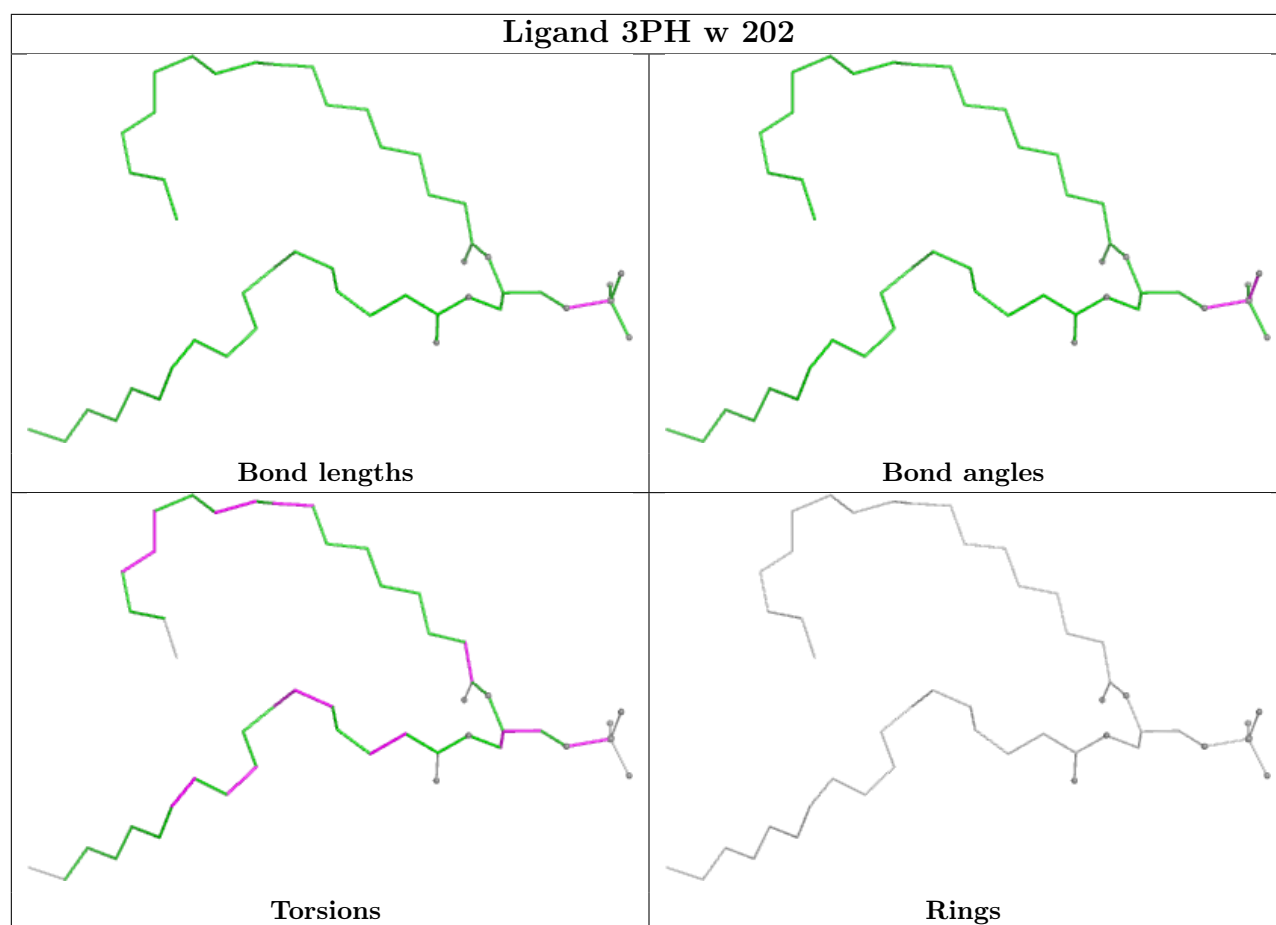


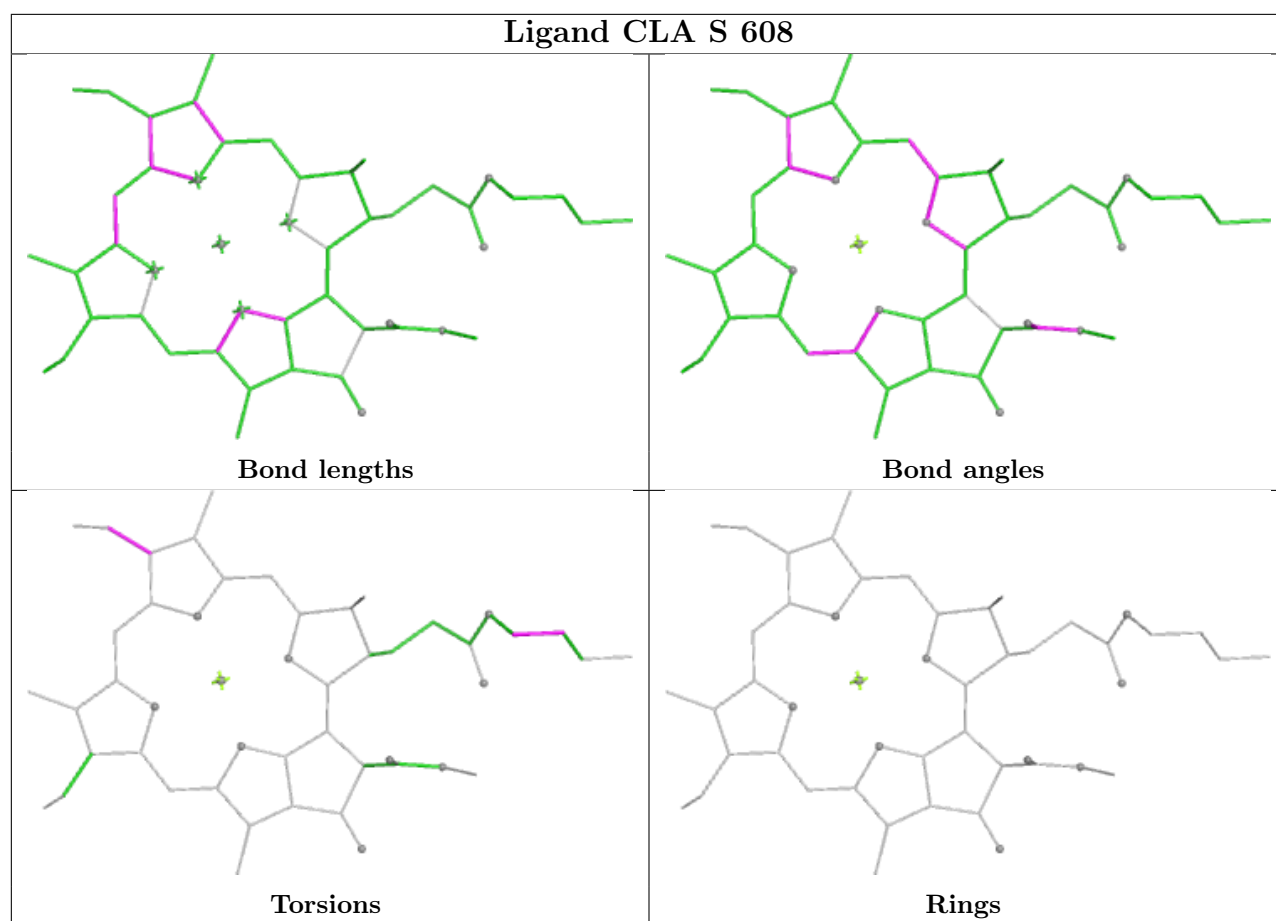


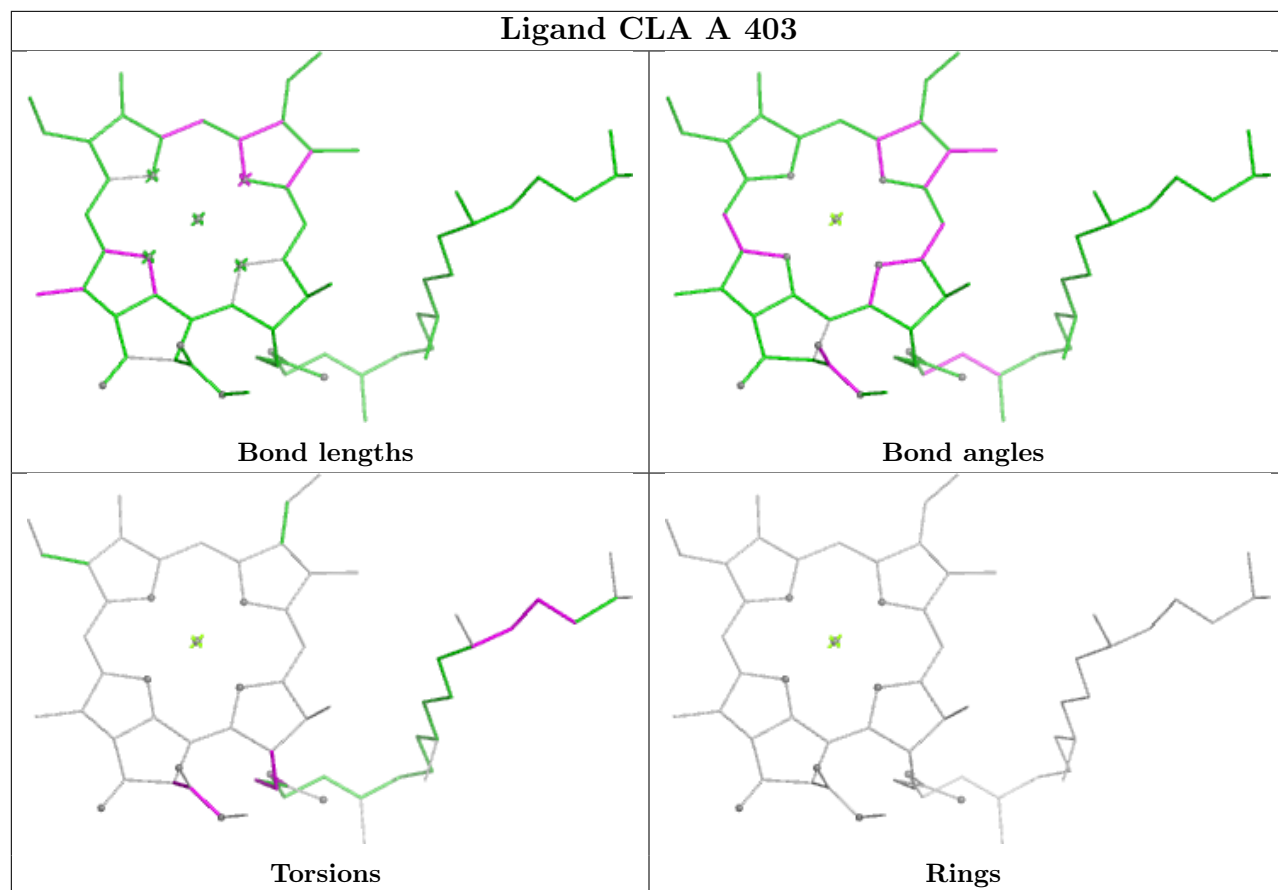


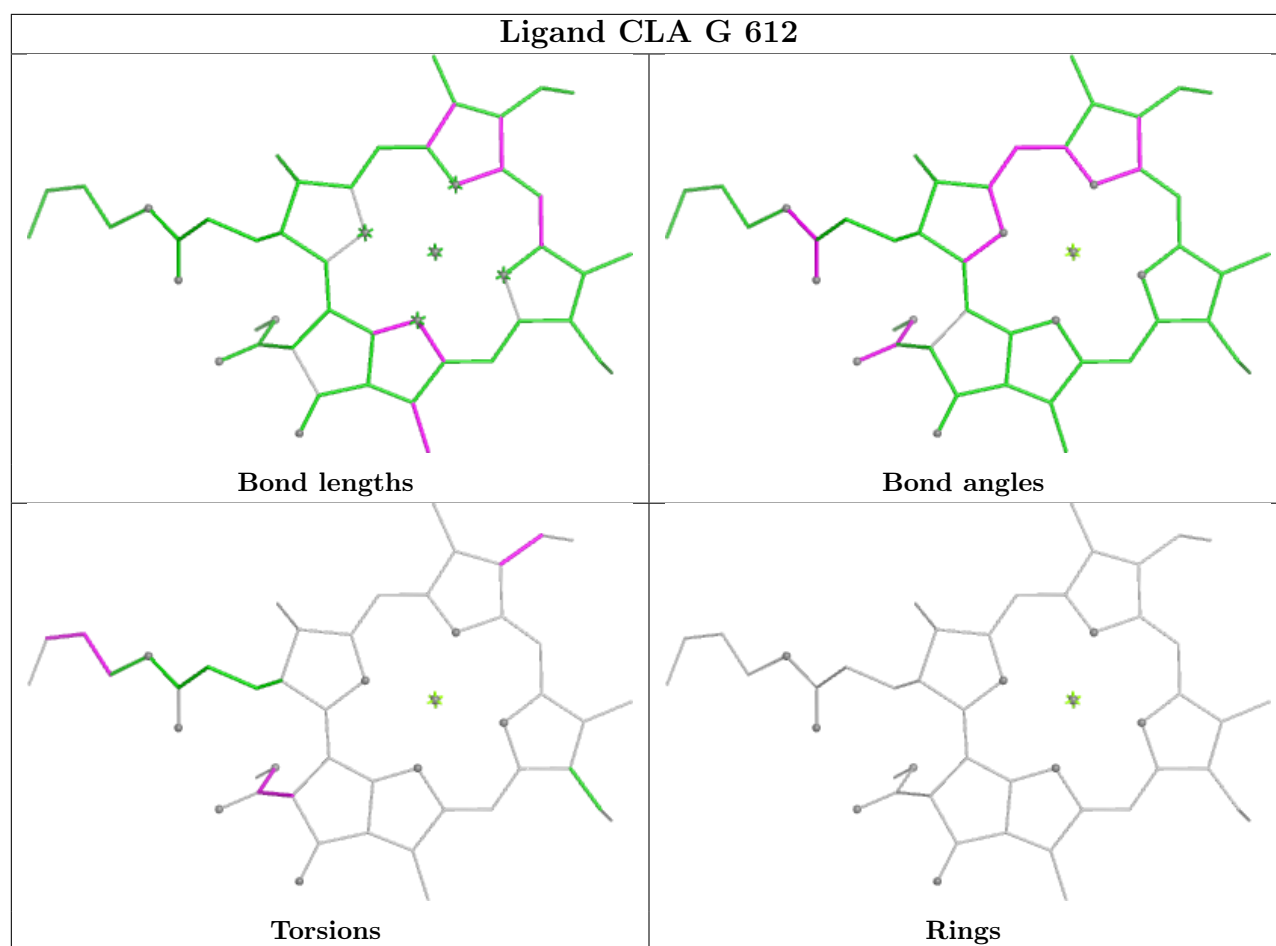


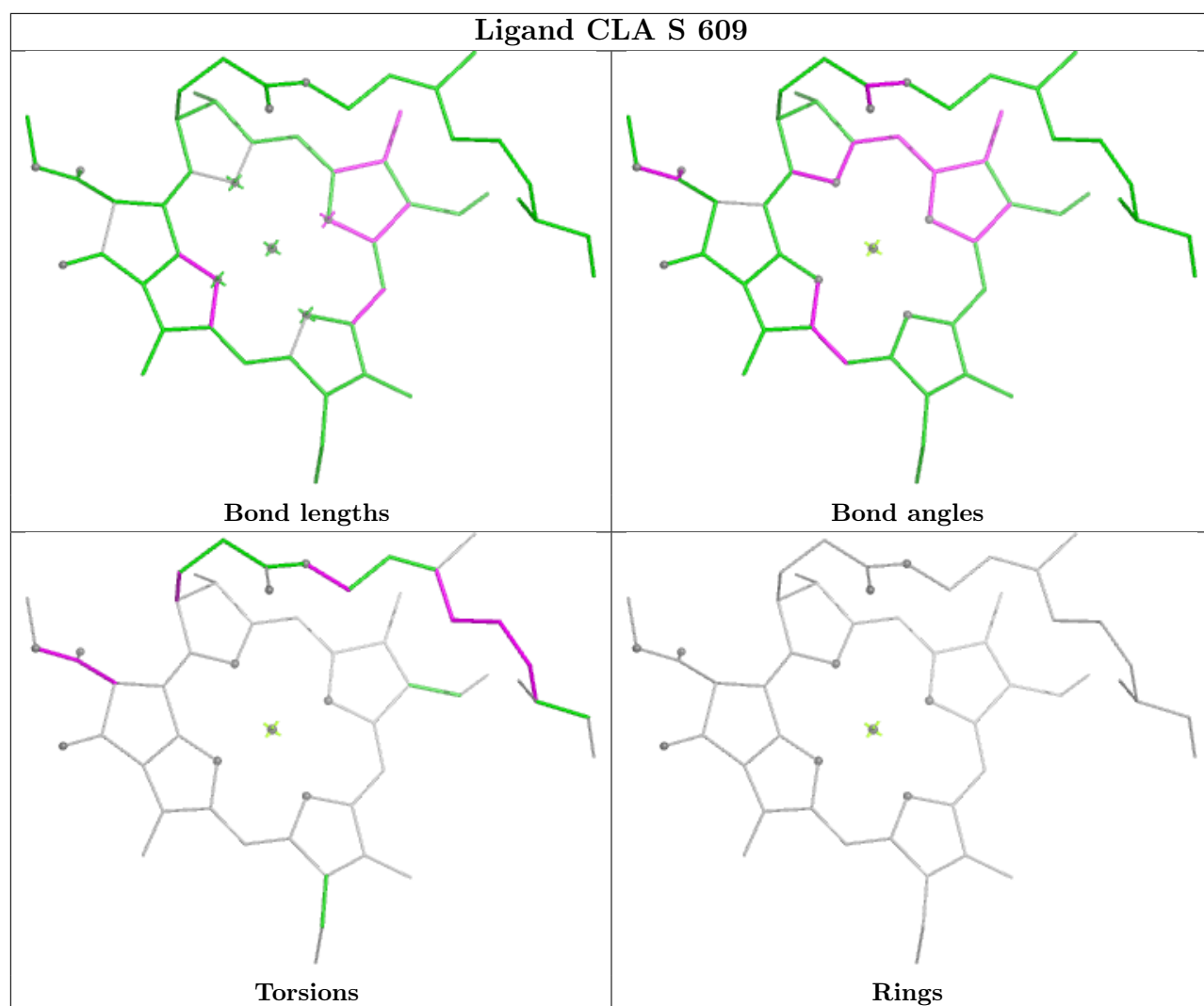


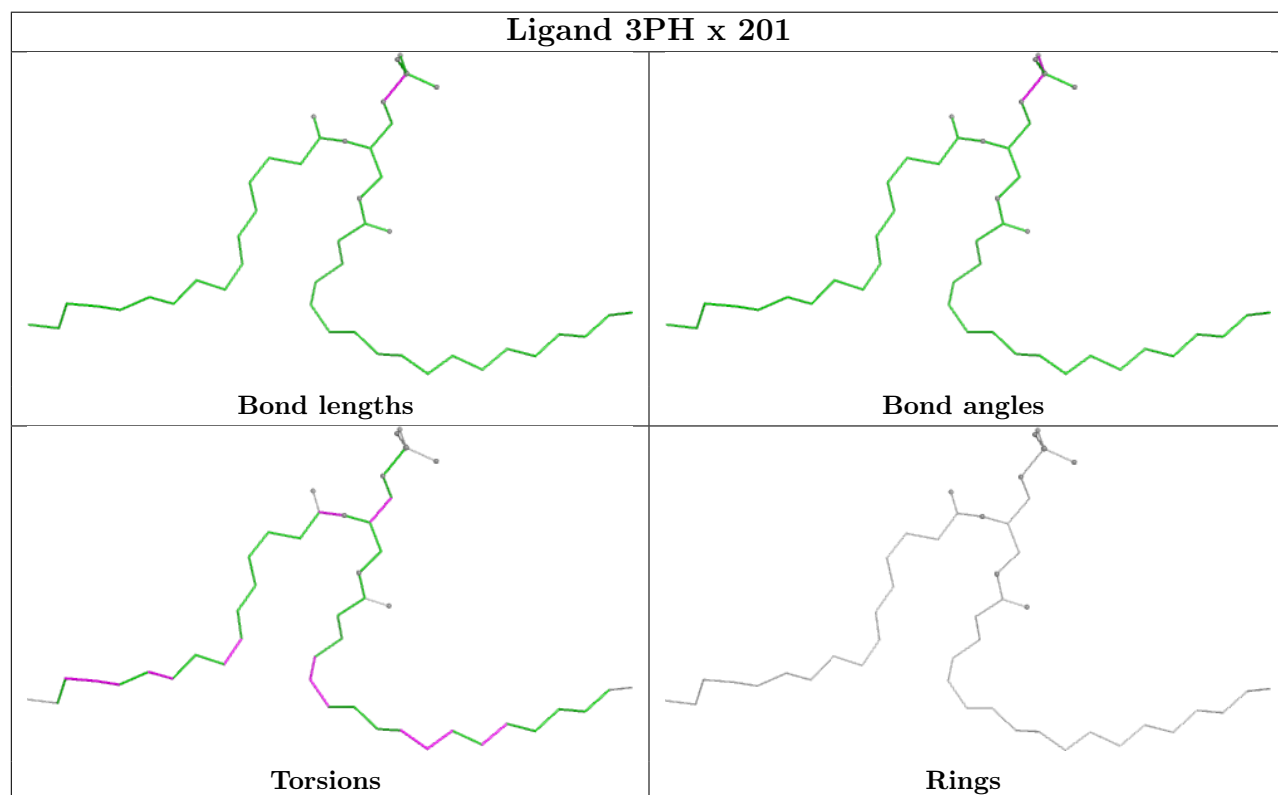
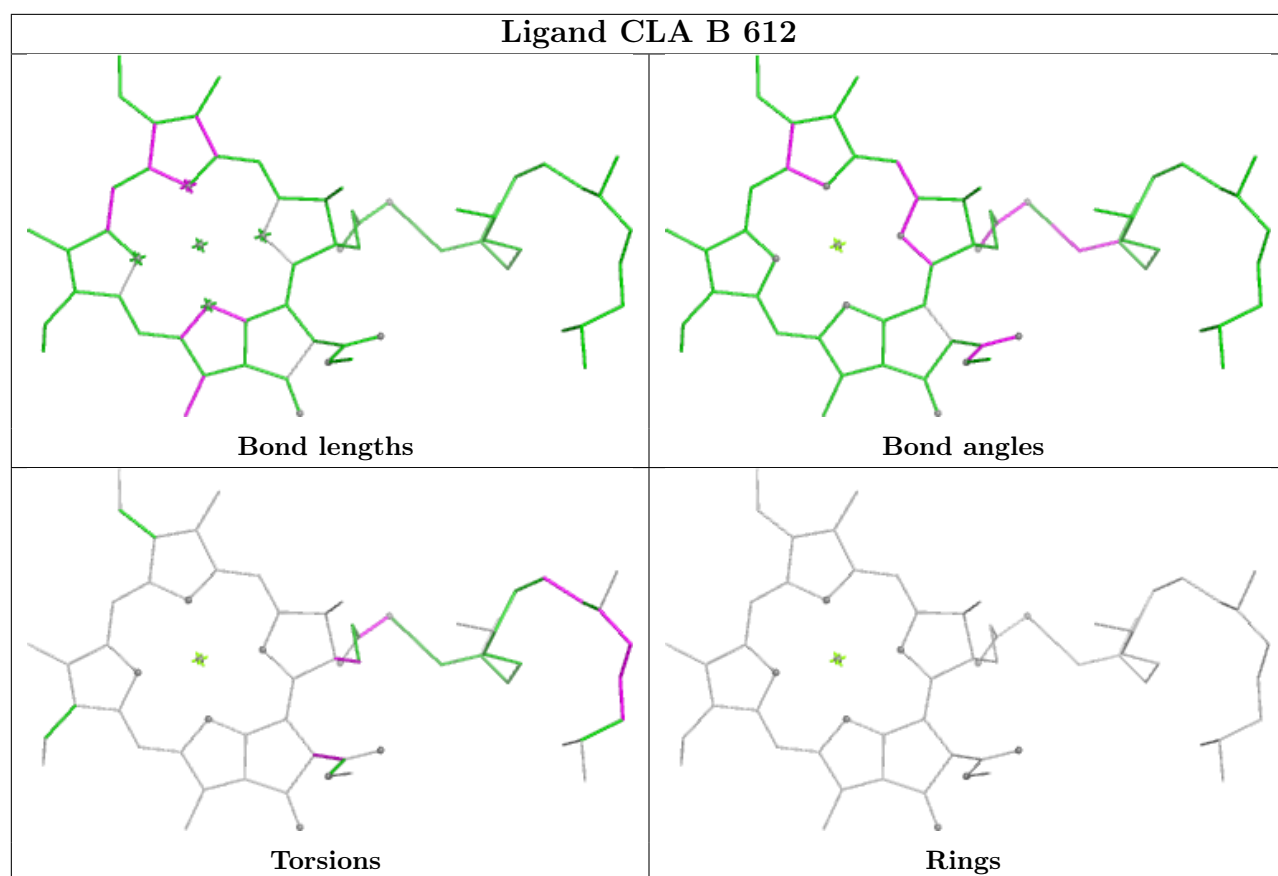


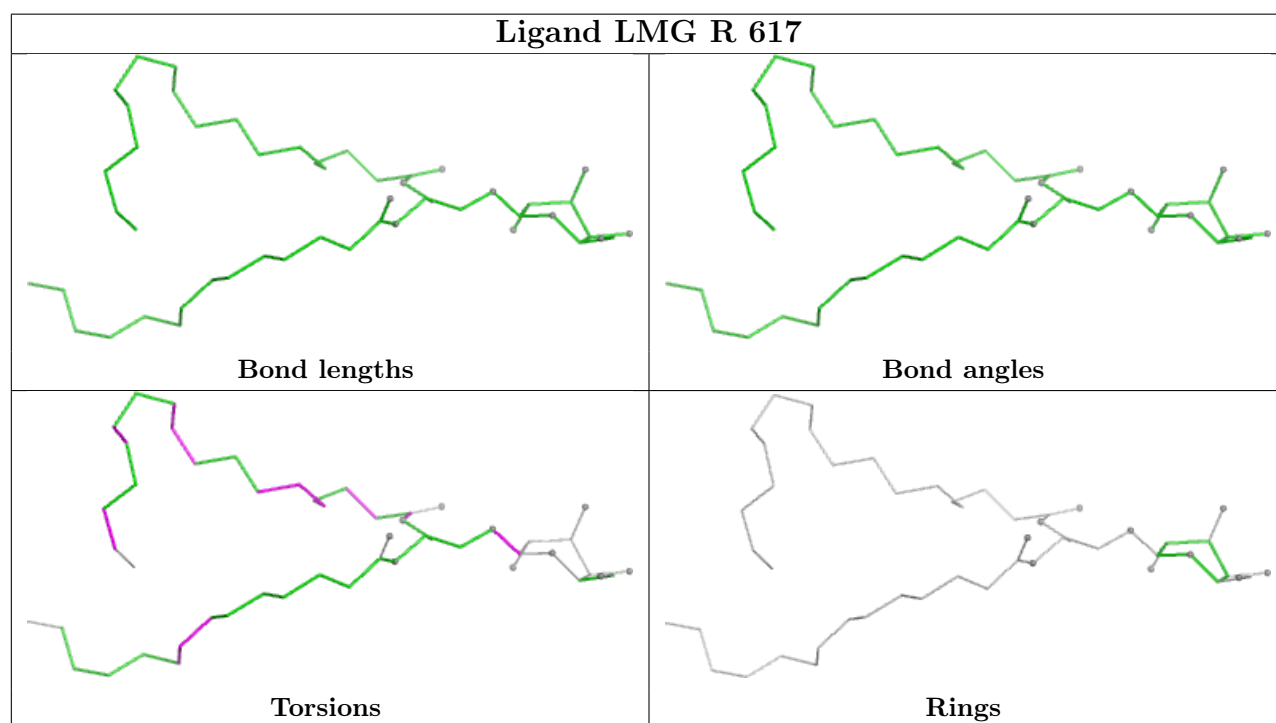
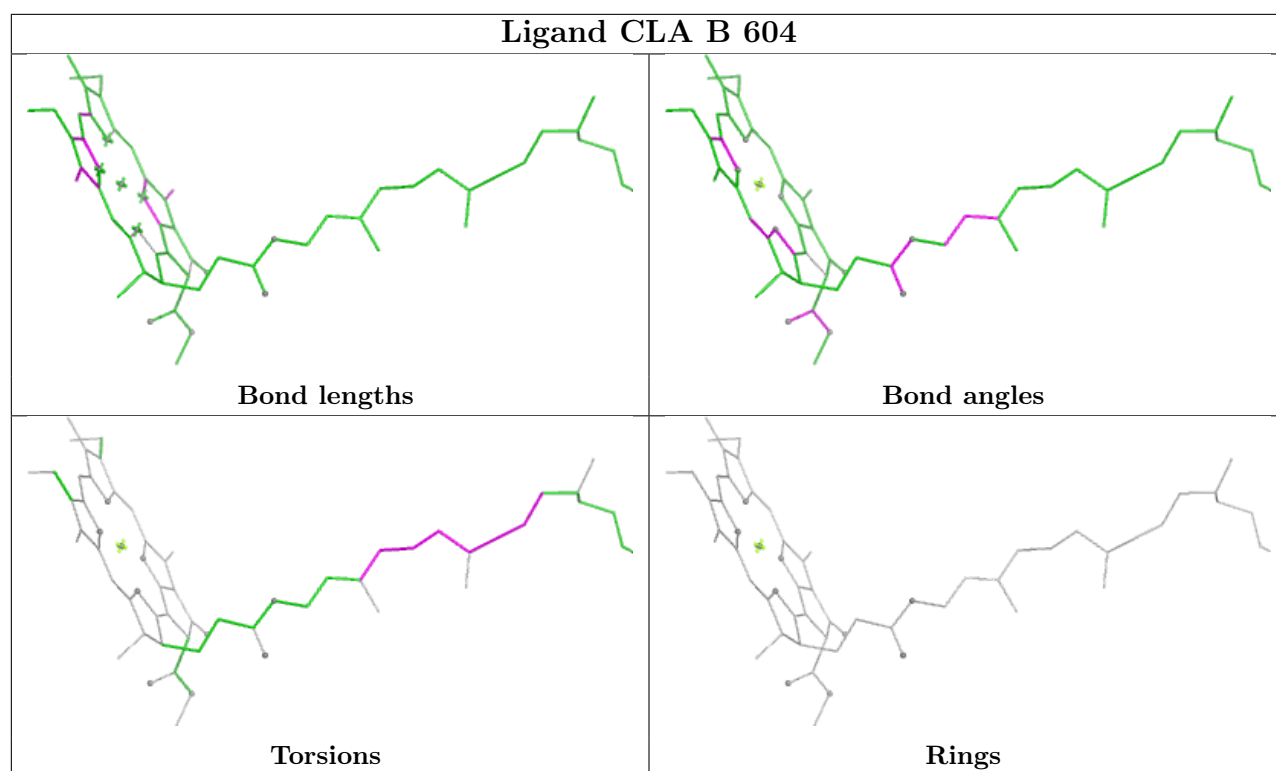


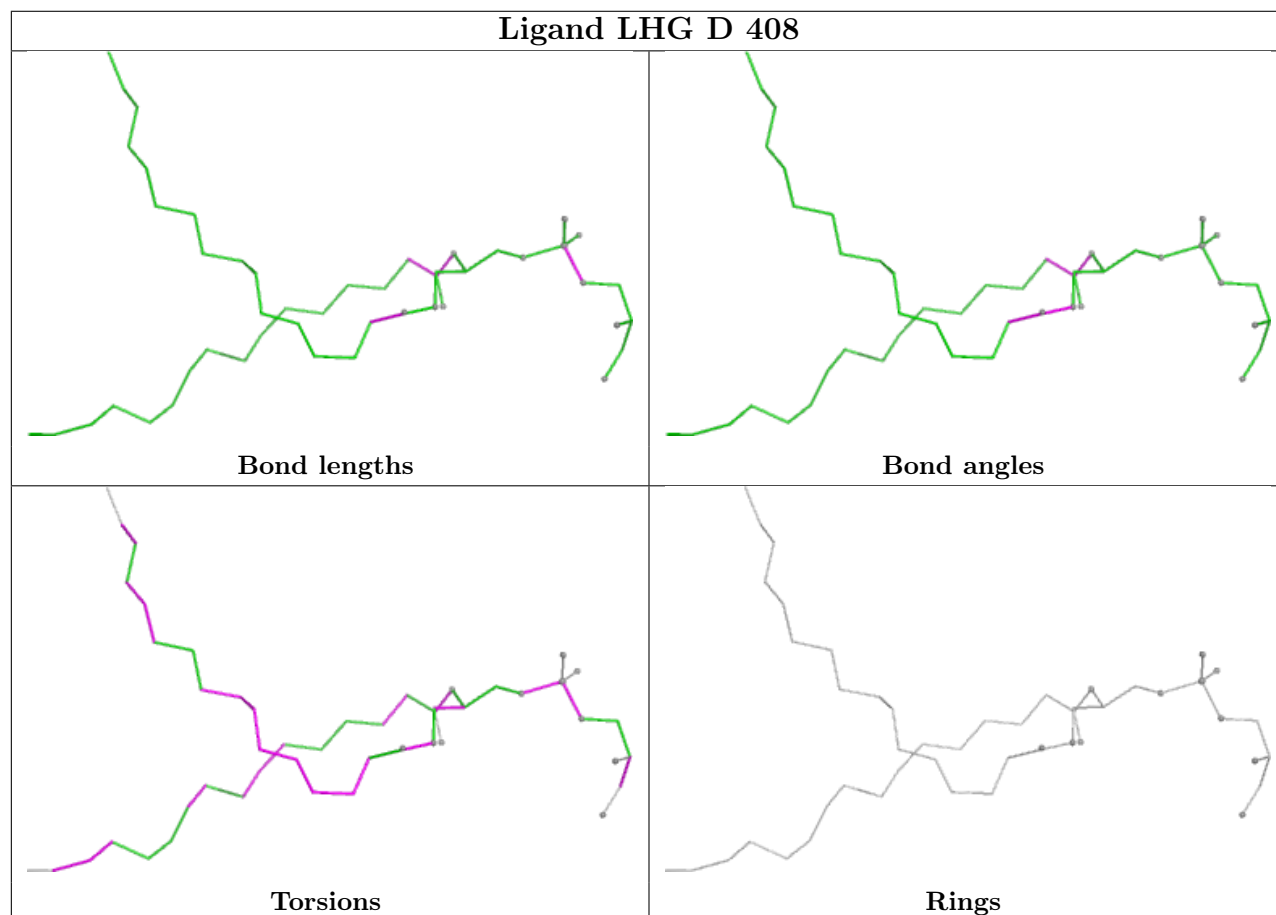
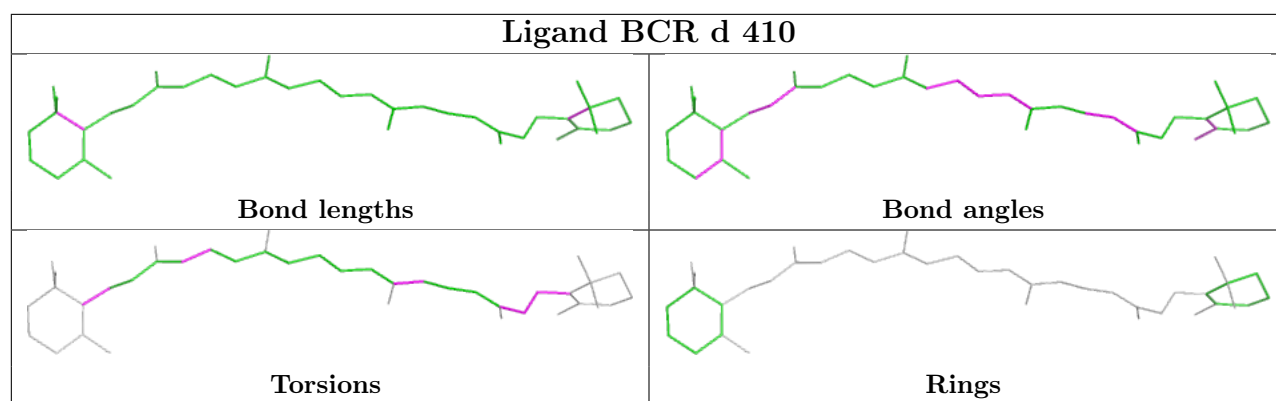


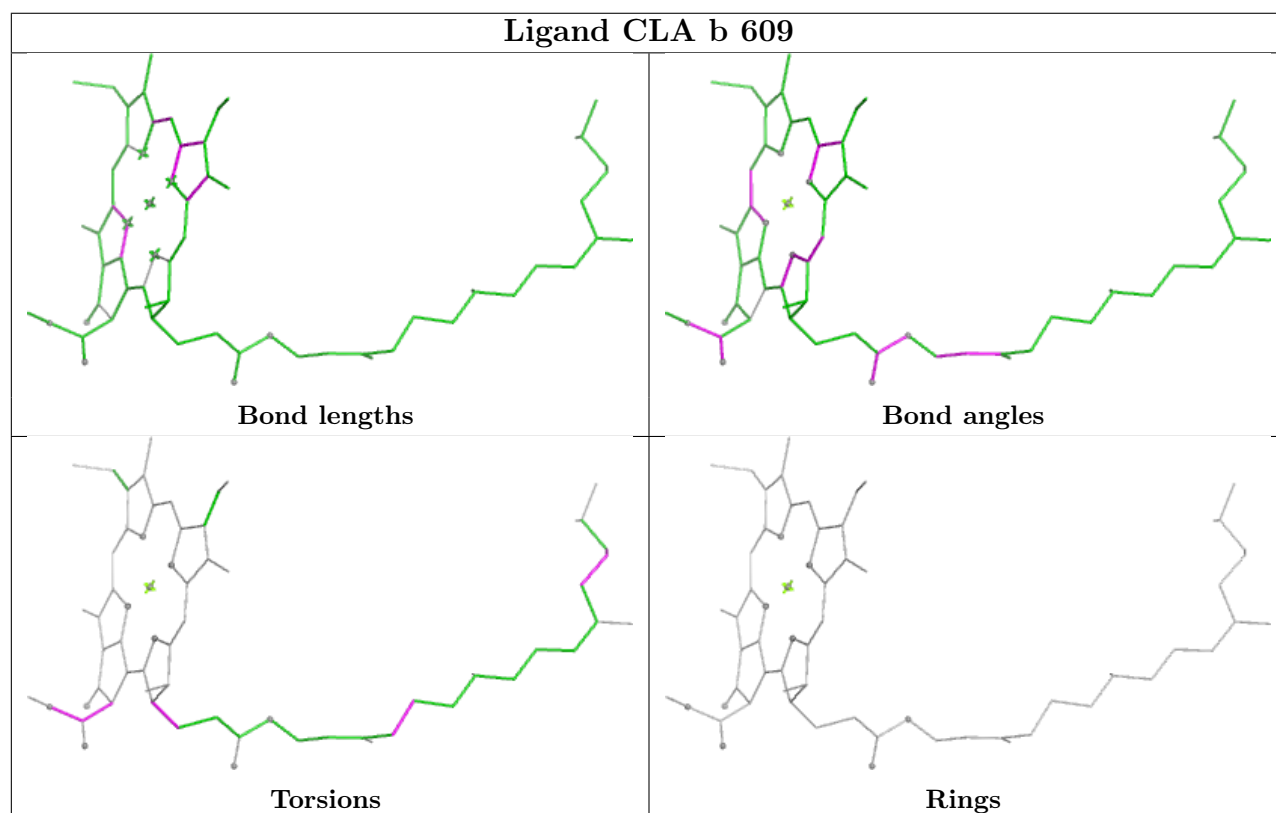
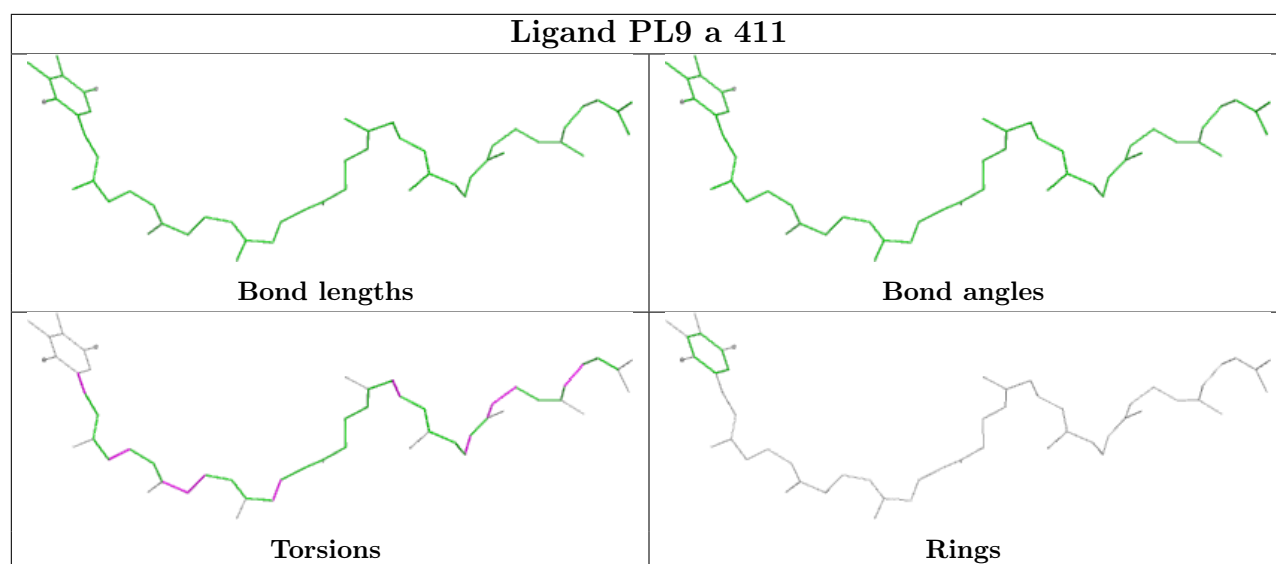


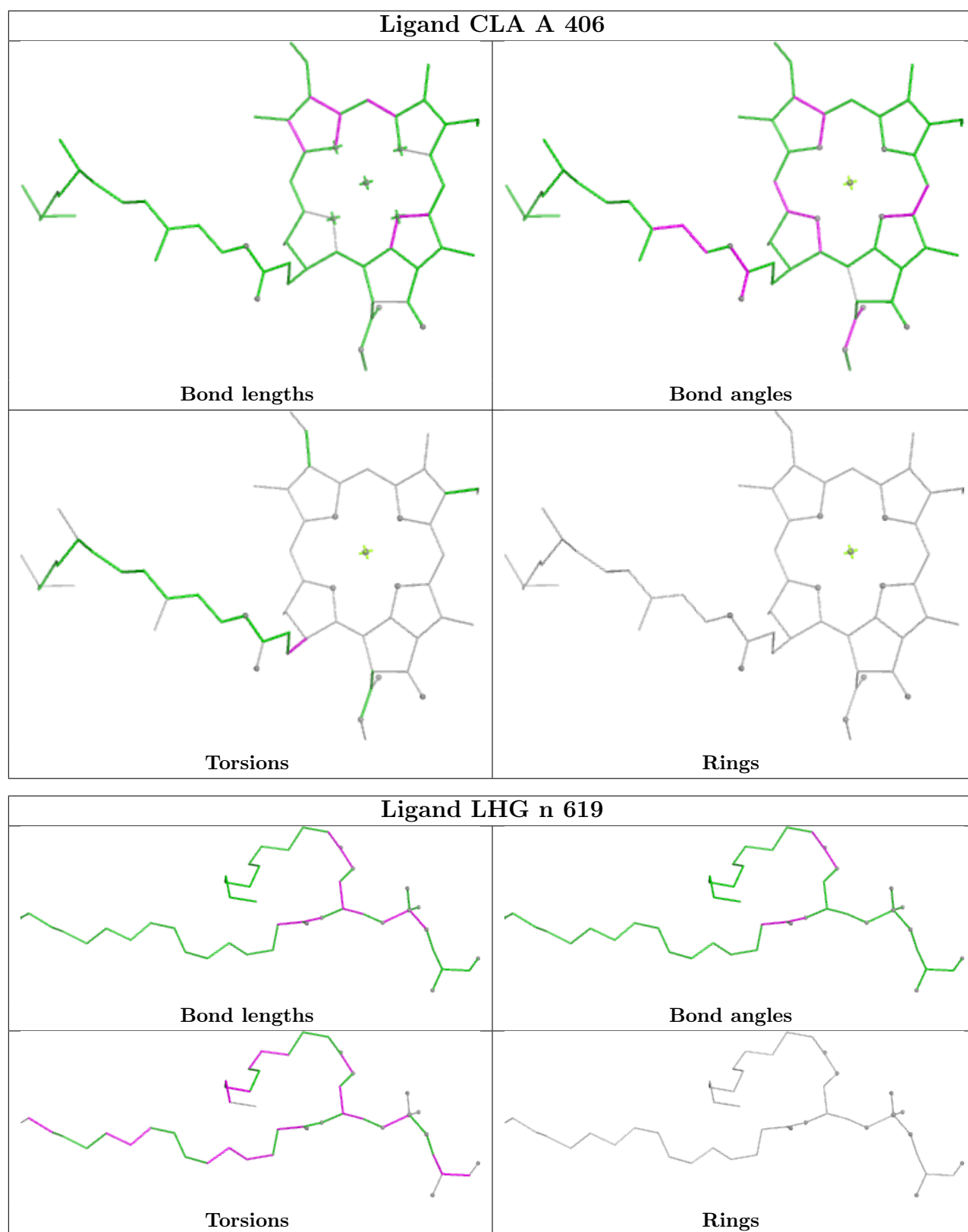


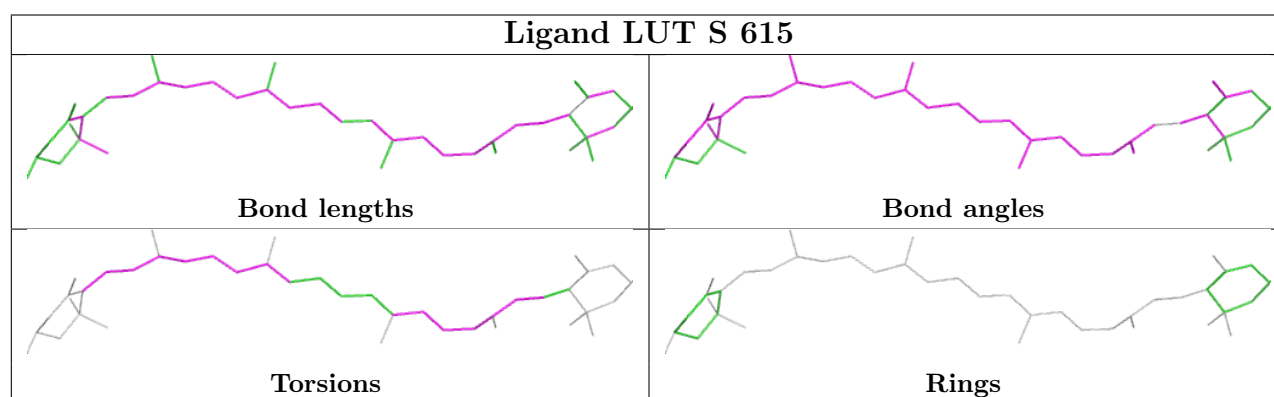
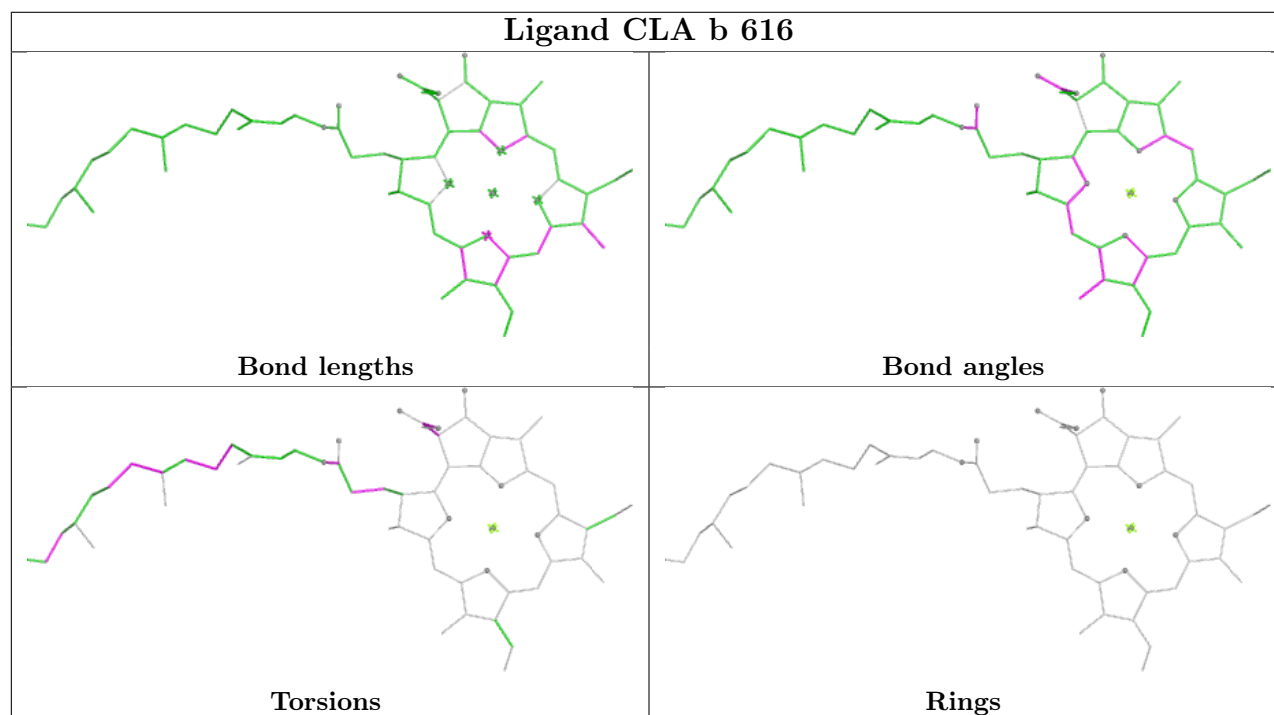
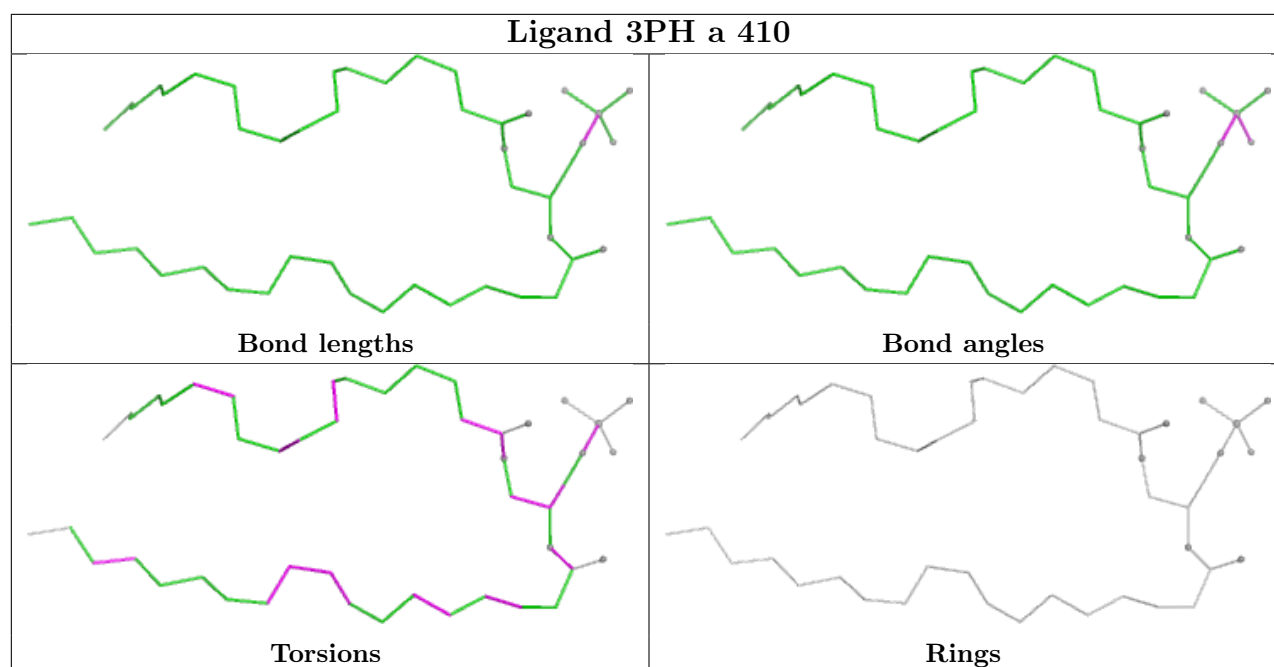


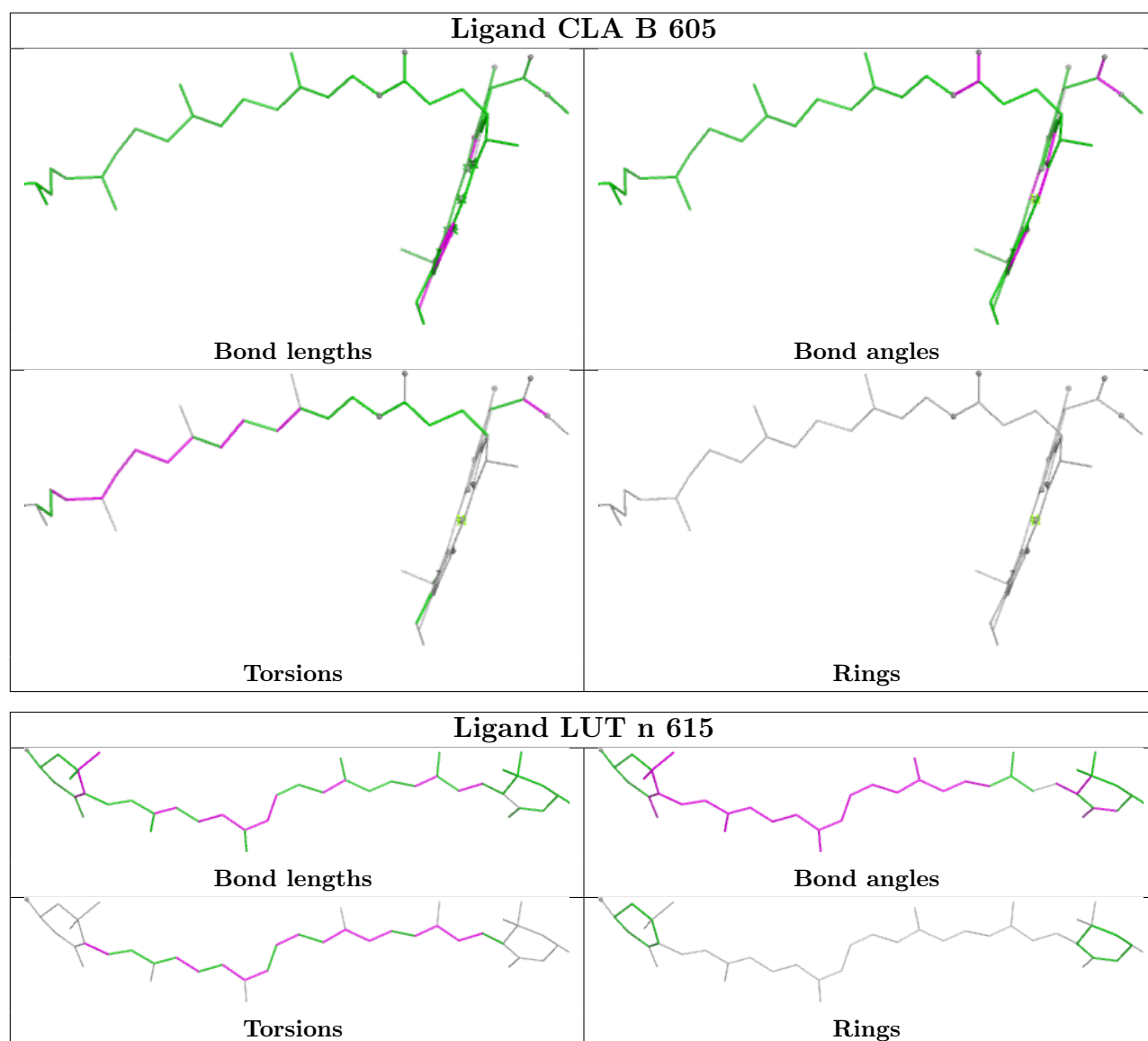


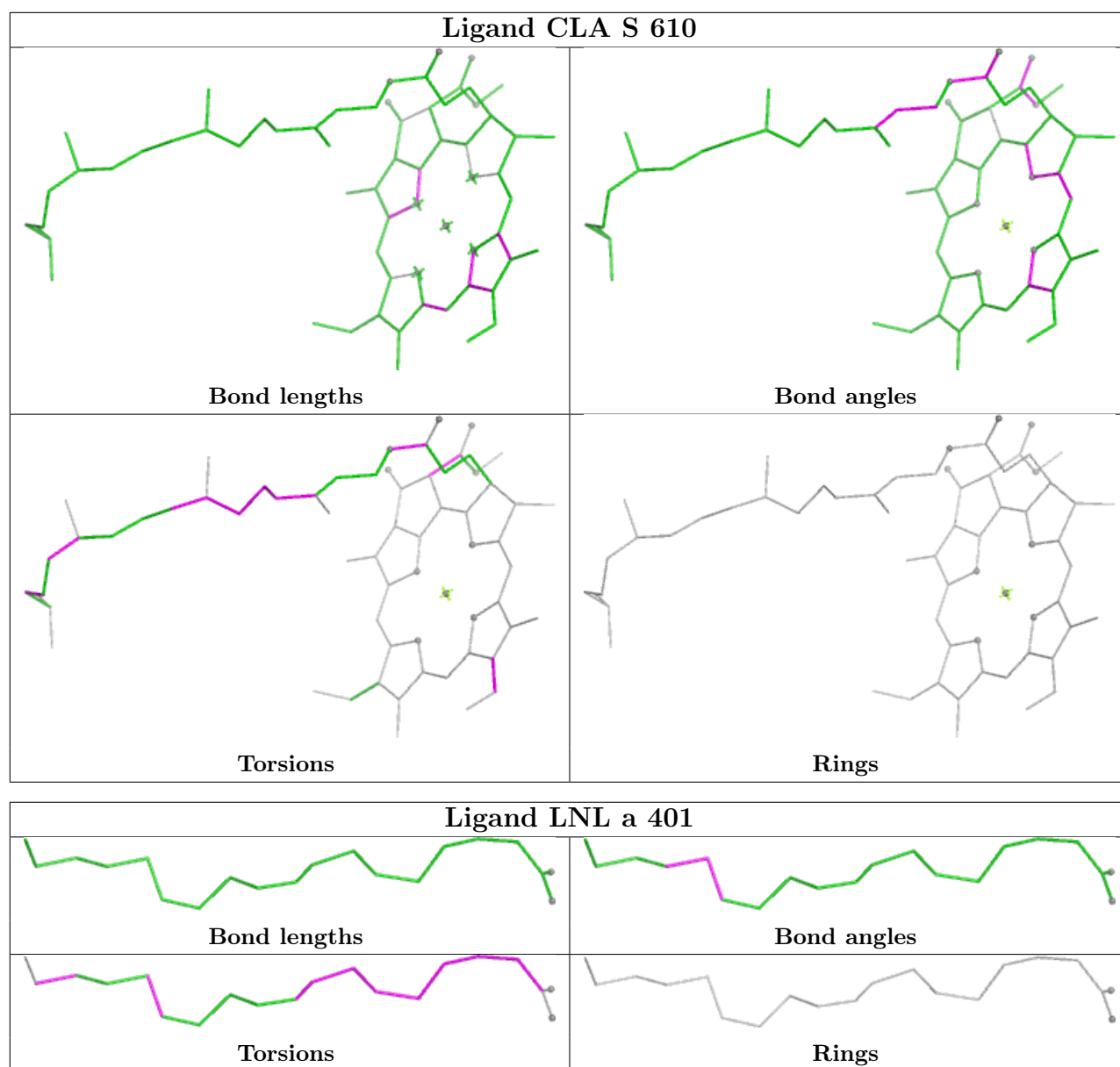


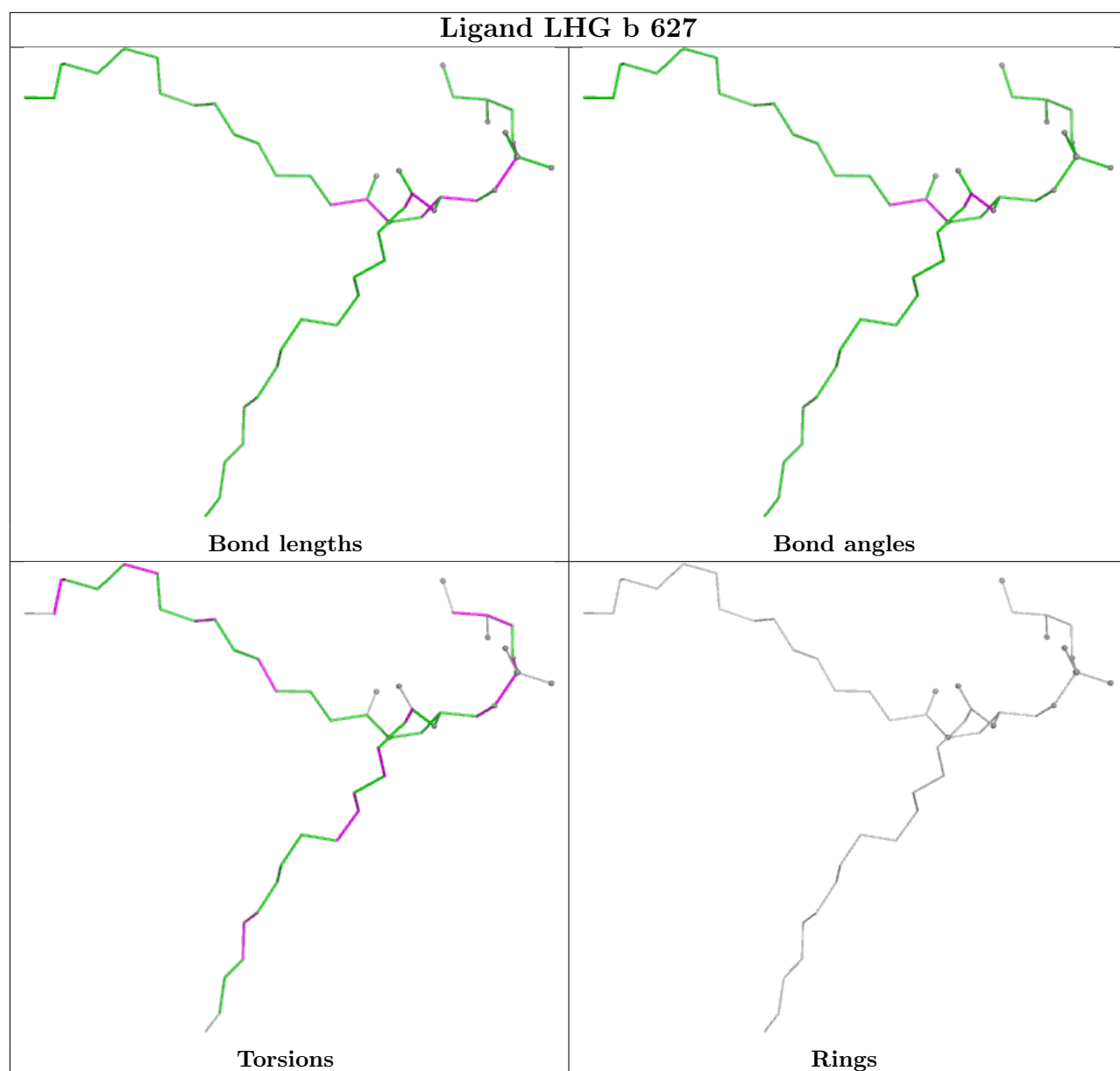


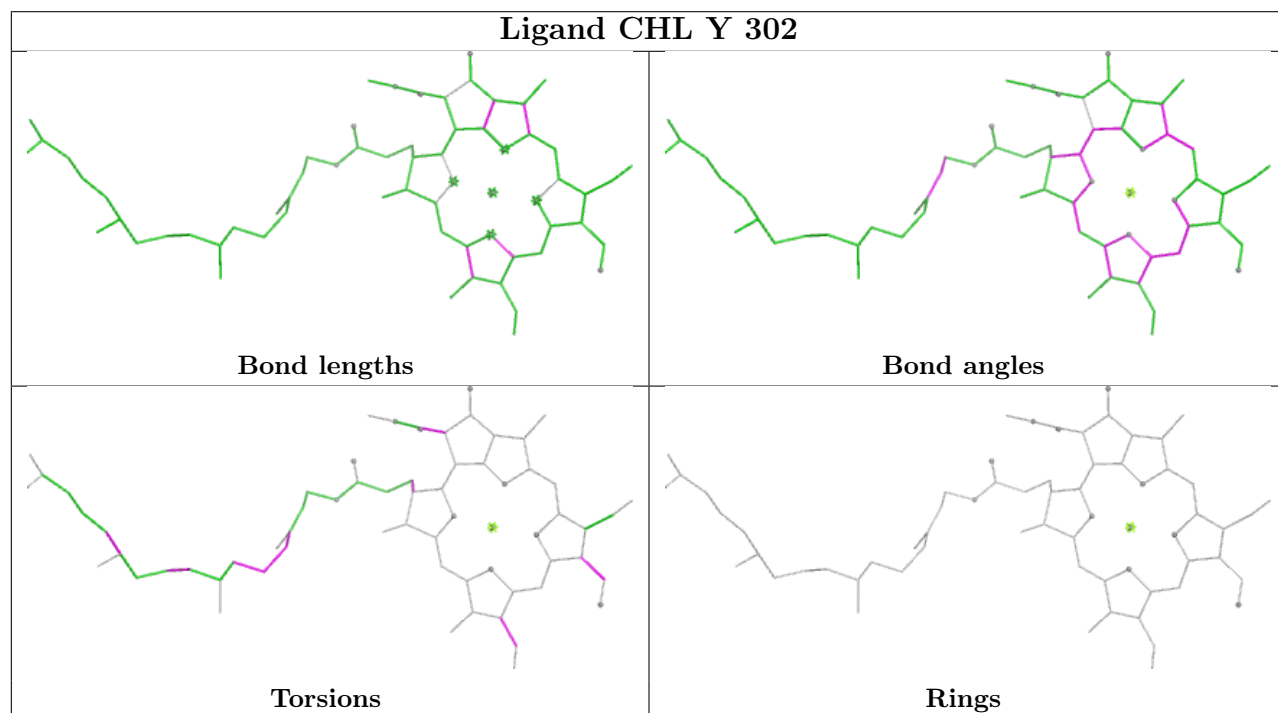
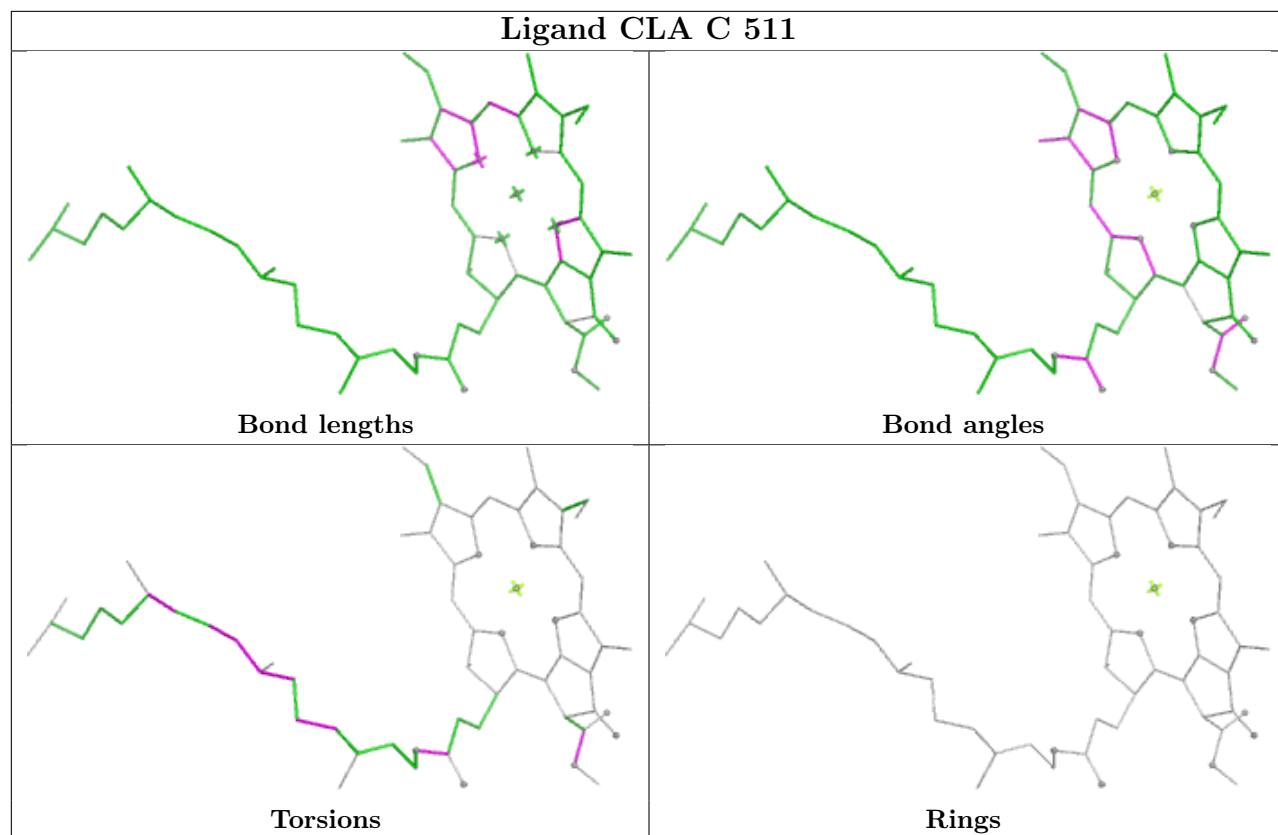


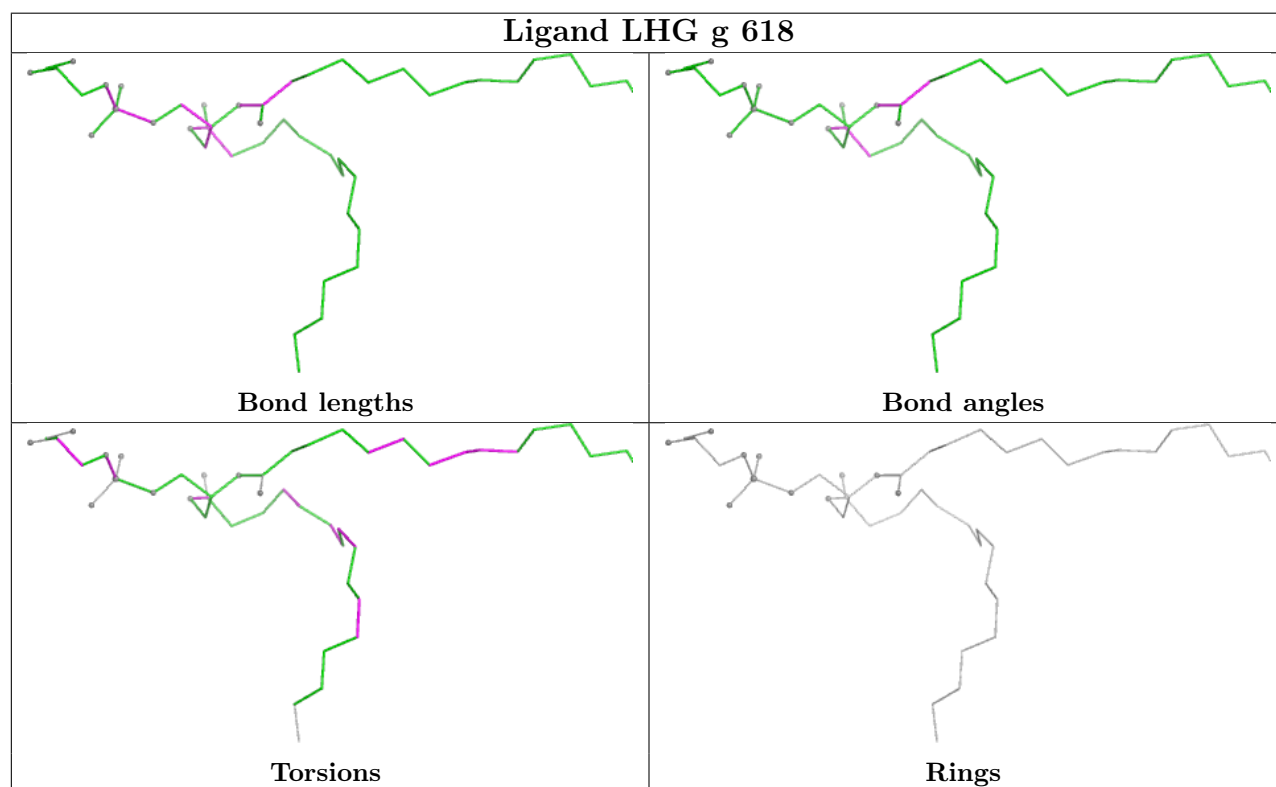
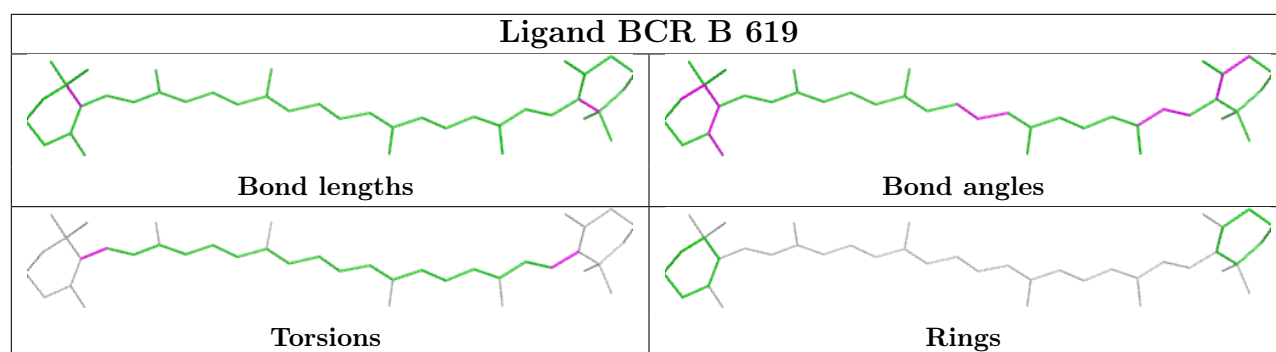


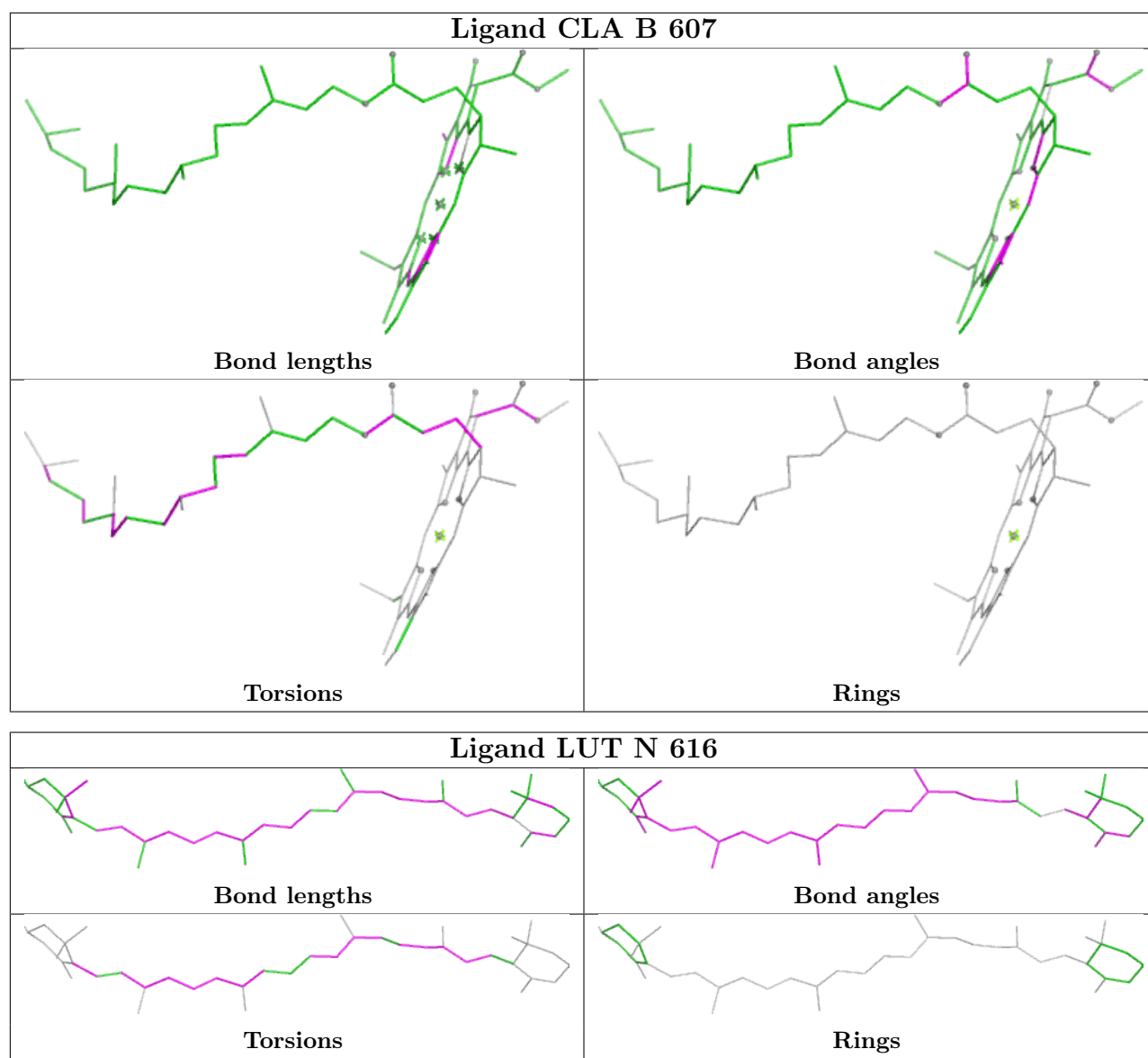


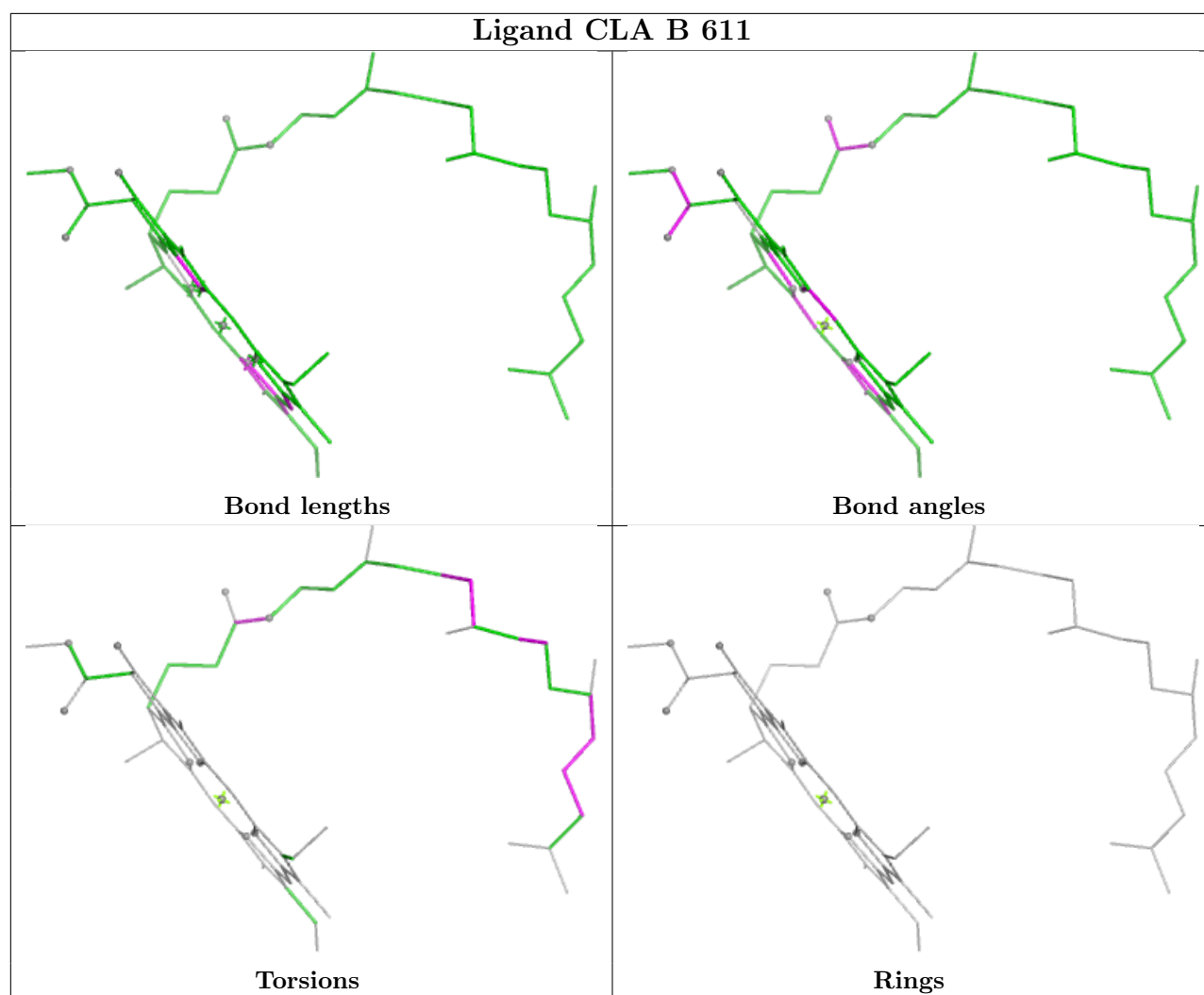


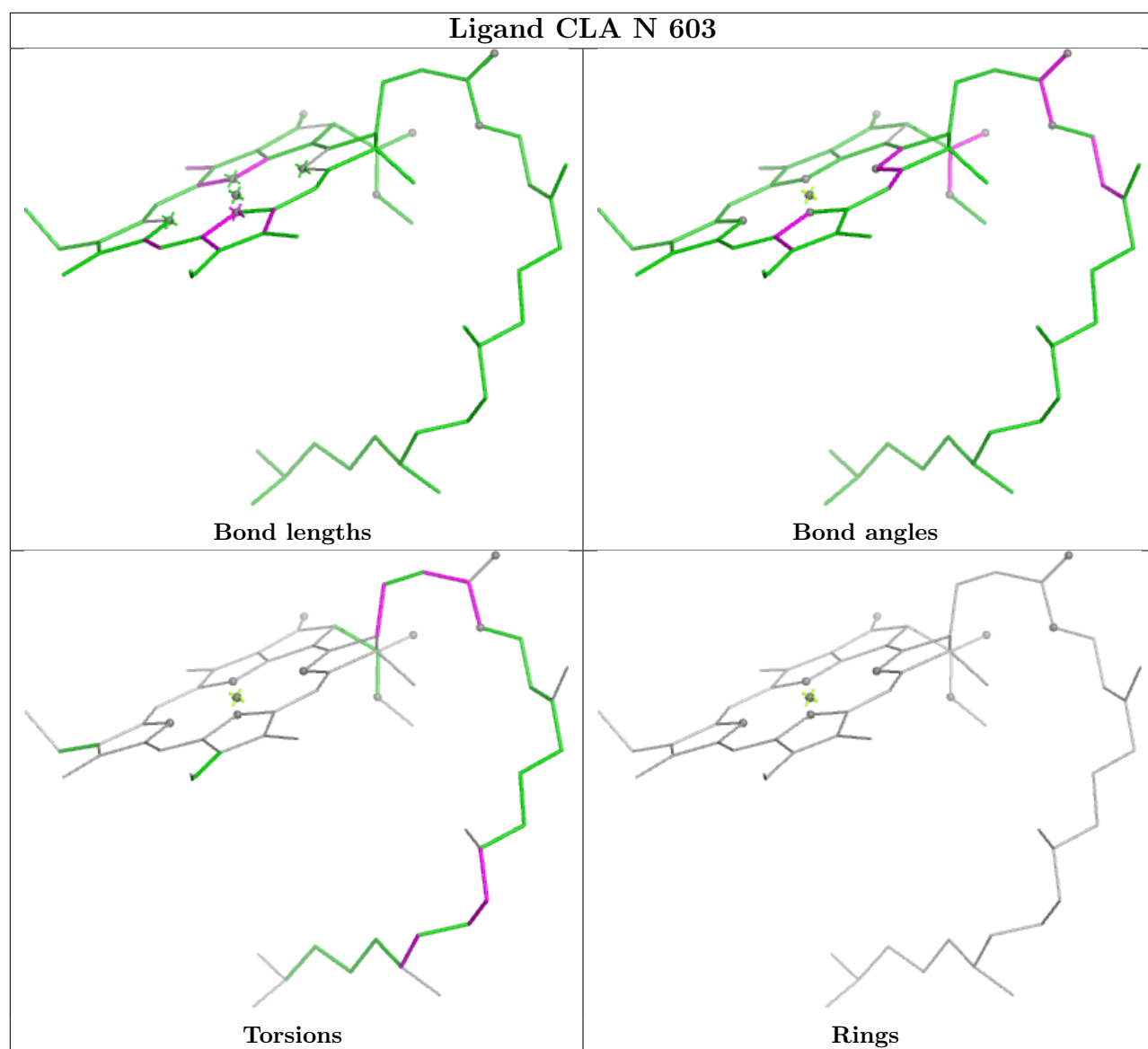


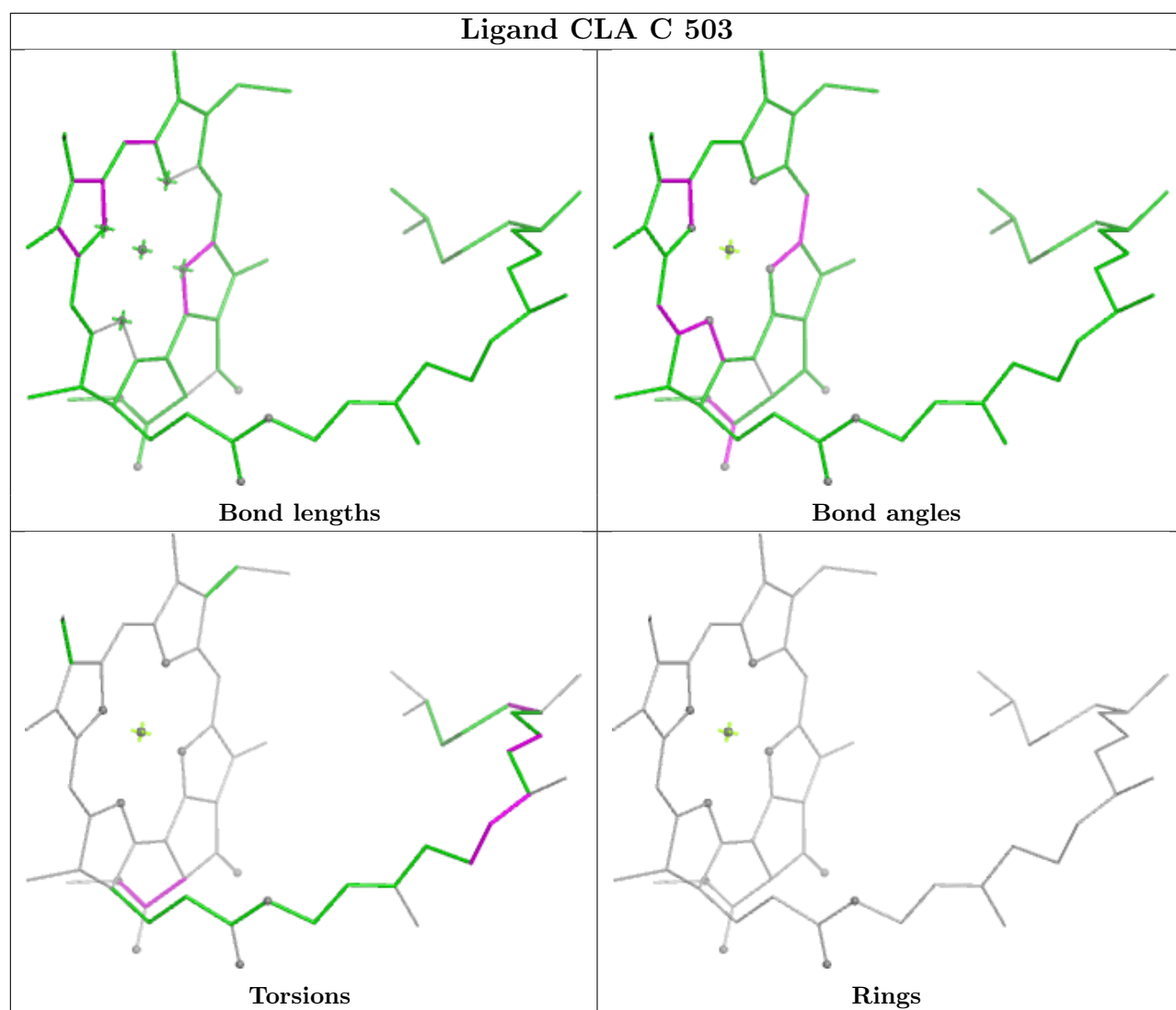




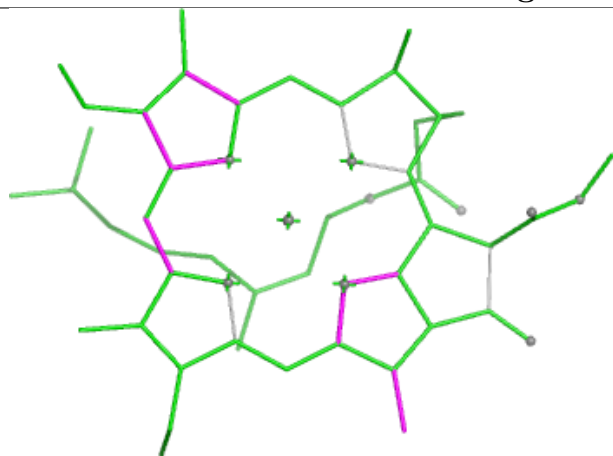




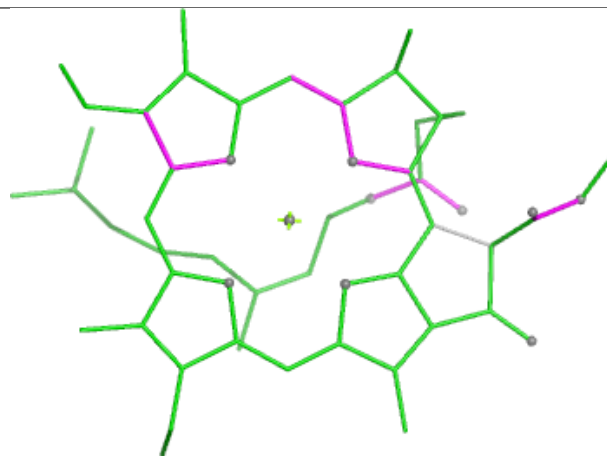




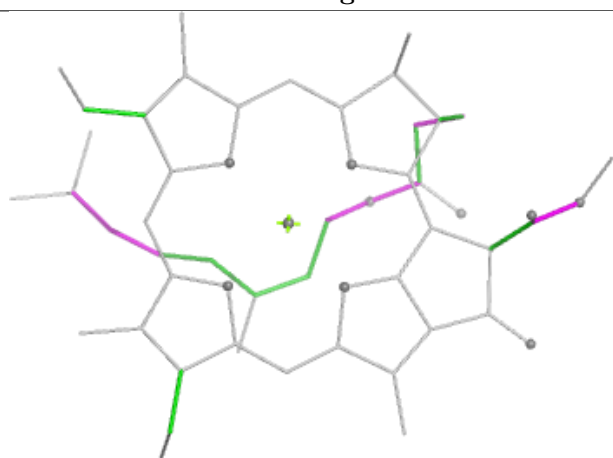
Ligand CLA S 612



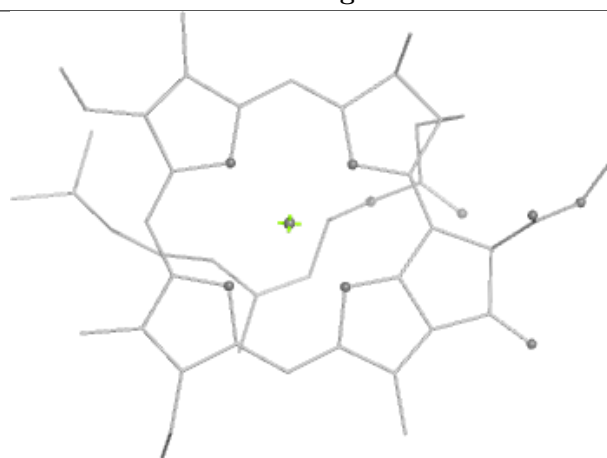
Bond lengths



Bond angles

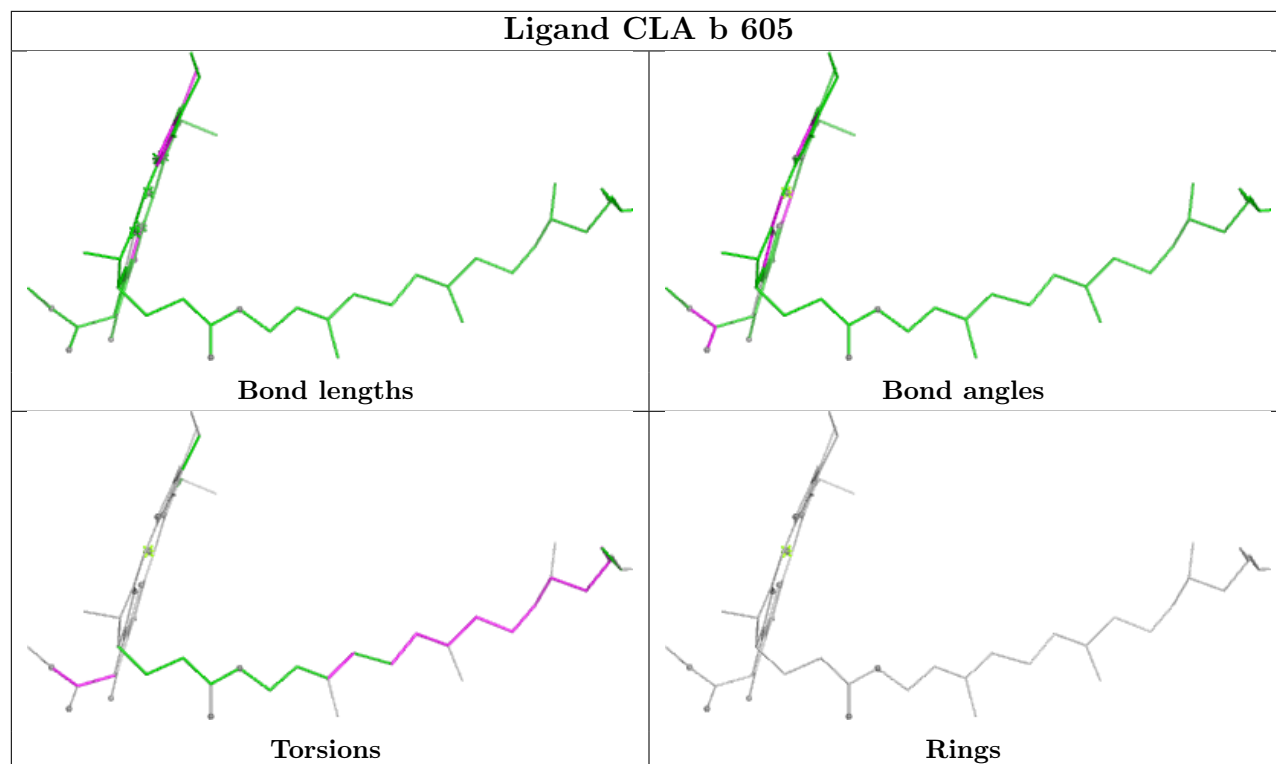


Torsions

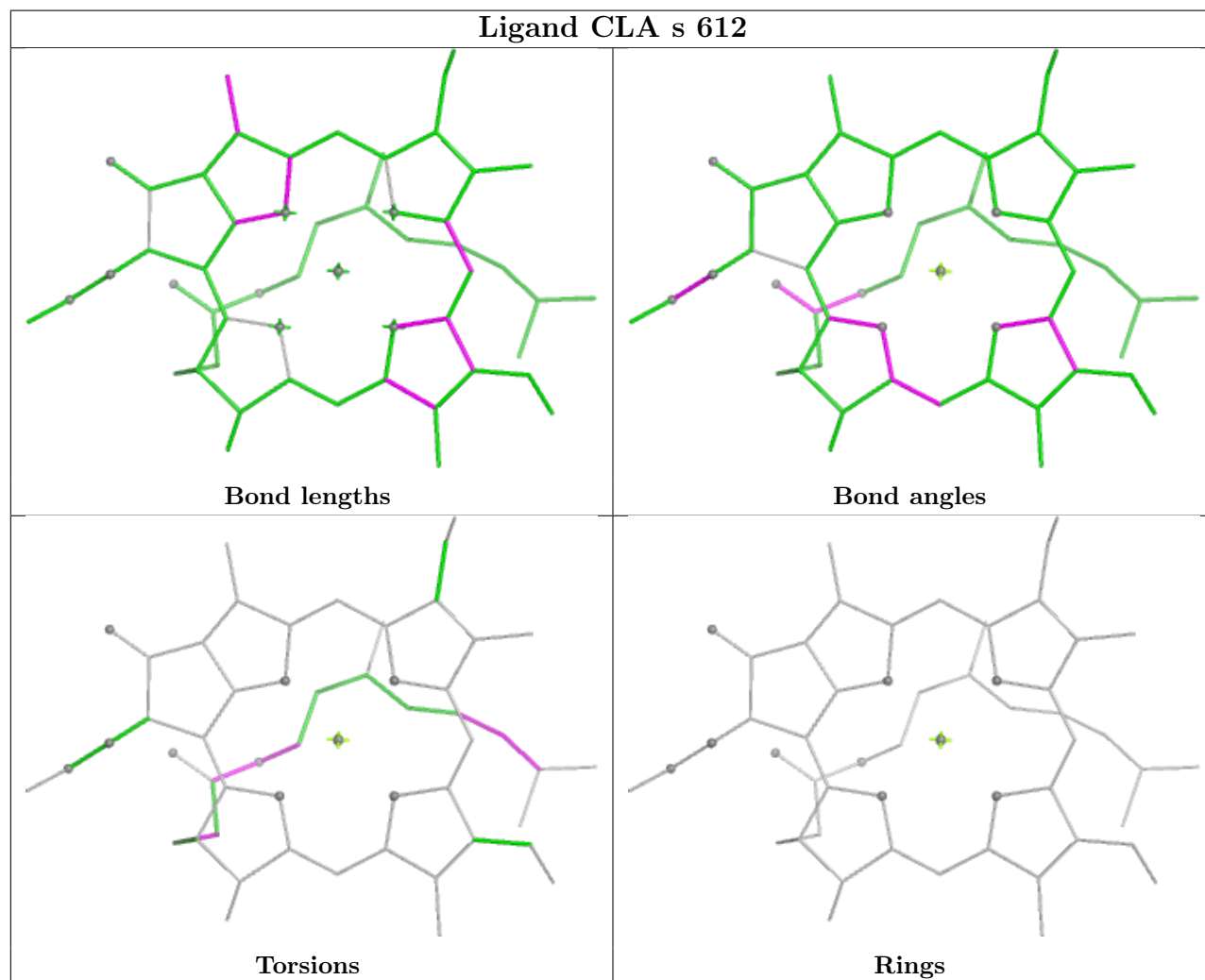


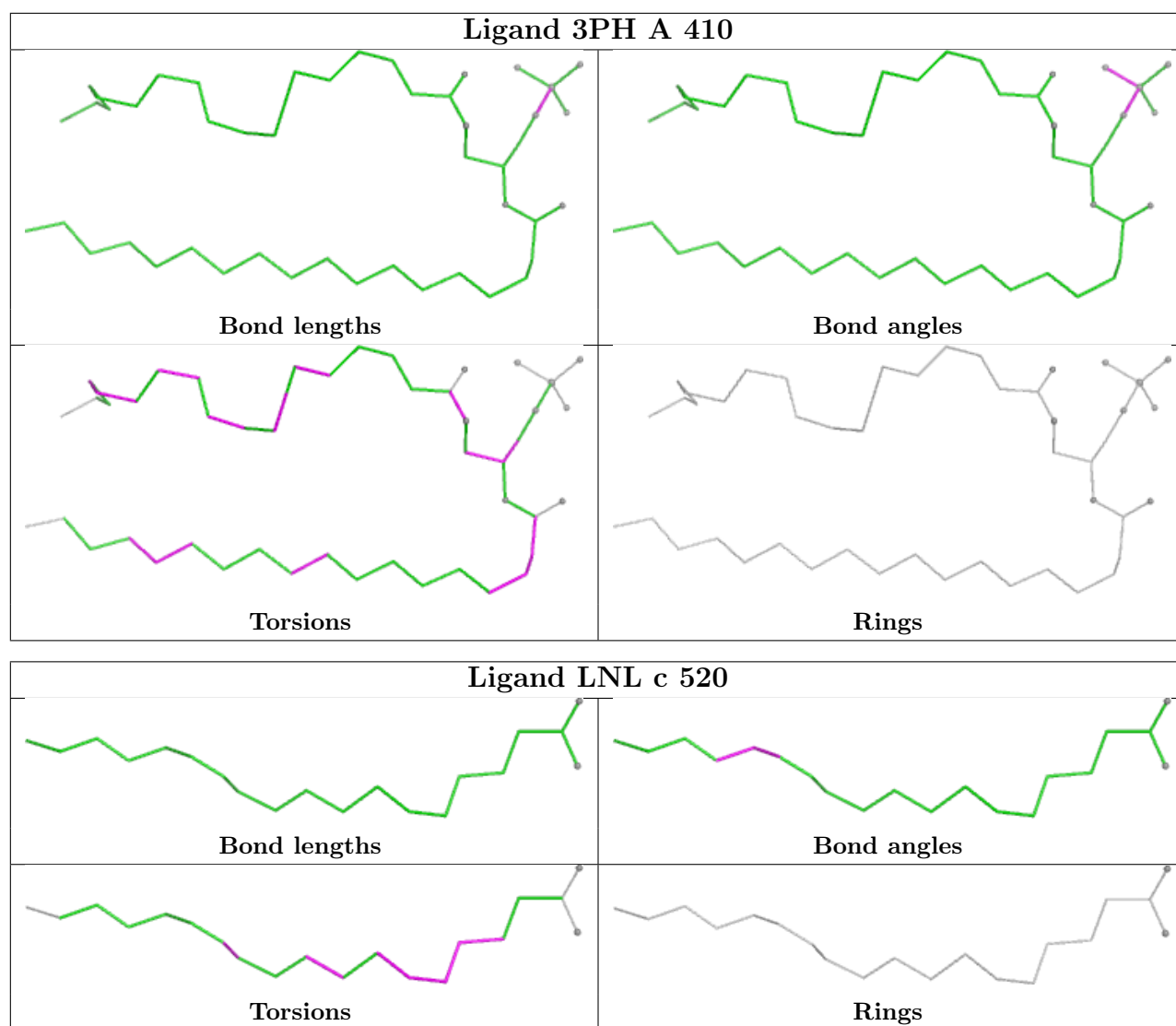
Rings

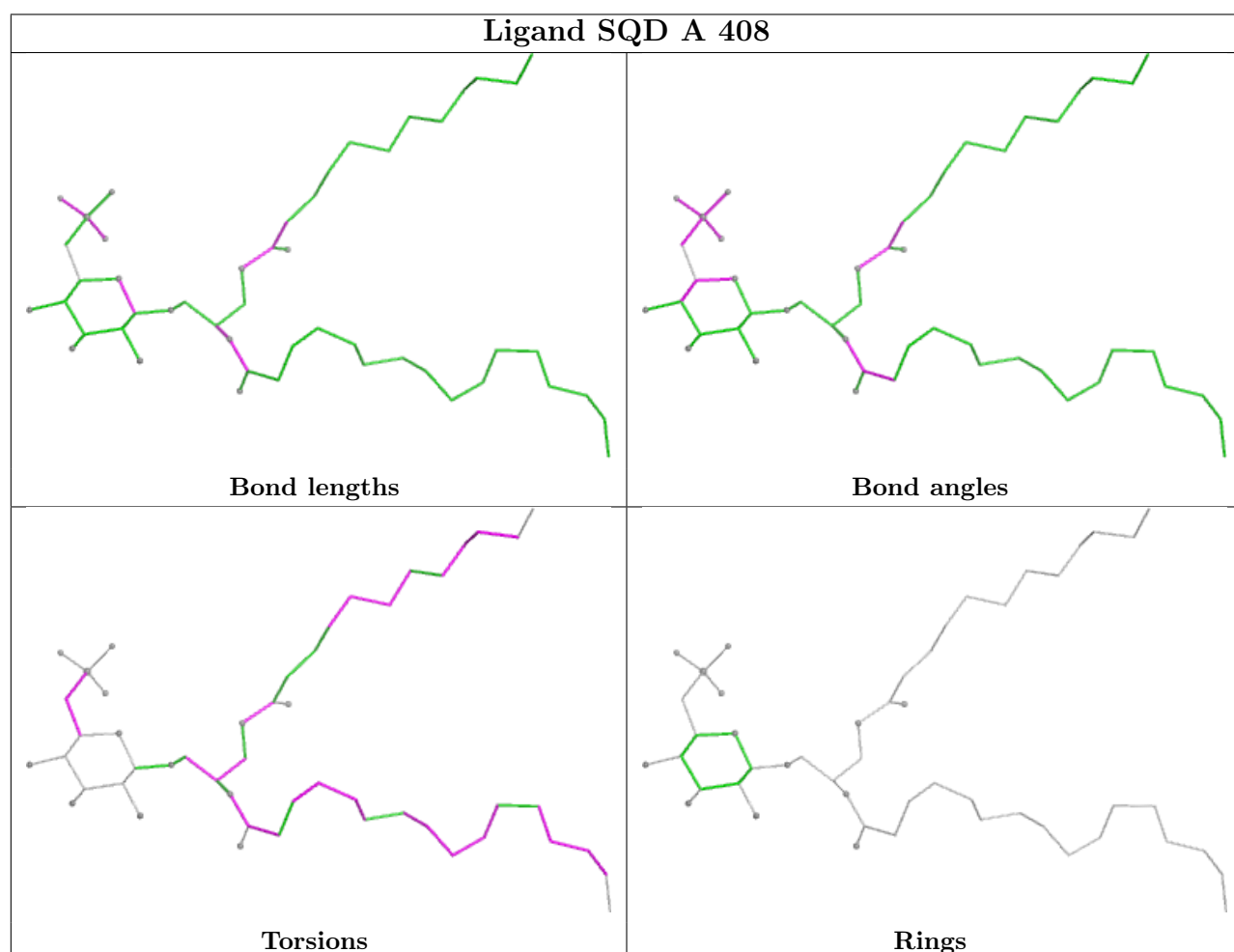
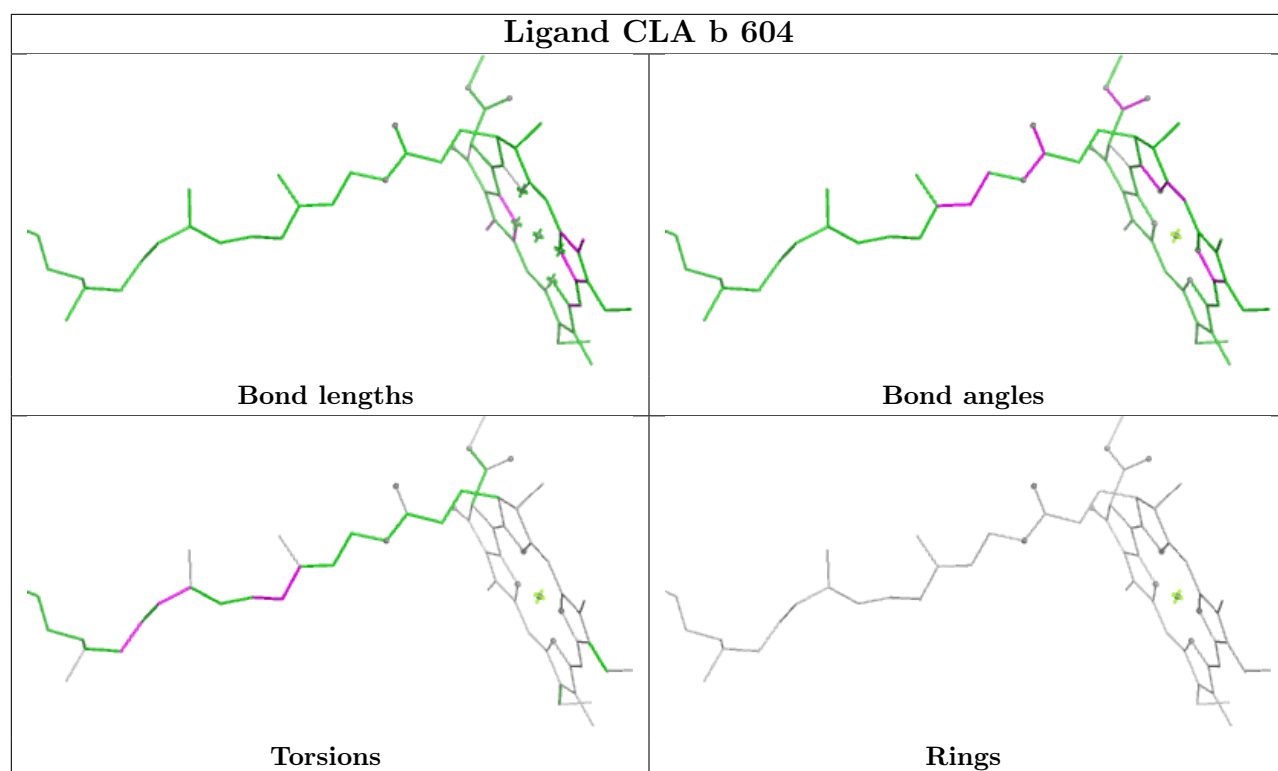
Ligand CLA b 605

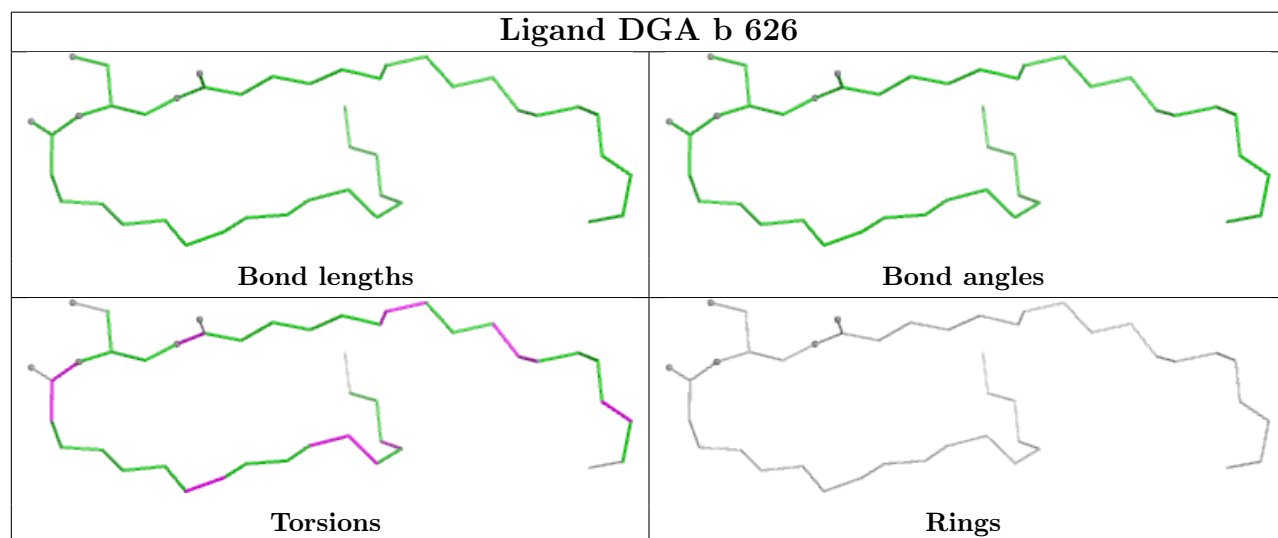
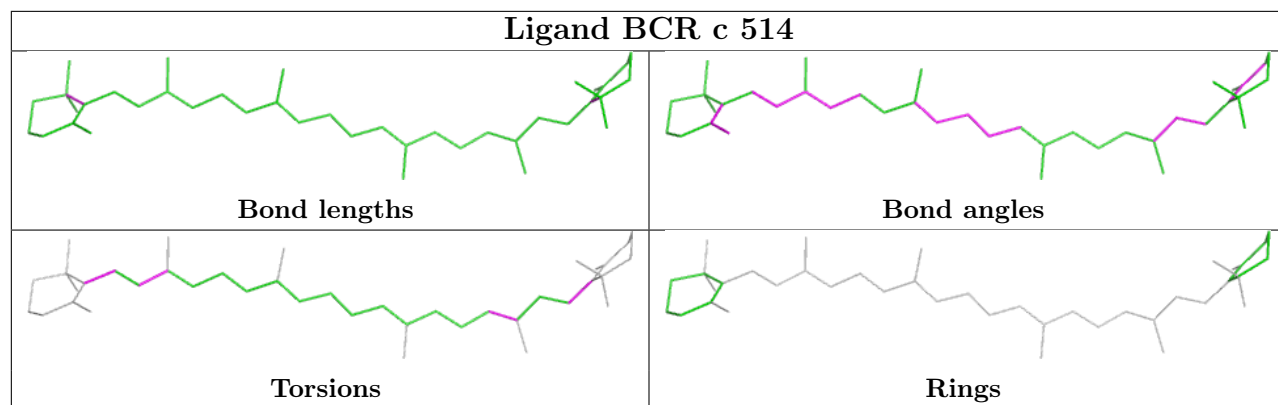


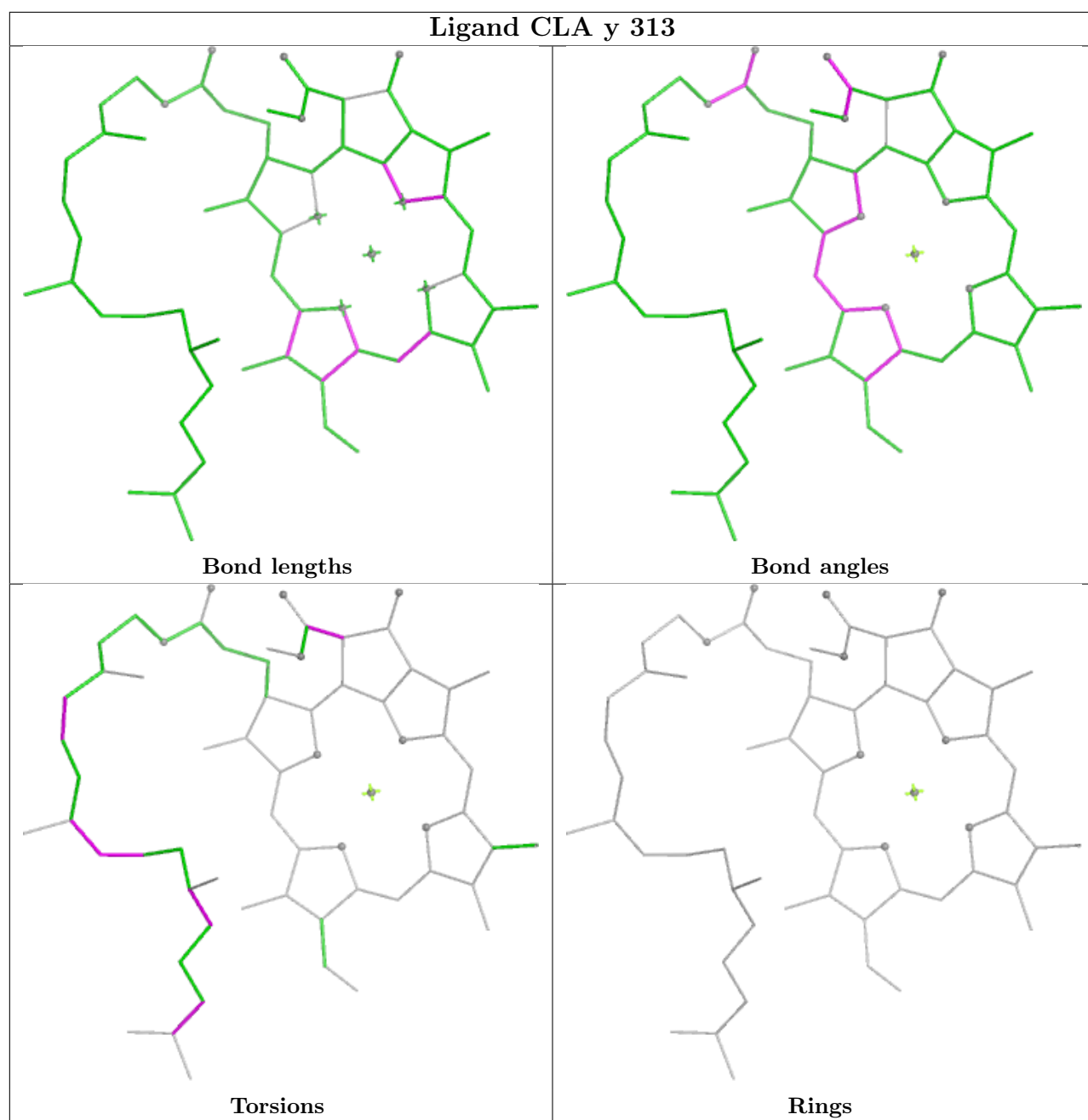
Ligand CLA s 612



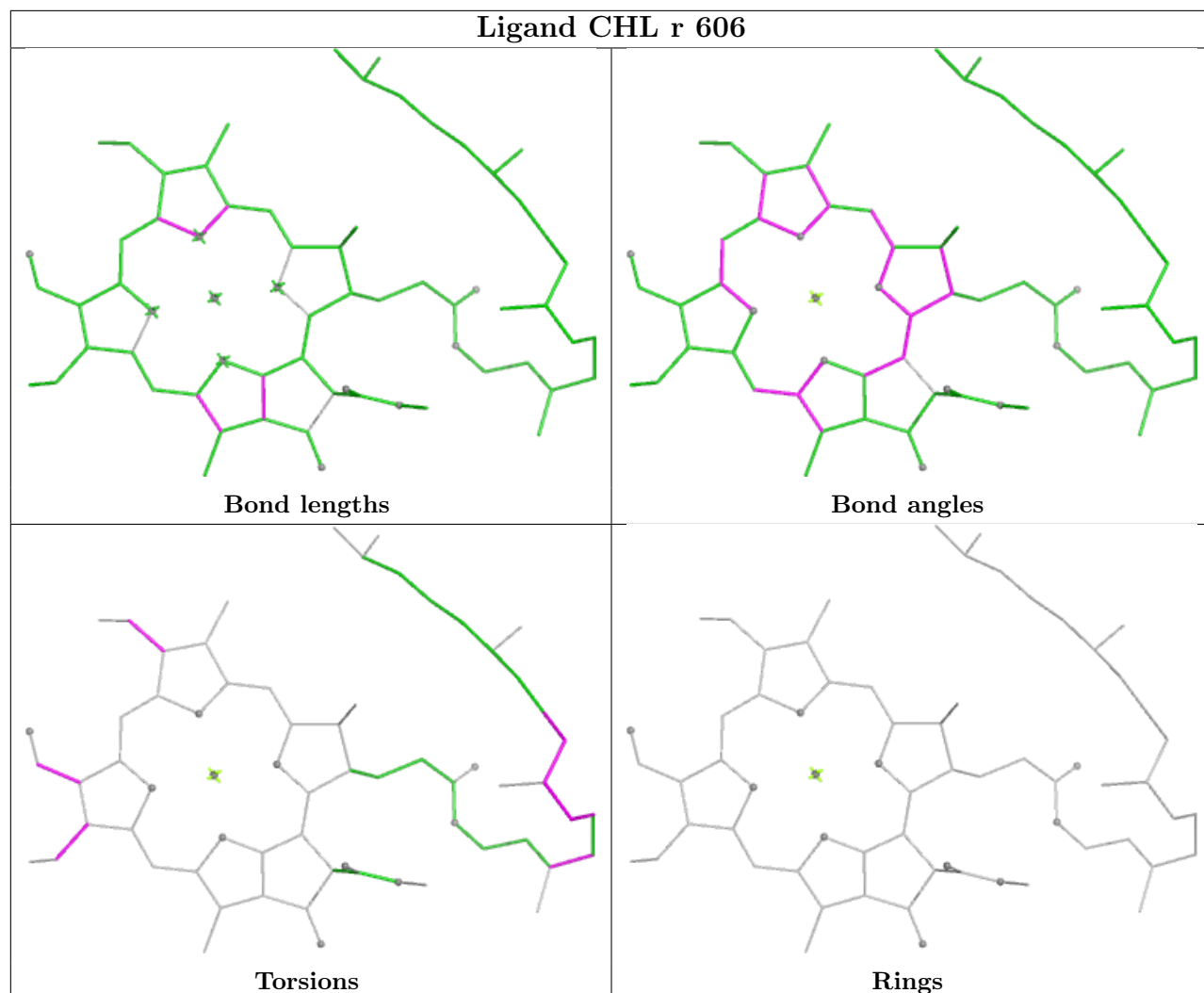




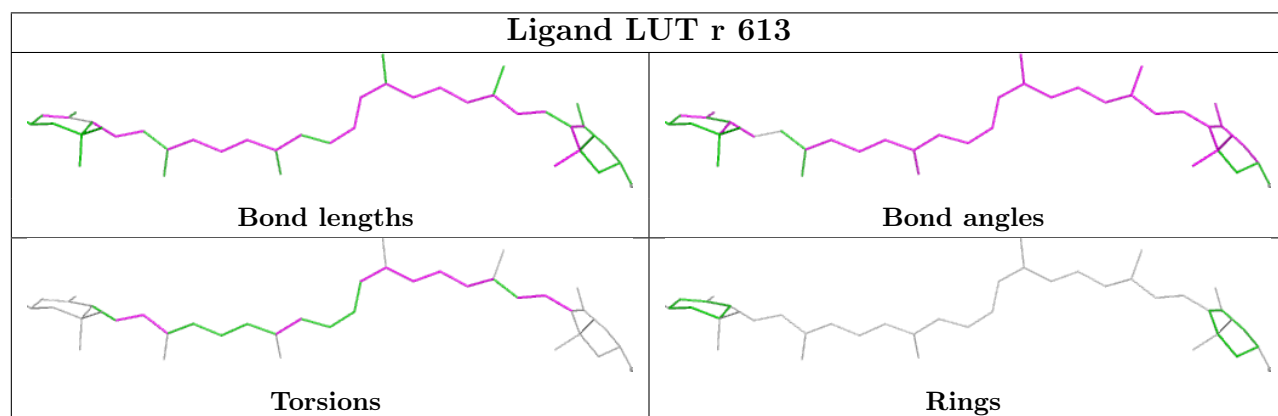




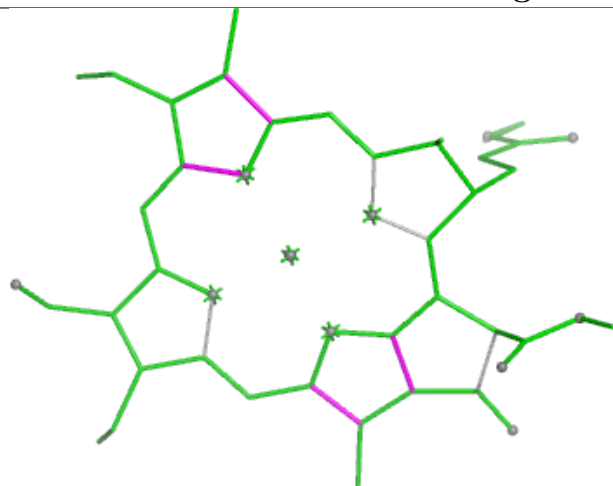
Ligand CHL r 606



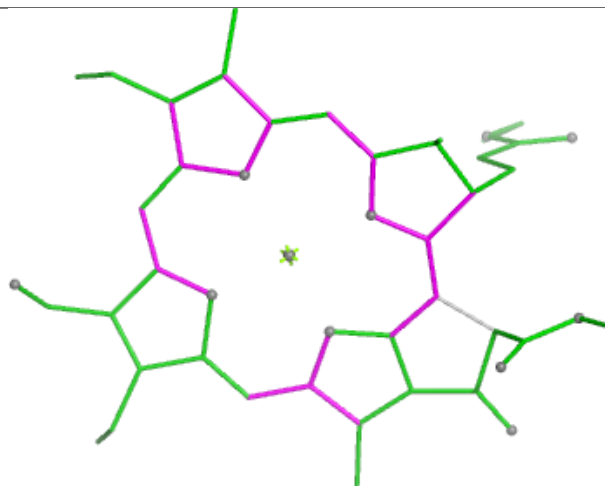
Ligand LUT r 613



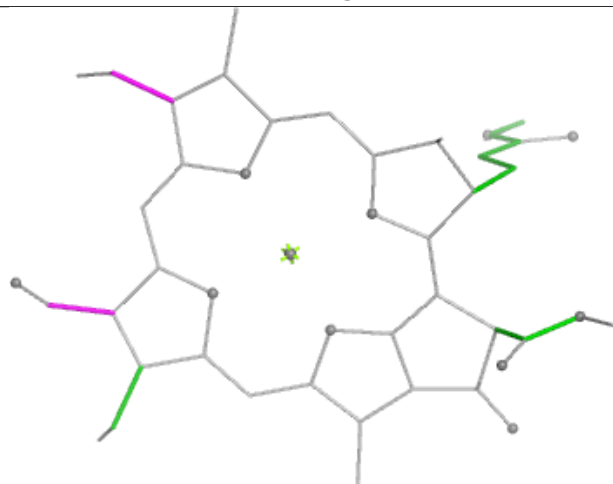
Ligand CHL Y 306



Bond lengths



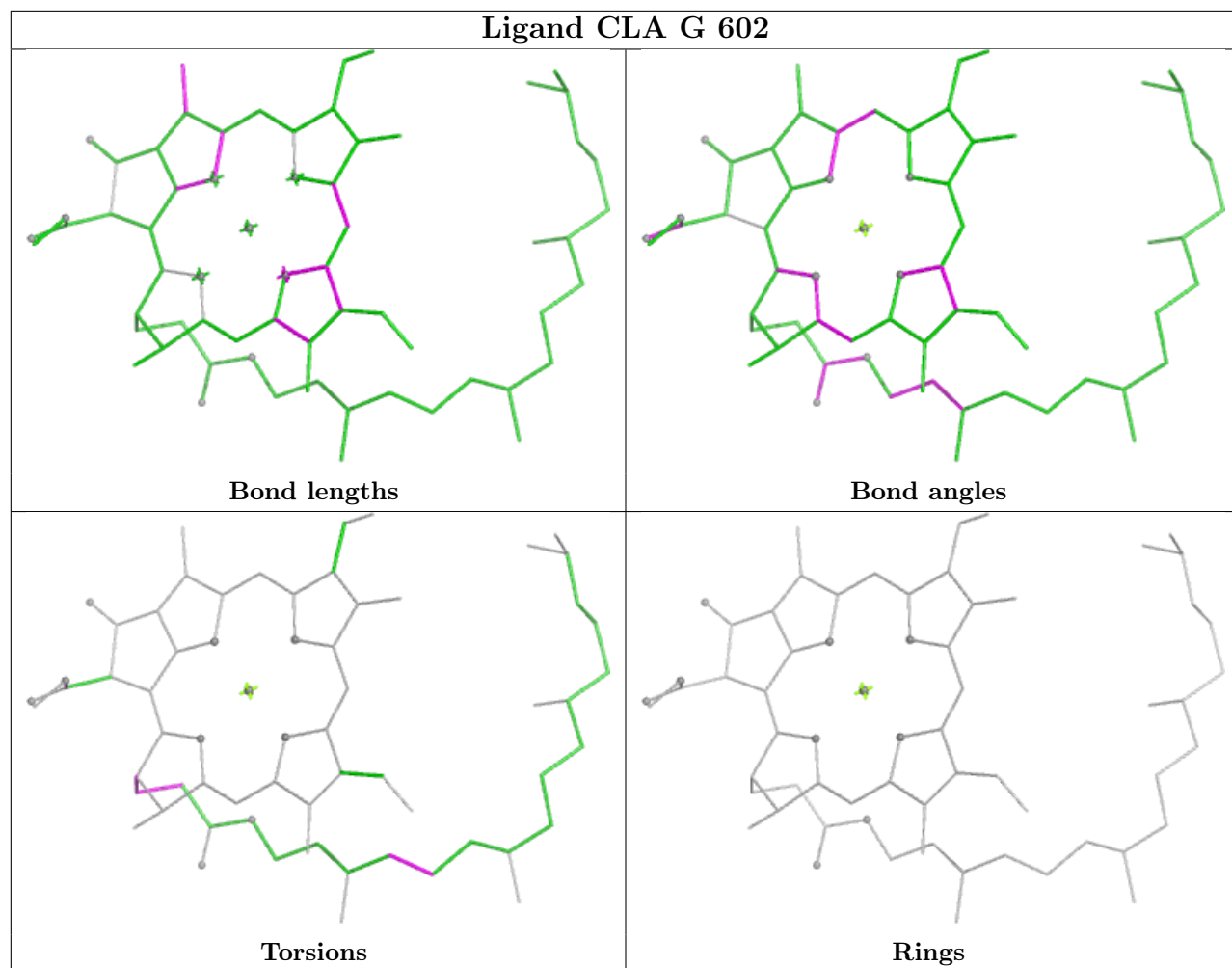
Bond angles



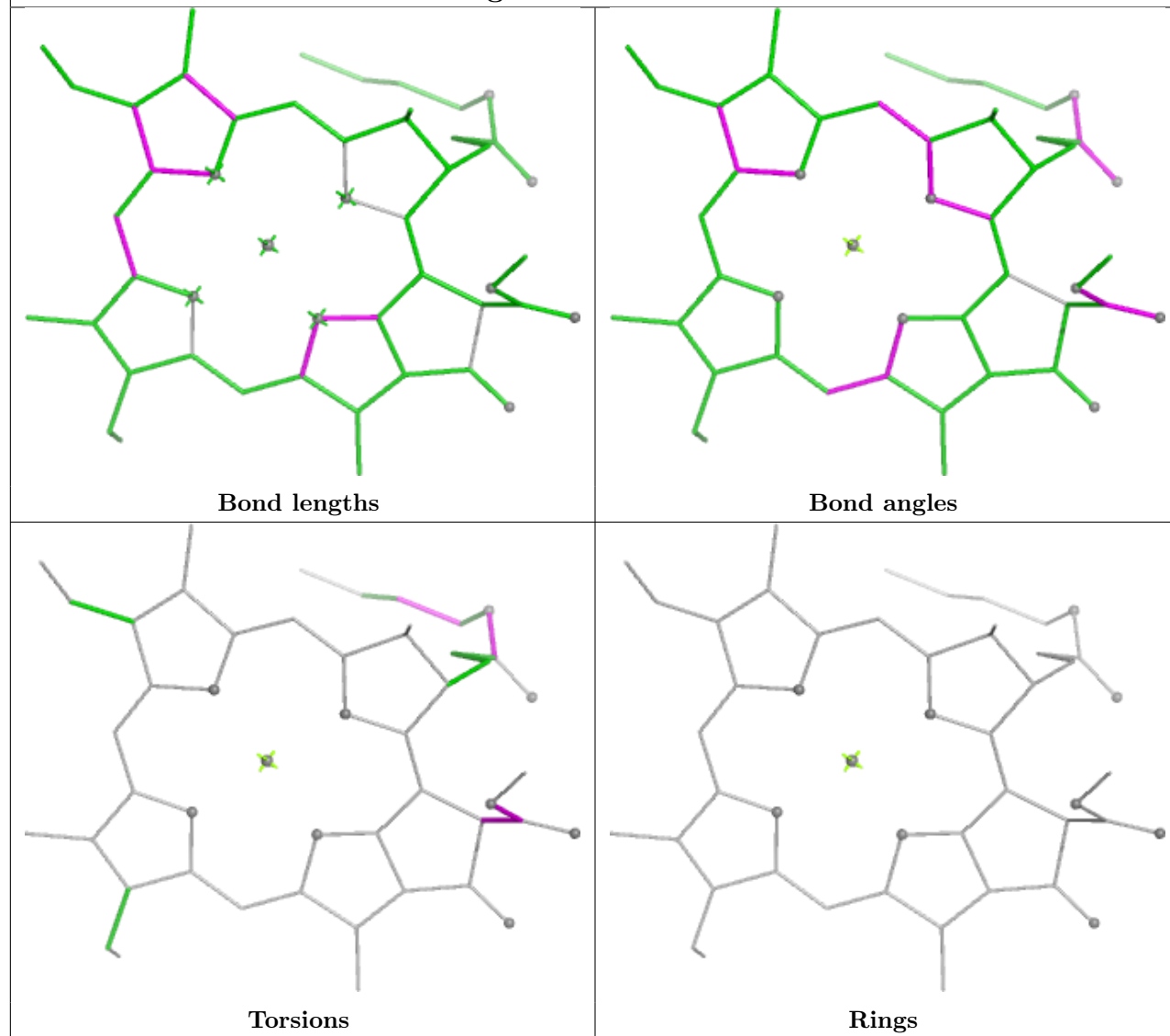
Torsions



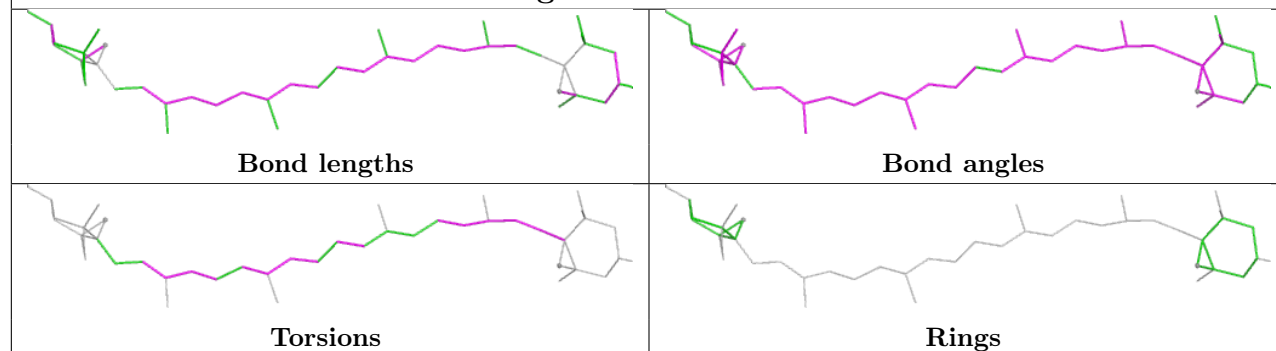
Rings



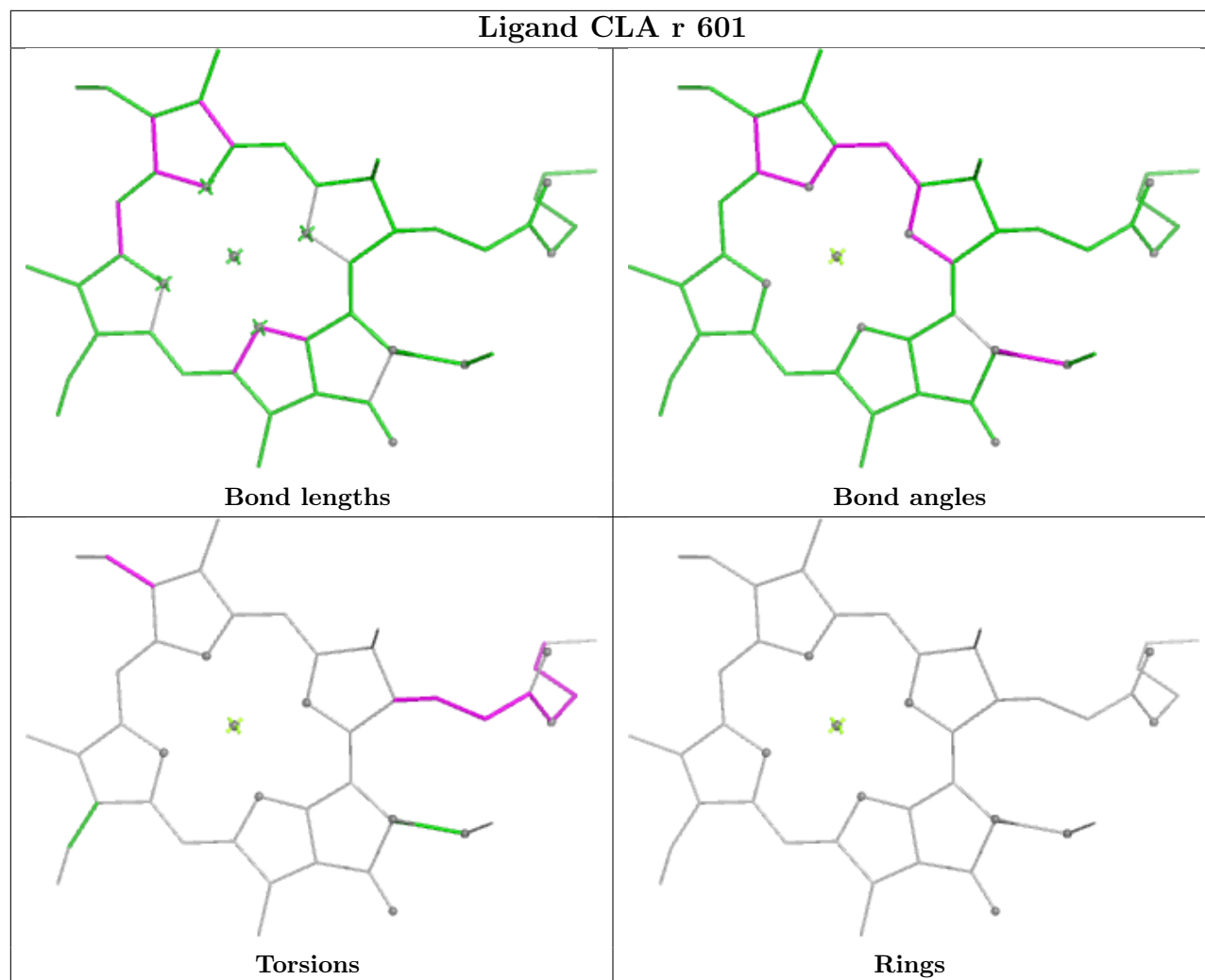
Ligand CLA N 614



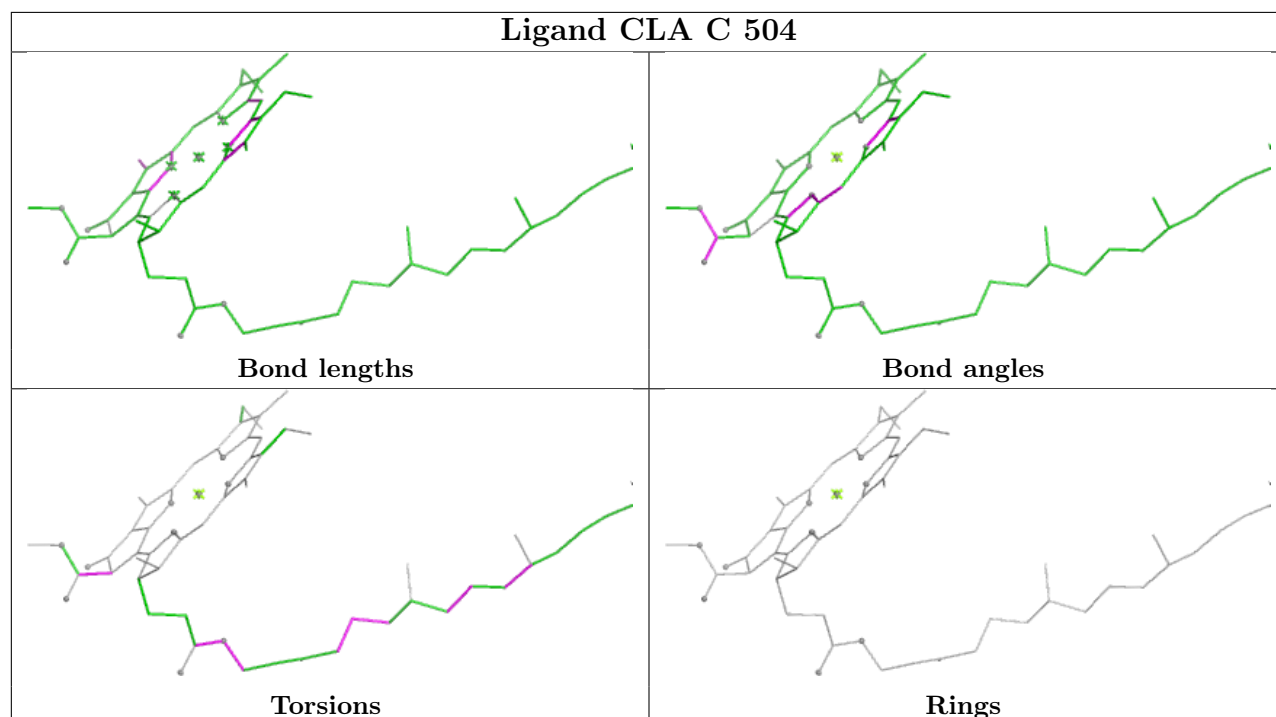
Ligand XAT r 615



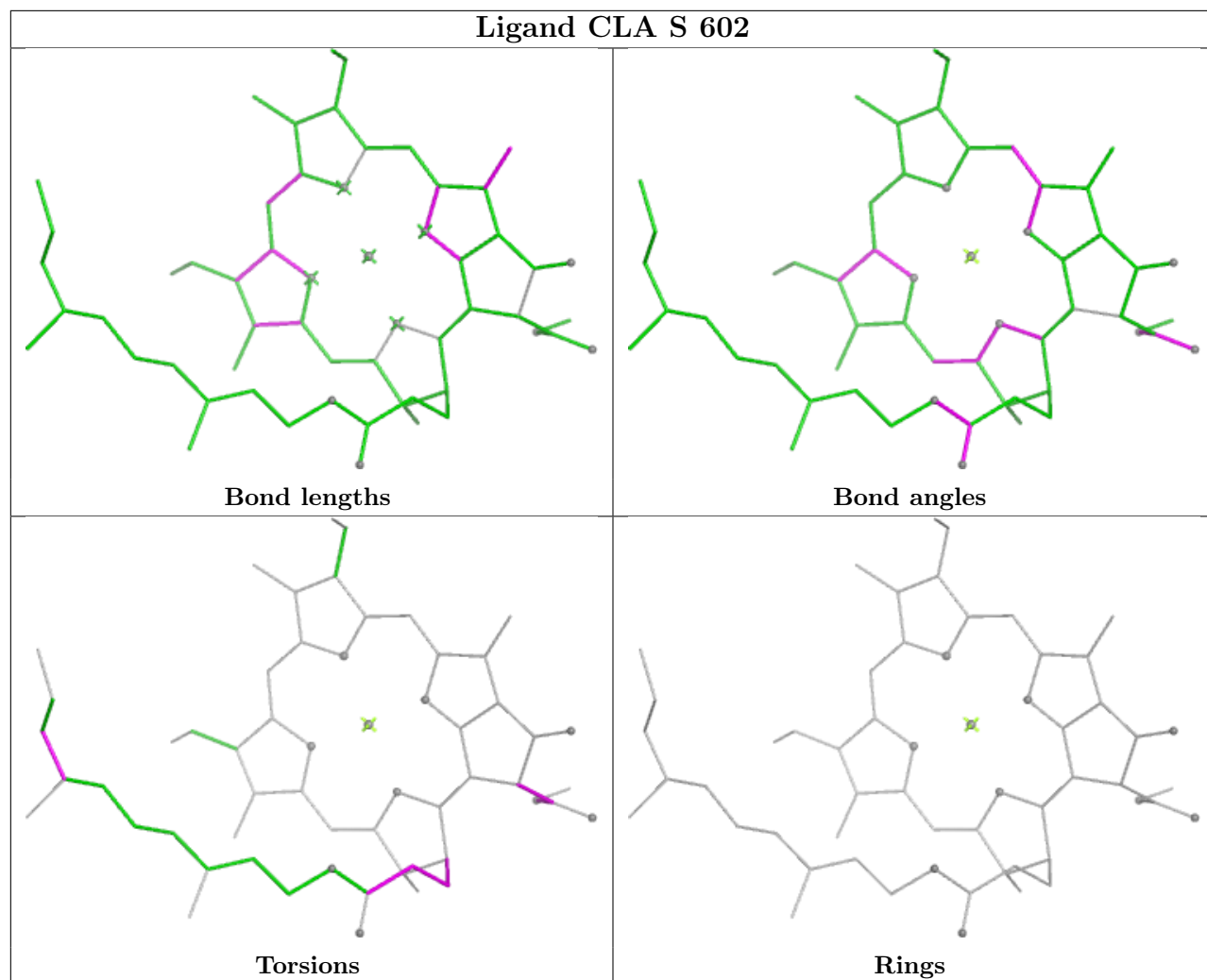
Ligand CLA r 601

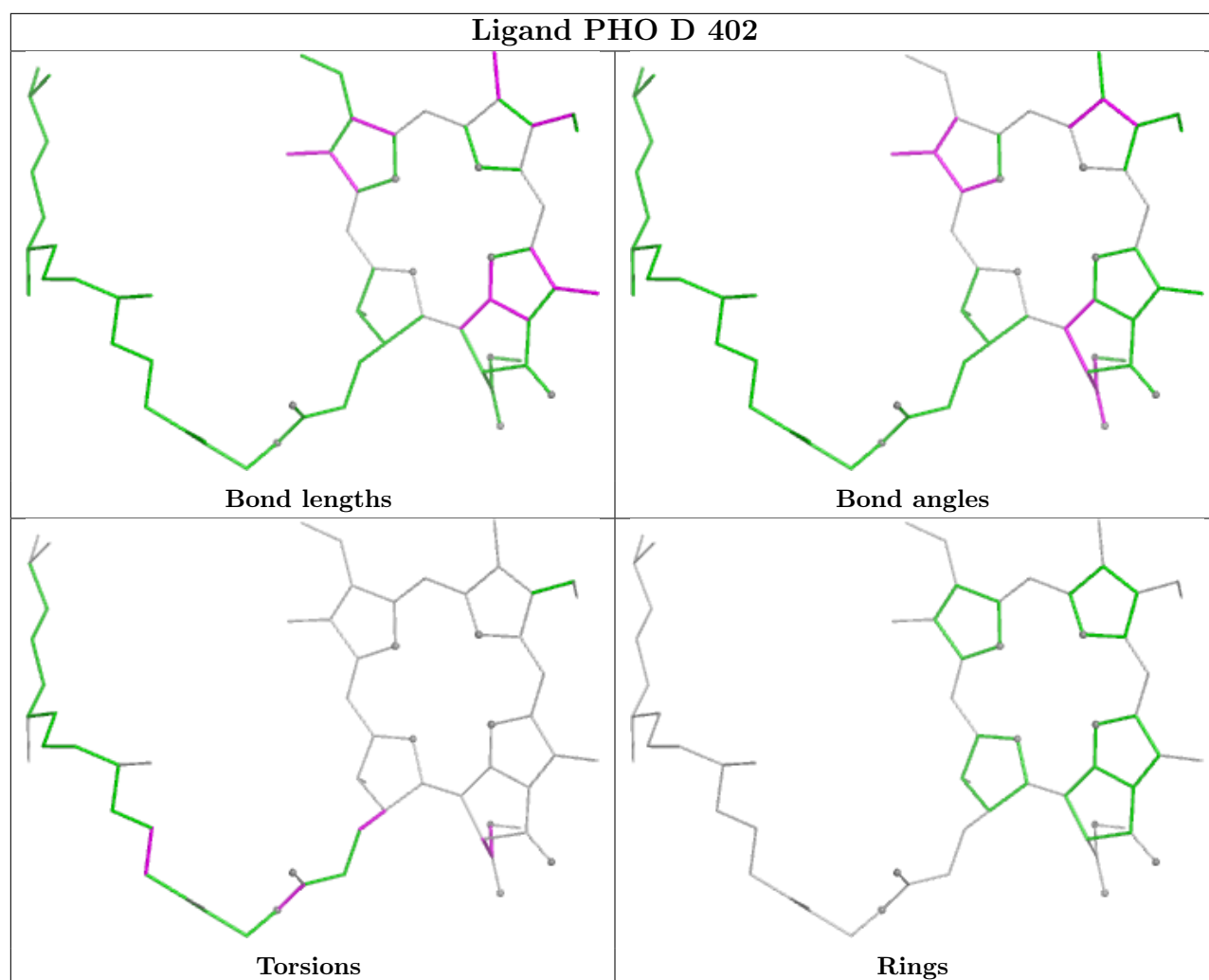


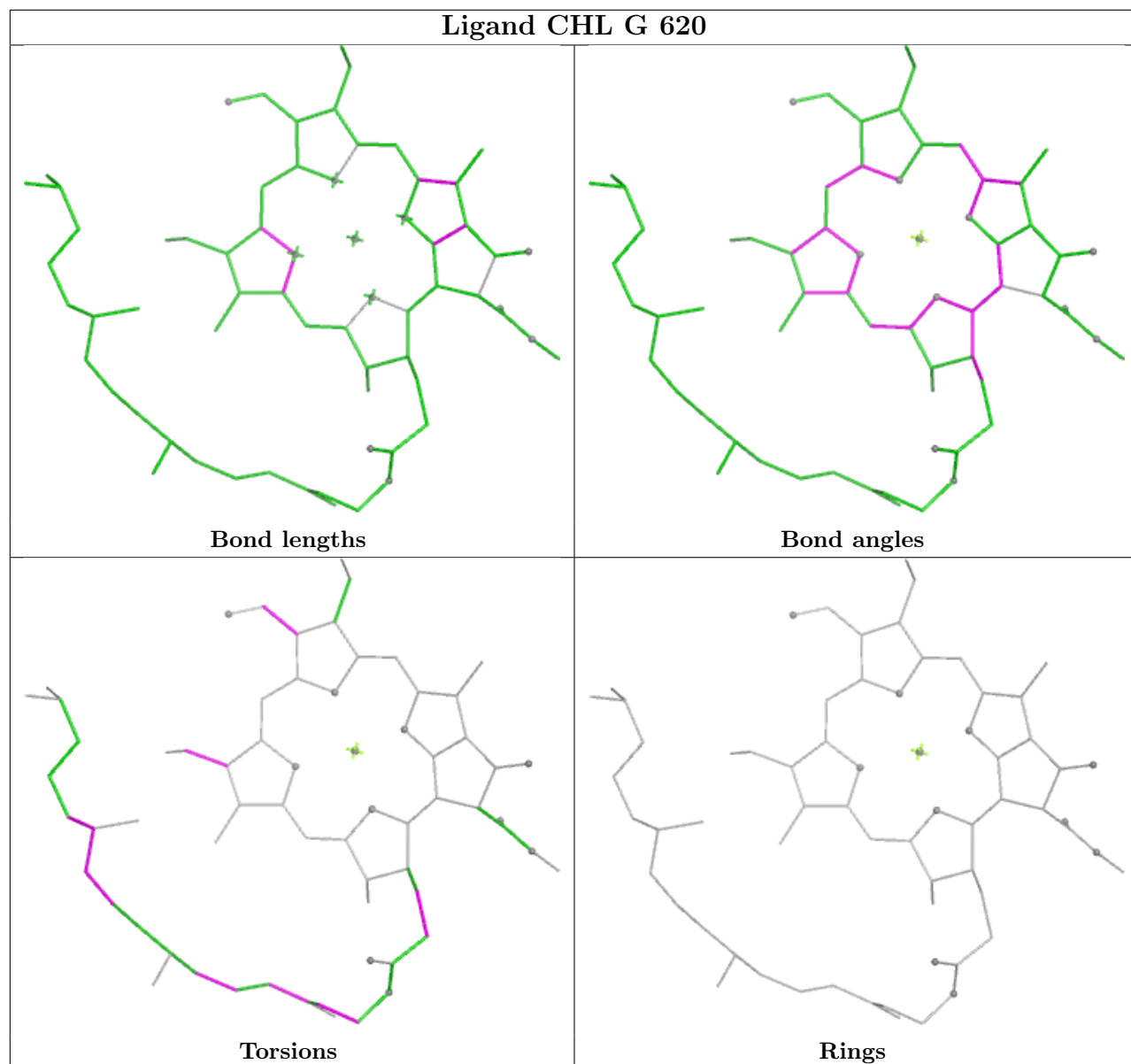
Ligand CLA C 504

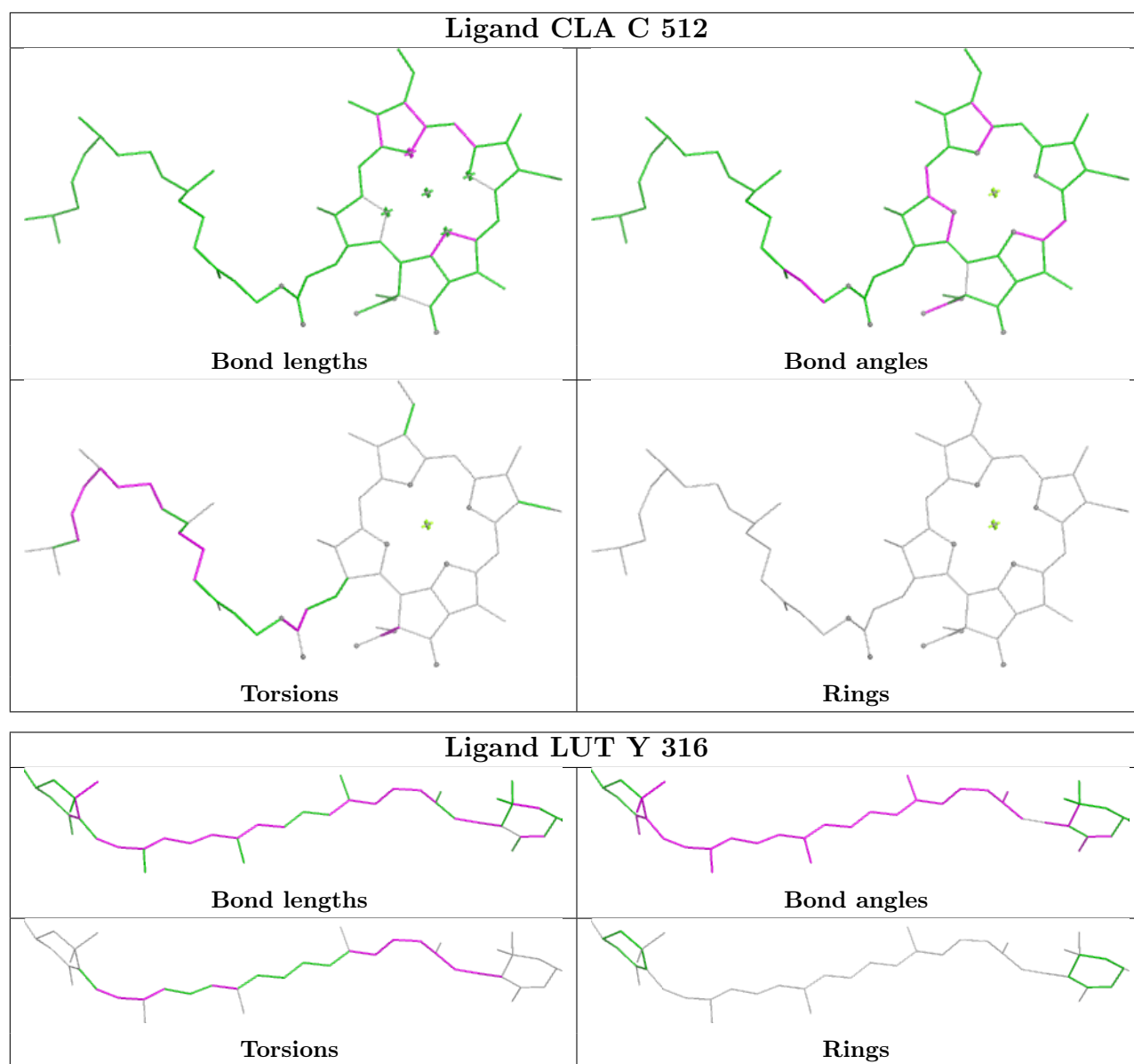


Ligand CLA S 602

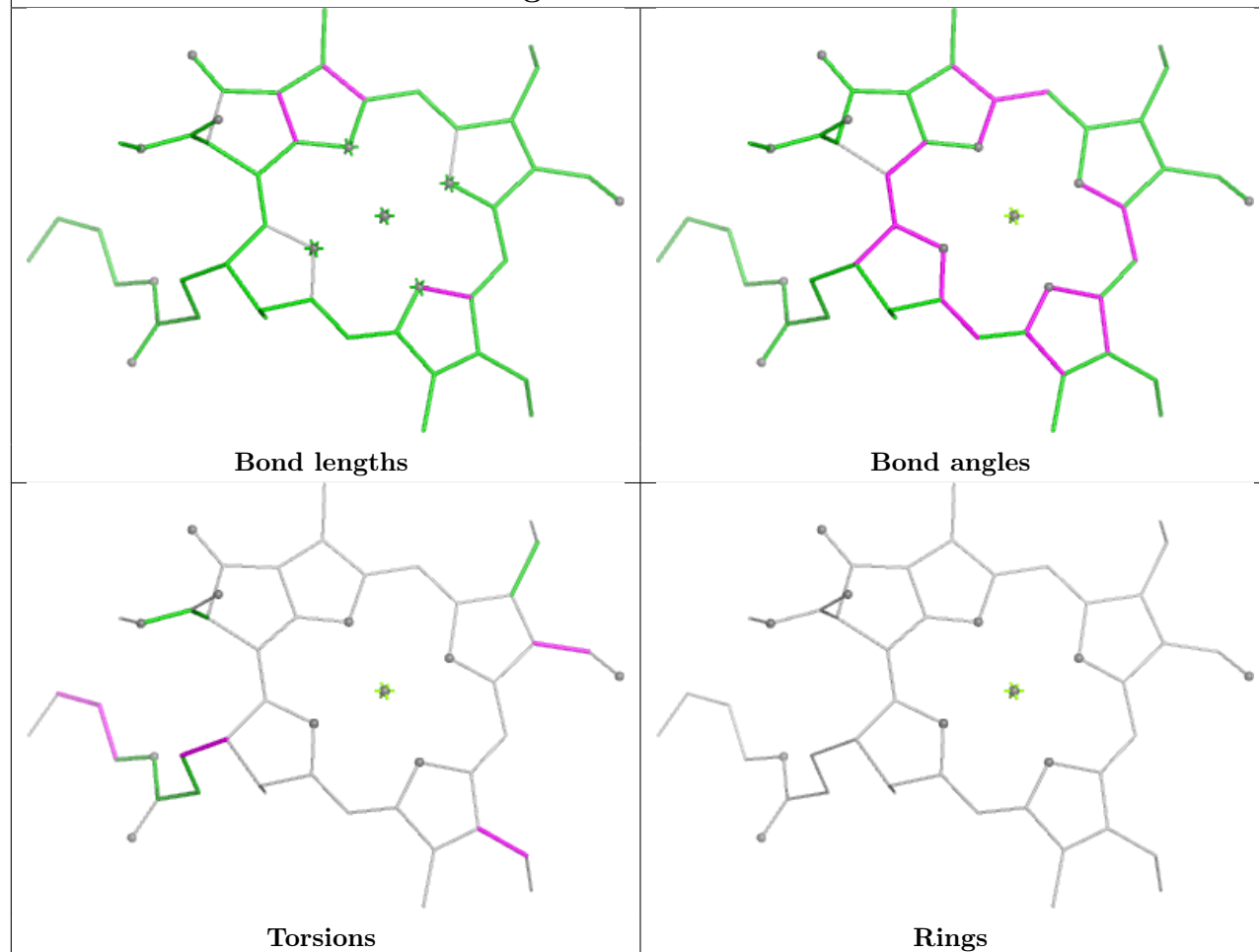




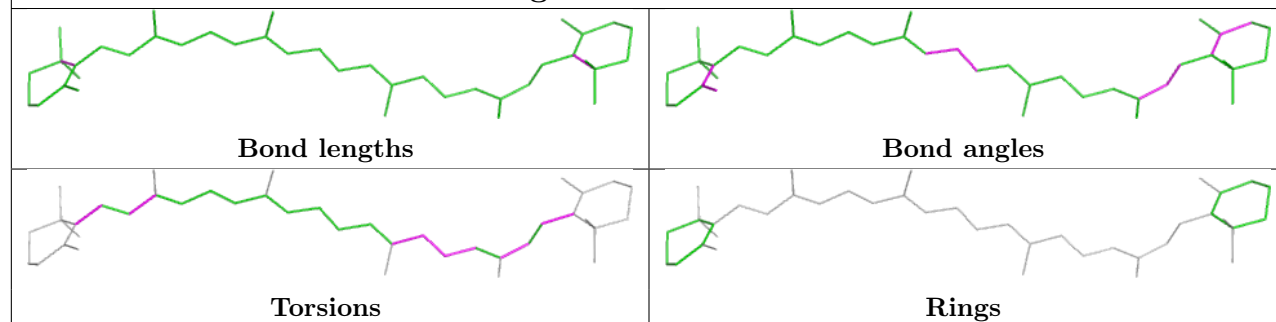


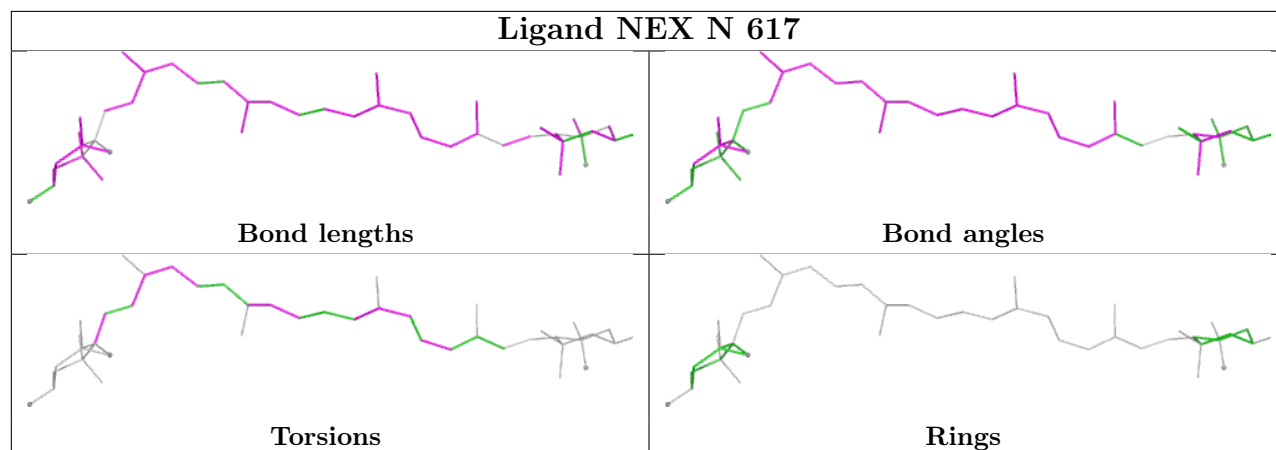
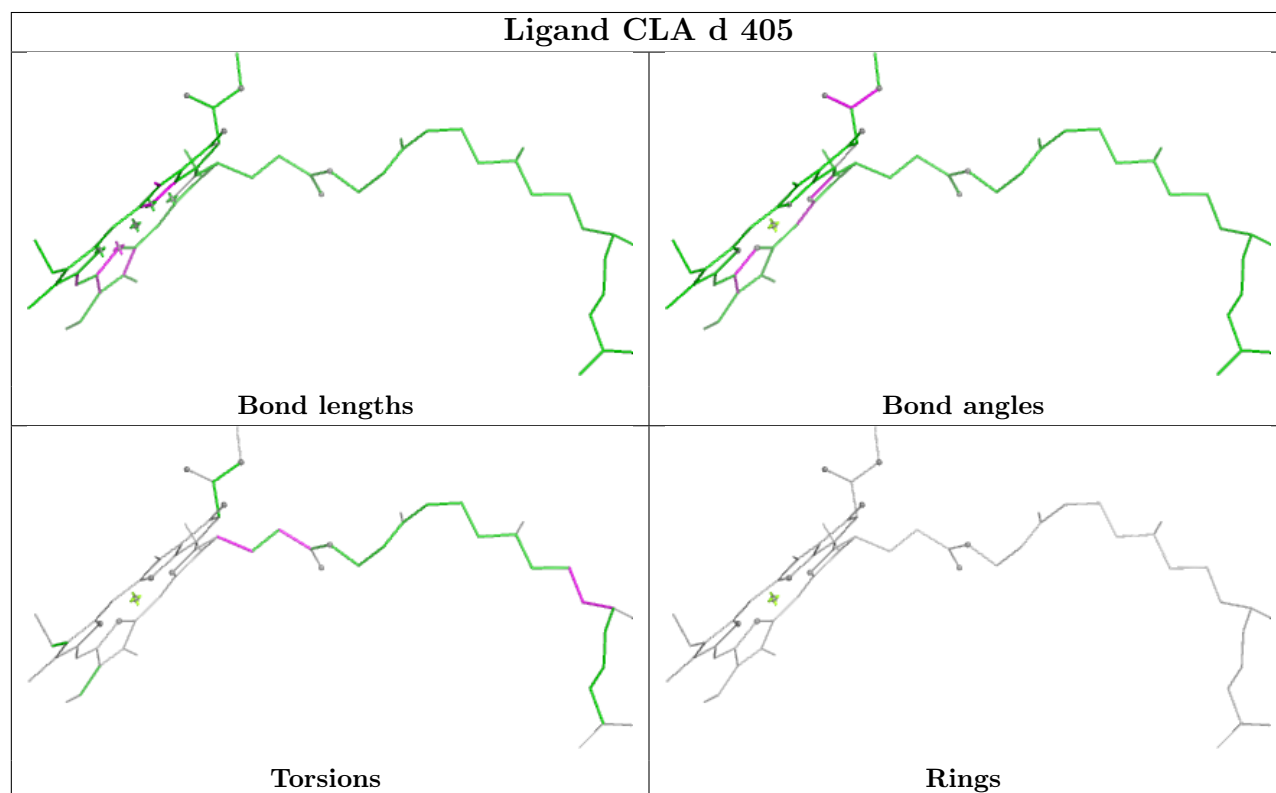
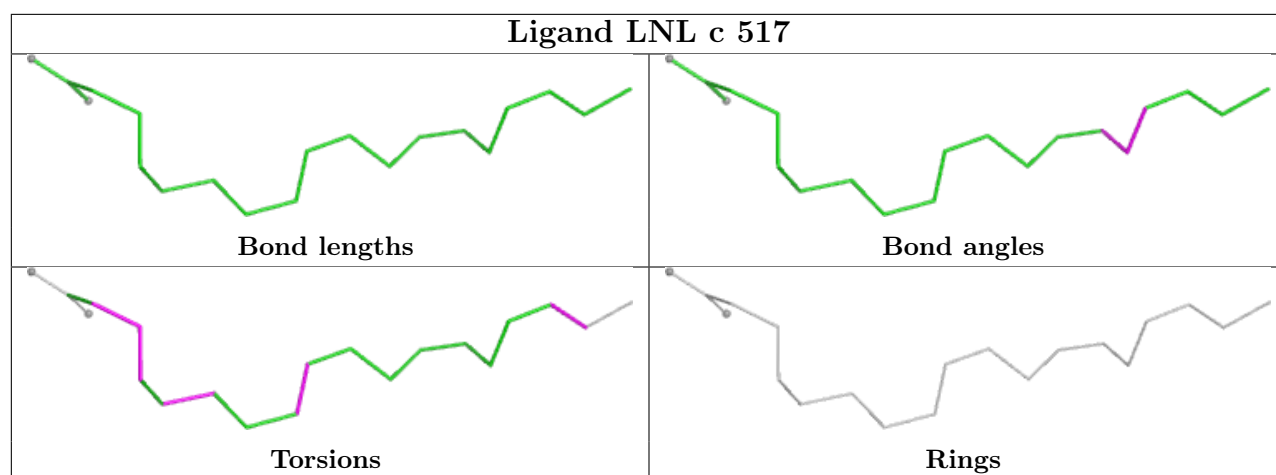


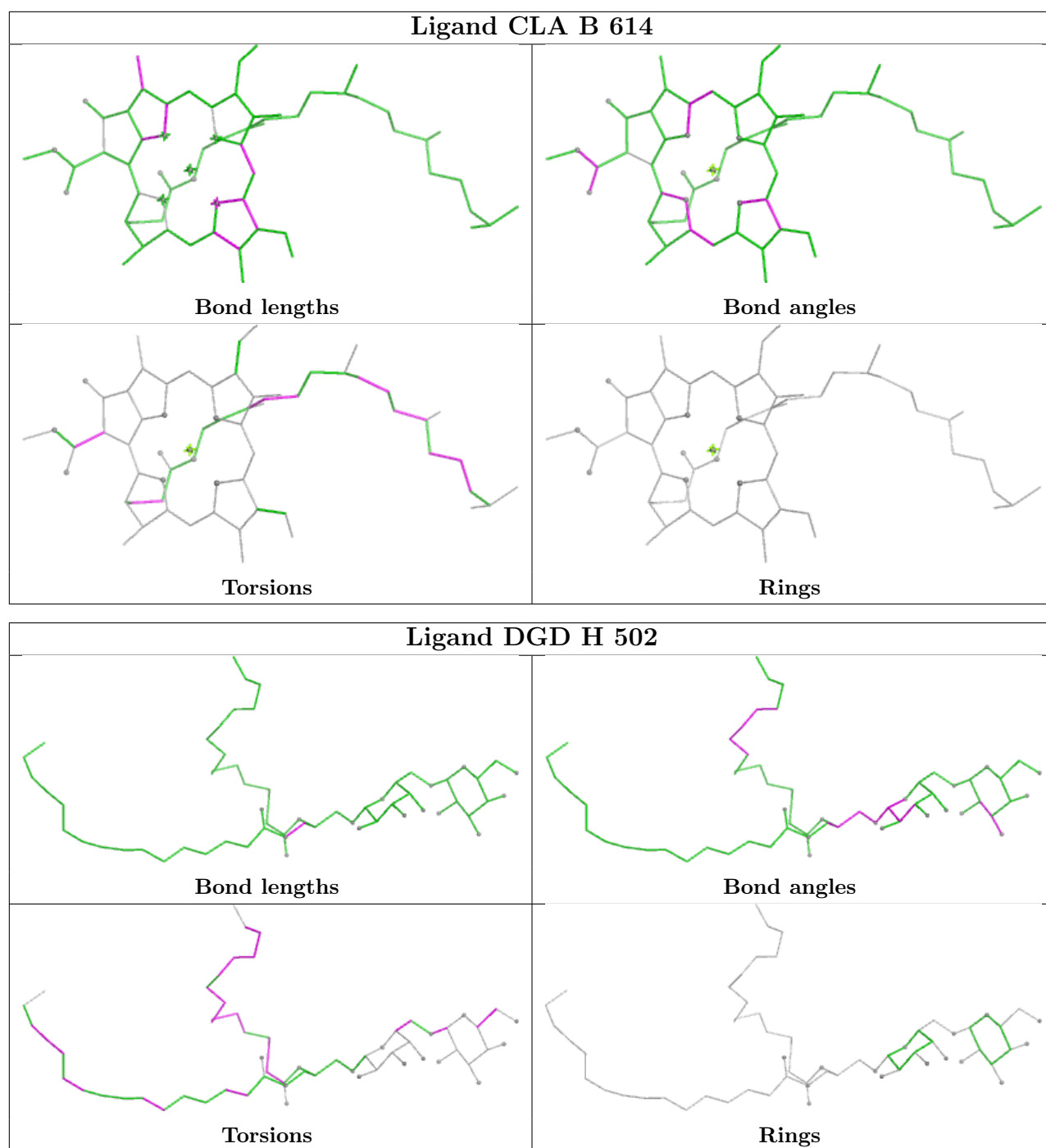
Ligand CHL N 605

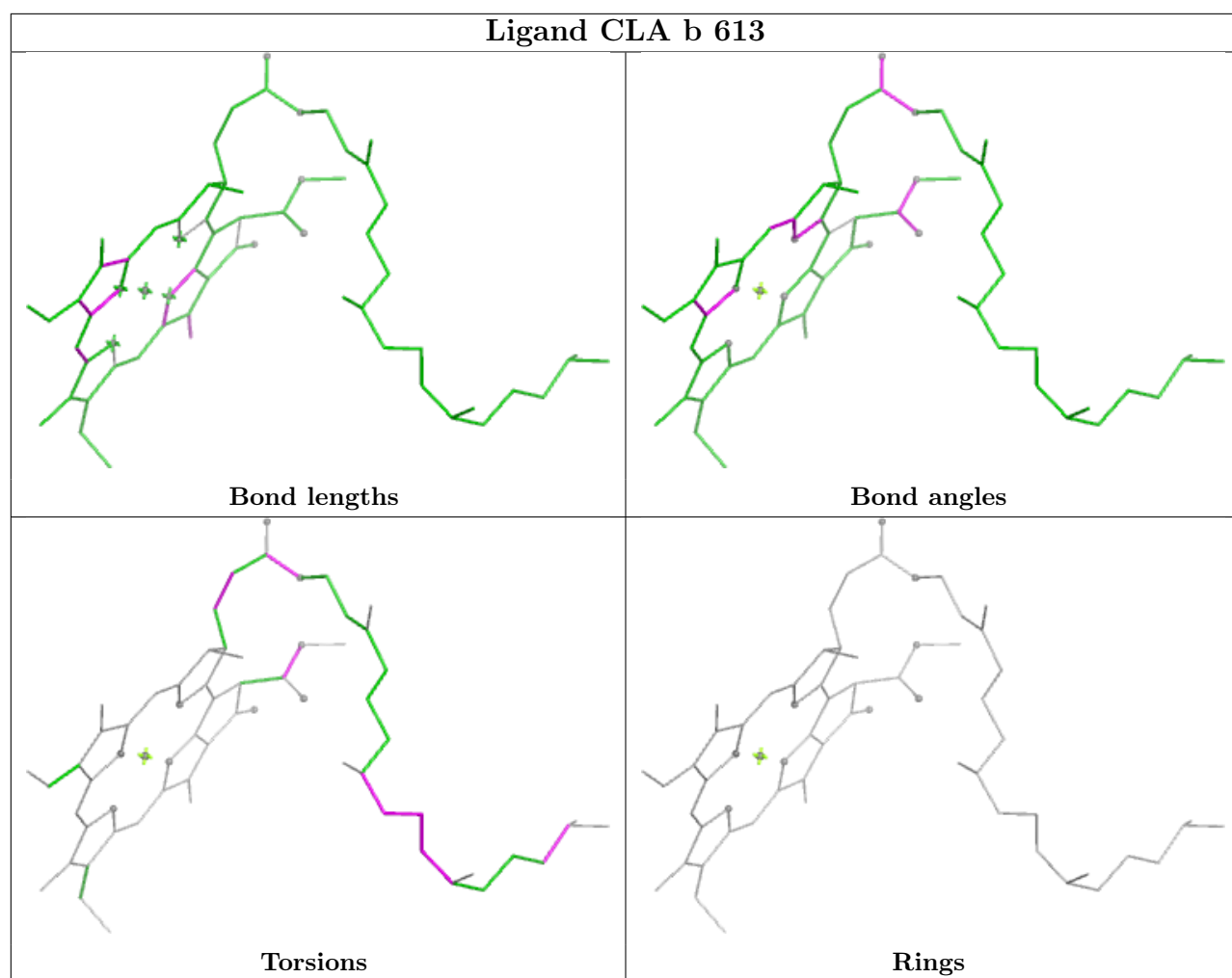


Ligand BCR V 101

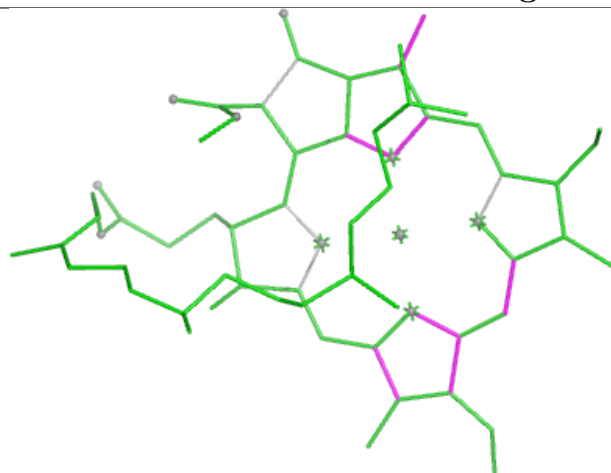




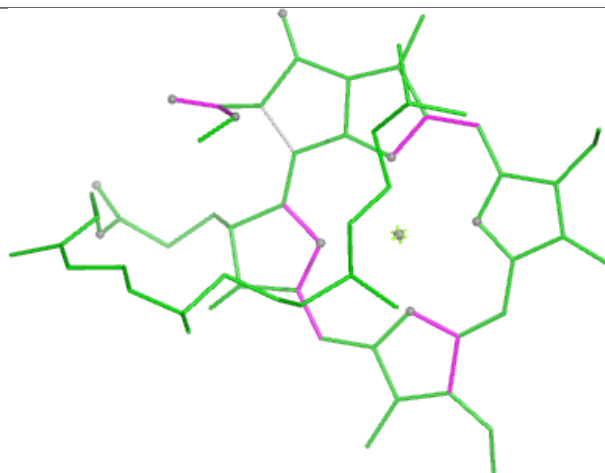




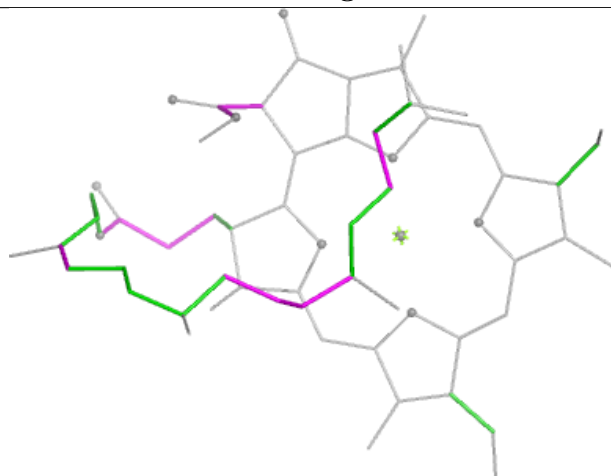
Ligand CLA c 510



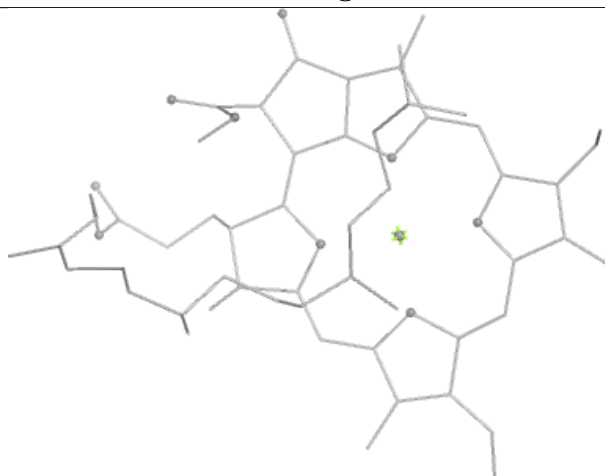
Bond lengths



Bond angles

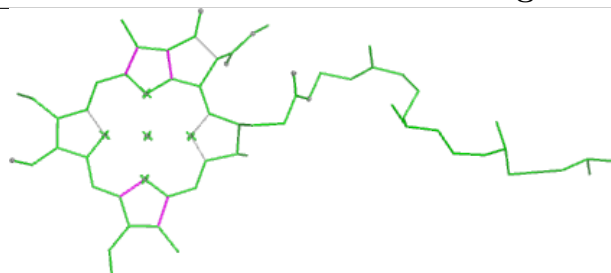


Torsions

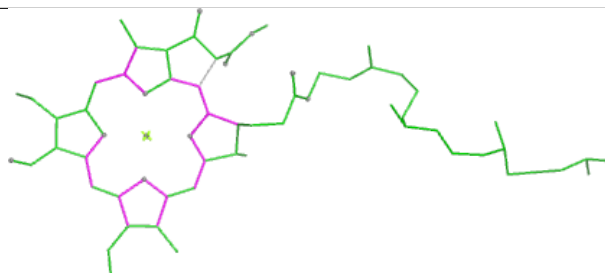


Rings

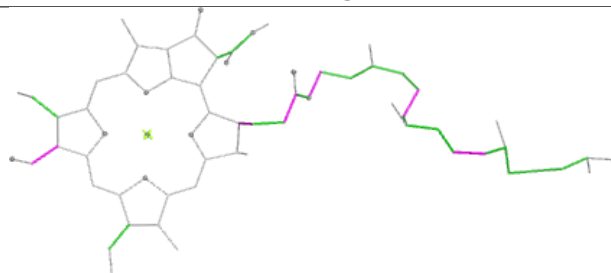
Ligand CHL n 606



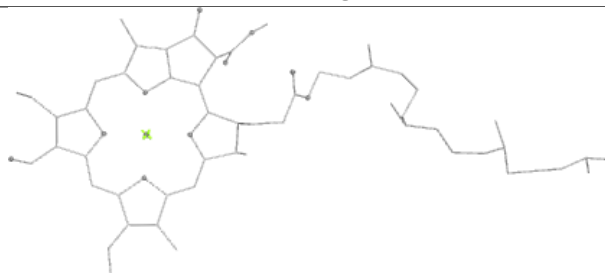
Bond lengths



Bond angles

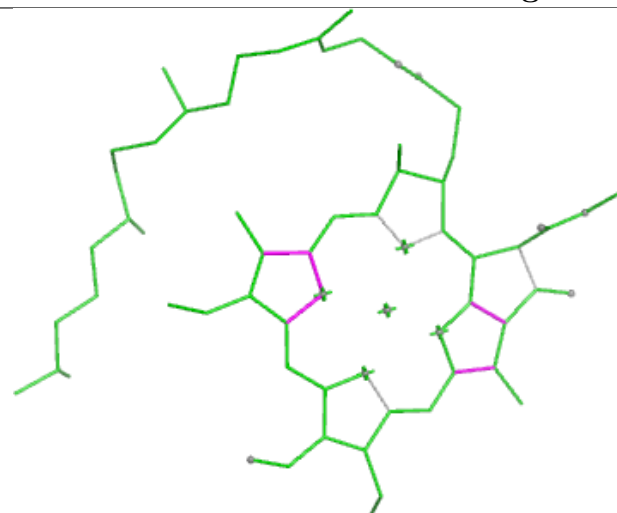


Torsions

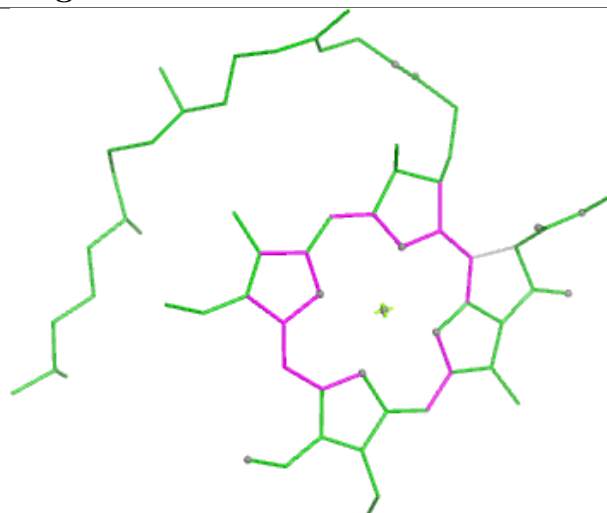


Rings

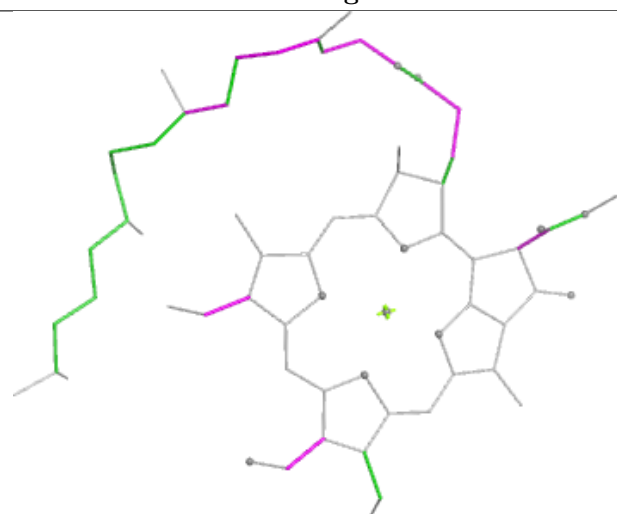
Ligand CHL g 607



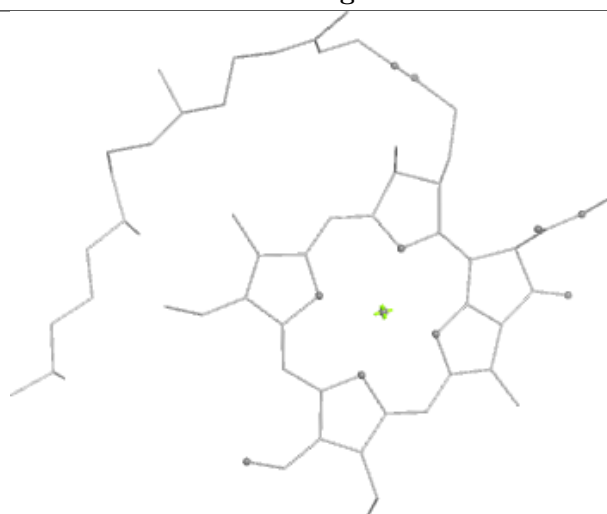
Bond lengths



Bond angles

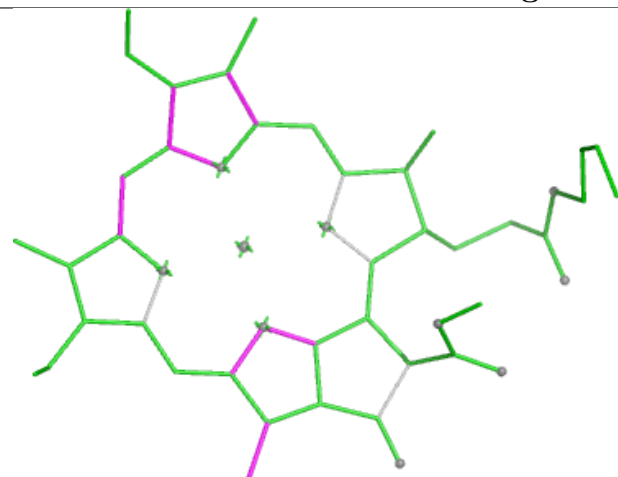


Torsions

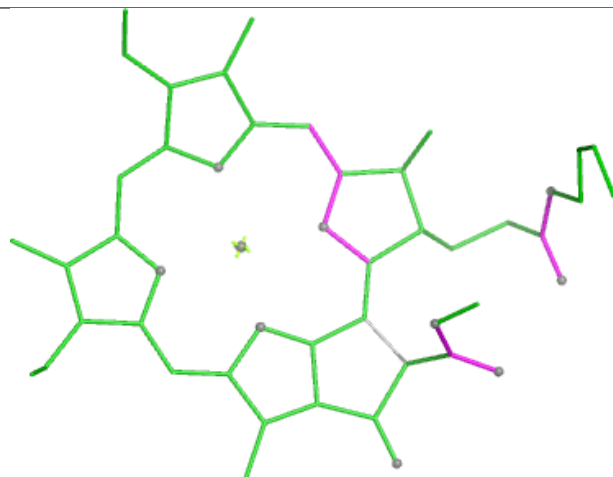


Rings

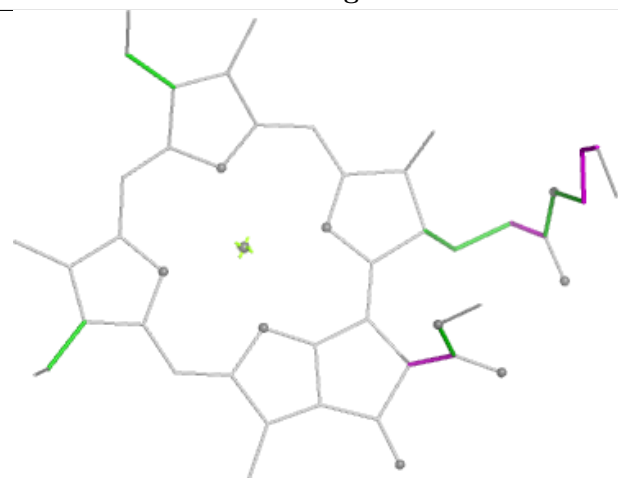
Ligand CLA n 612



Bond lengths



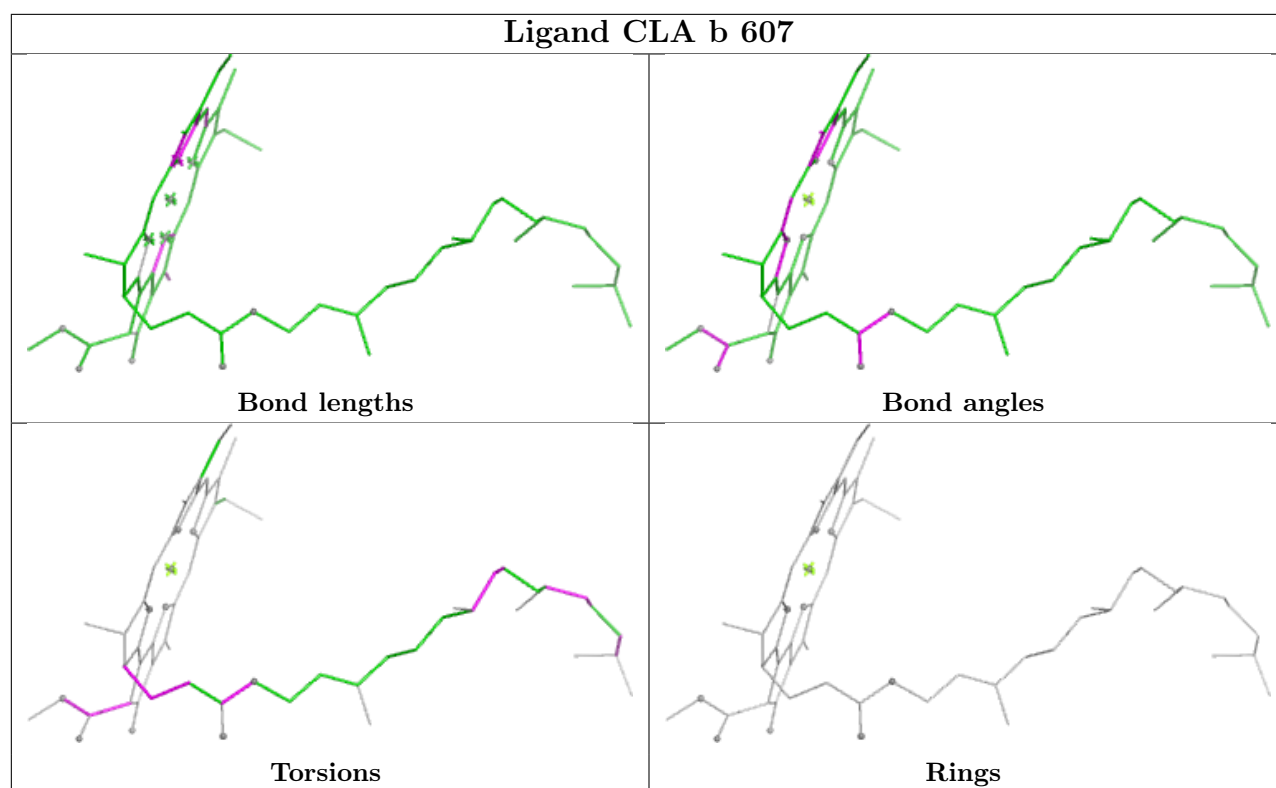
Bond angles

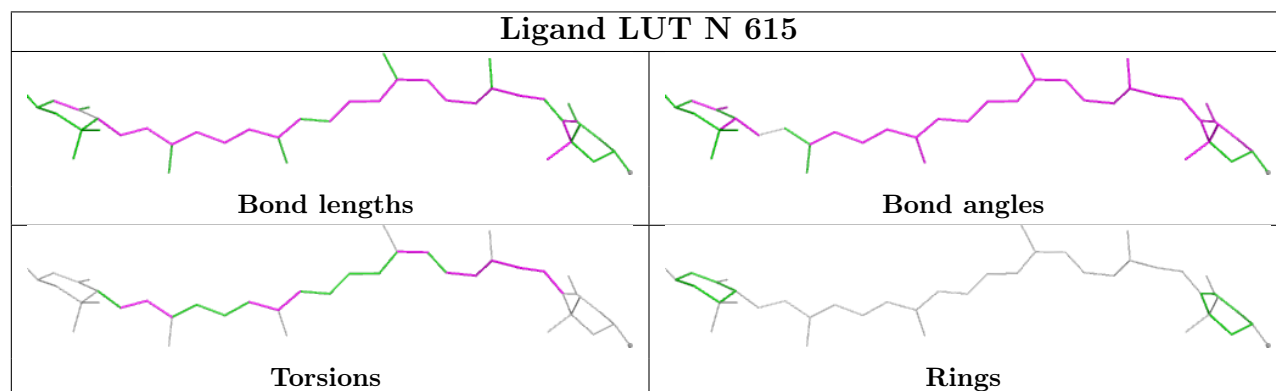
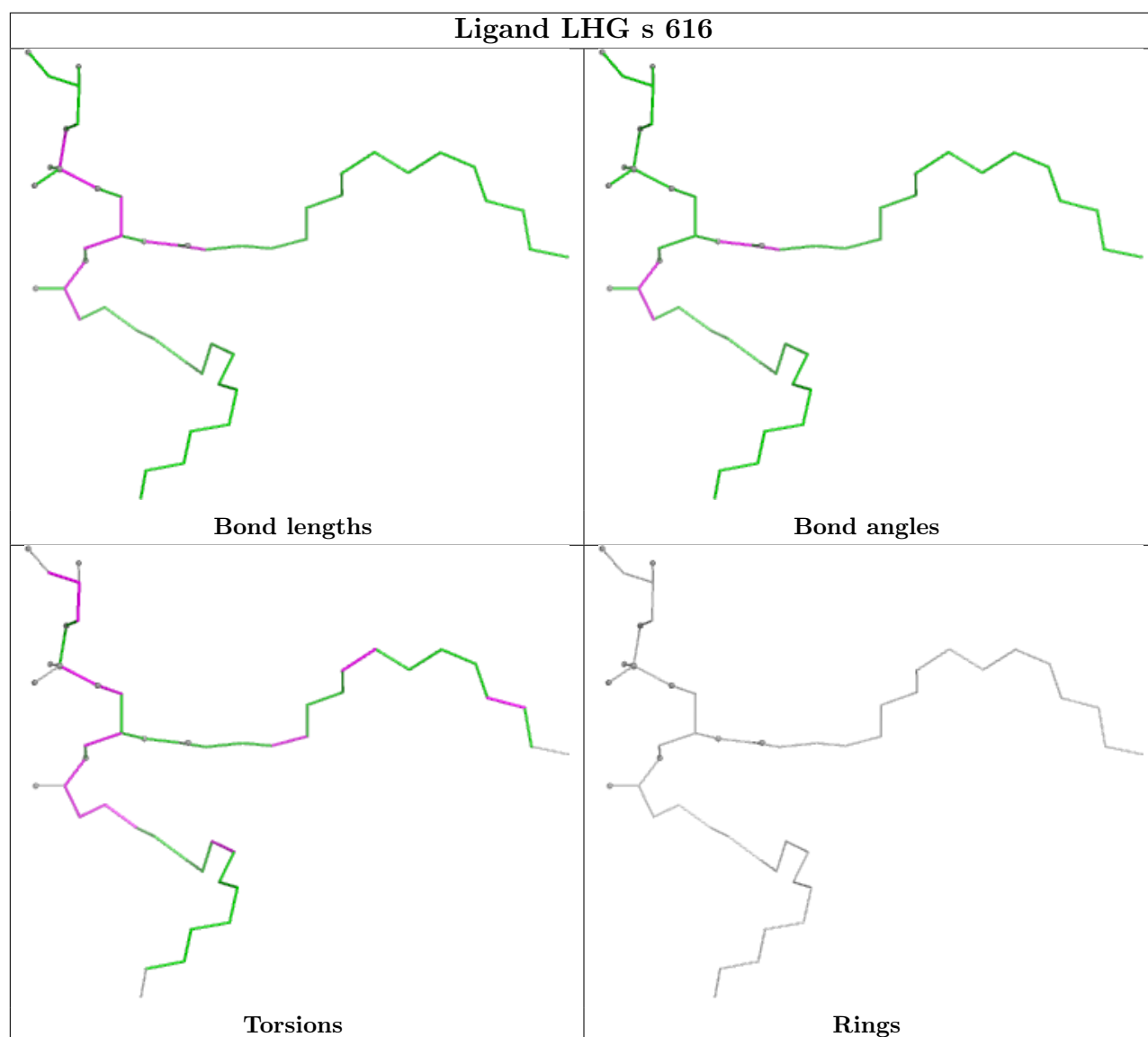


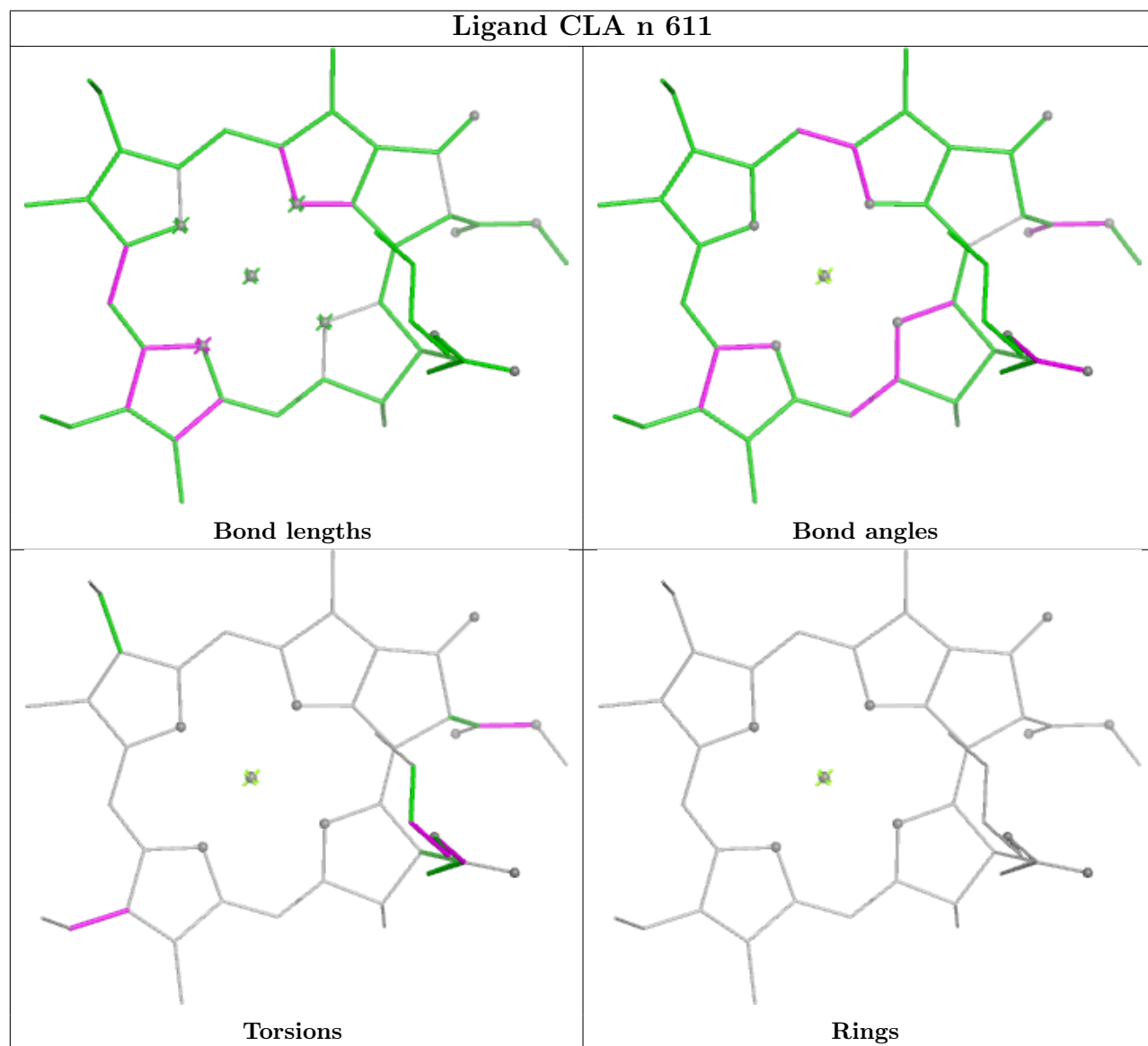
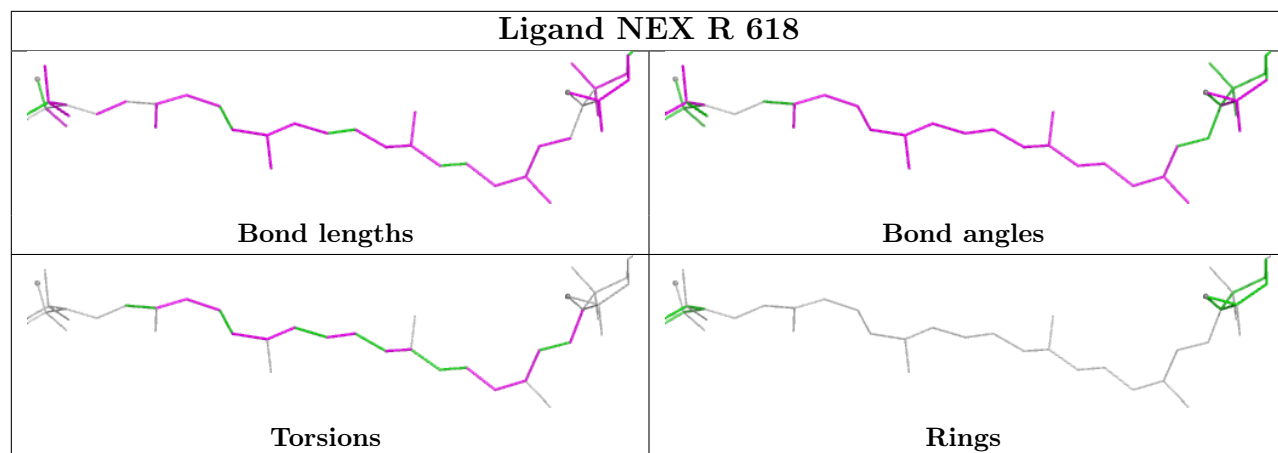
Torsions

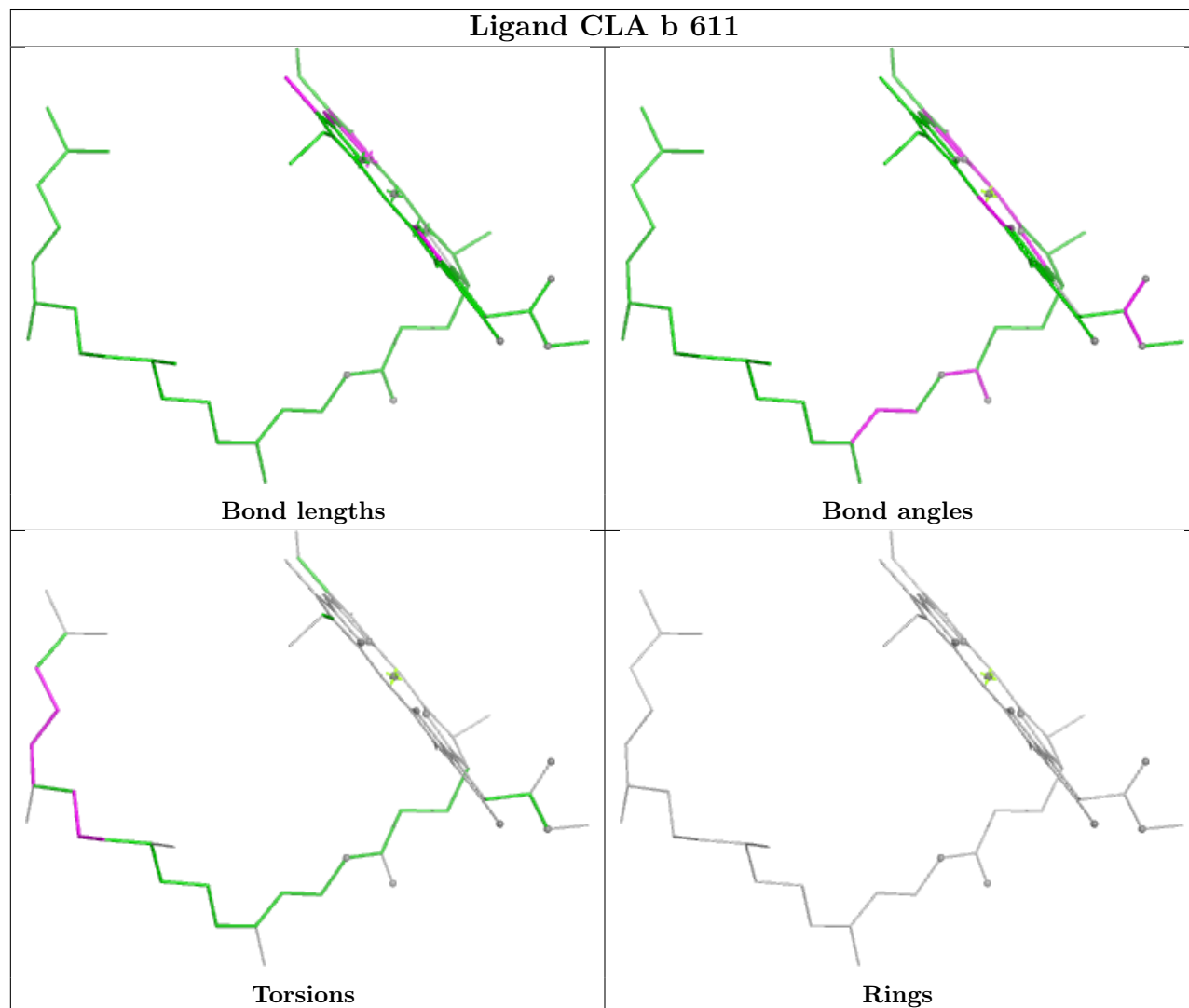
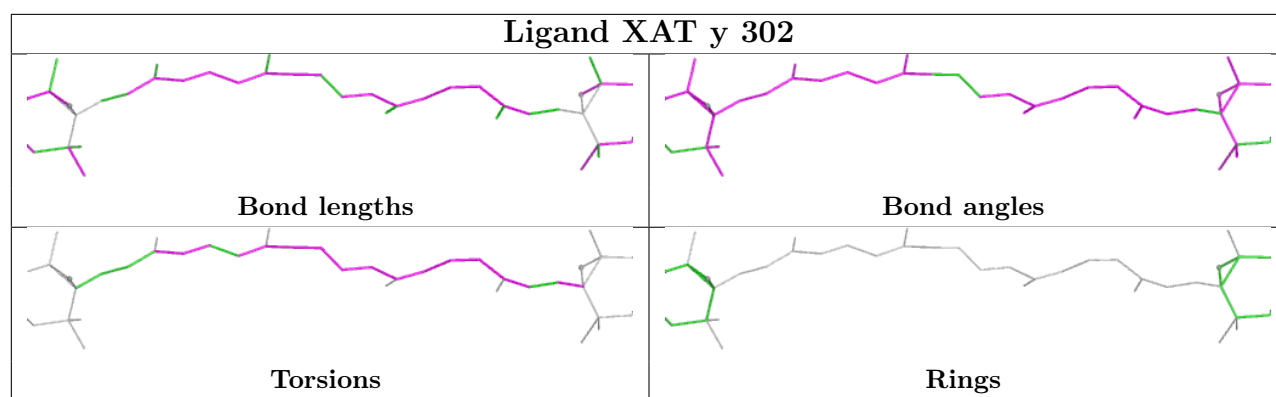


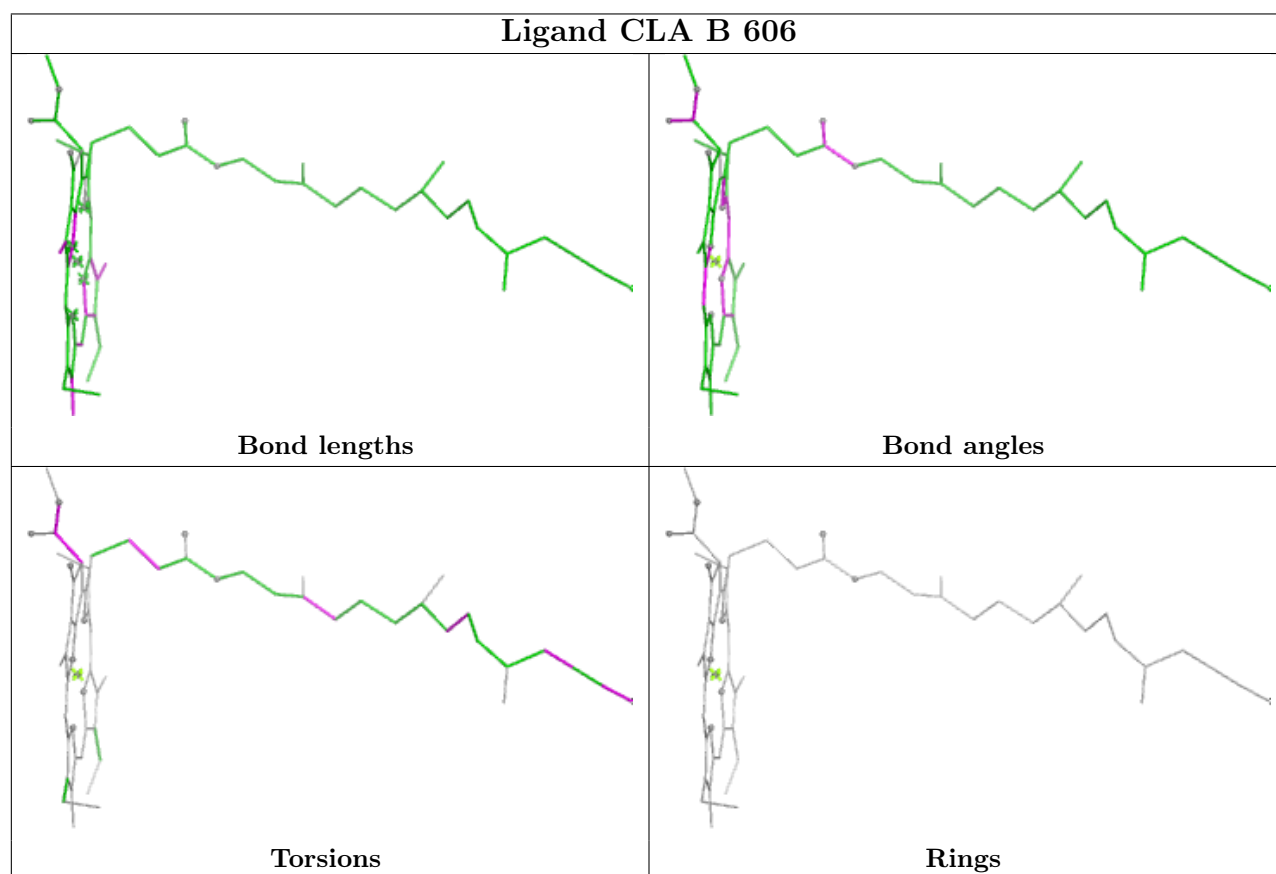
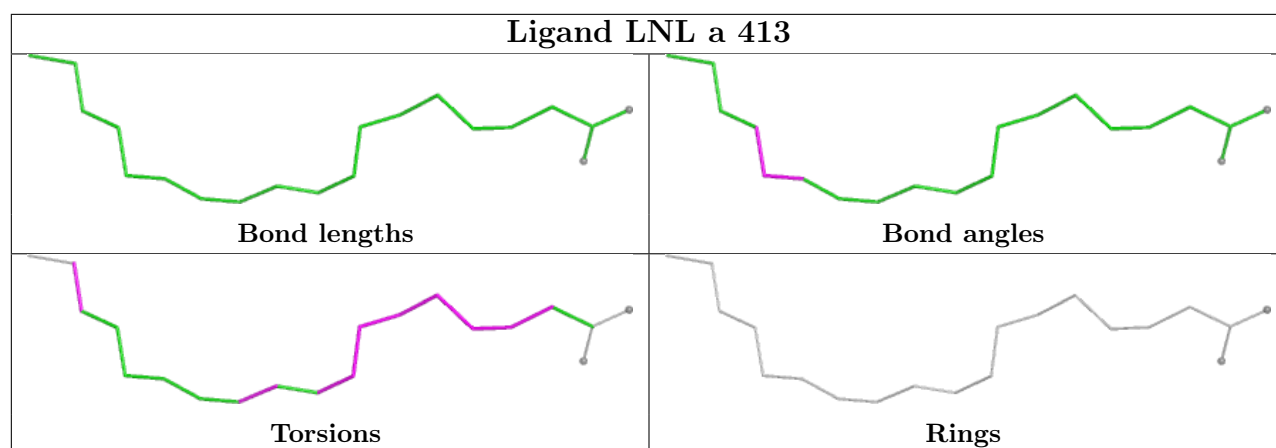
Rings



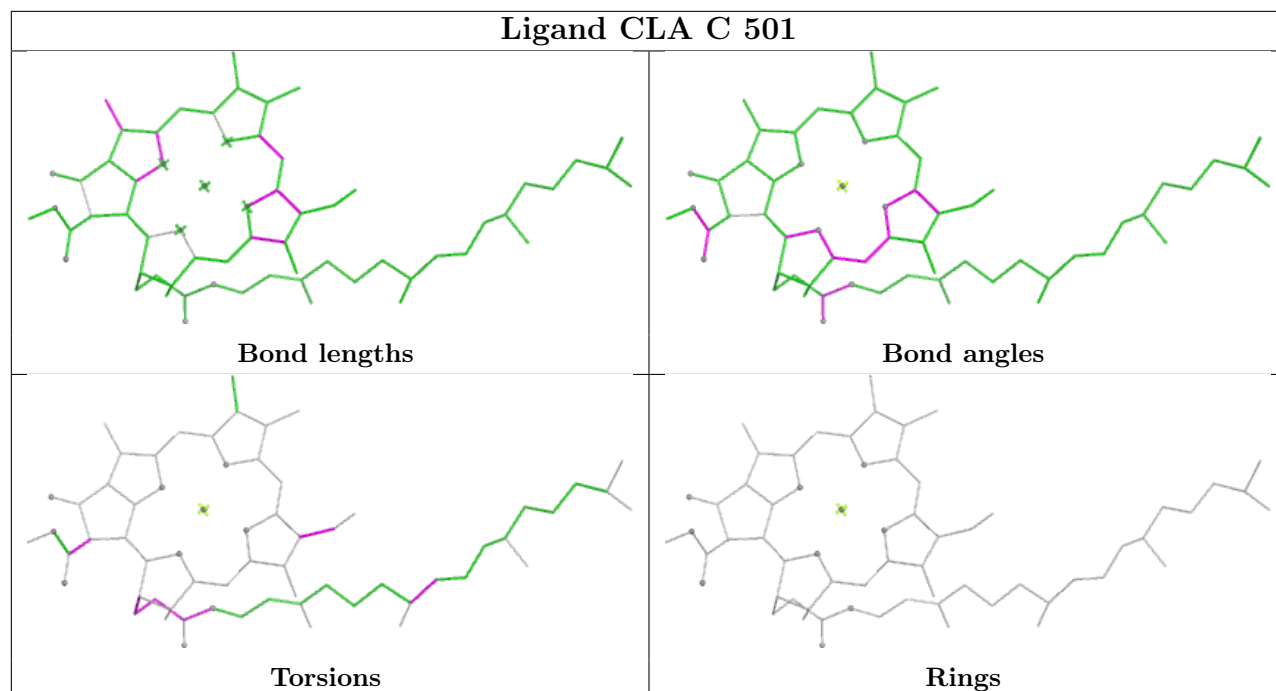




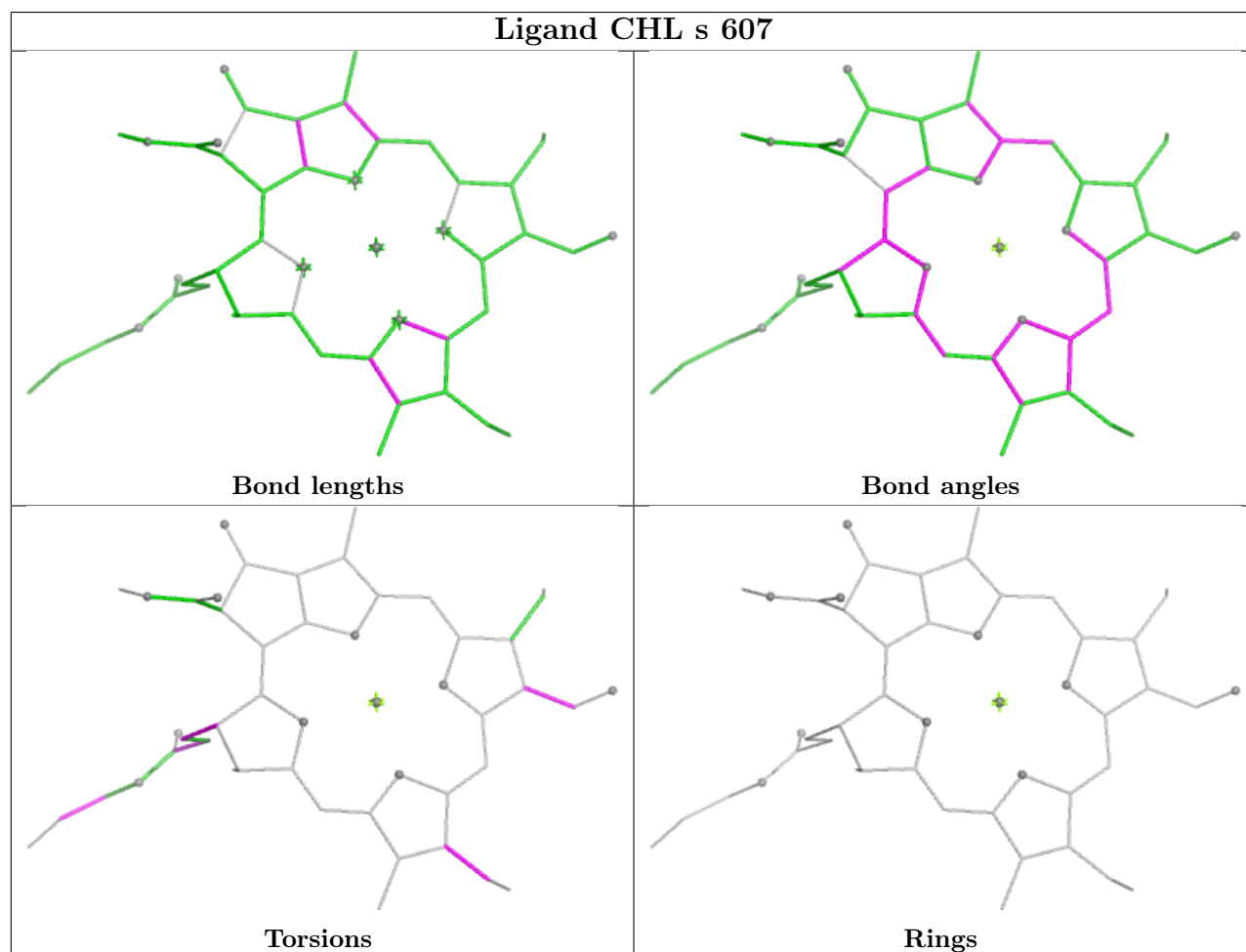


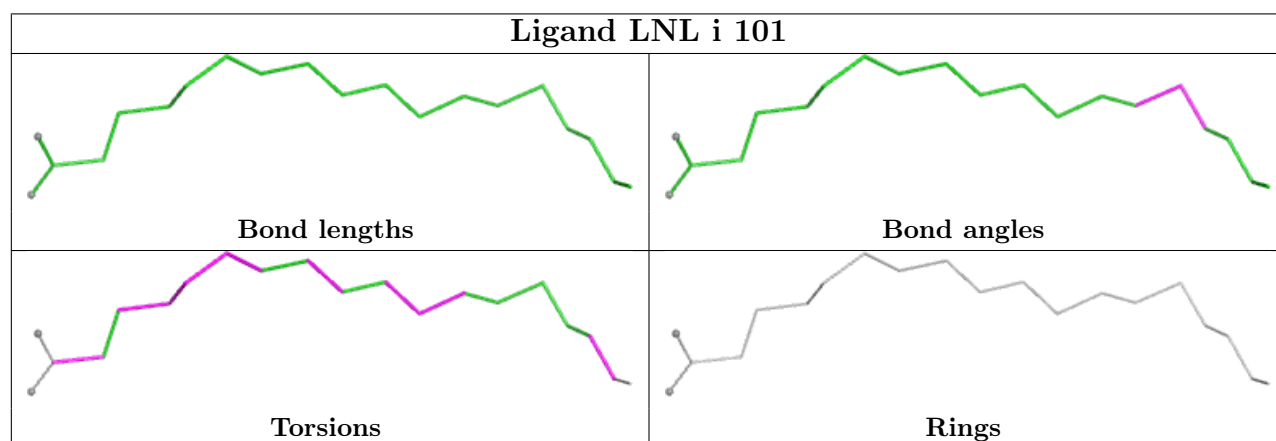
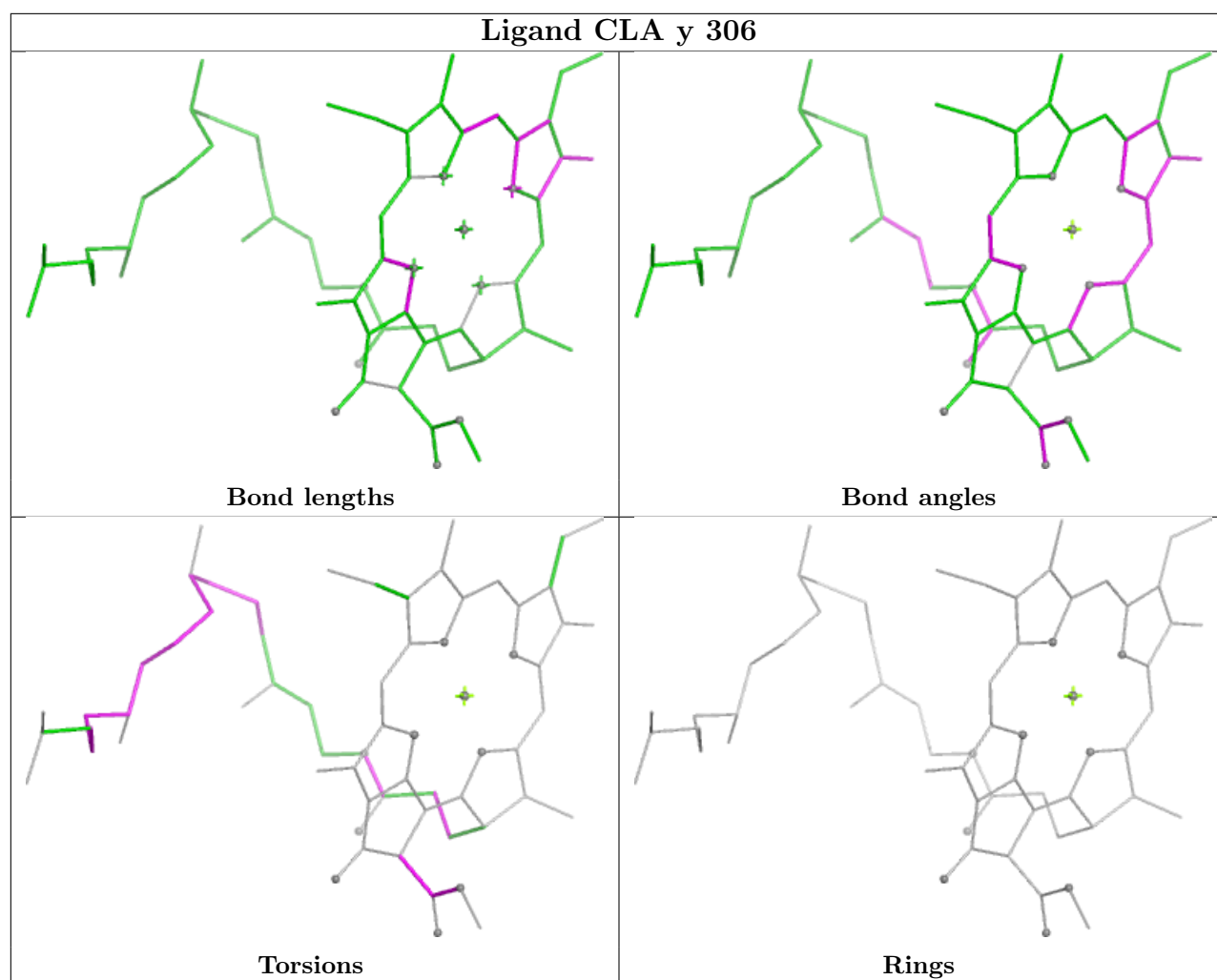


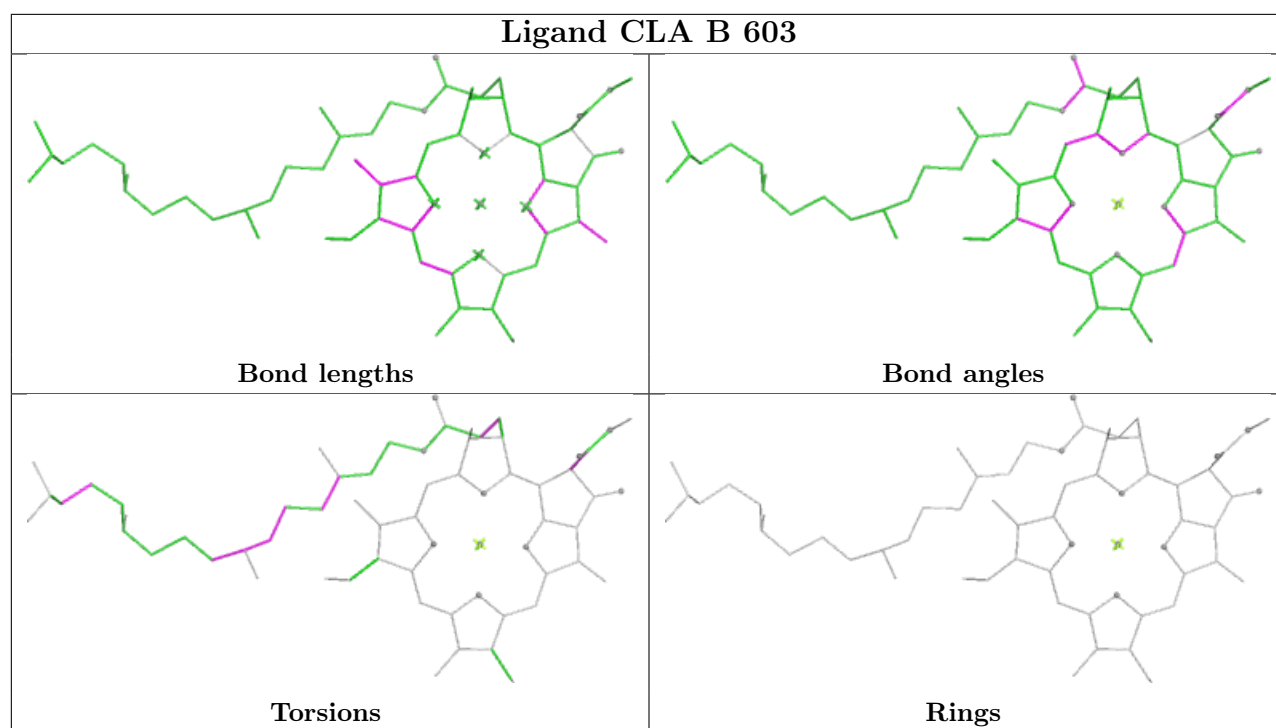
Ligand CLA C 501

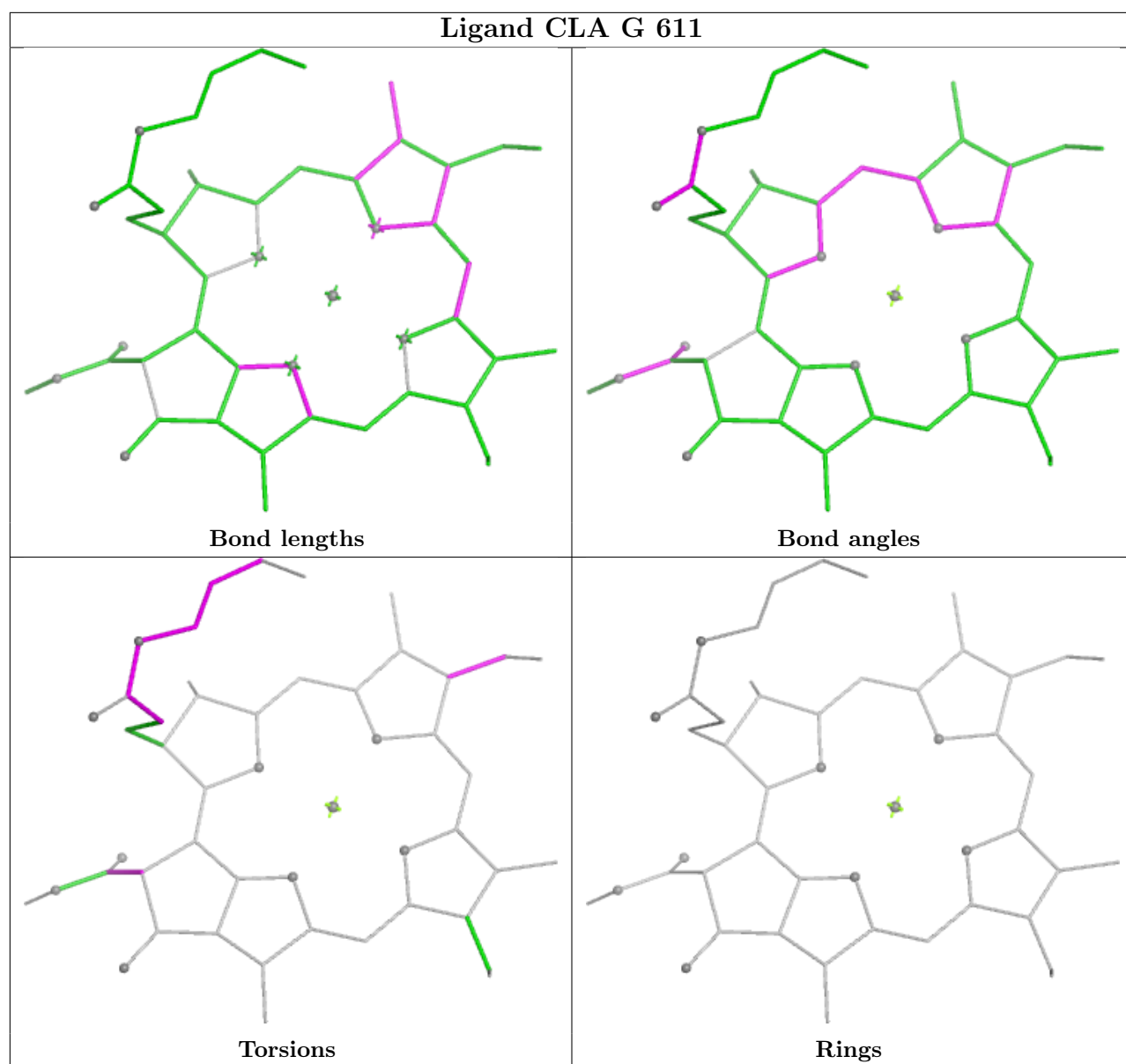


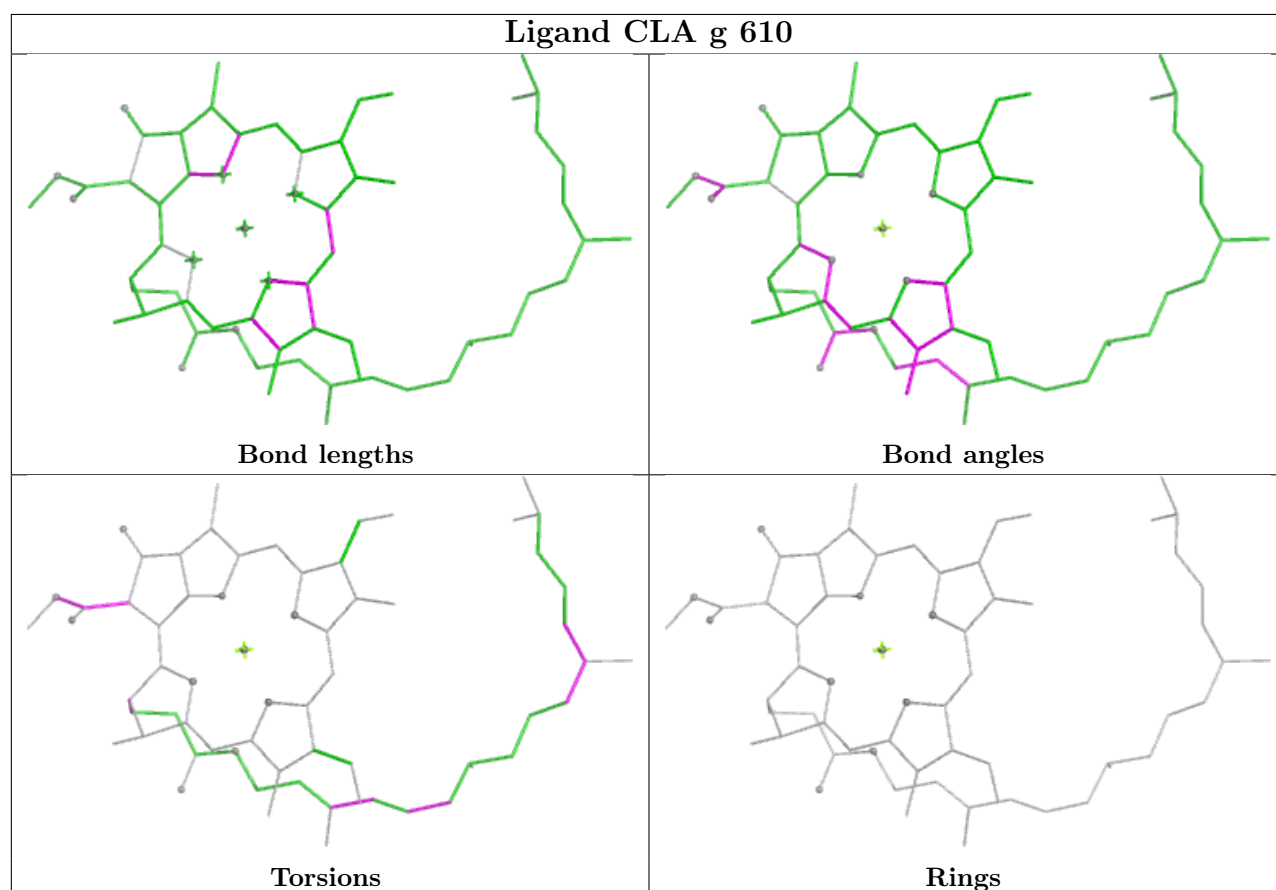
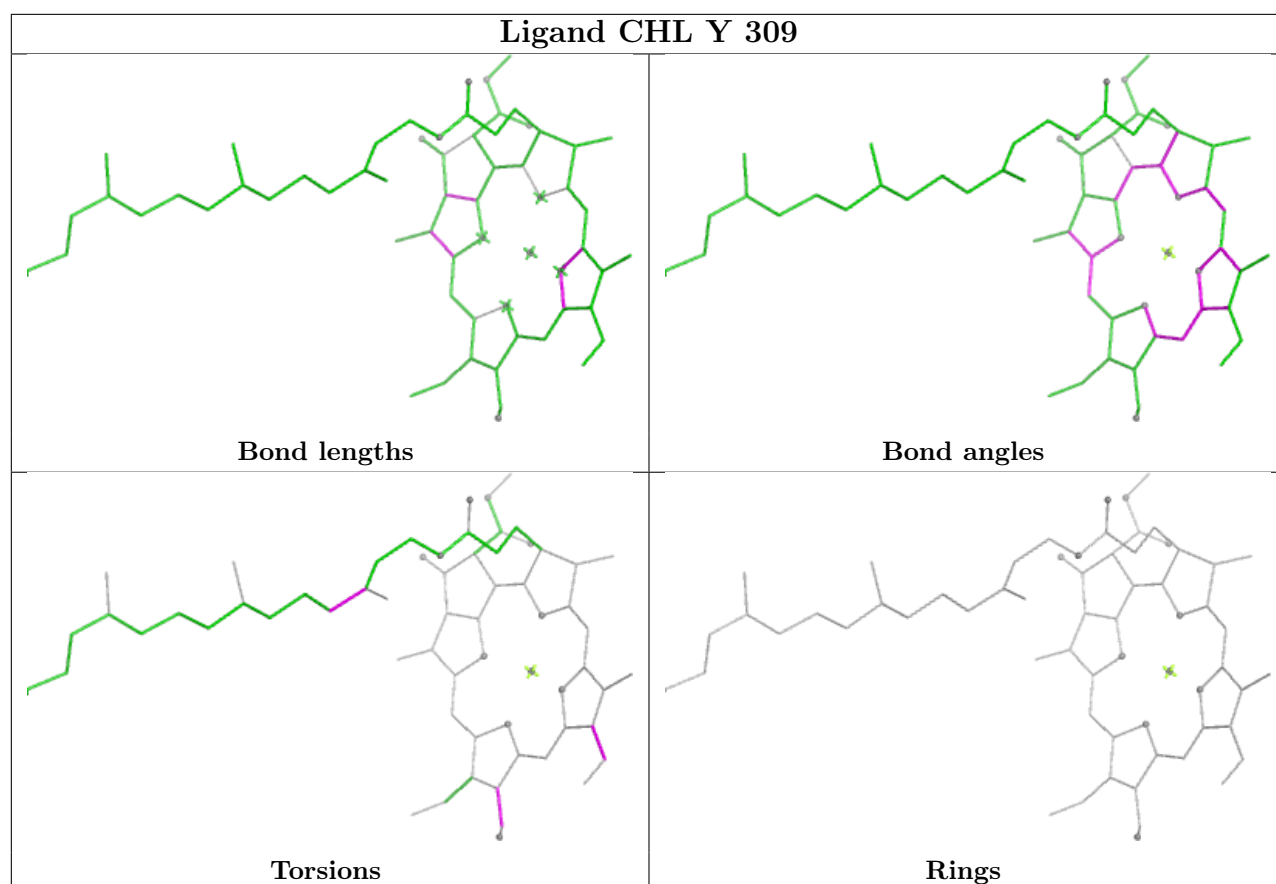
Ligand CHL s 607

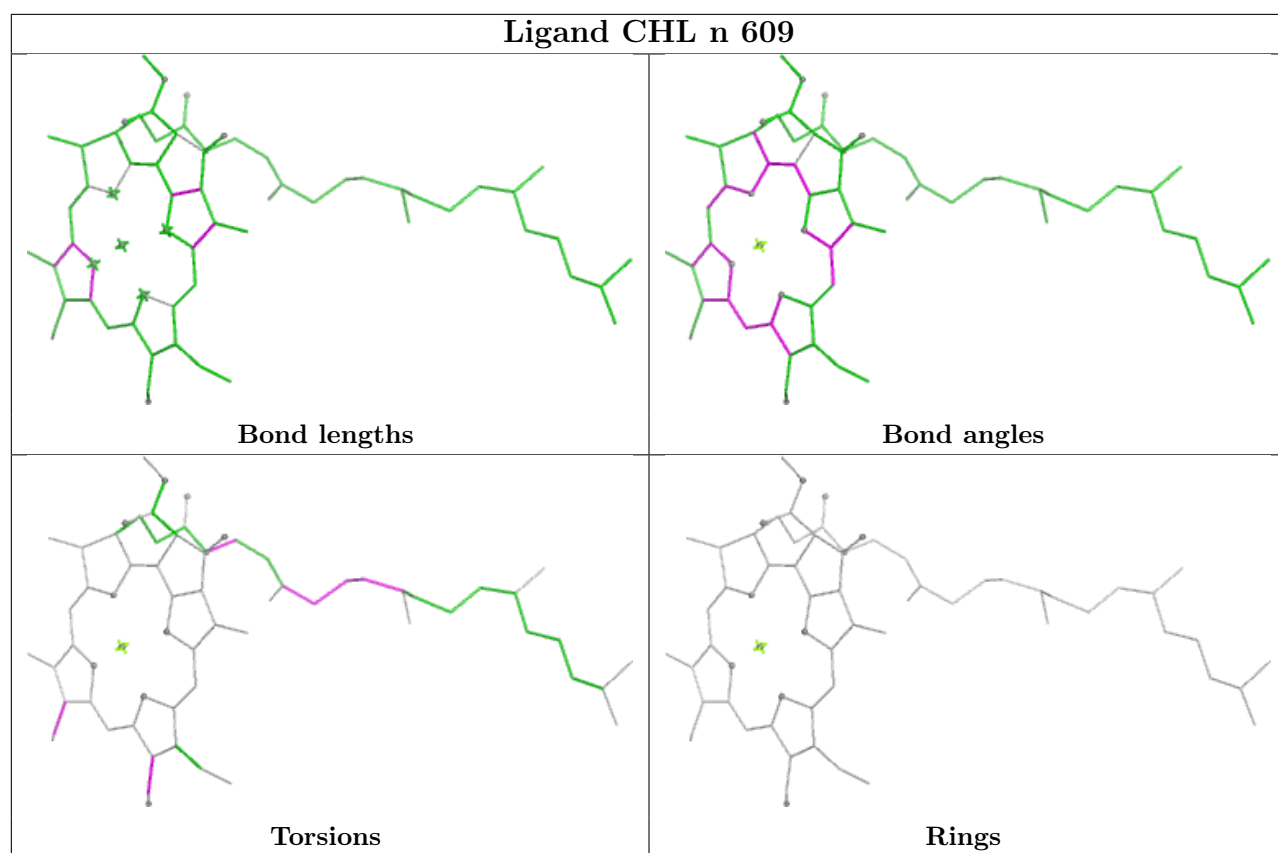




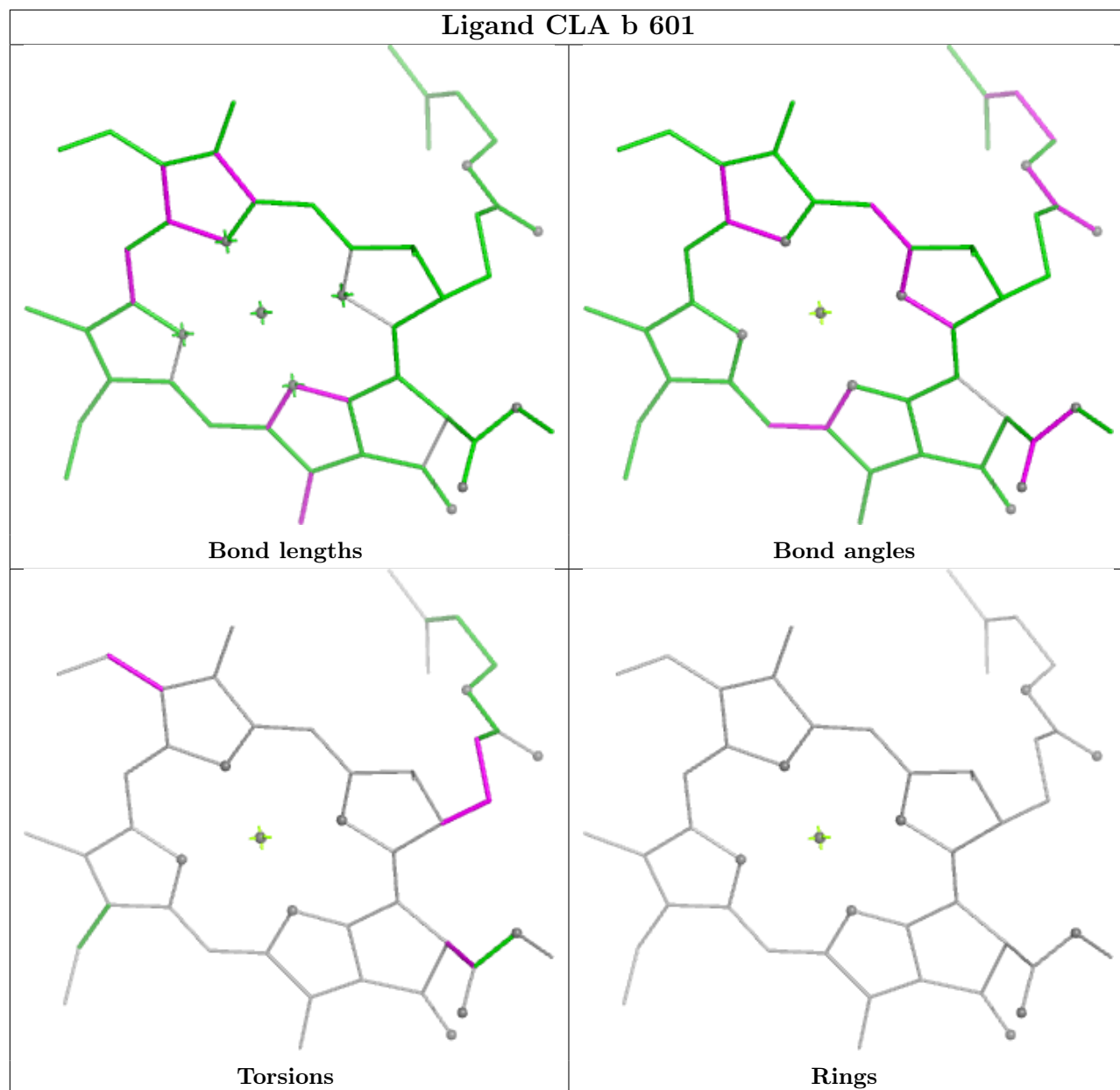


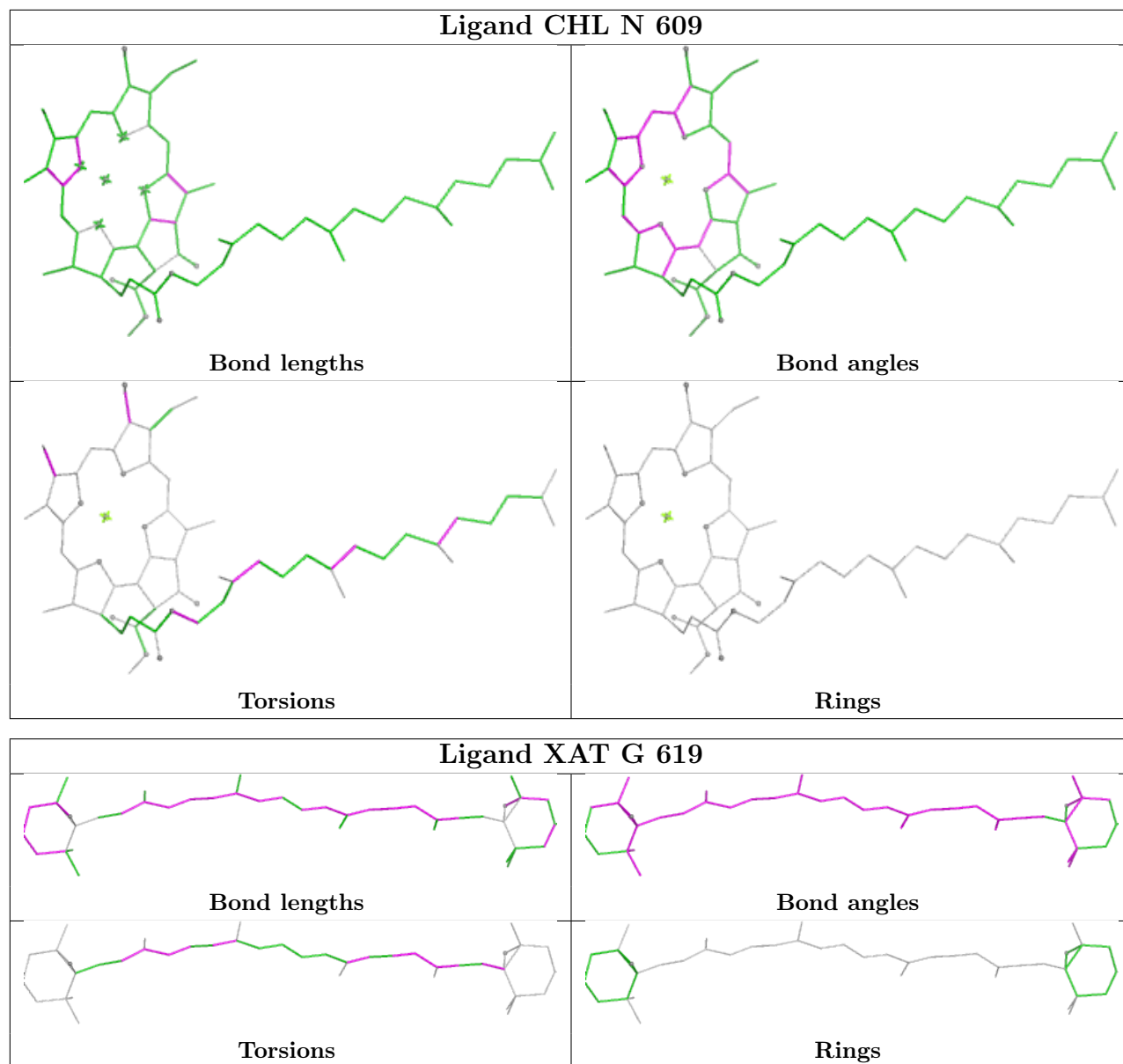


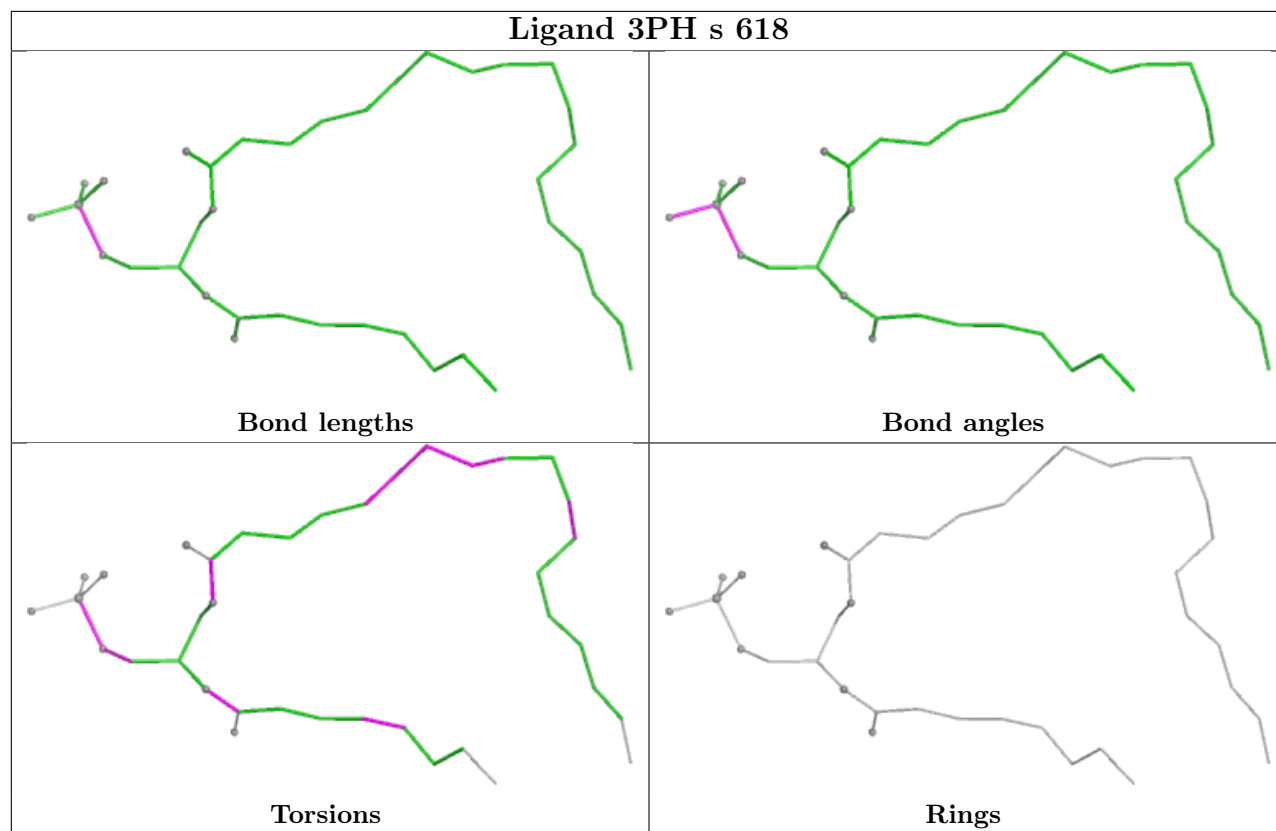


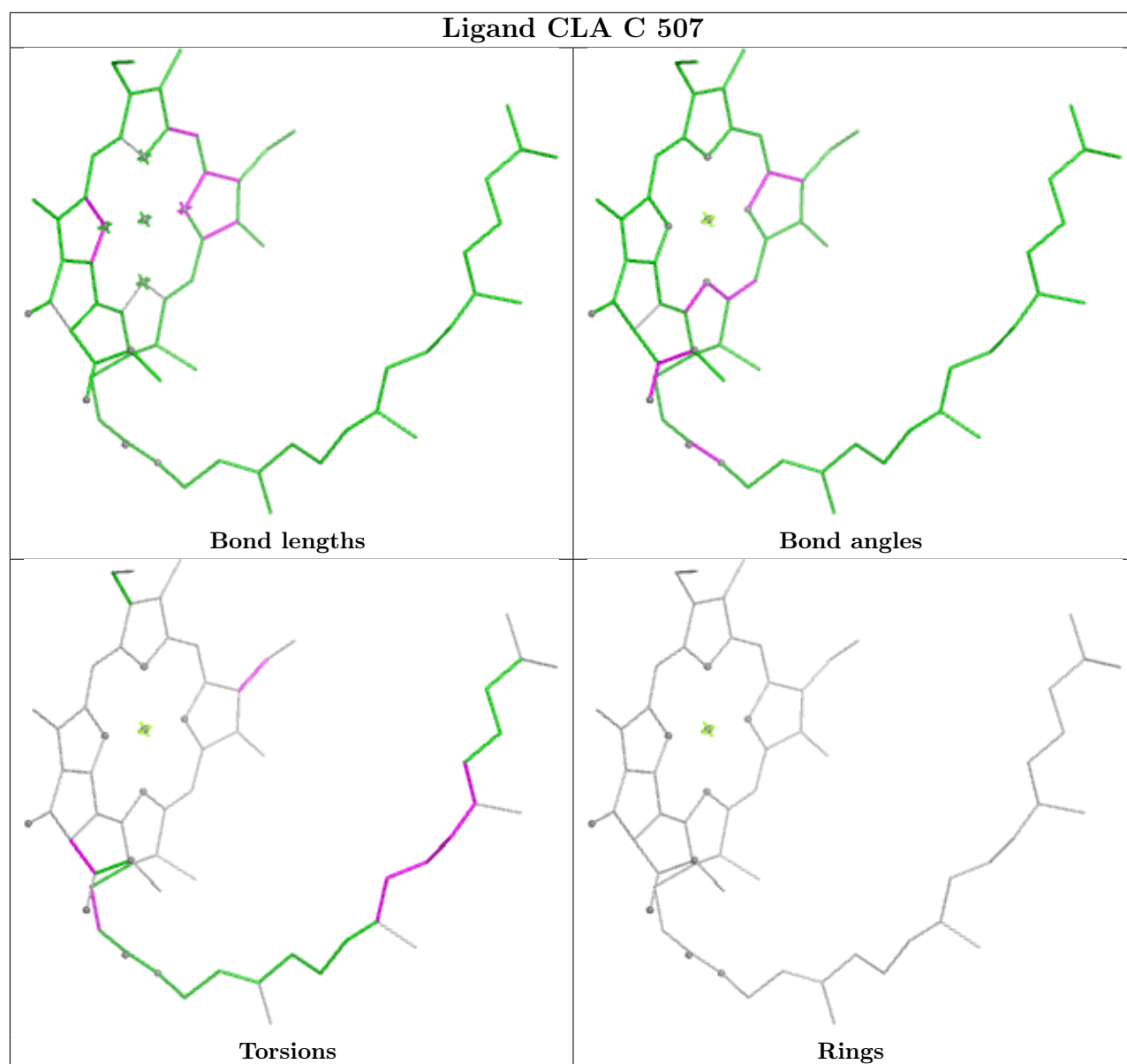


Ligand CLA b 601

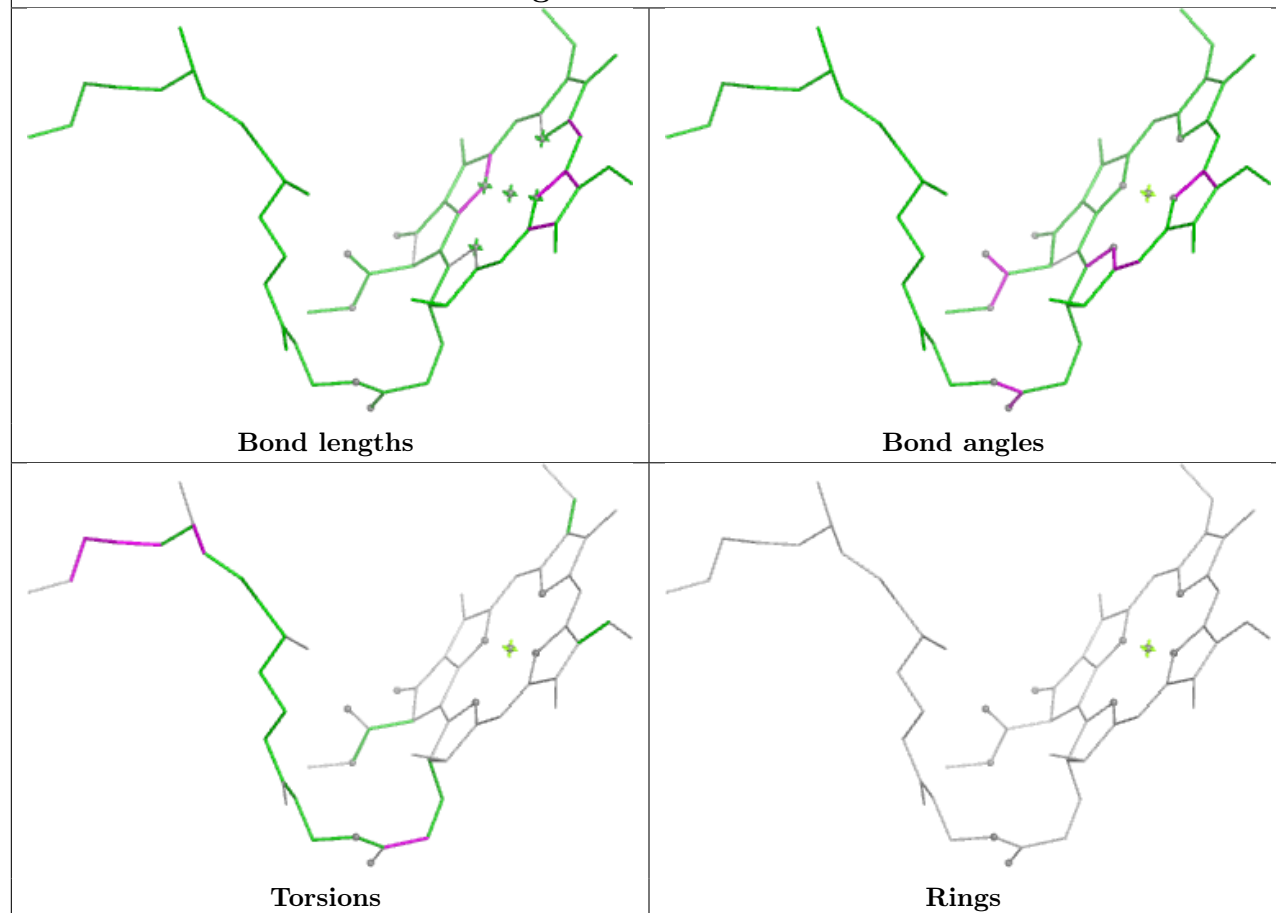




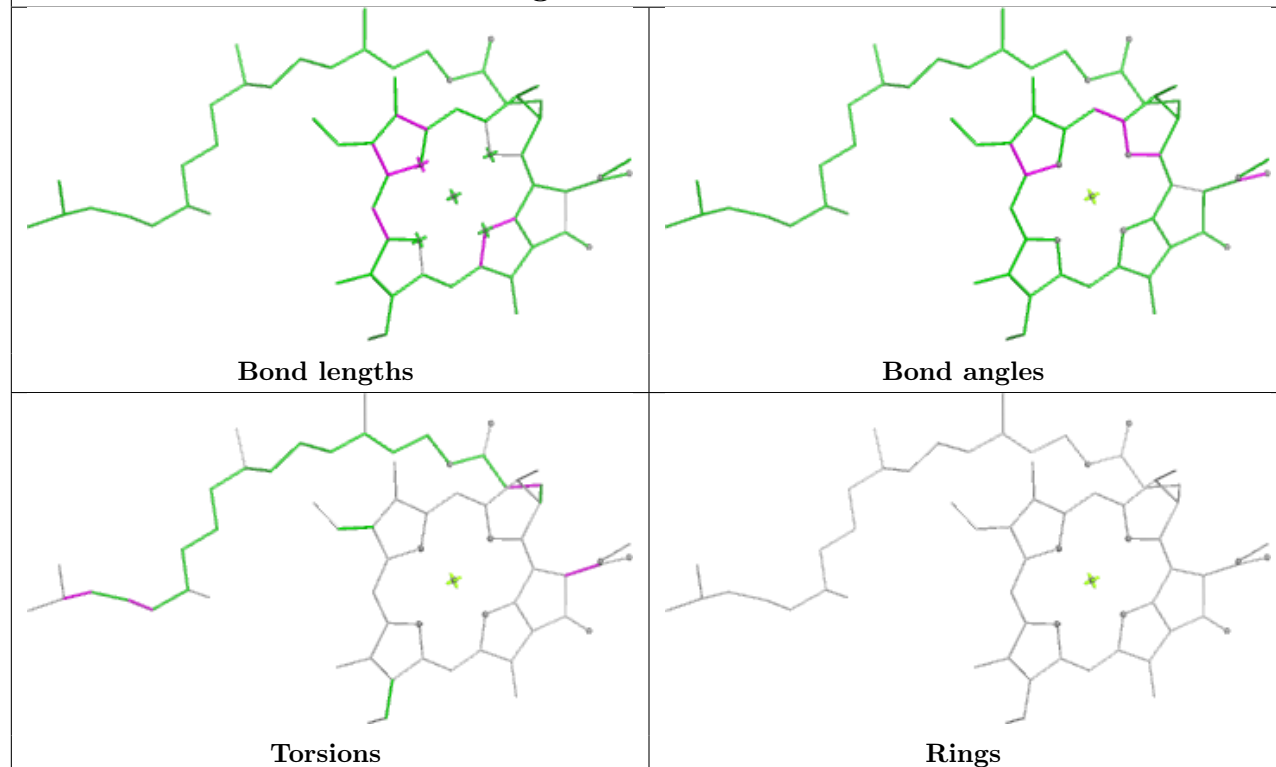


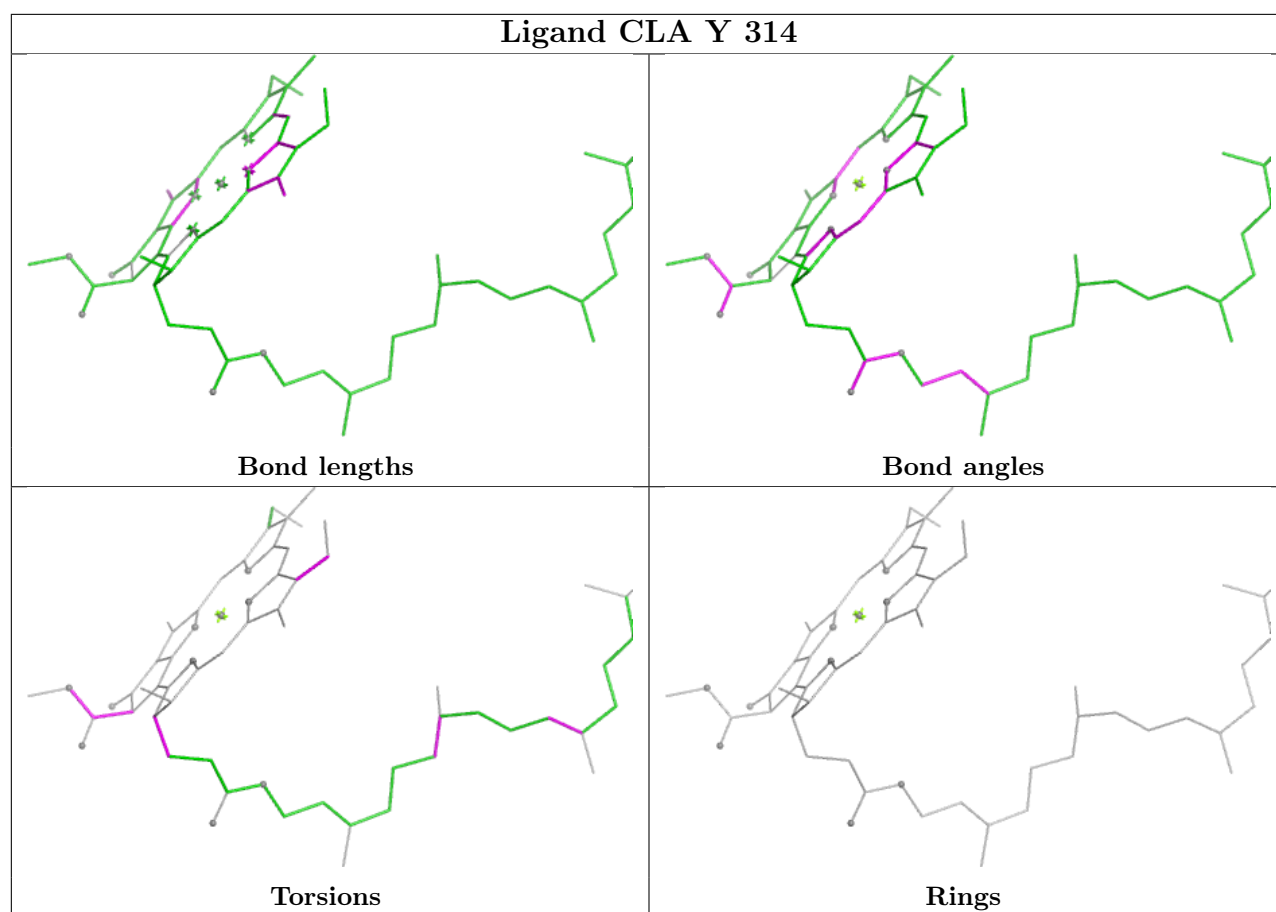


Ligand CLA B 613

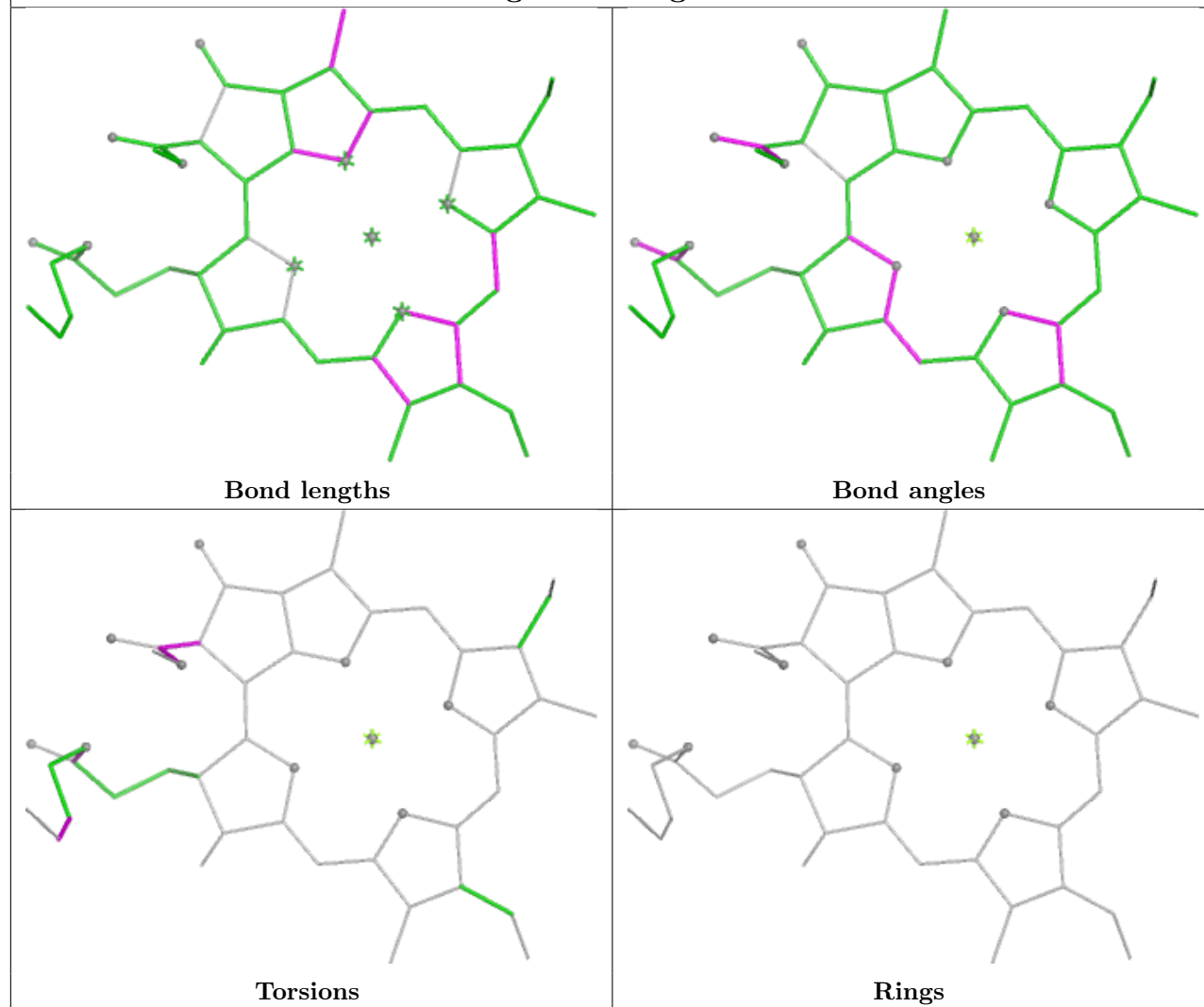


Ligand CLA R 602

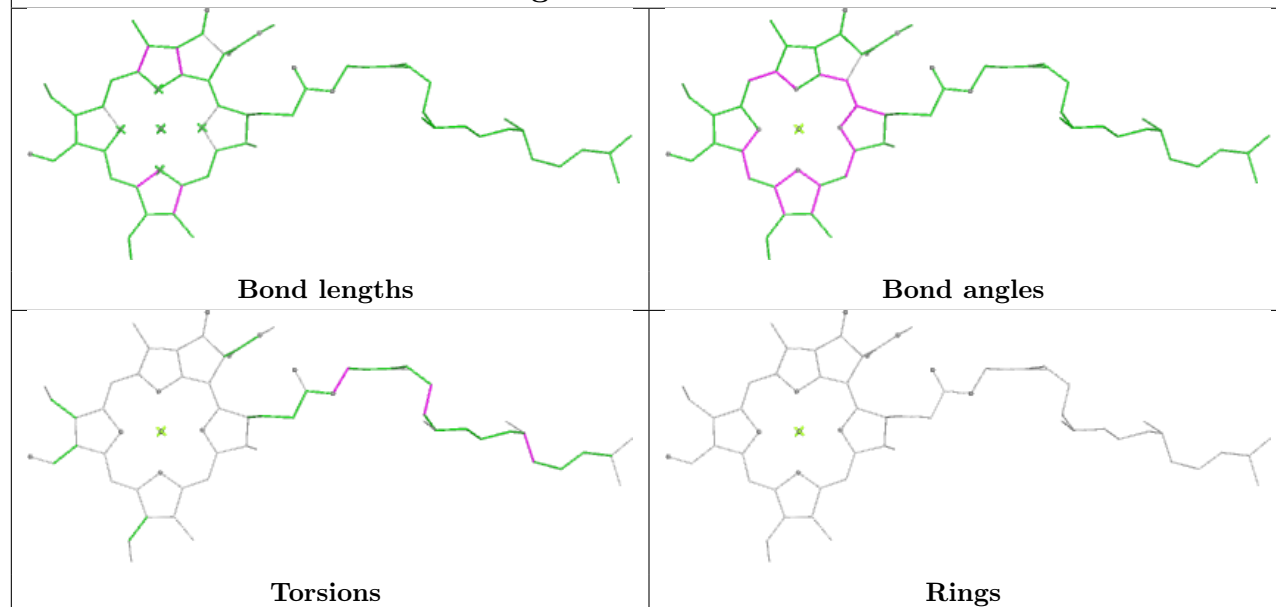


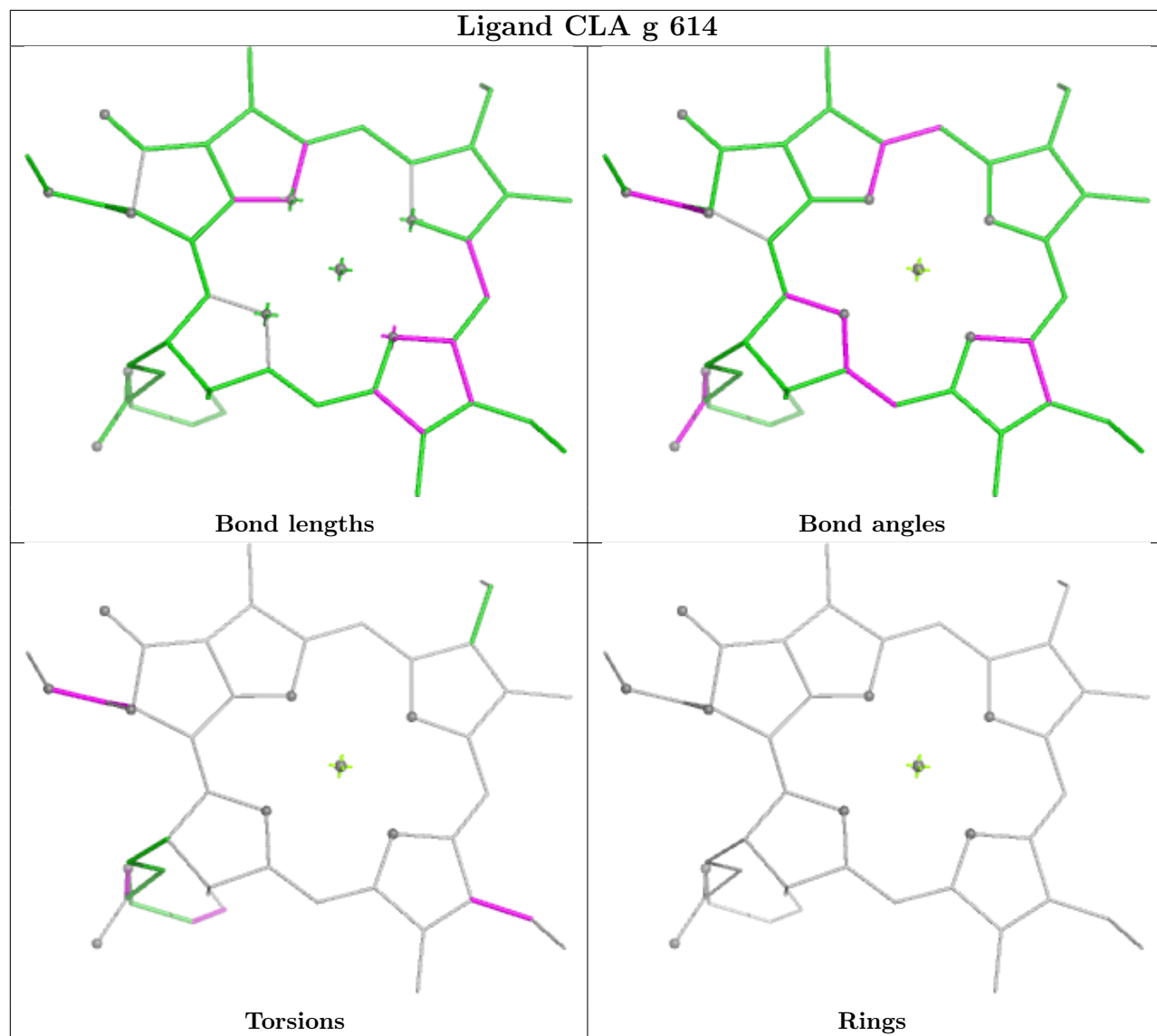


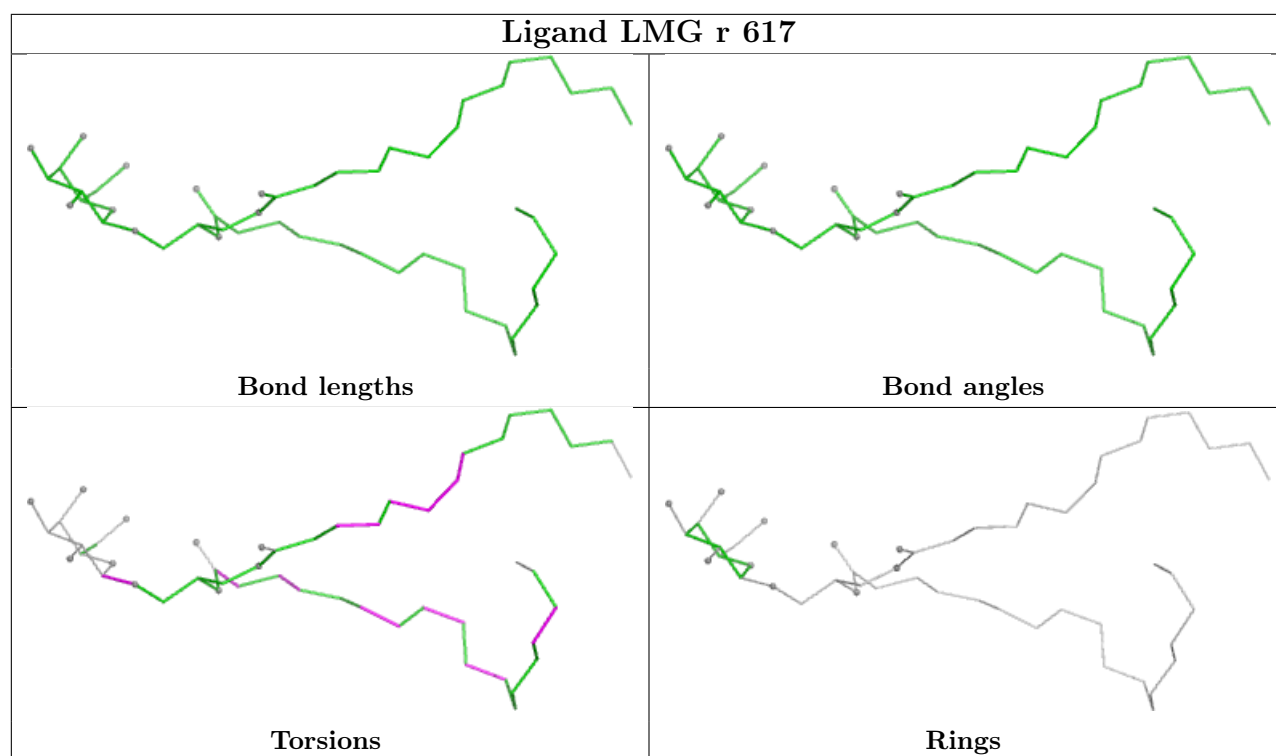
Ligand CLA g 612



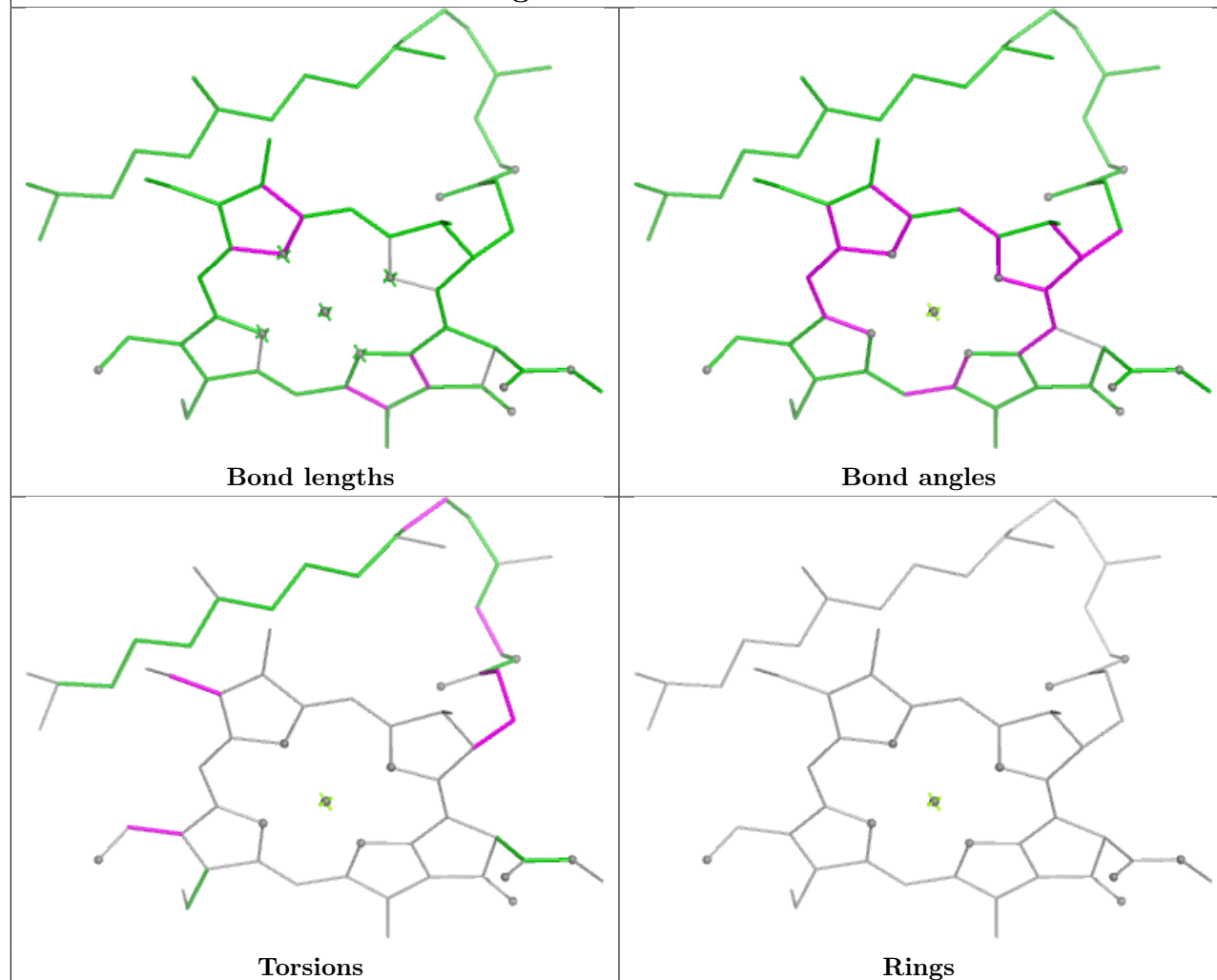
Ligand CHL Y 307



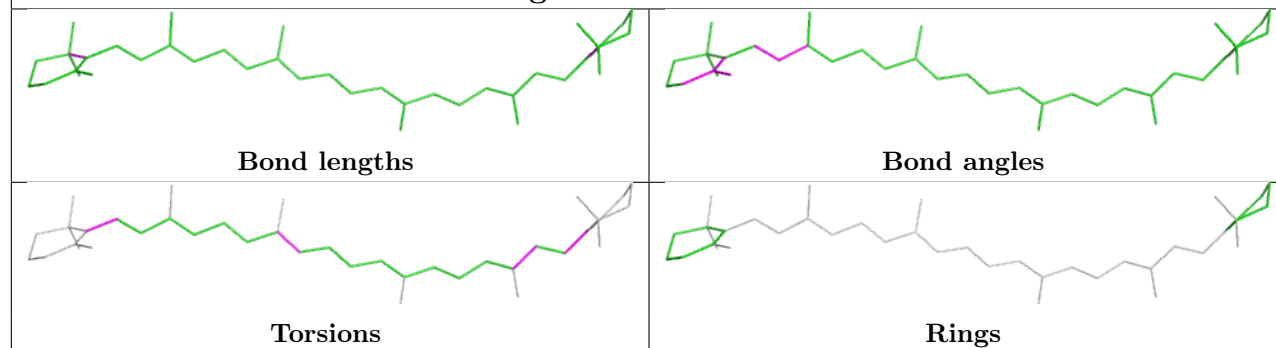




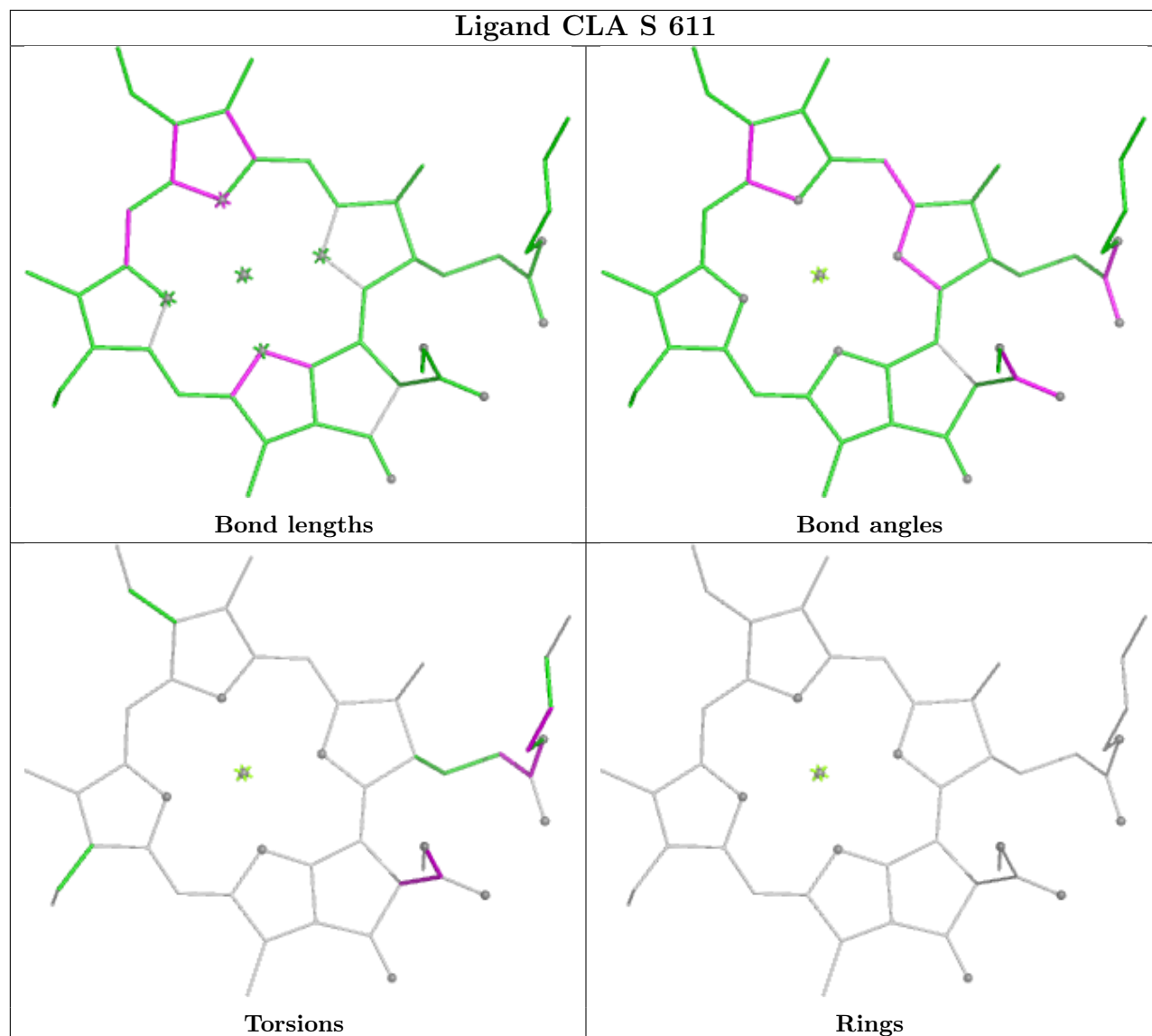
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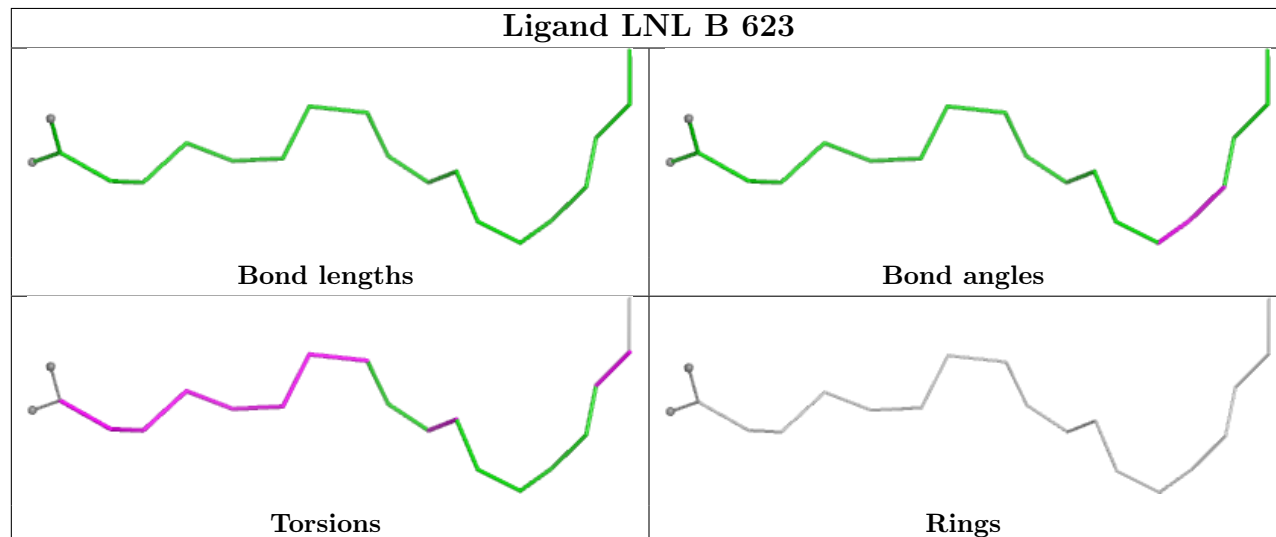
Ligand BCR H 501

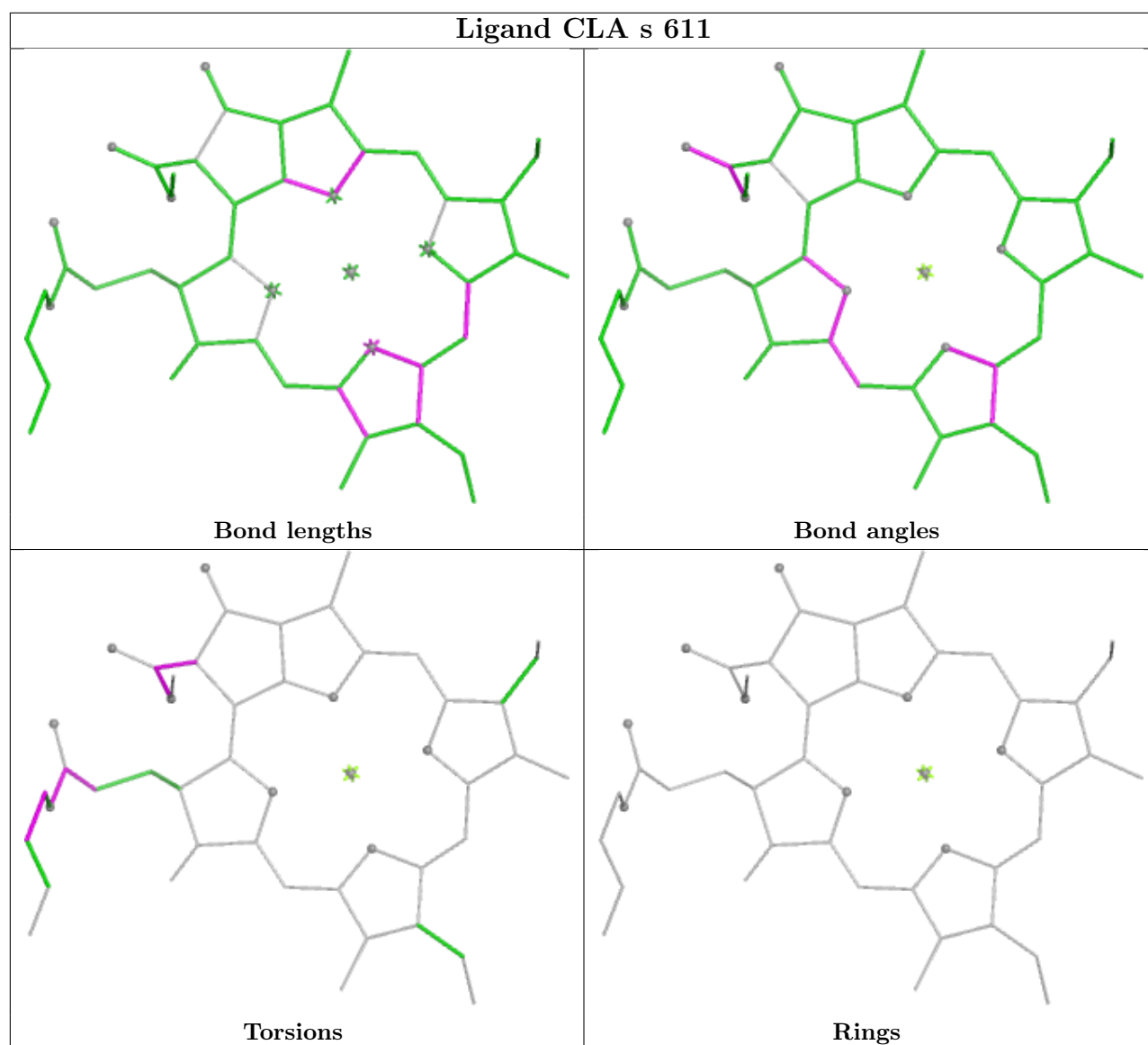


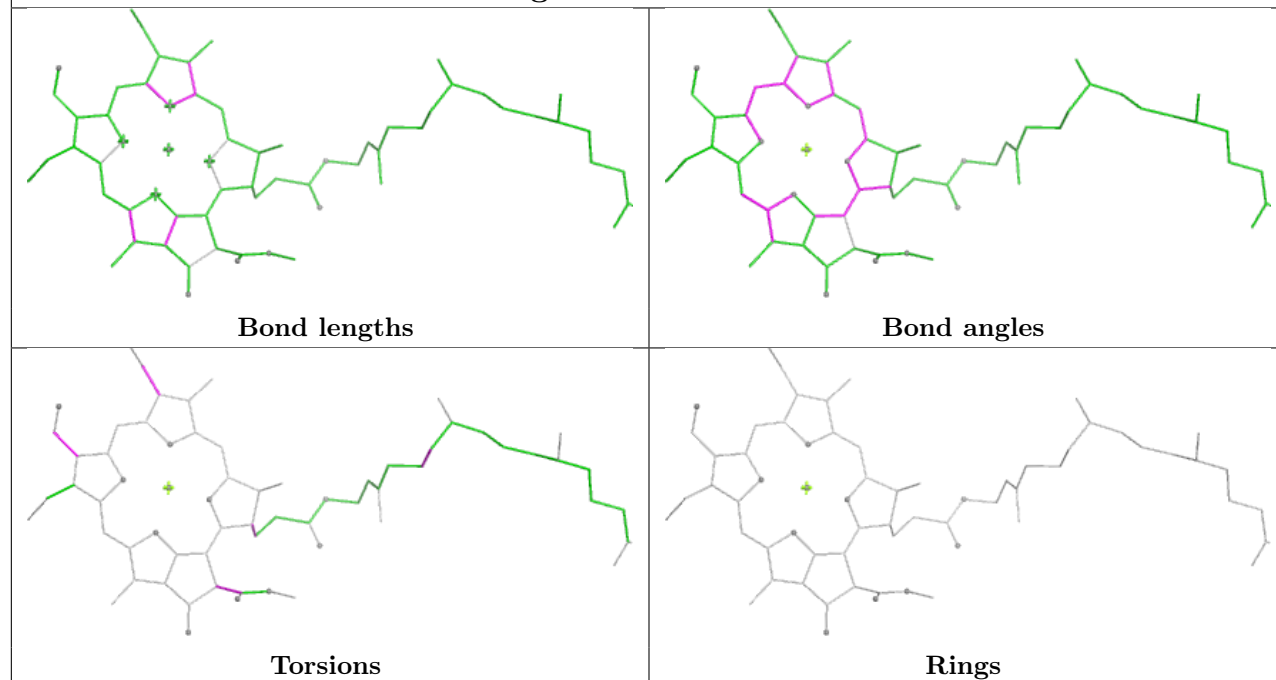
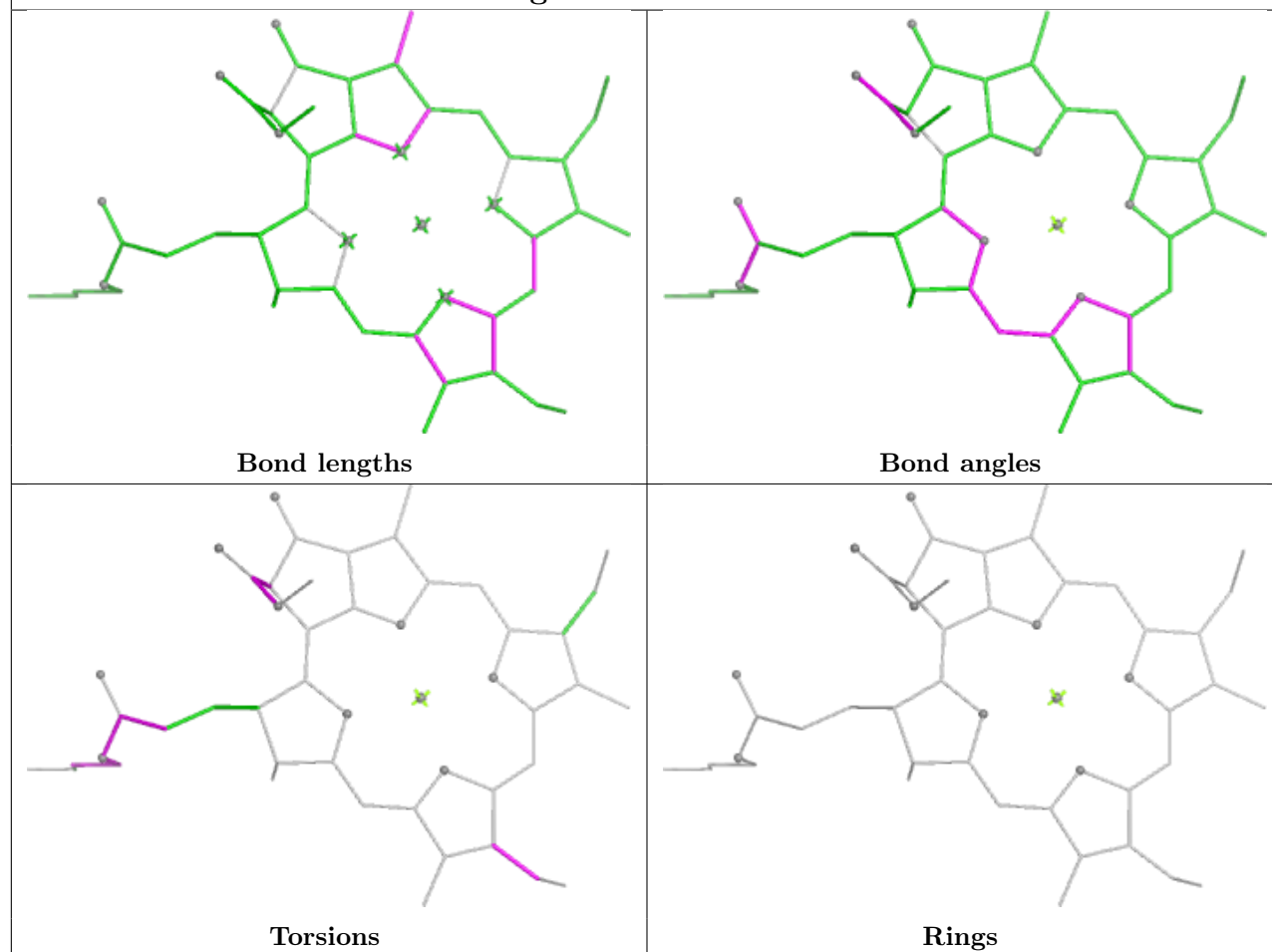
Ligand CLA S 611

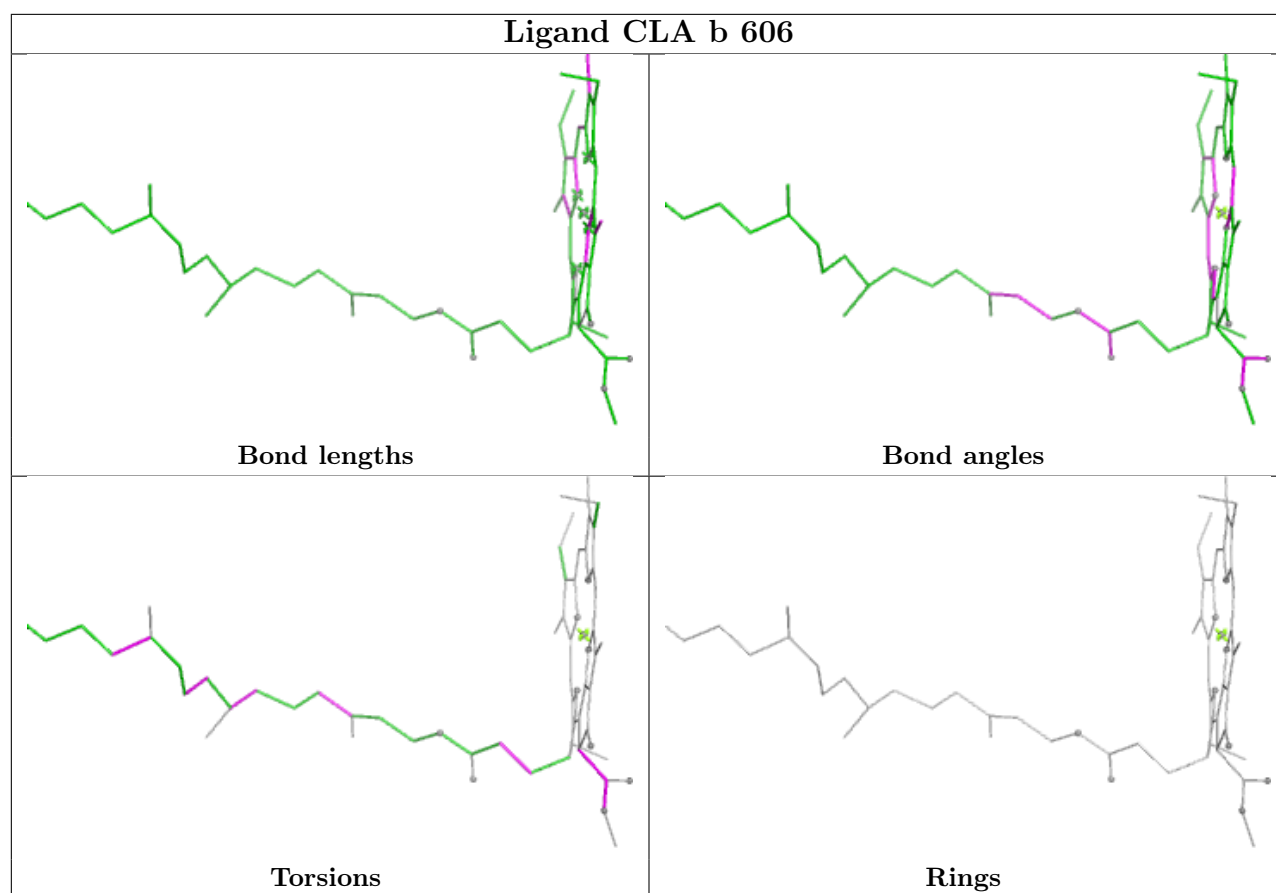


Ligand LNL B 623

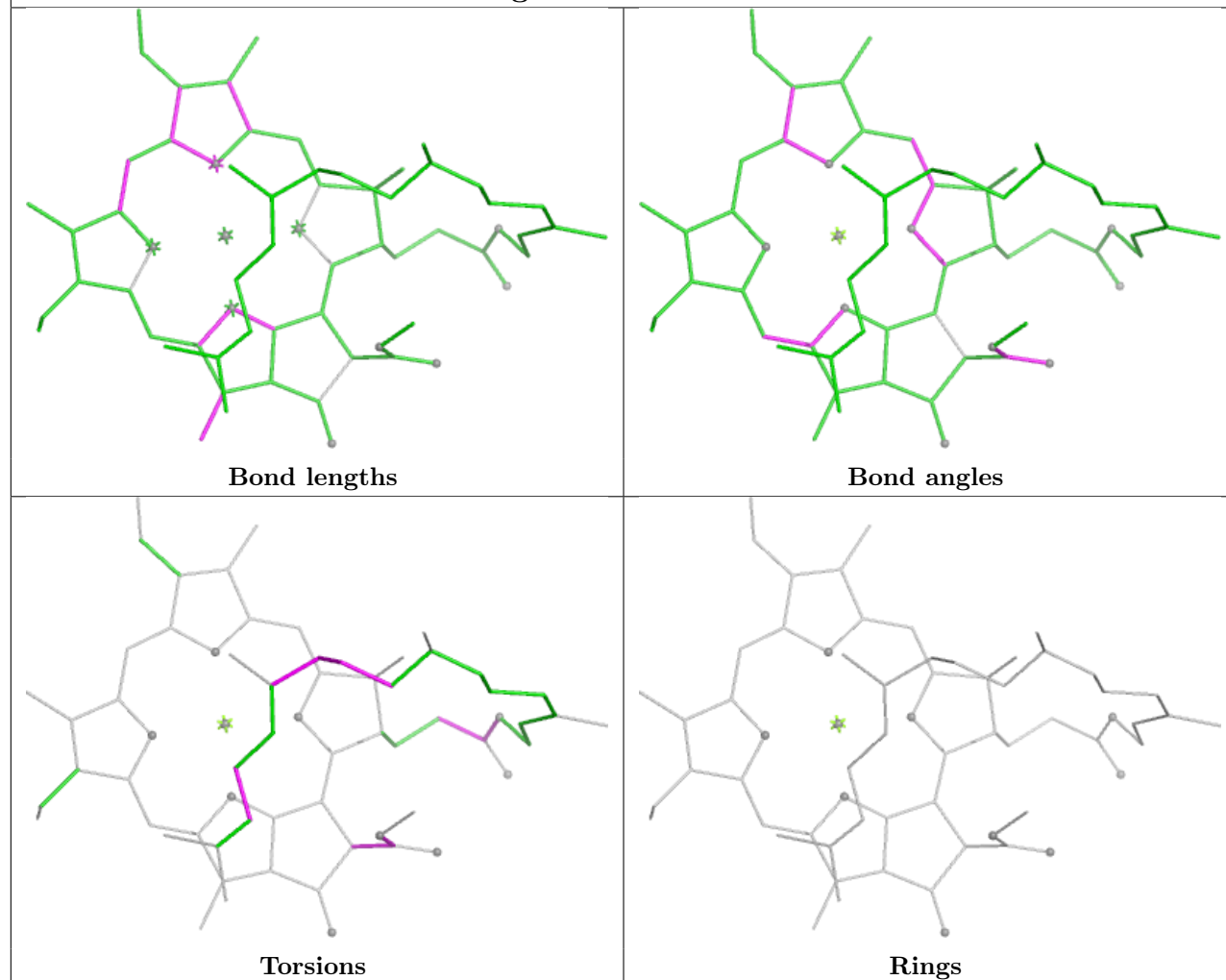




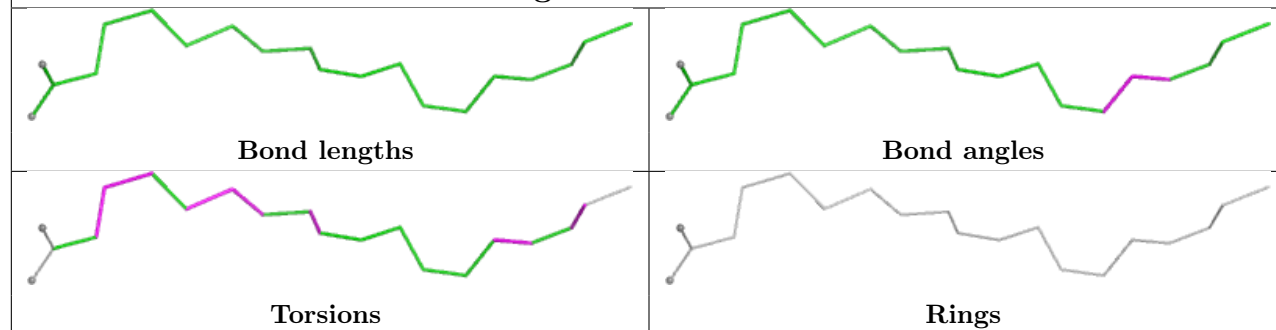
Ligand CHL N 601**Ligand CLA R 601**

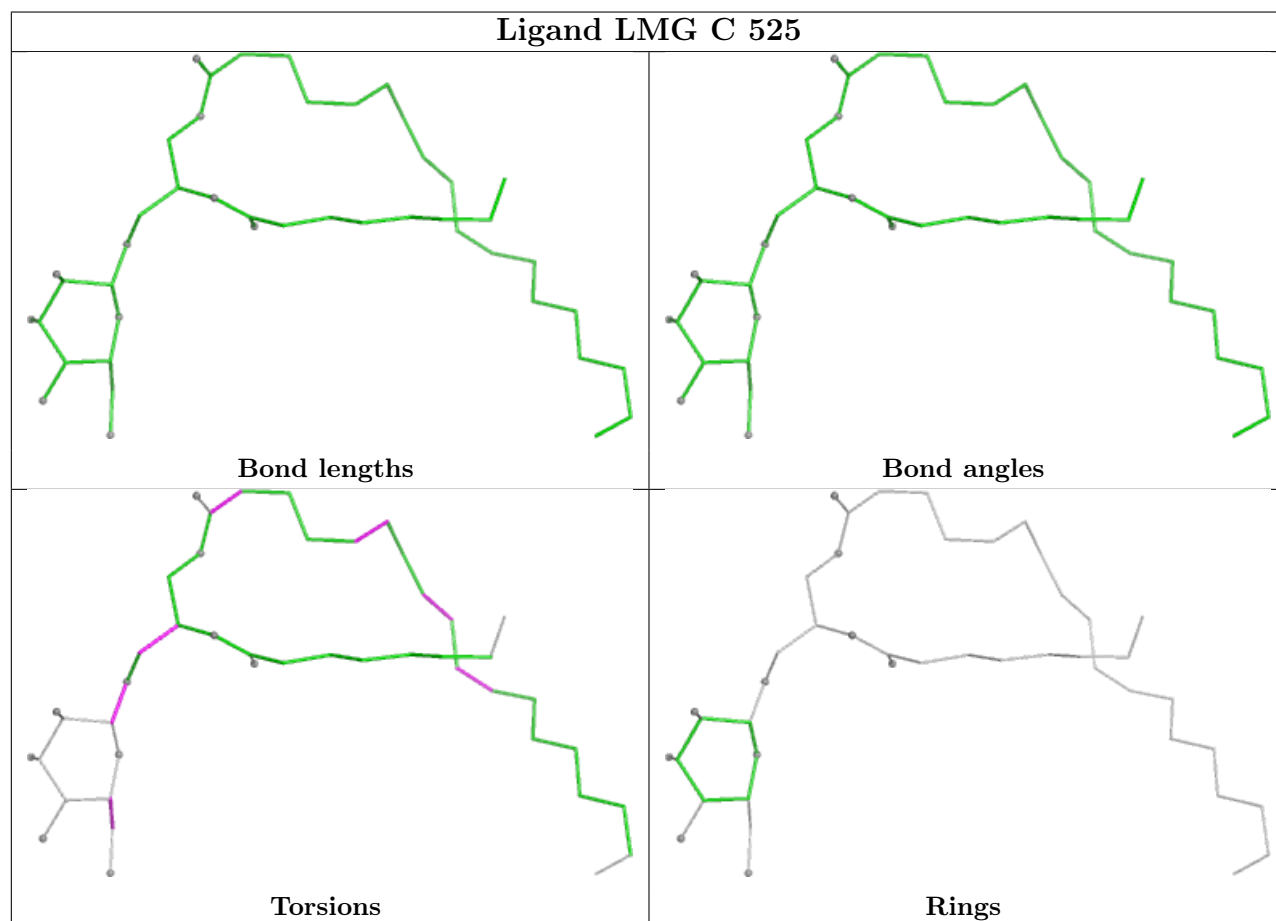
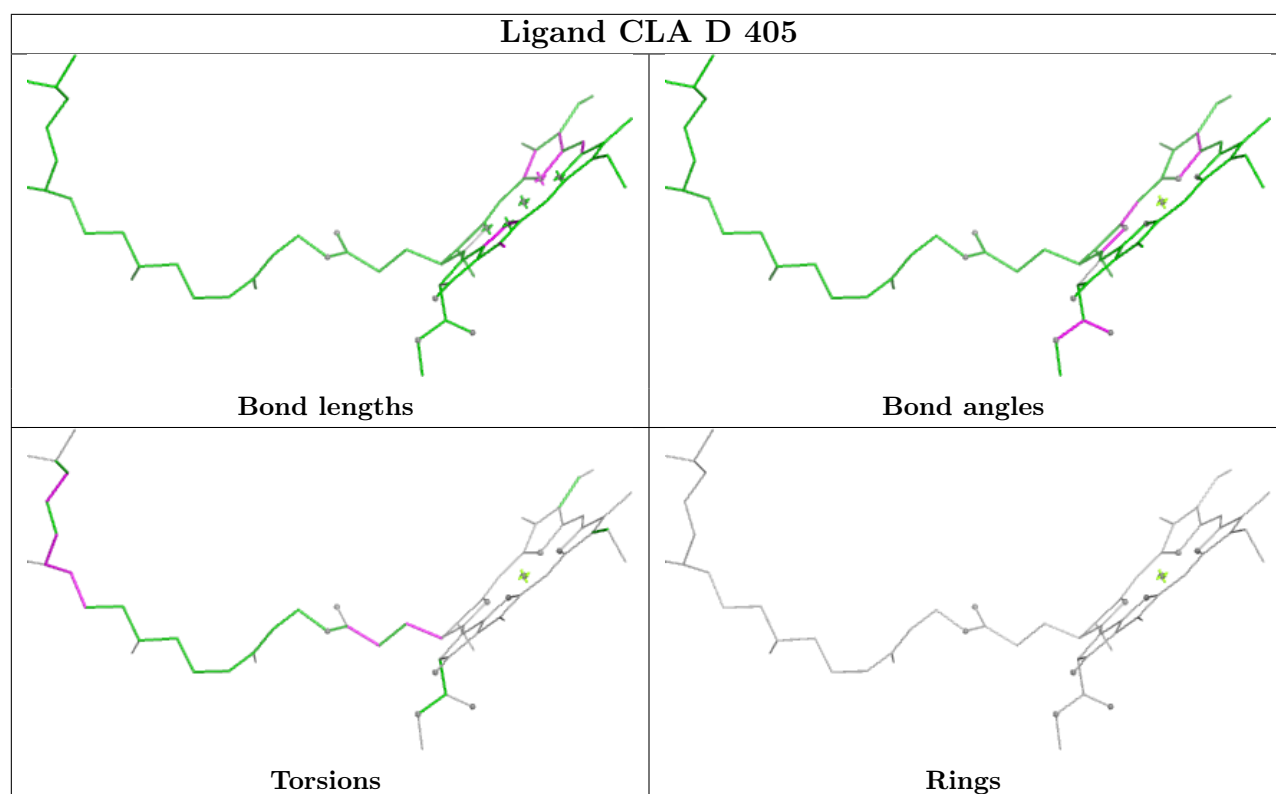


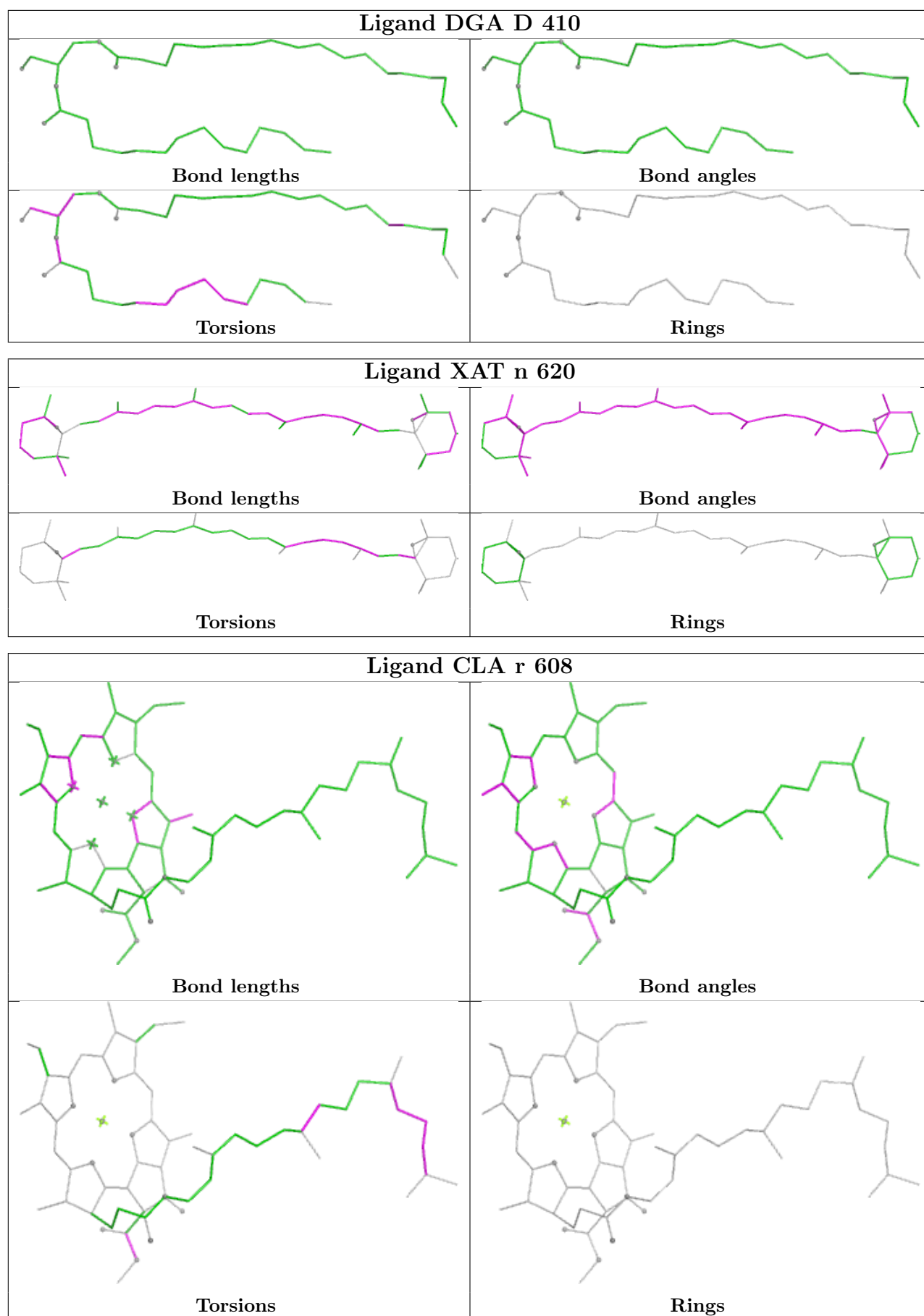
Ligand CLA C 510

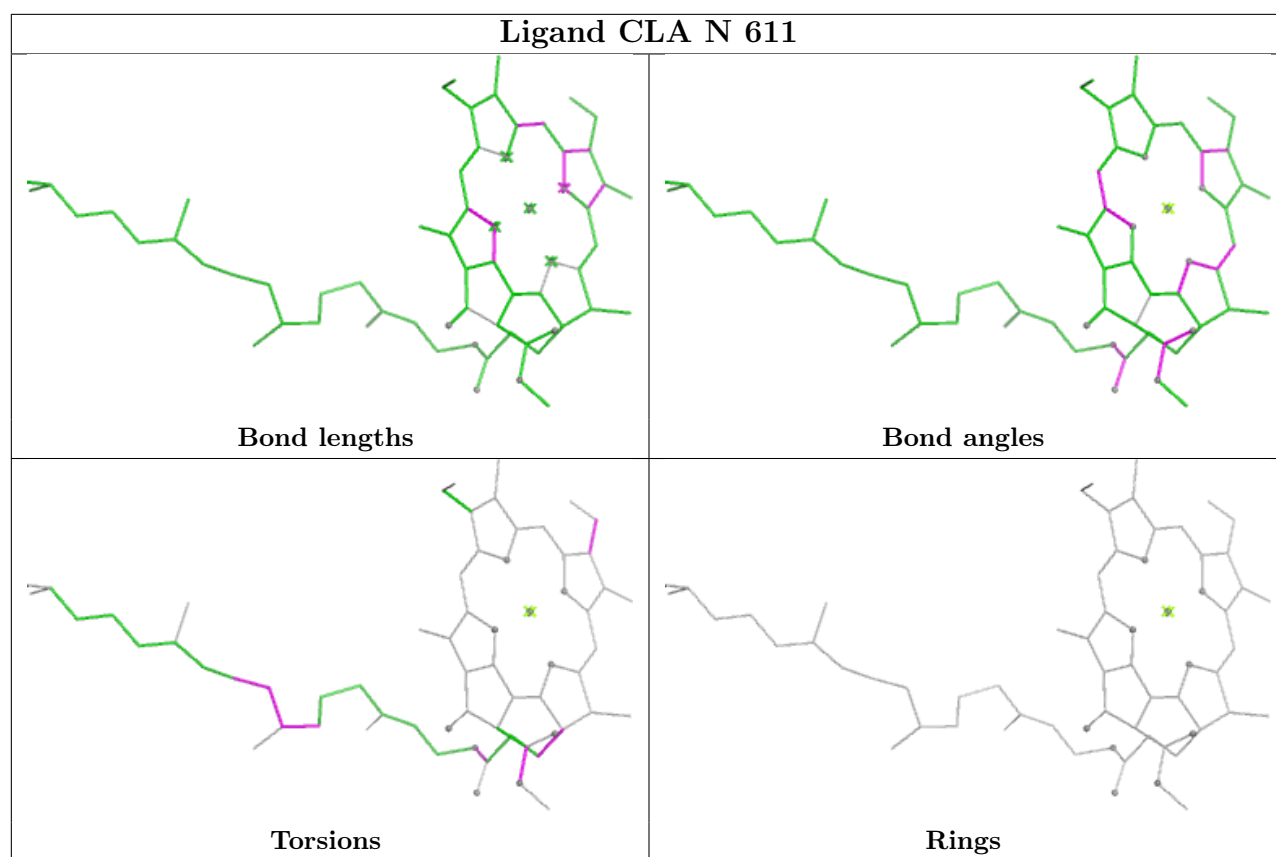


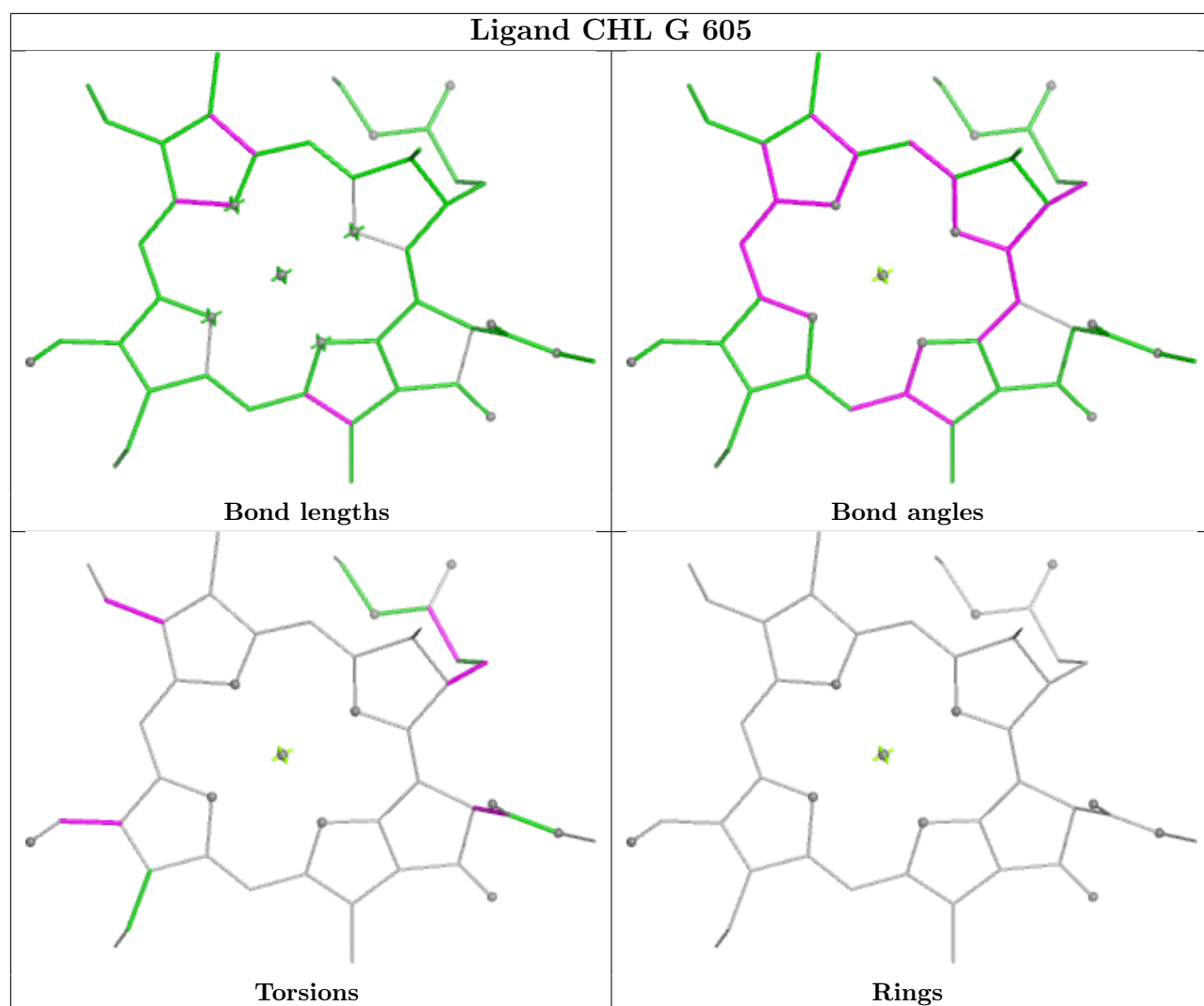
Ligand LNL B 622

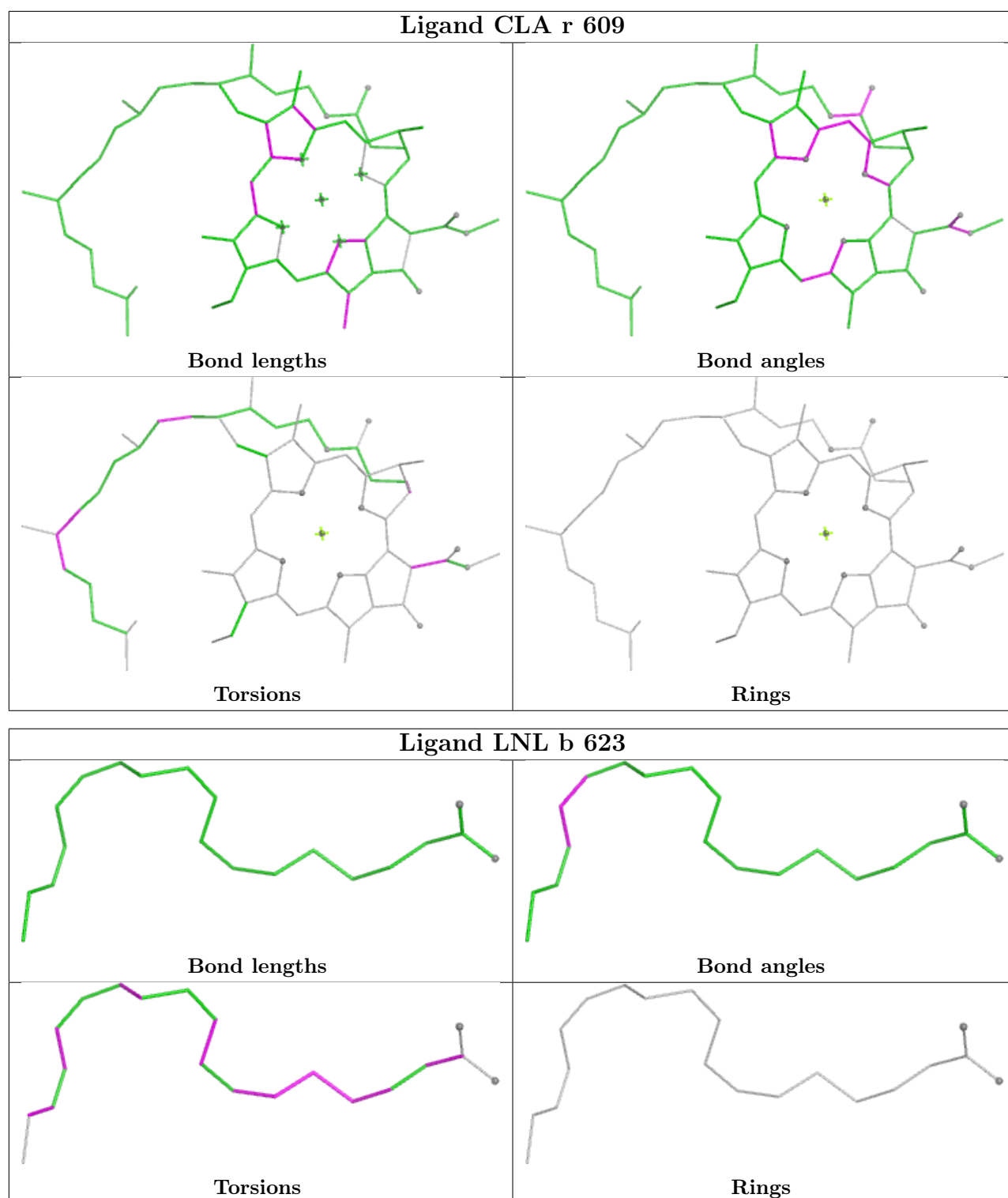


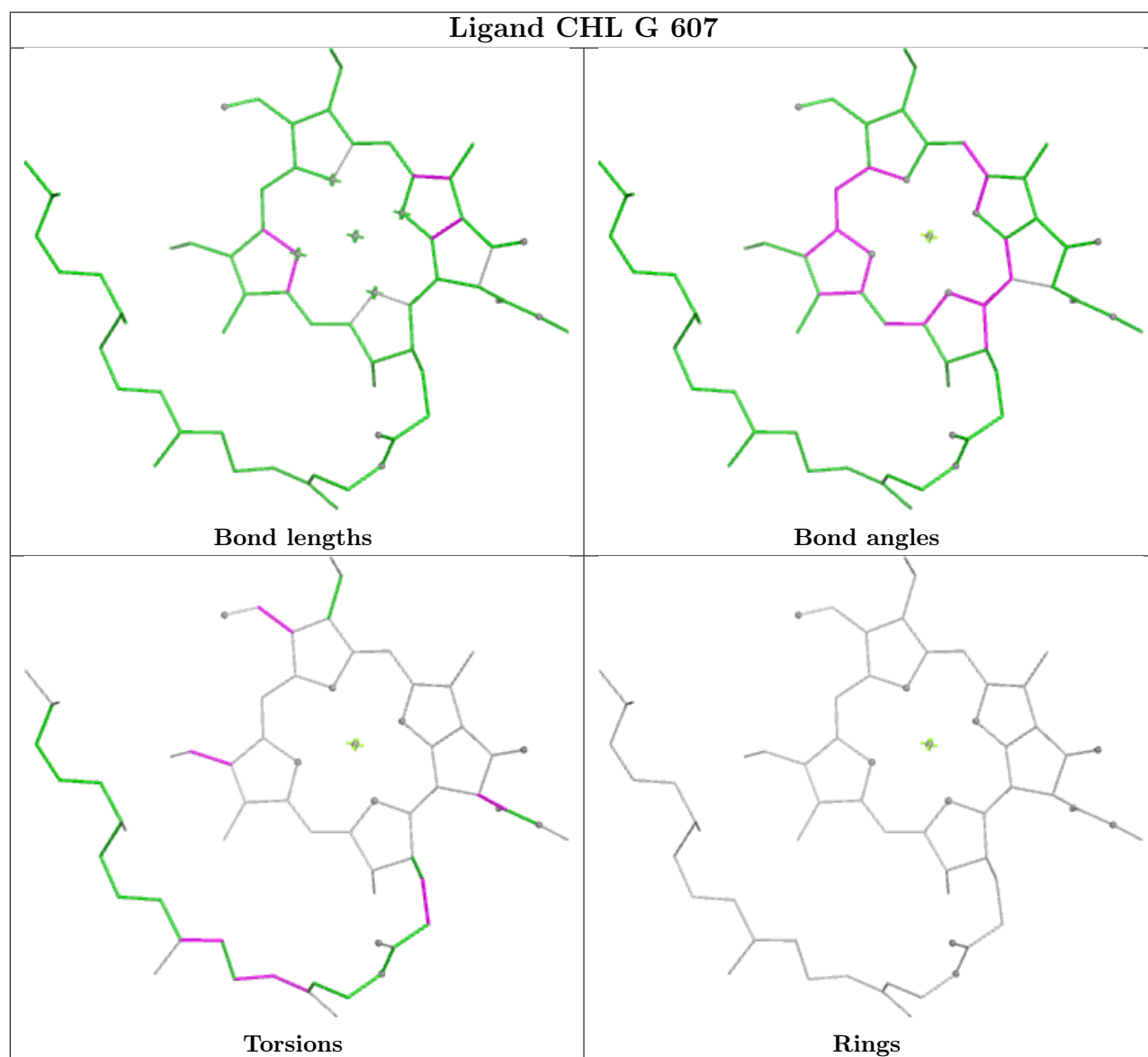
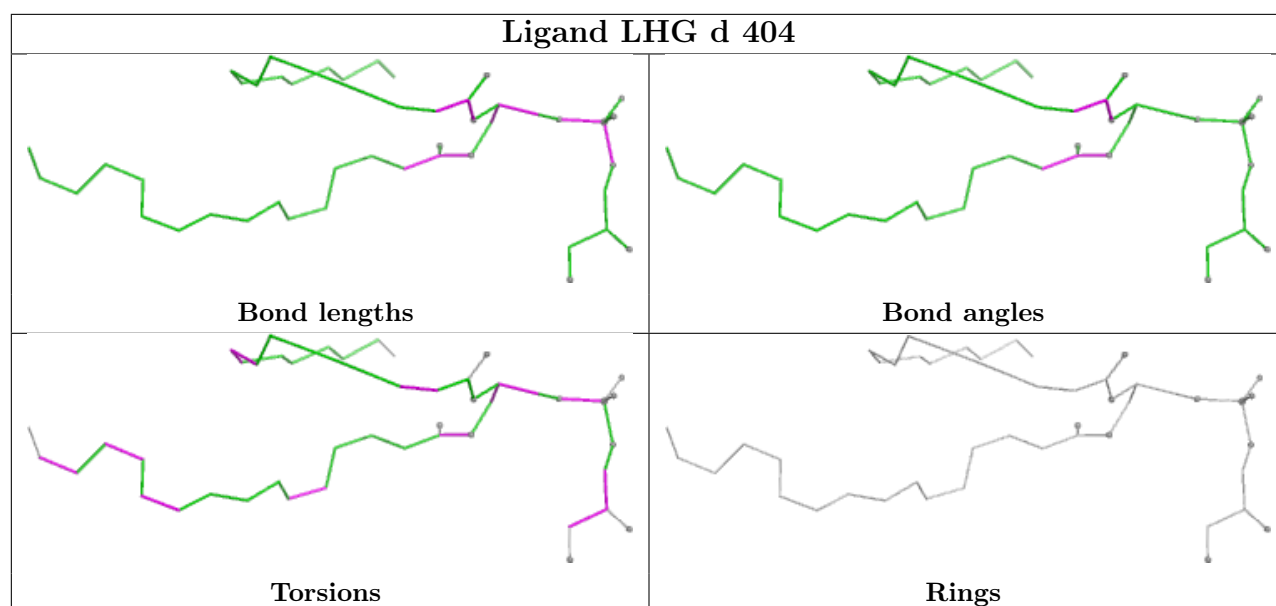


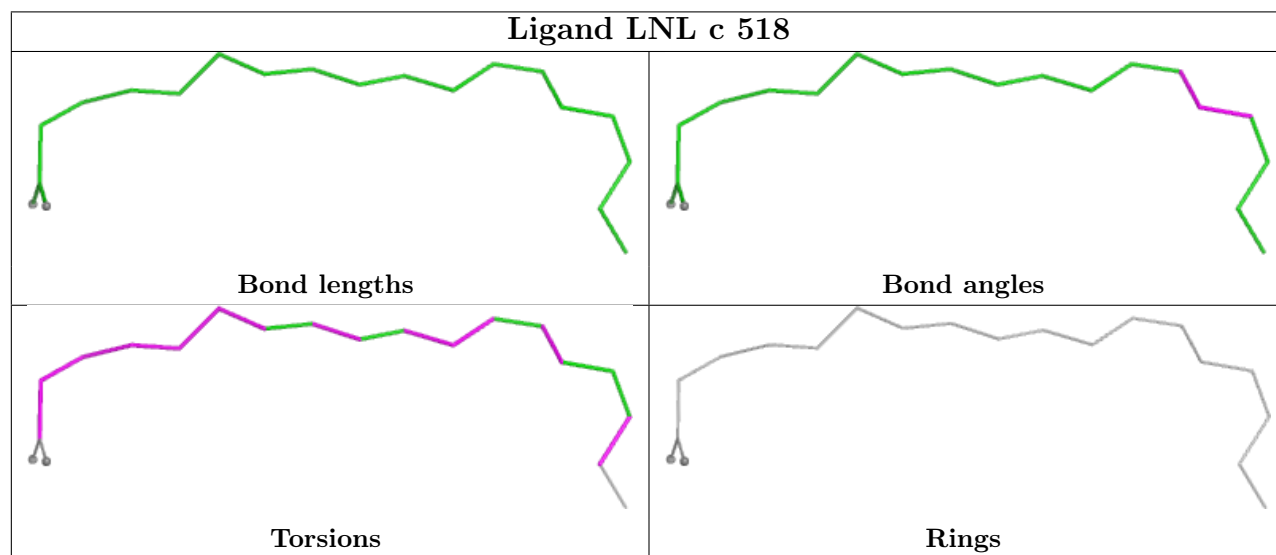
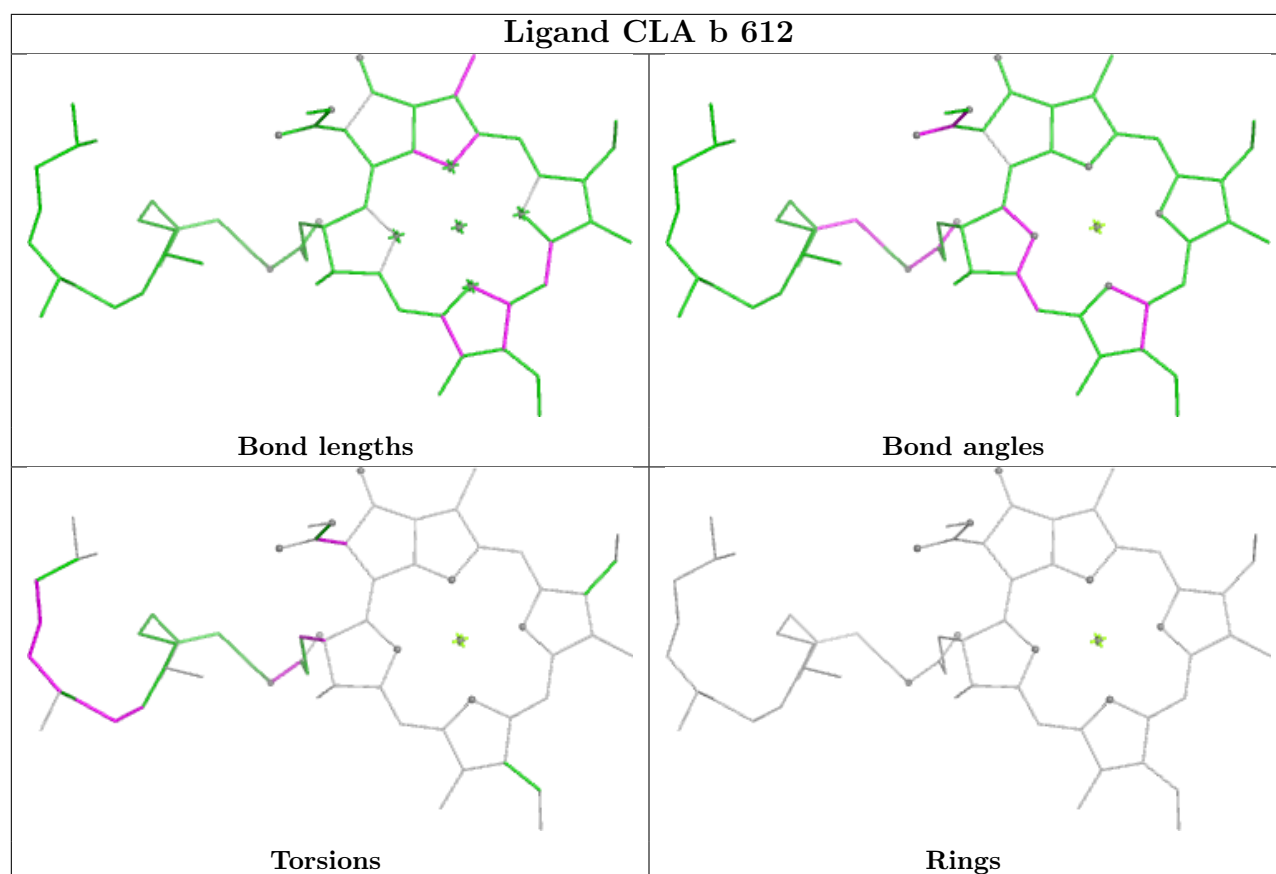


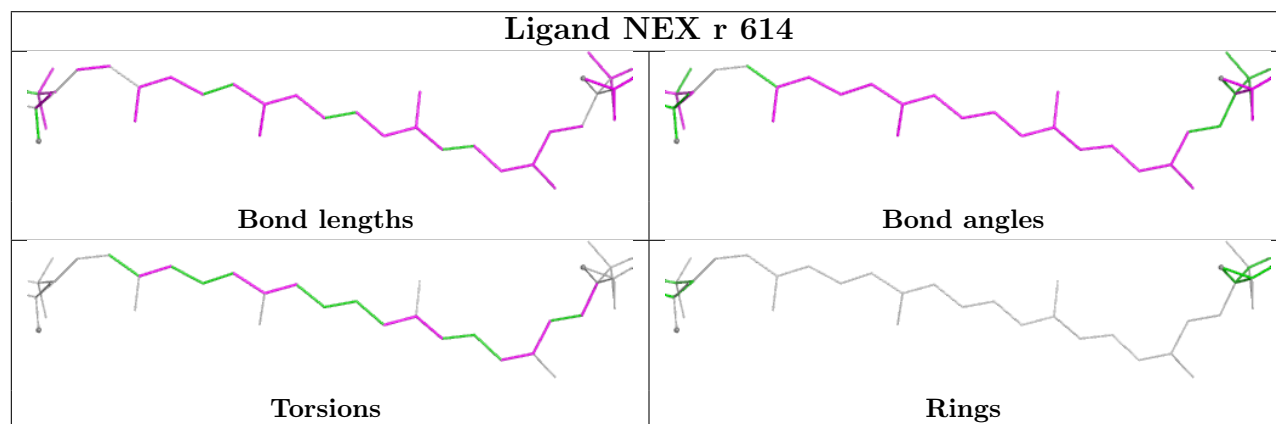
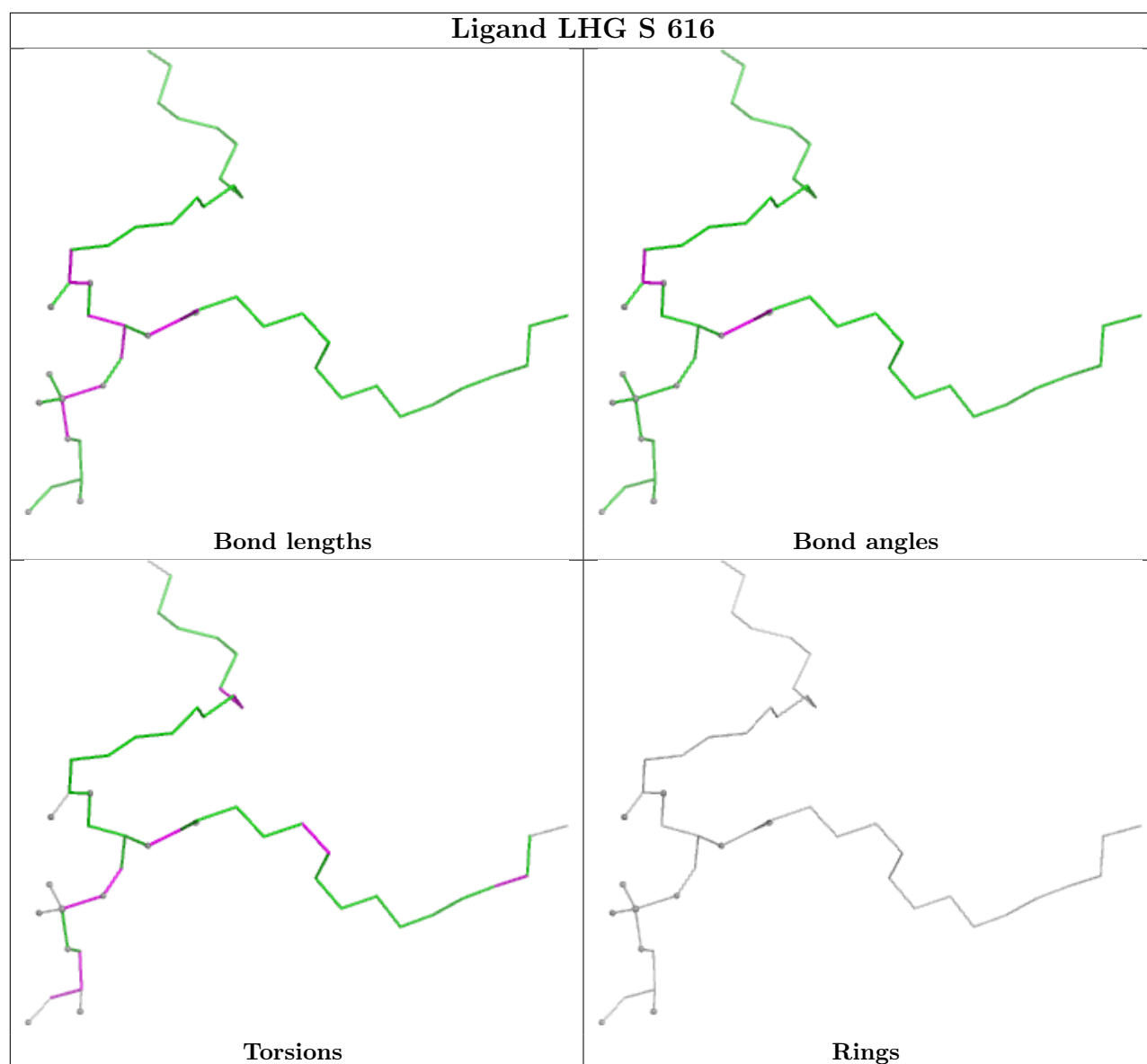


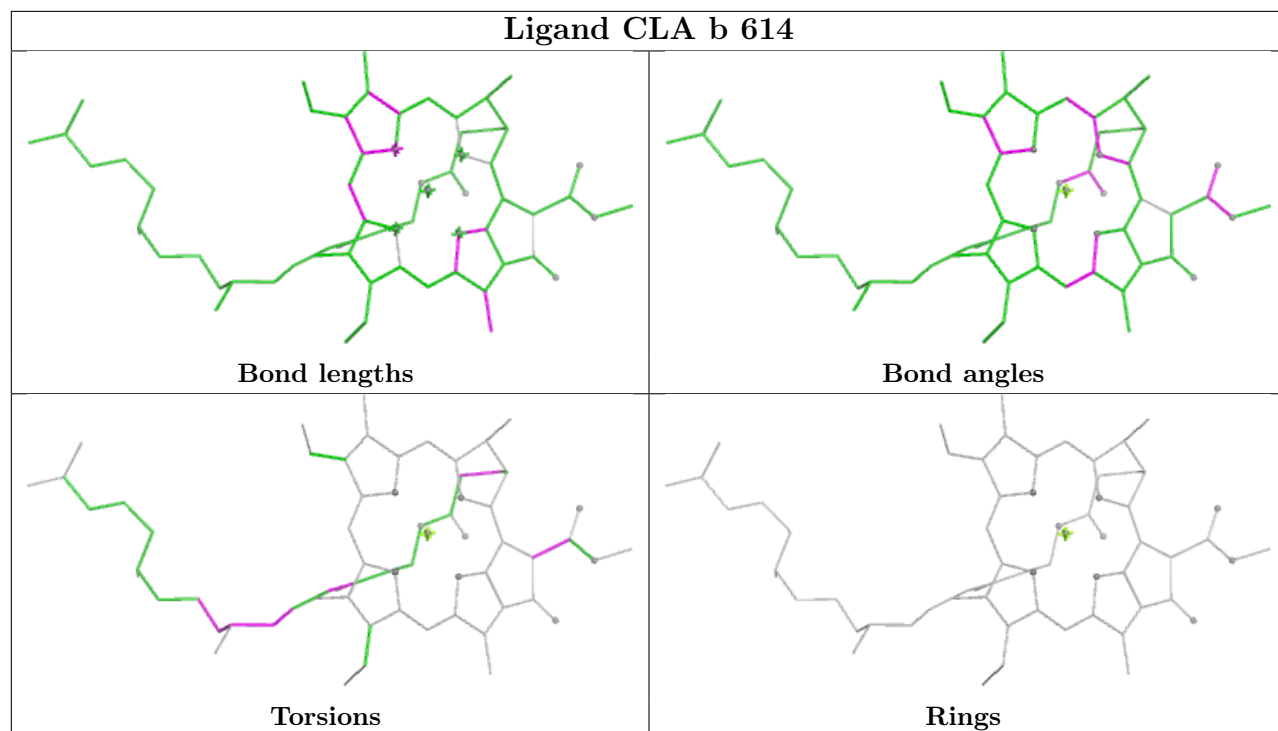


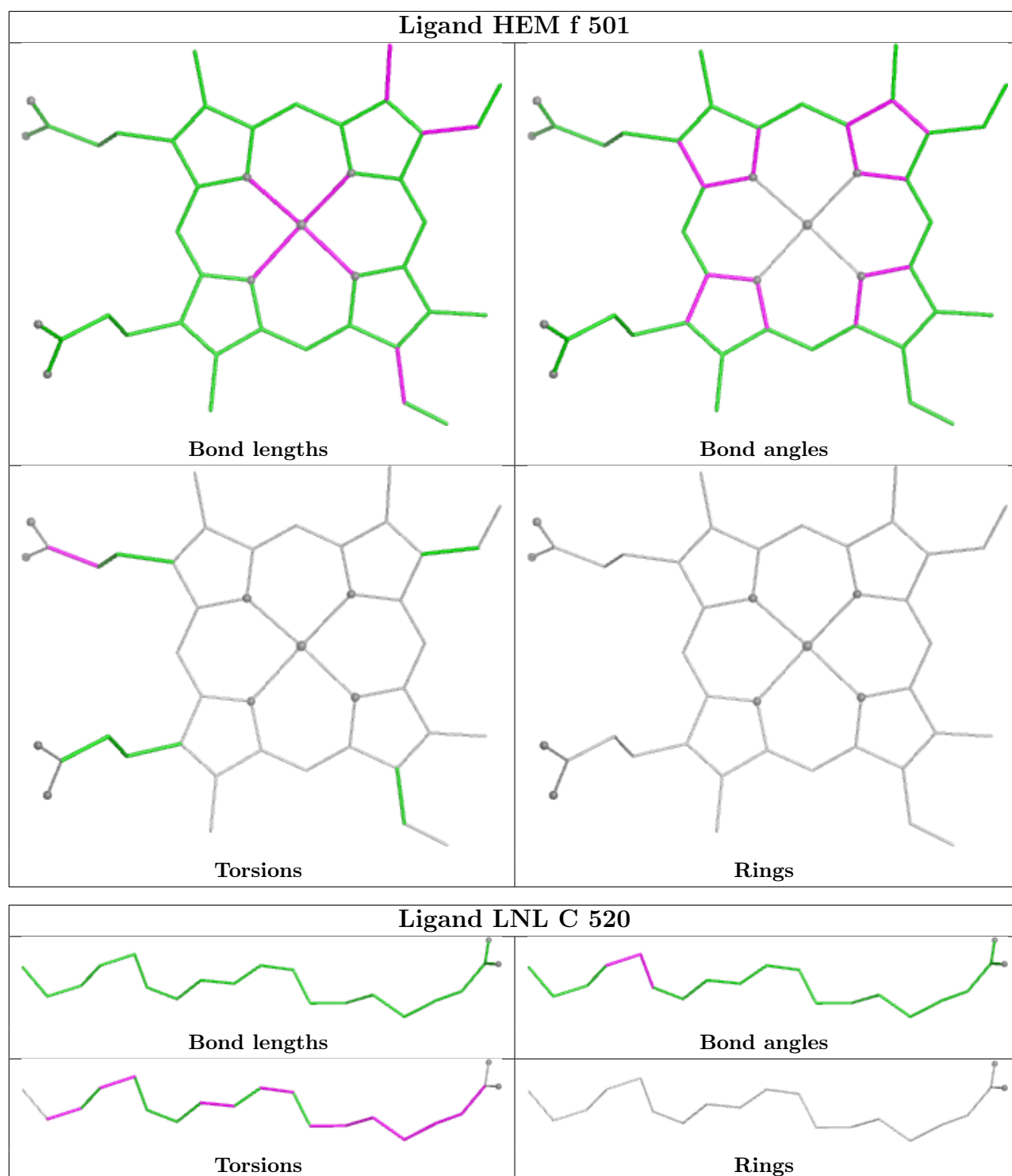


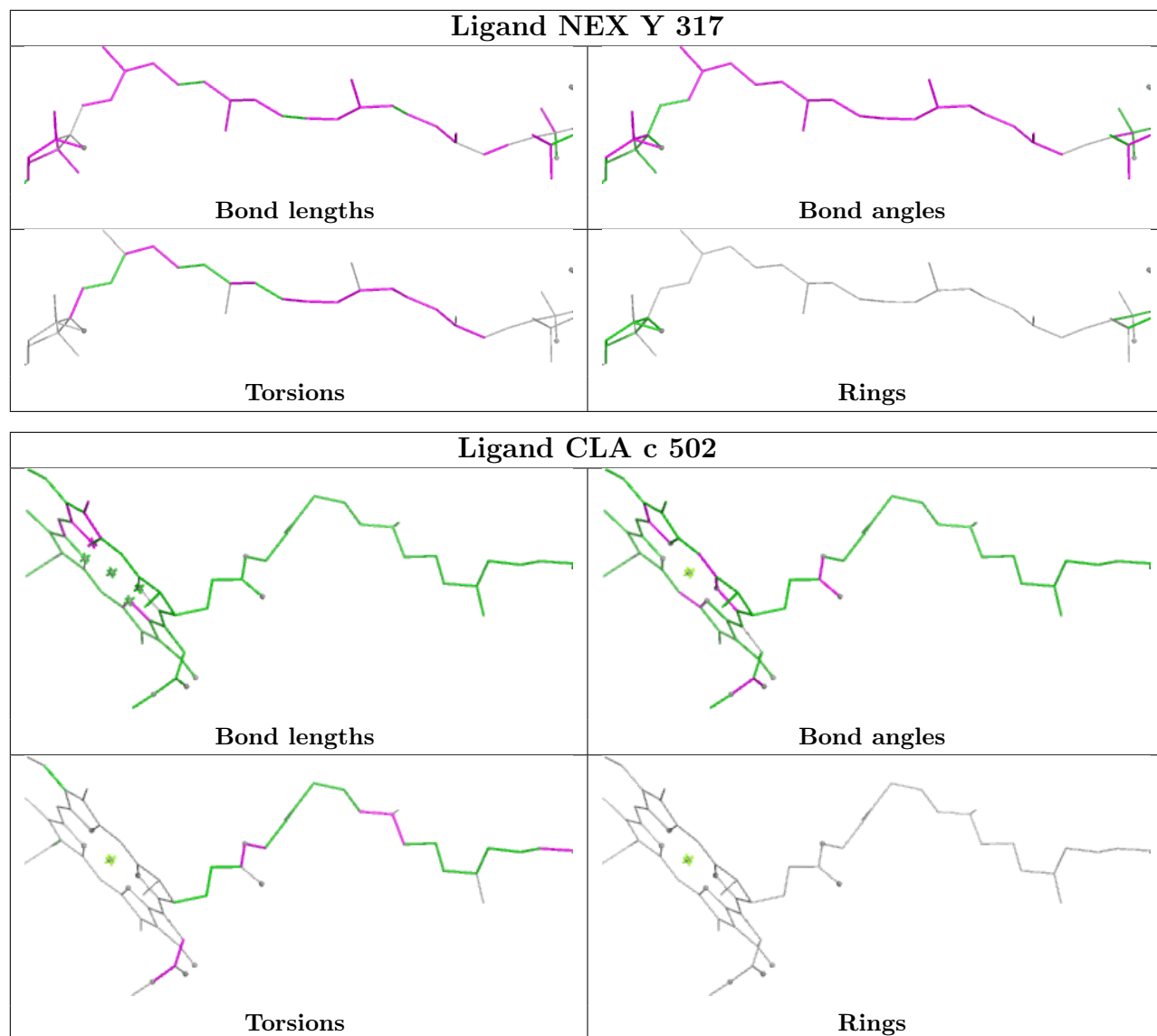




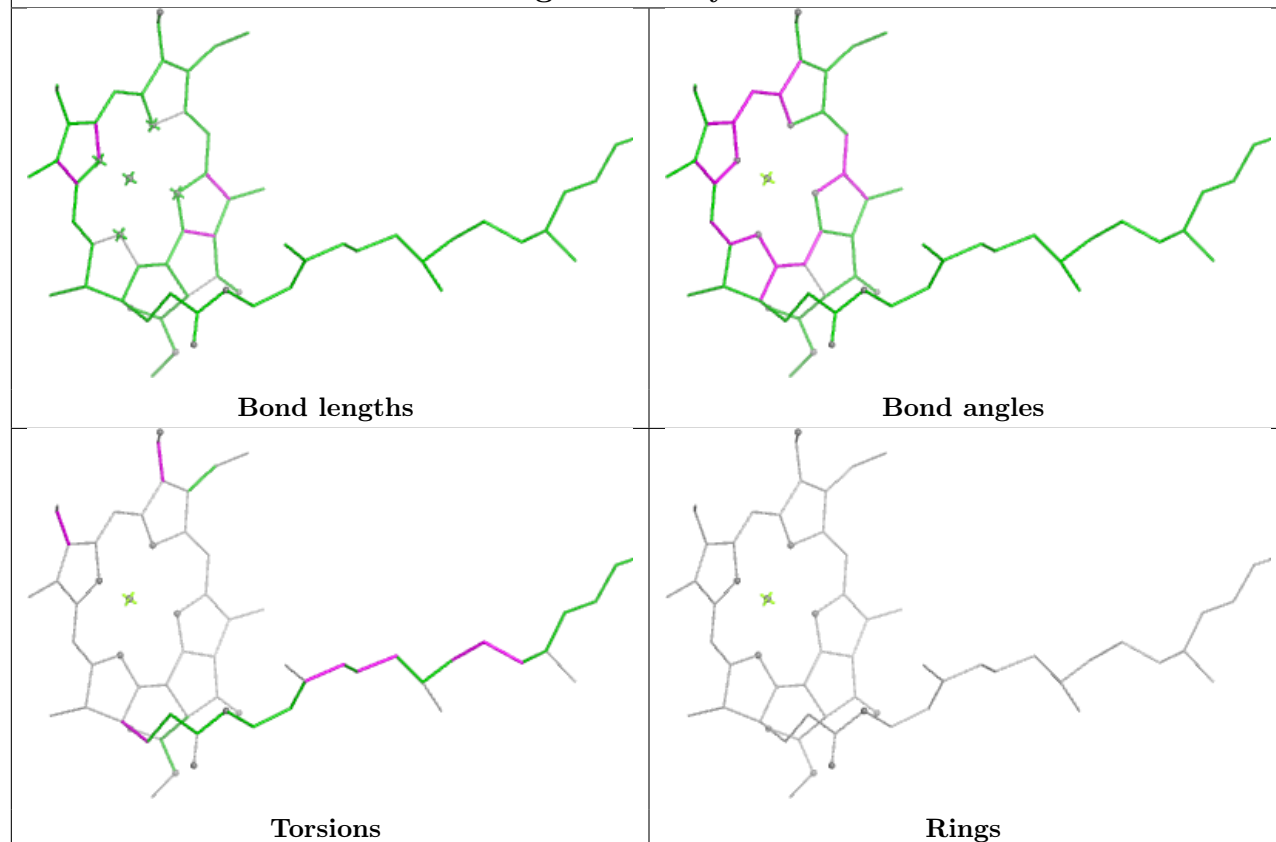




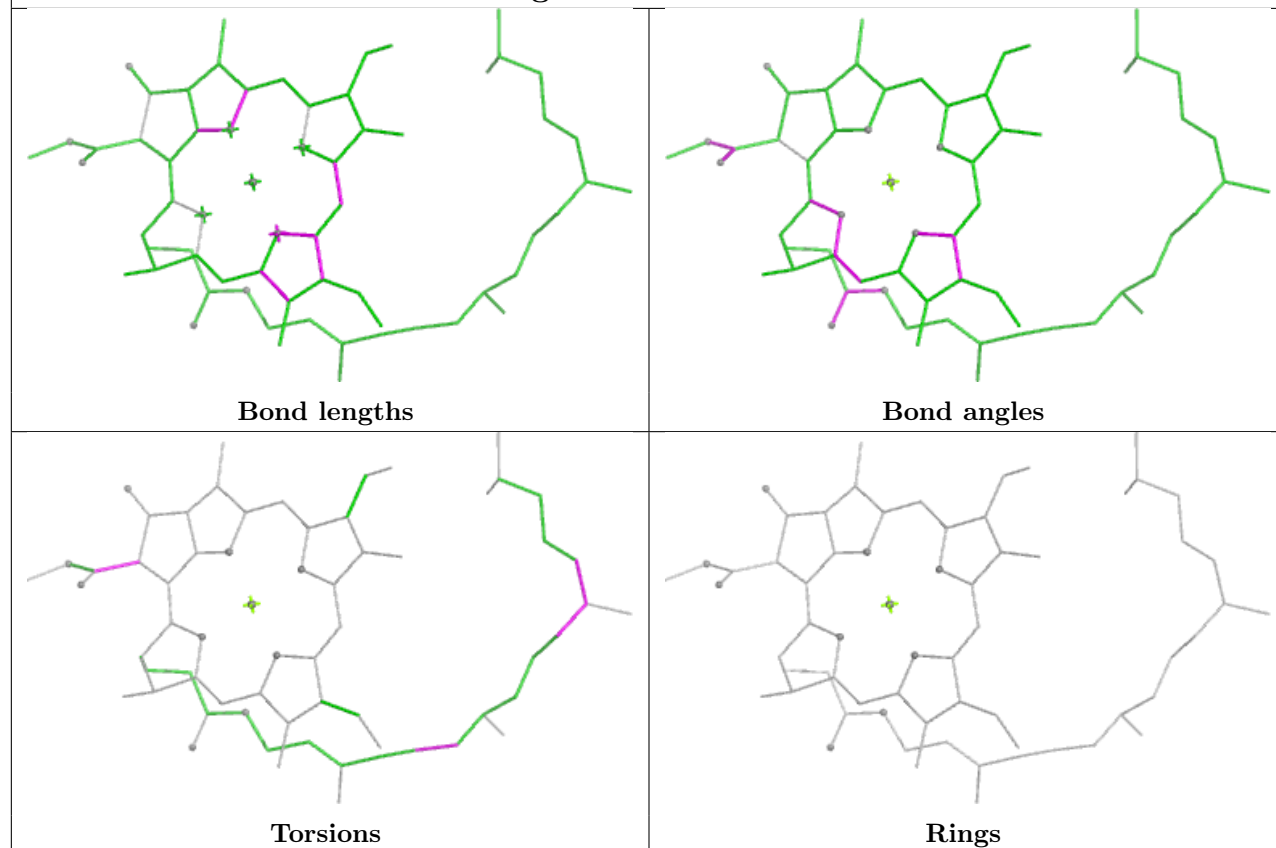


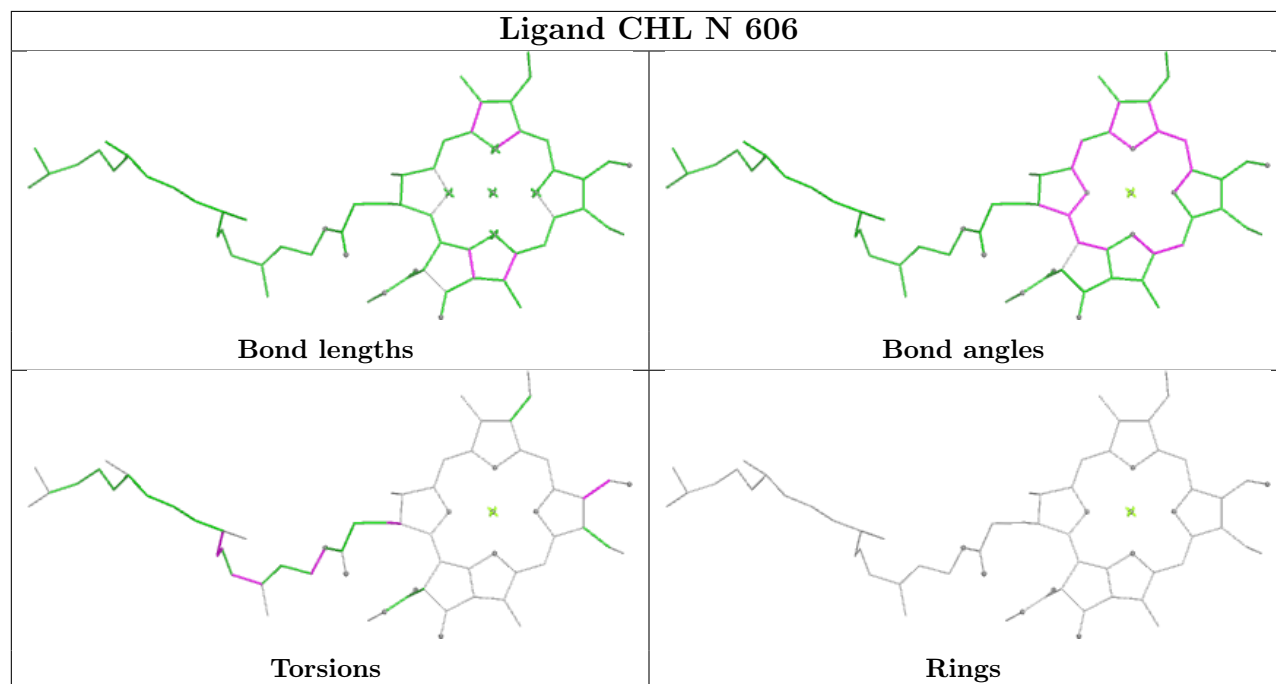
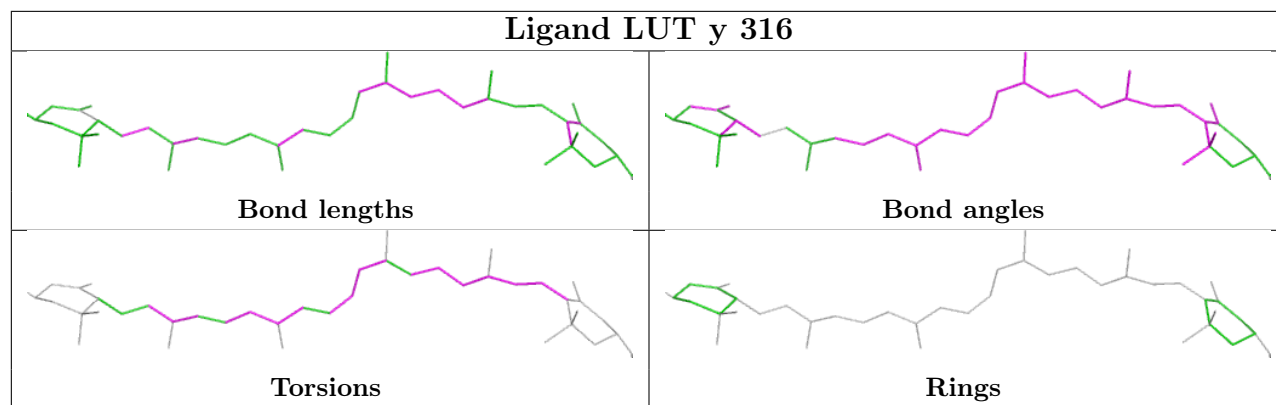


Ligand CHL y 310

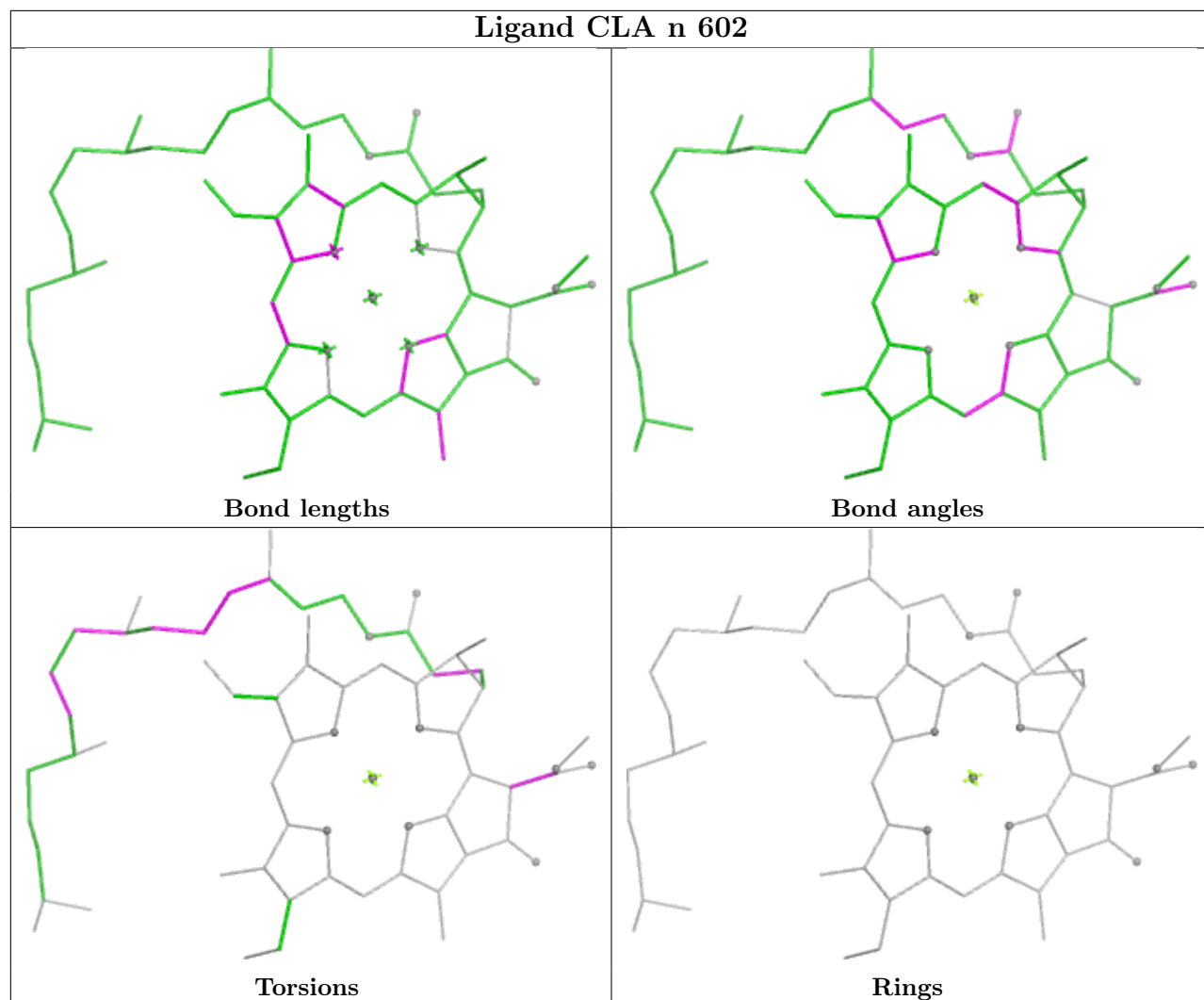


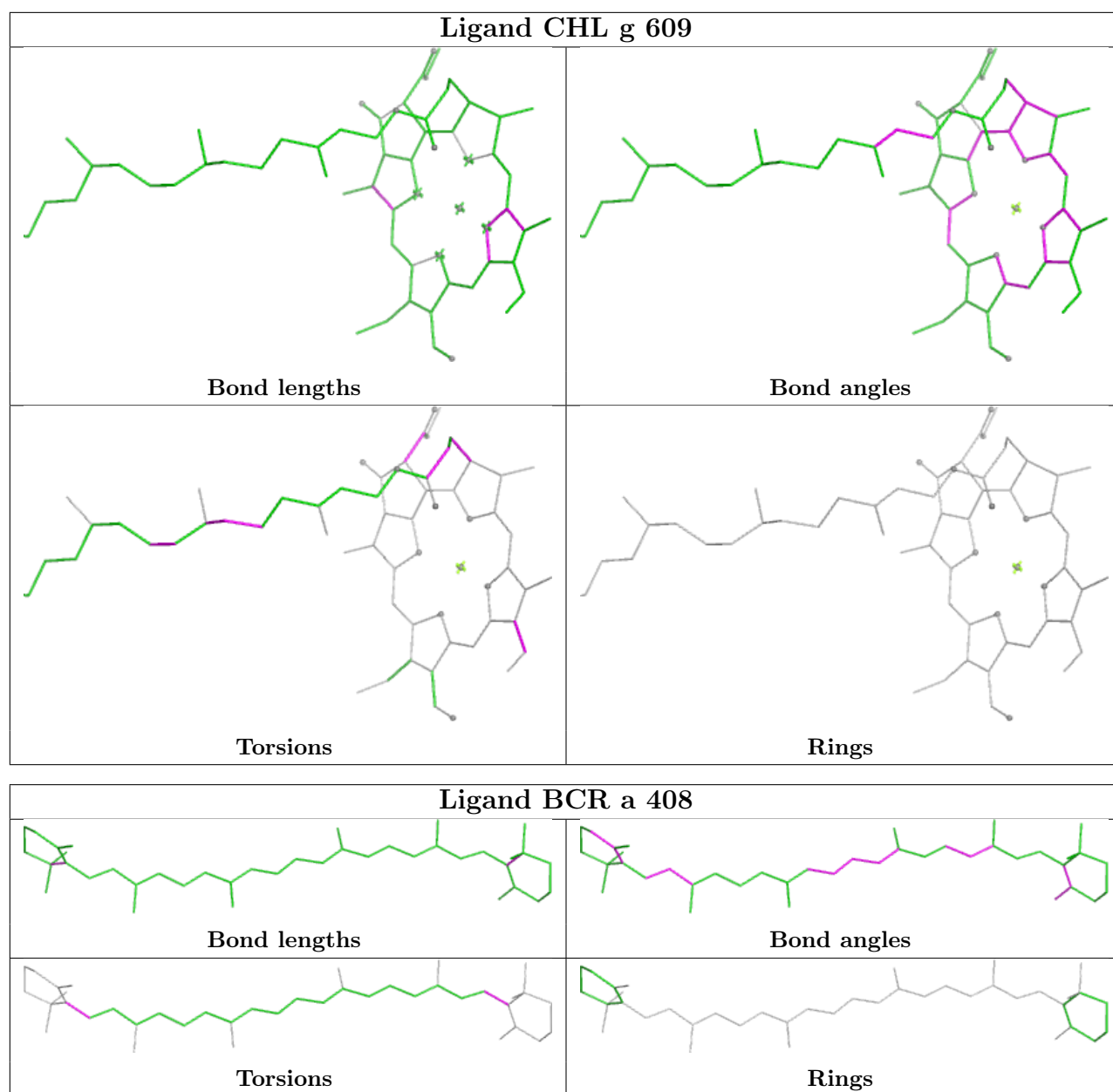
Ligand CLA R 609



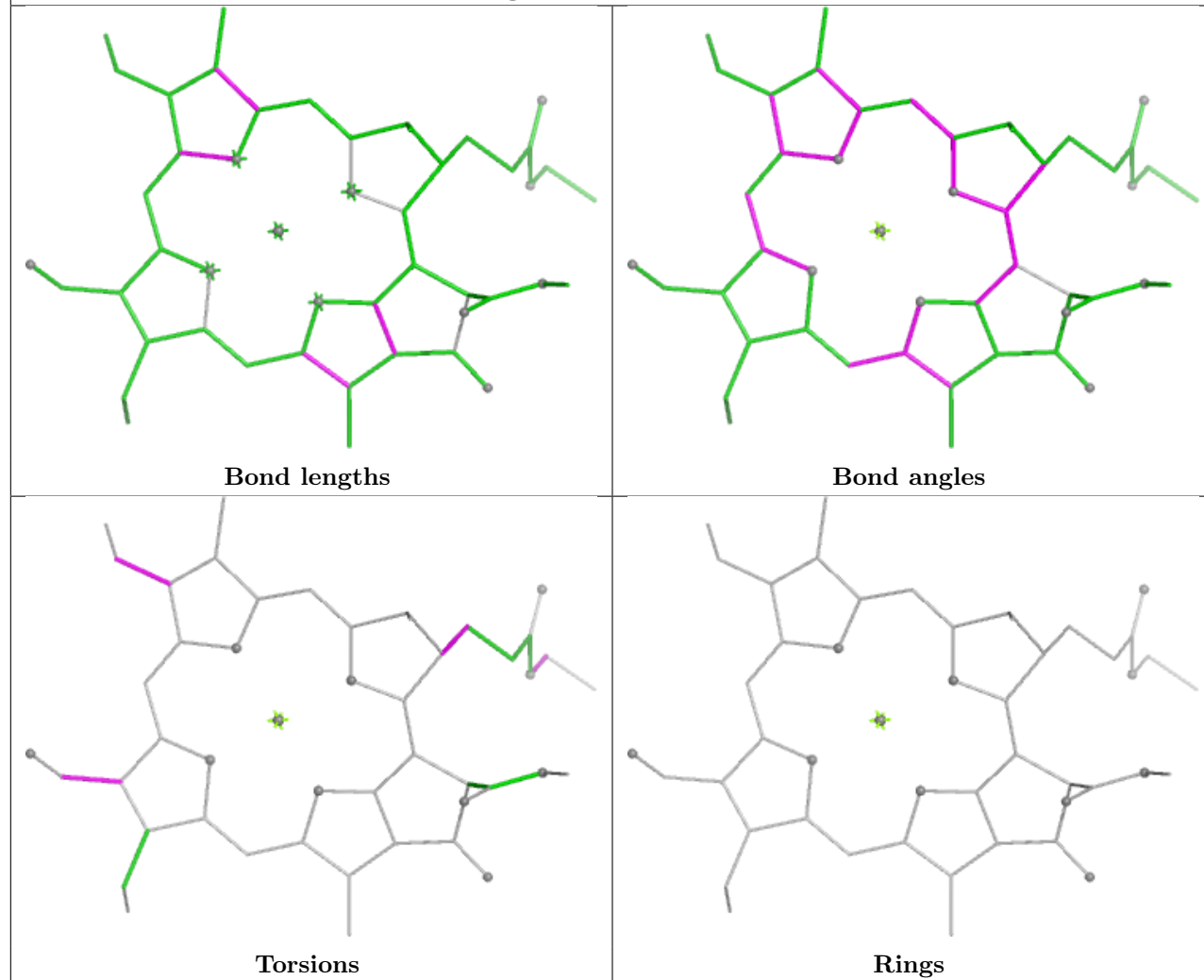


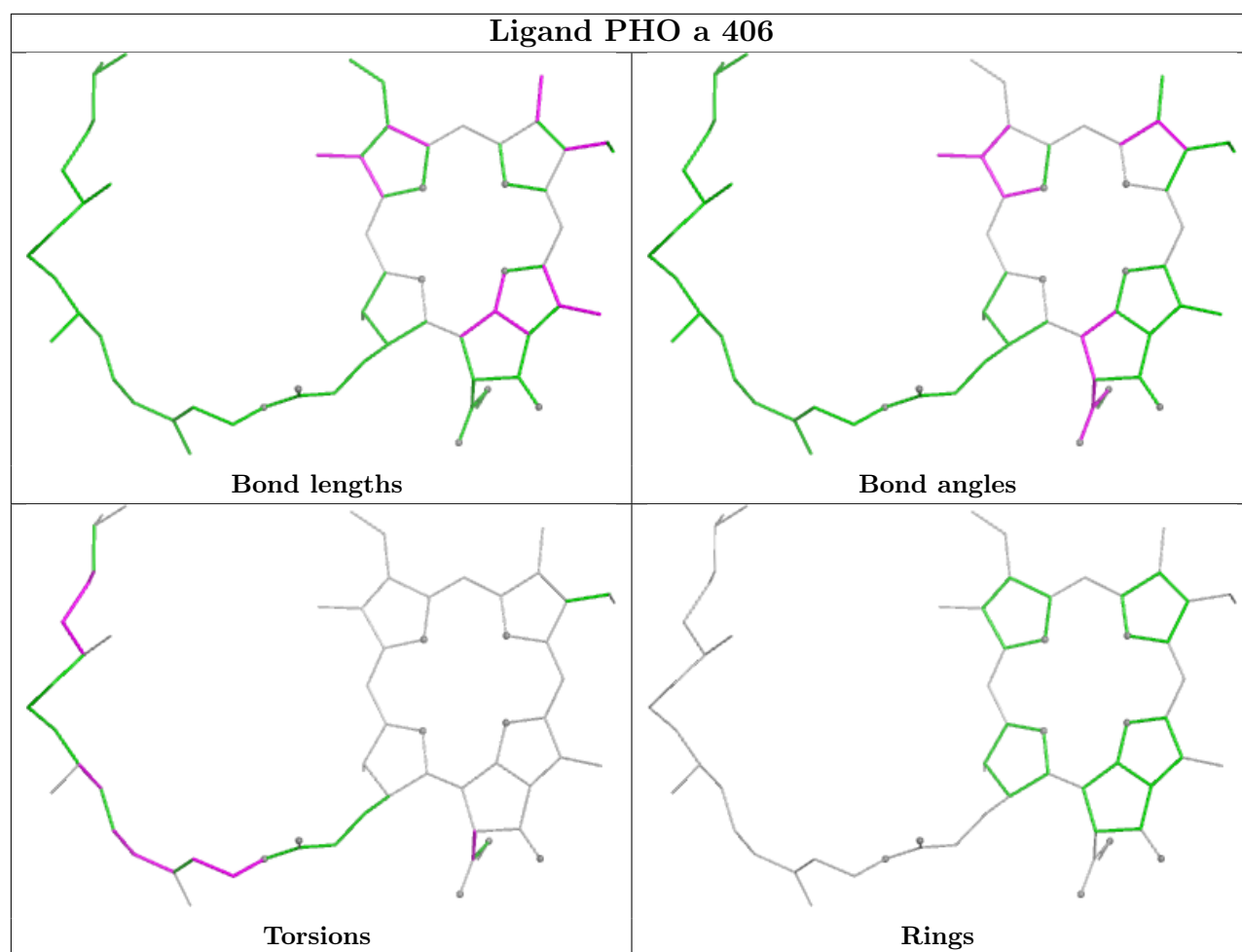
Ligand CLA n 602

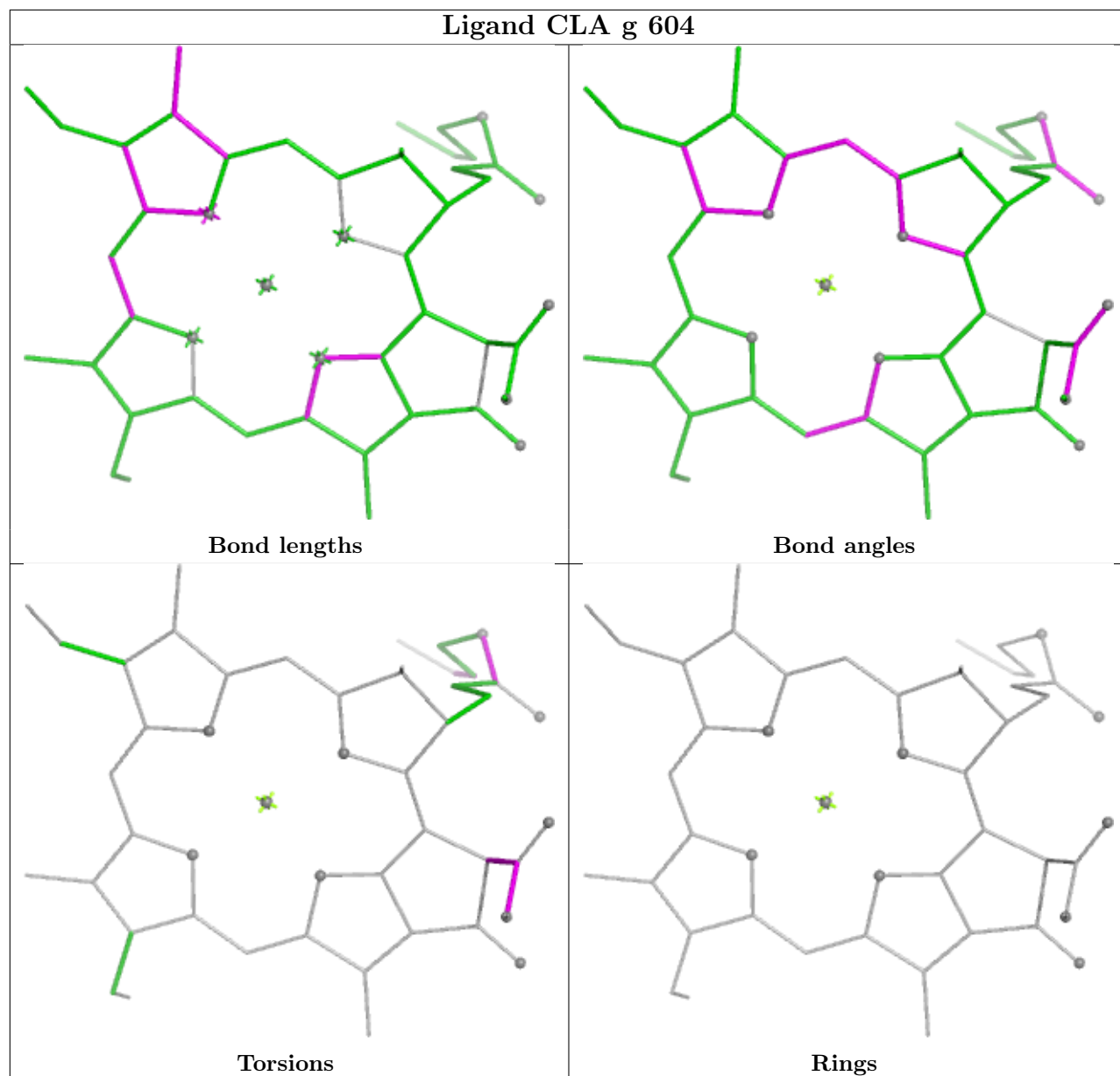




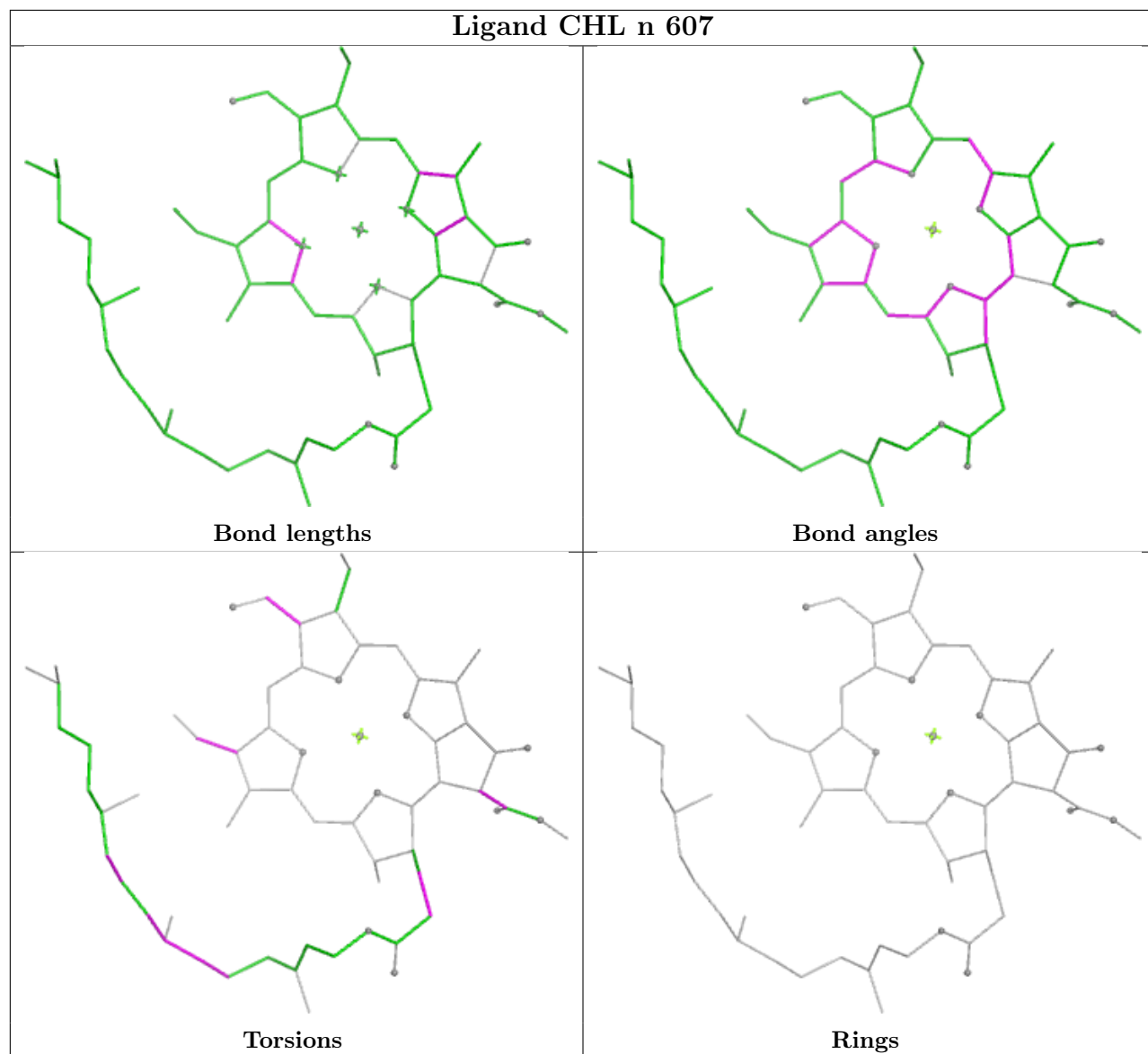
Ligand CHL n 605

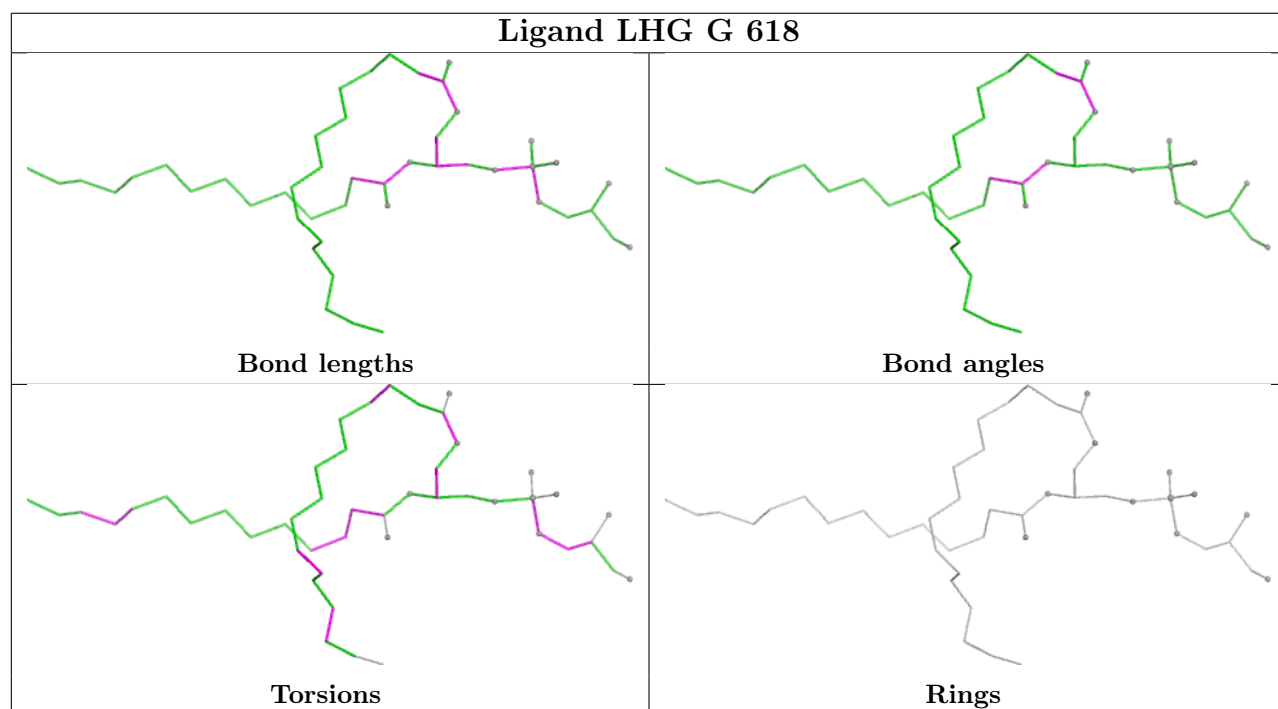
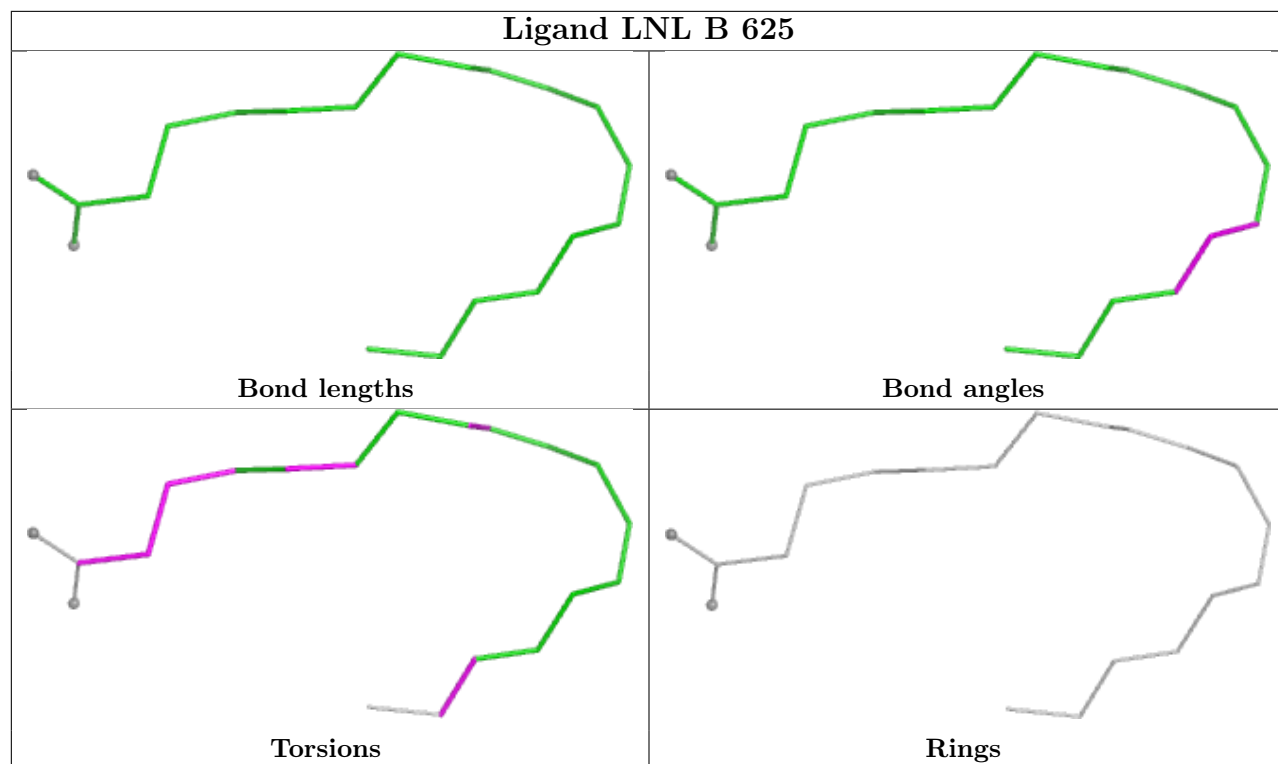


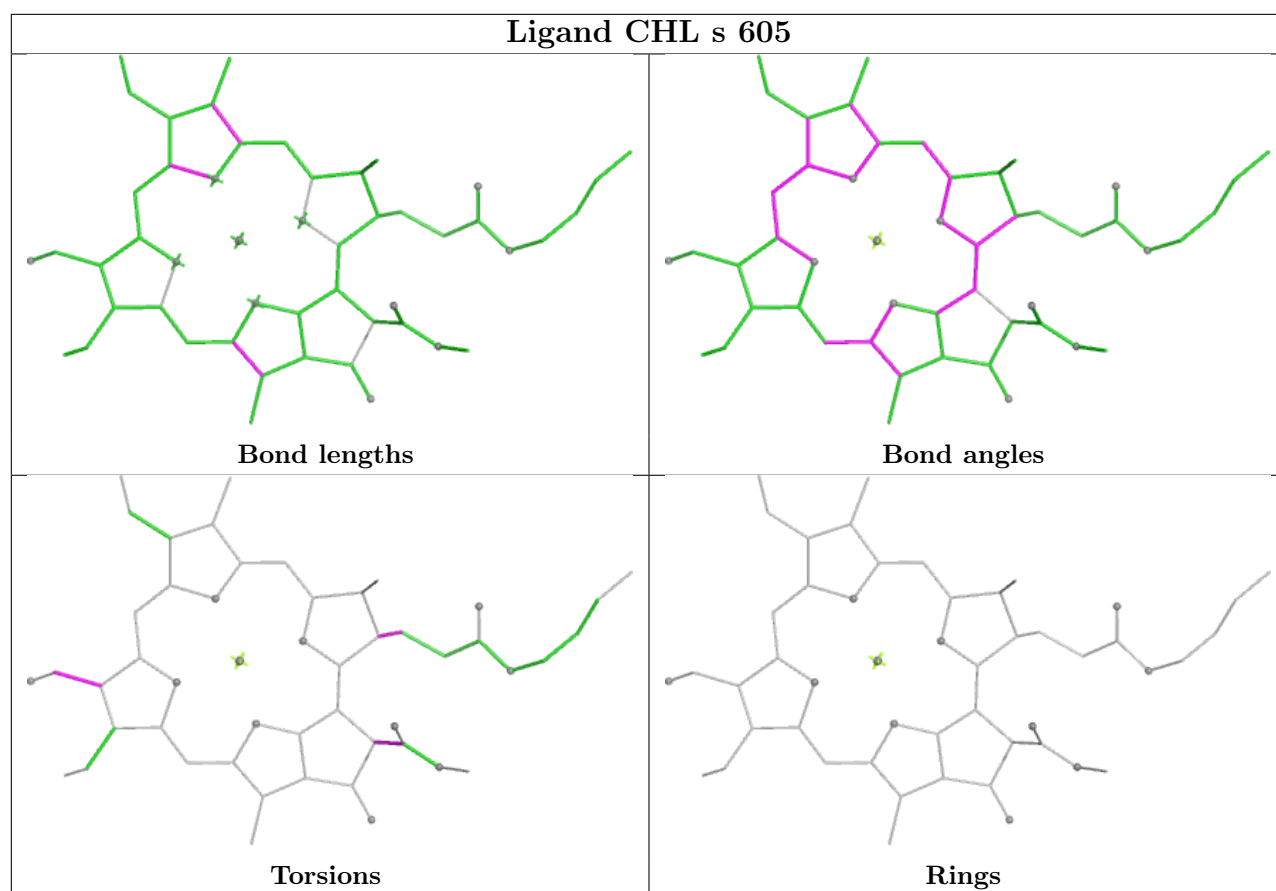




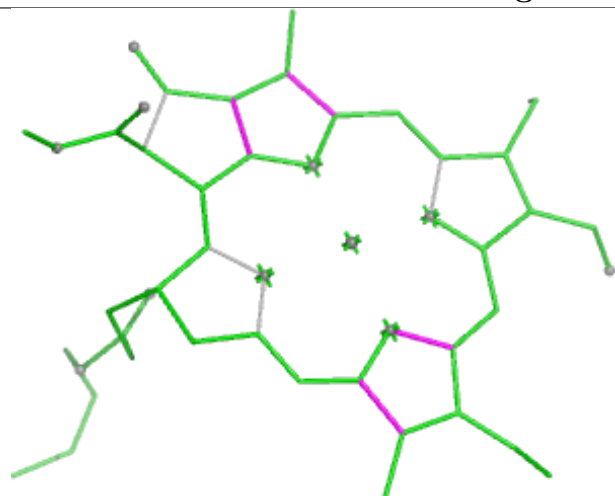
Ligand CHL n 607



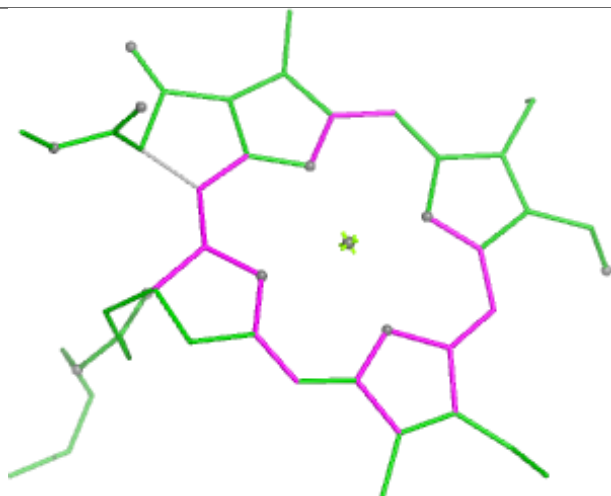




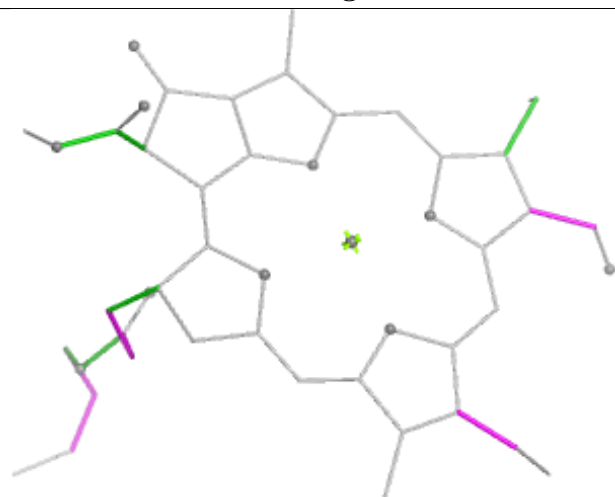
Ligand CHL Y 308



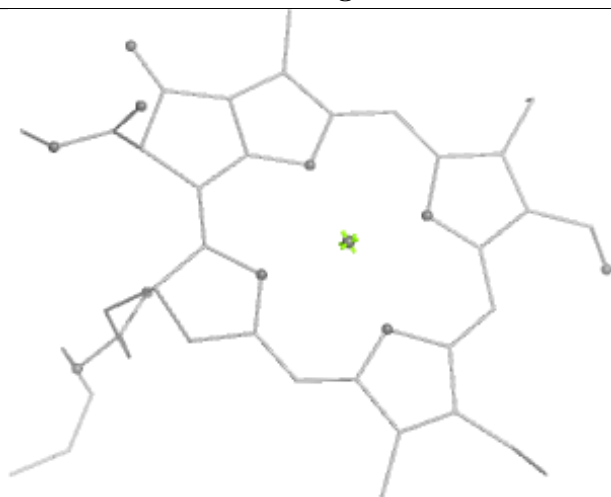
Bond lengths



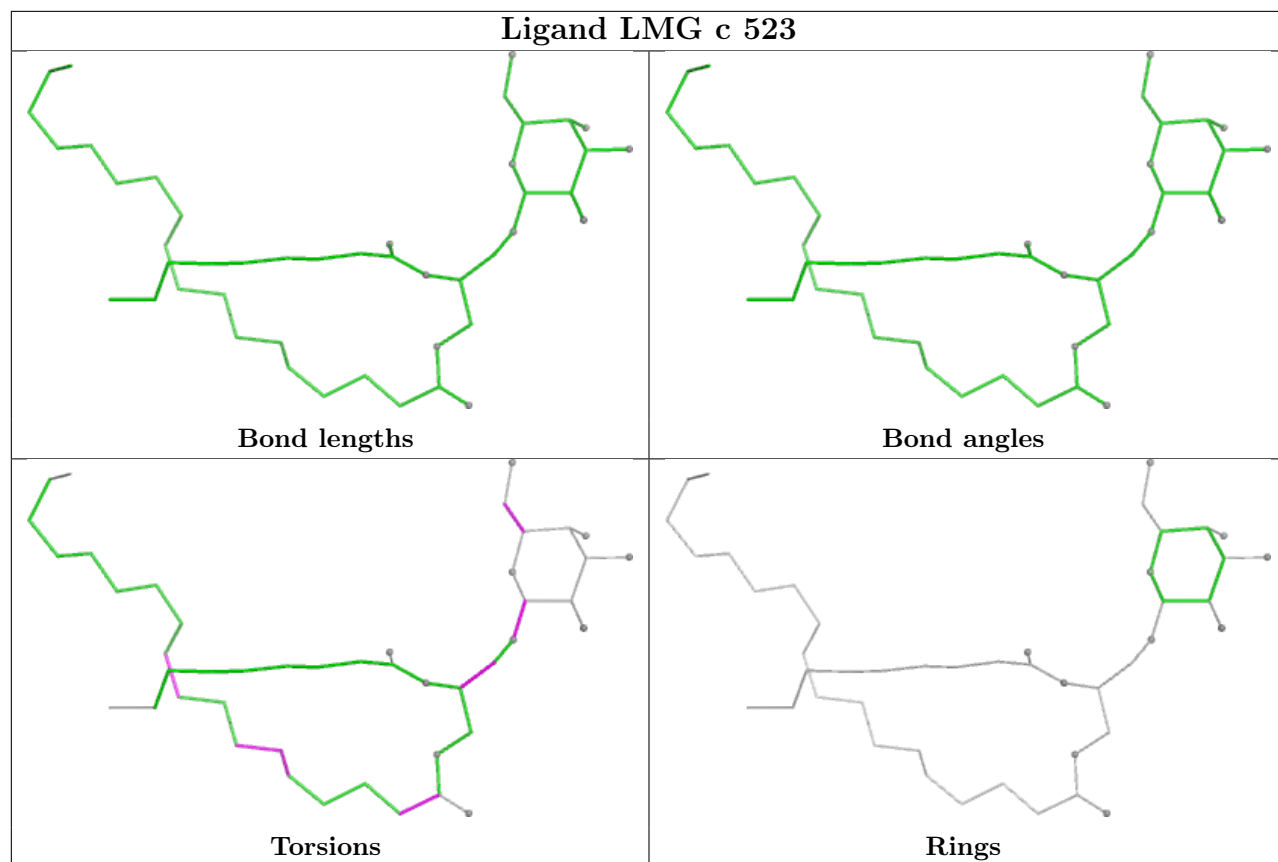
Bond angles

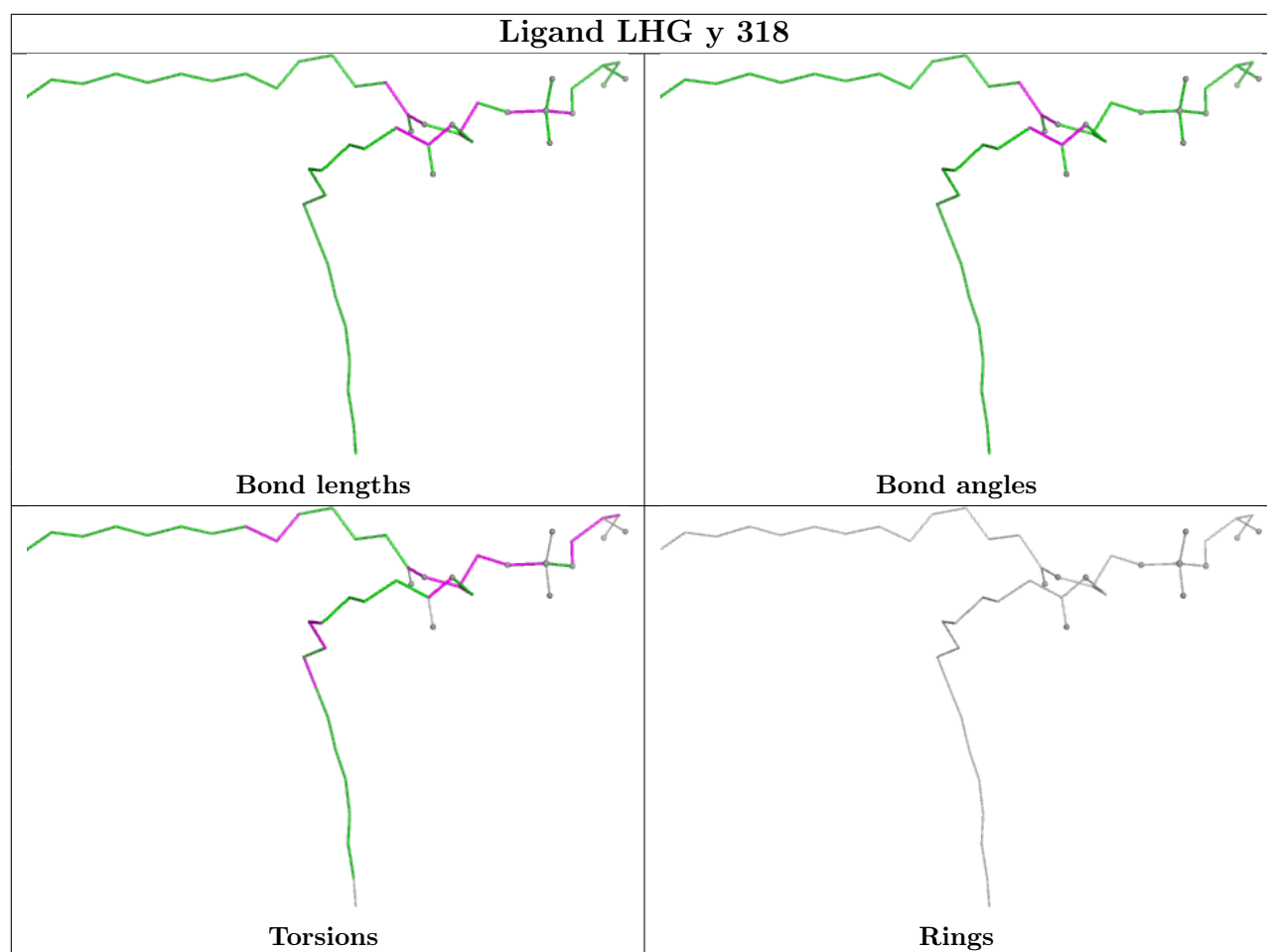


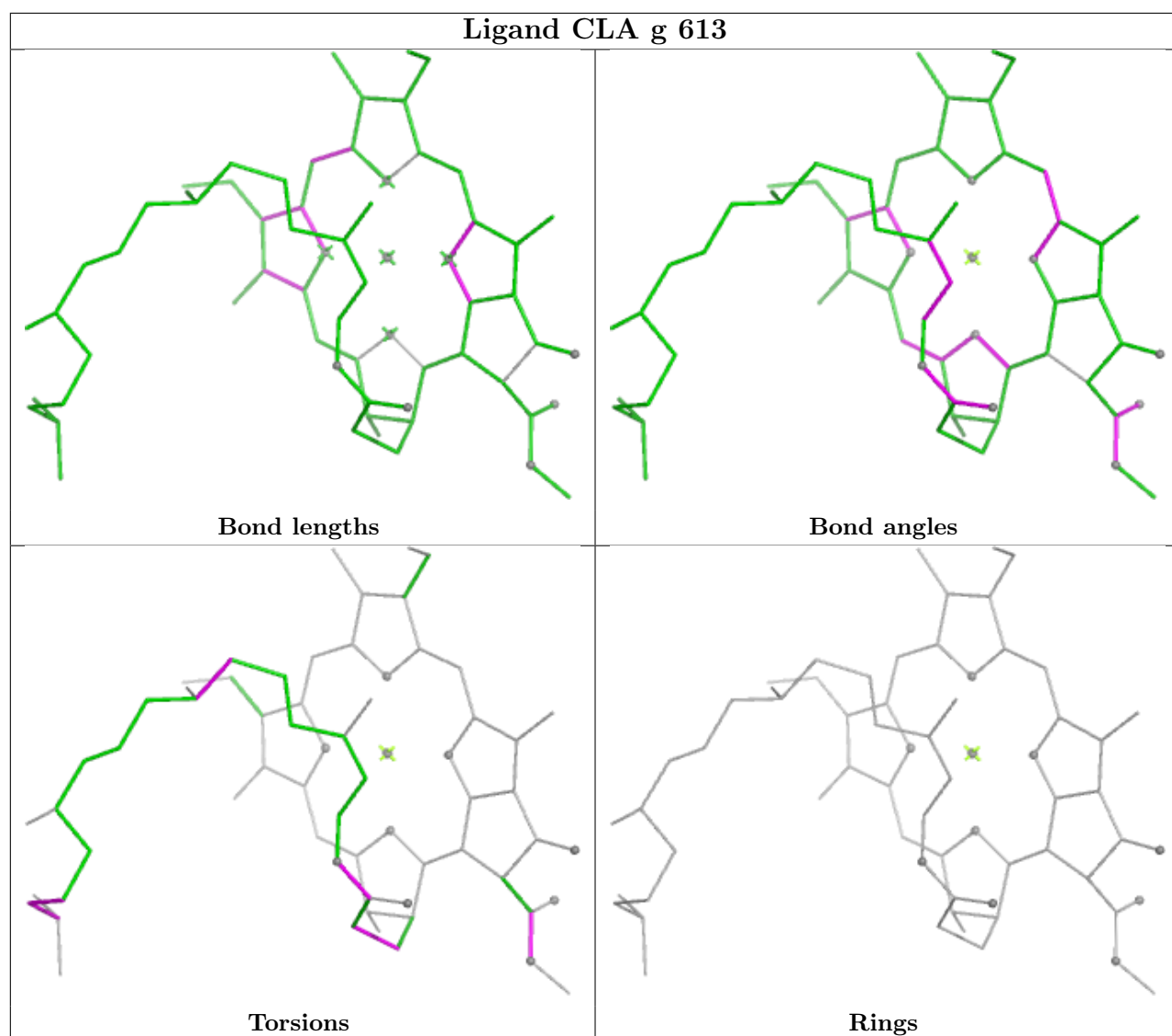
Torsions



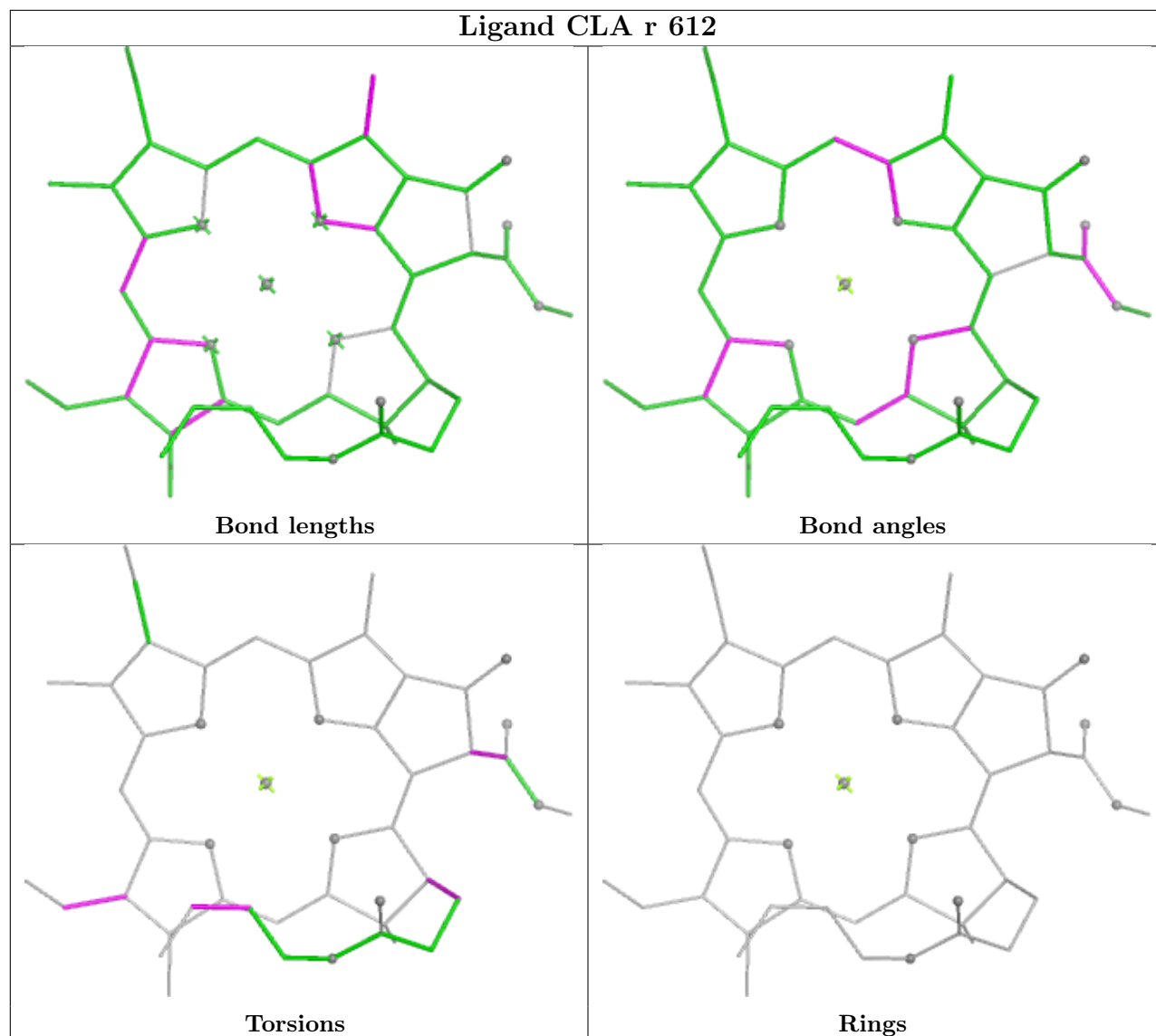
Rings

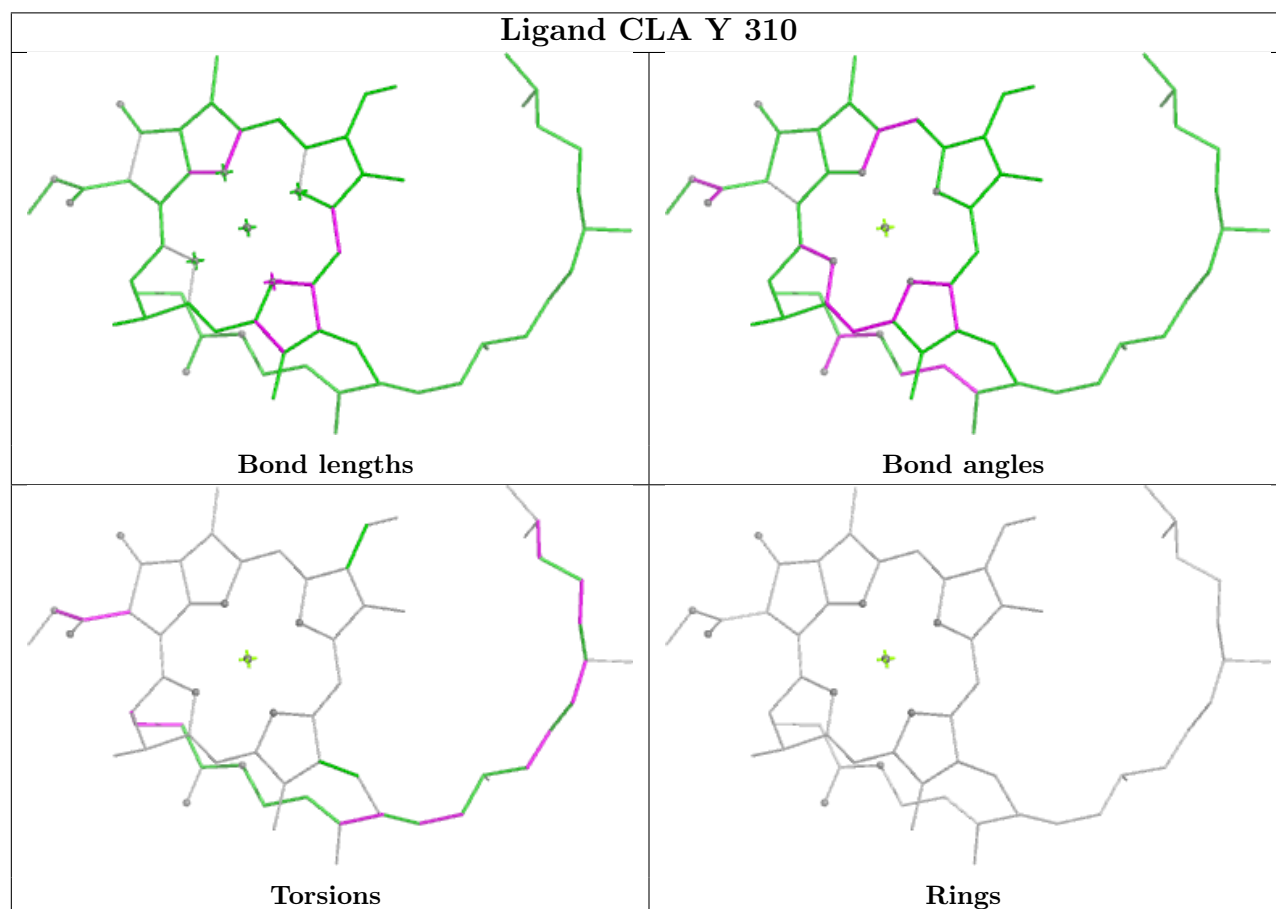
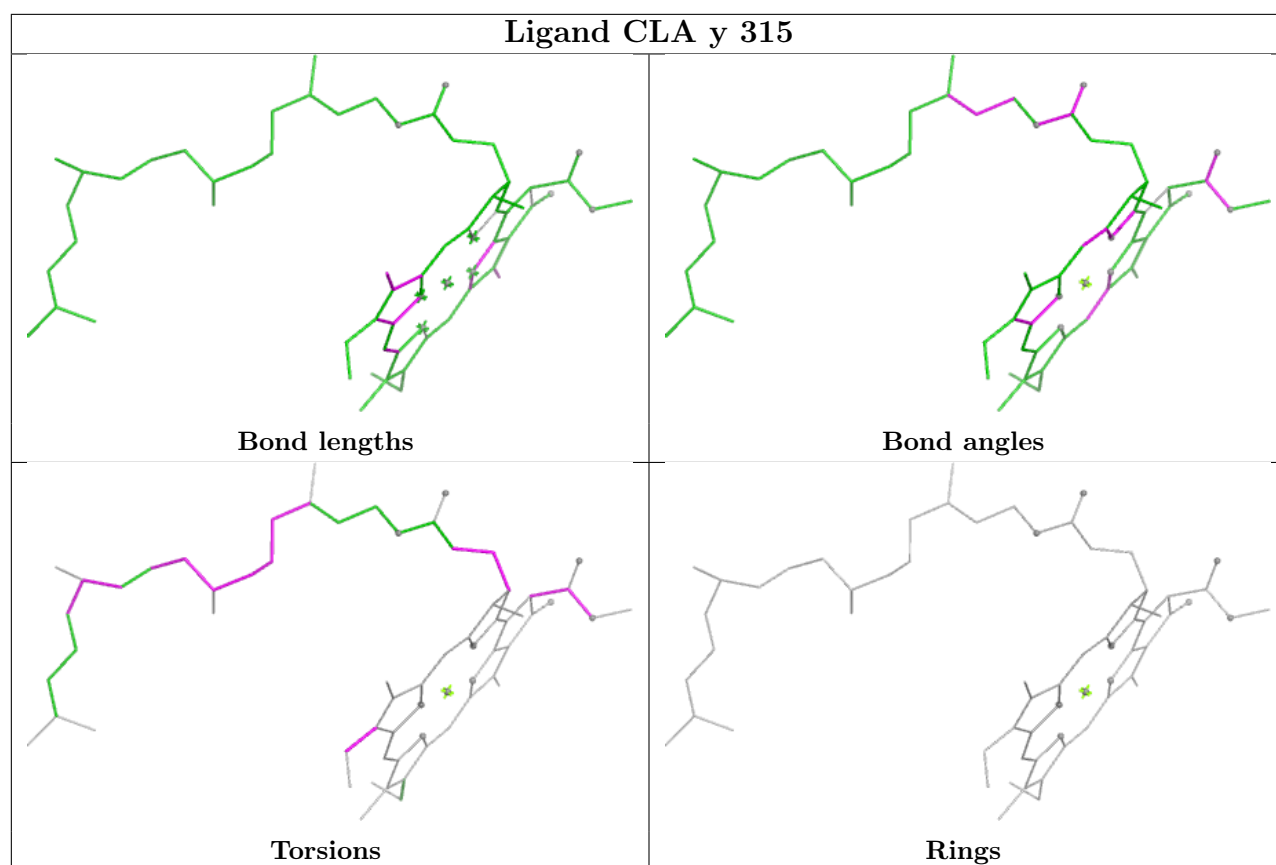


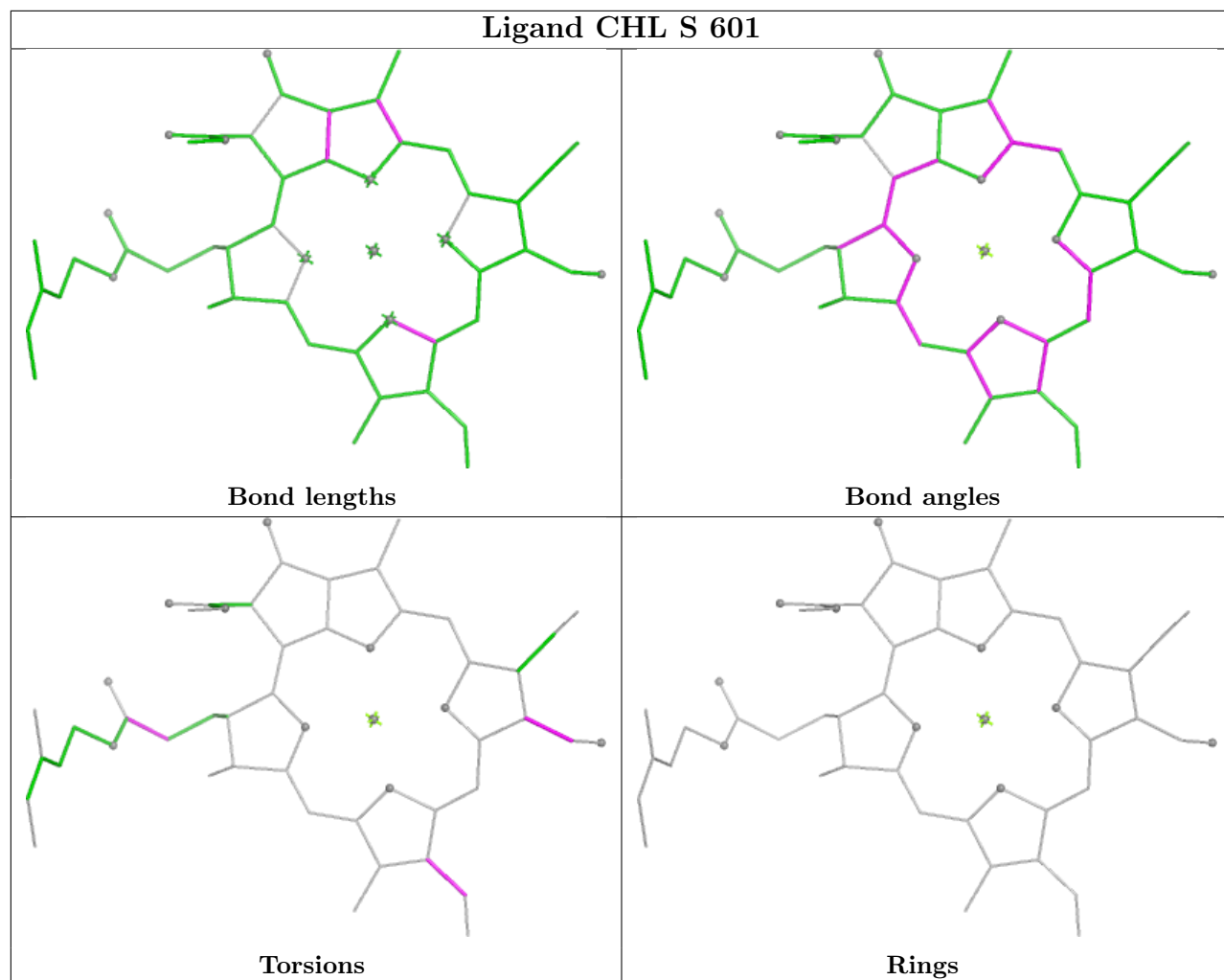


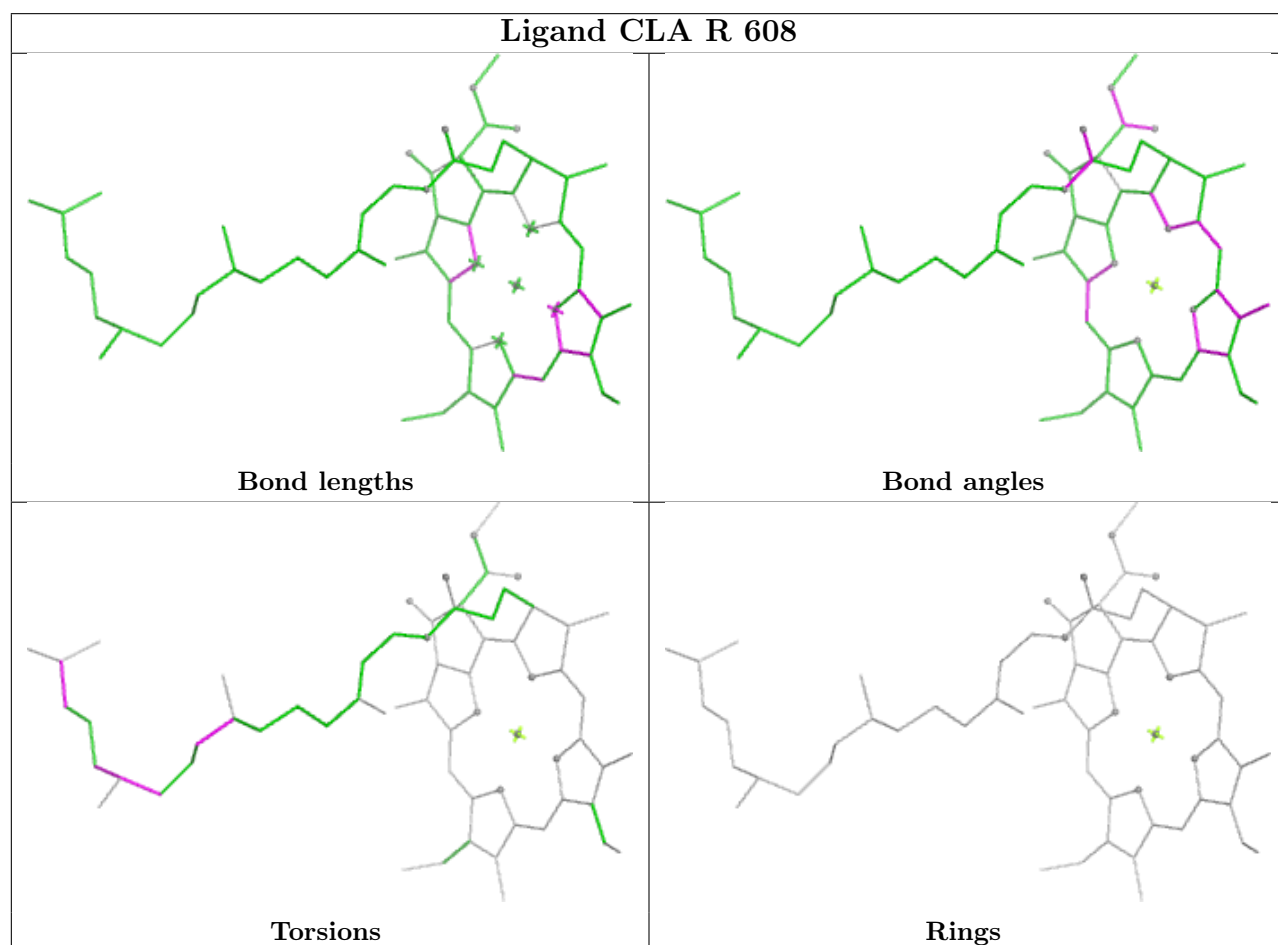
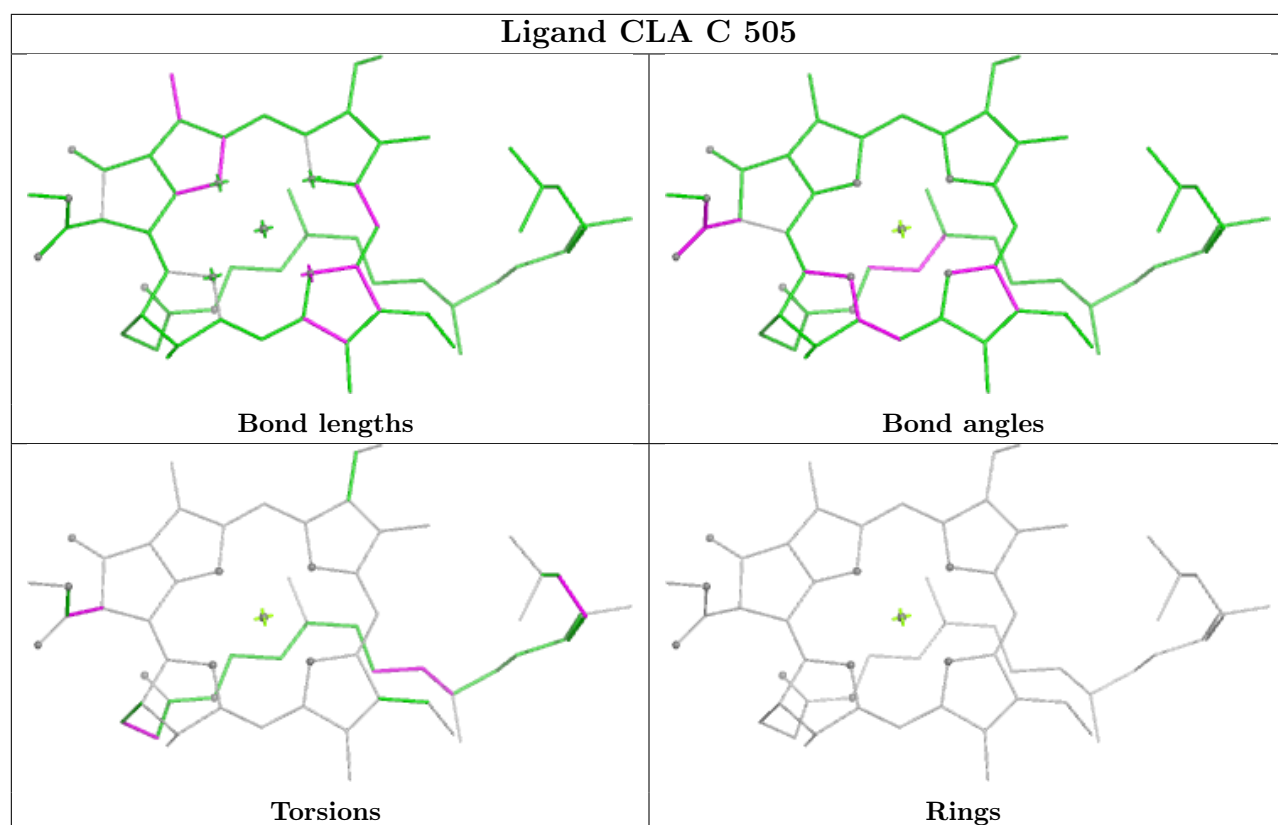


Ligand CLA r 612

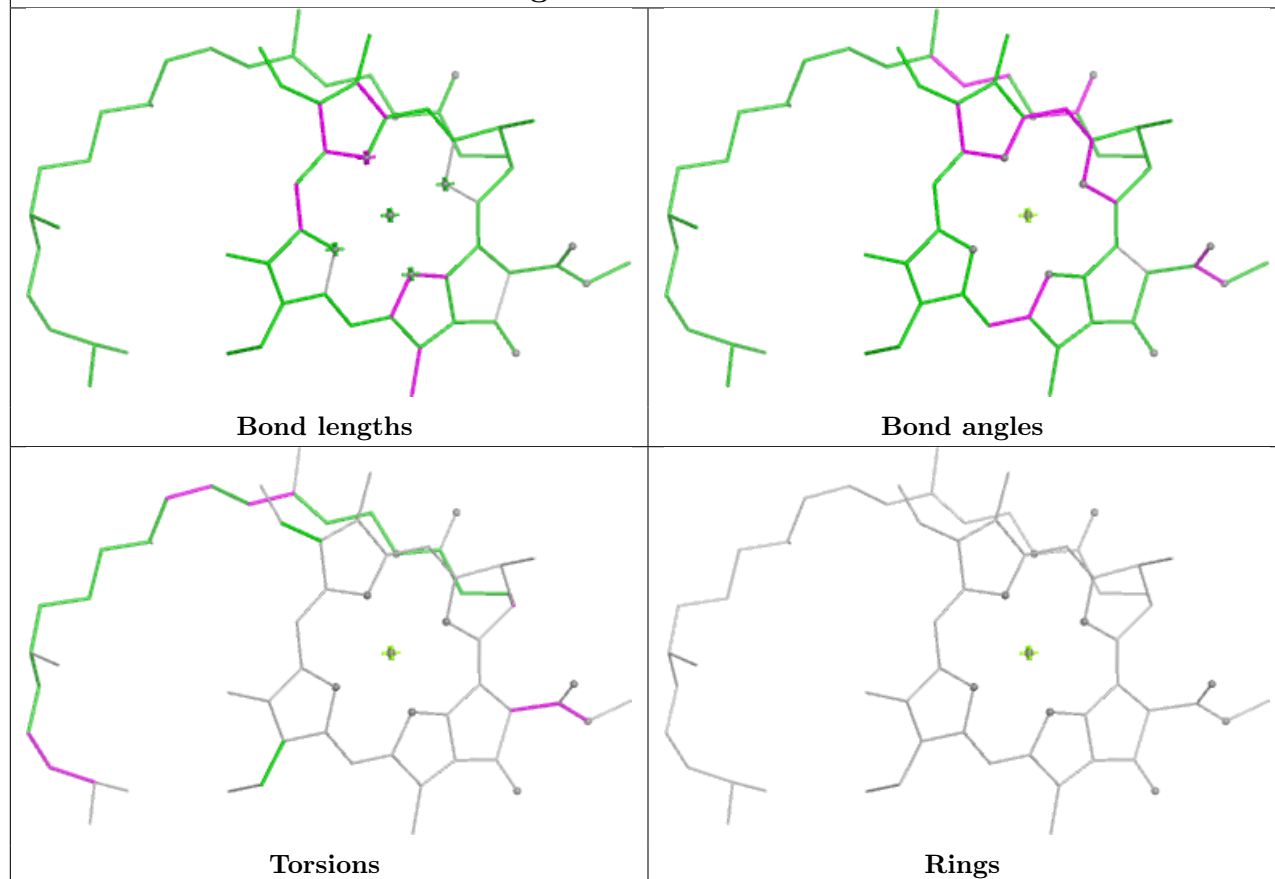




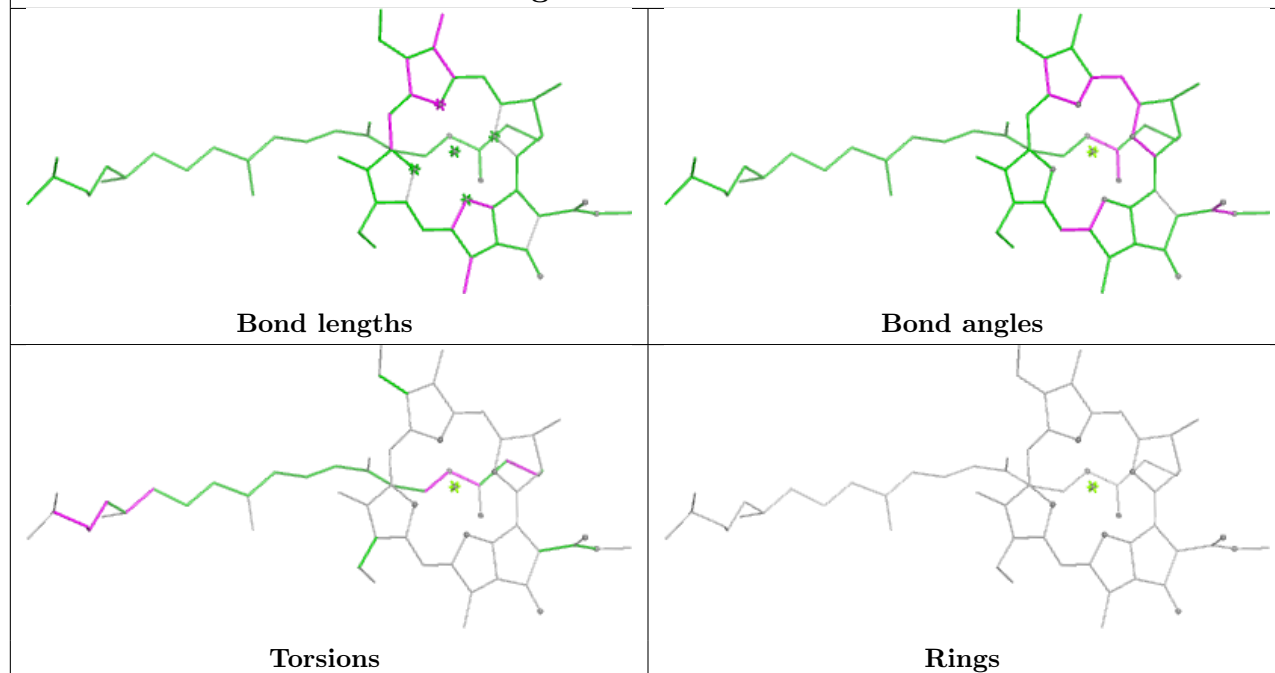


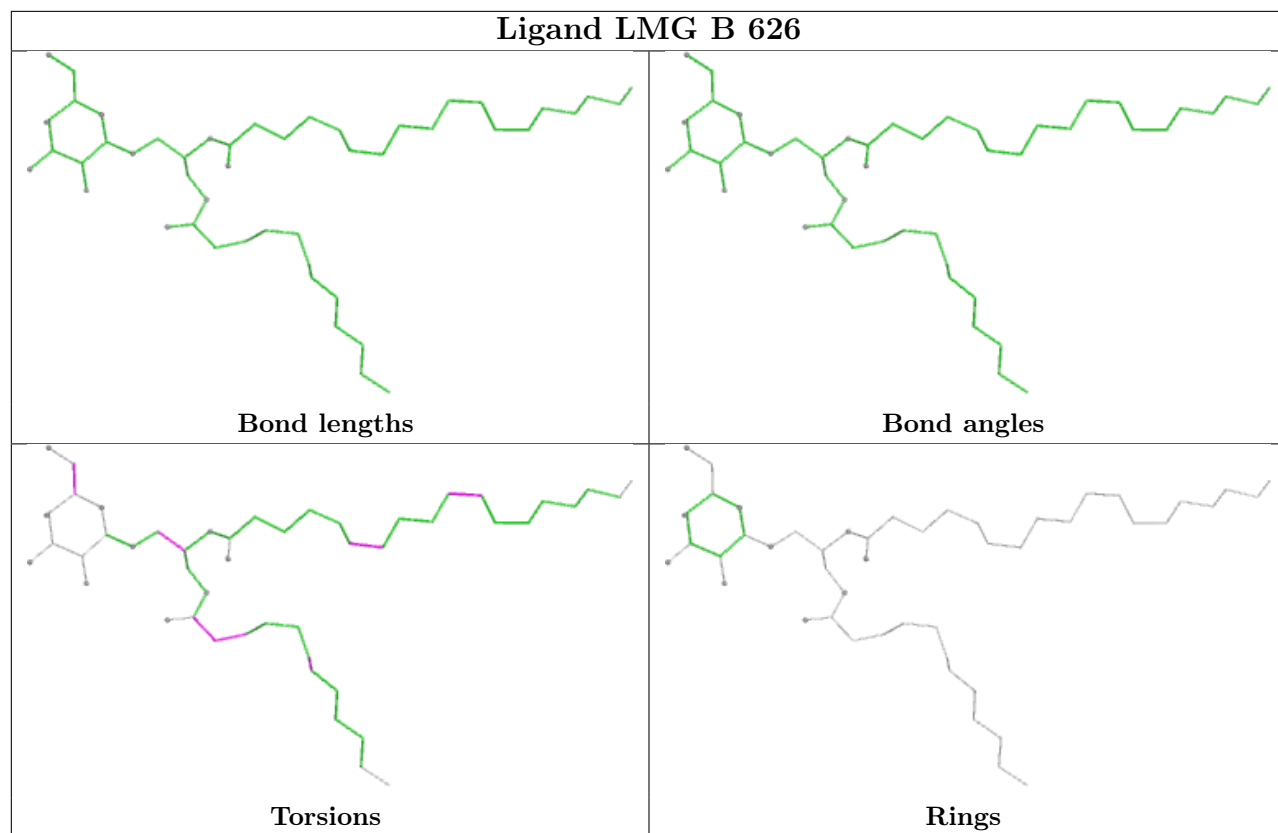


Ligand CLA N 610

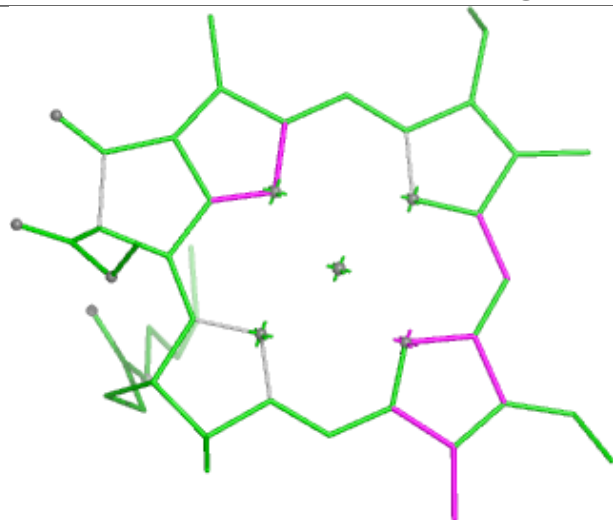


Ligand CLA B 608

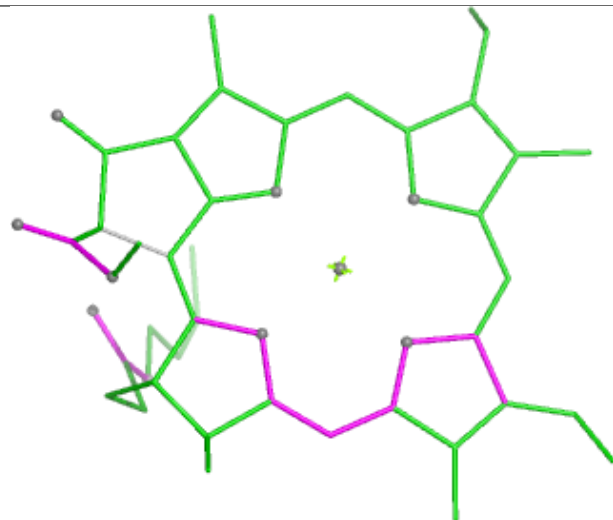




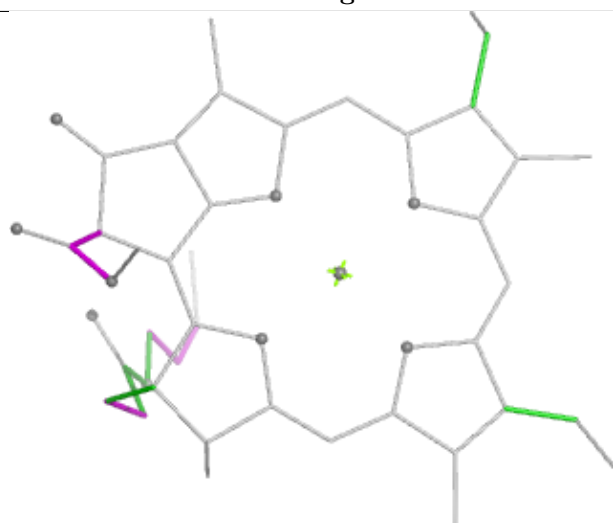
Ligand CLA S 604



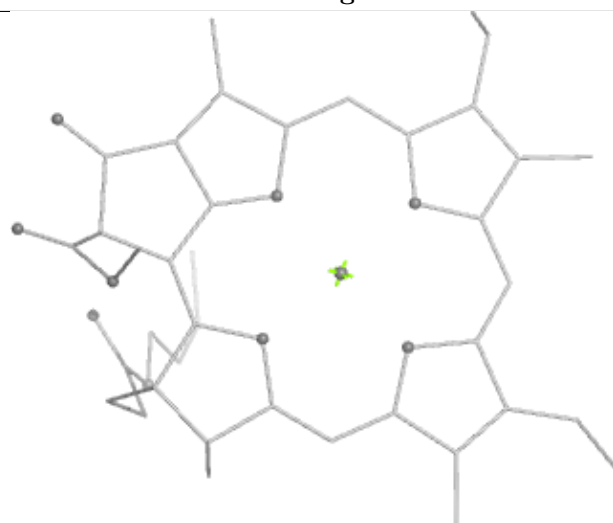
Bond lengths



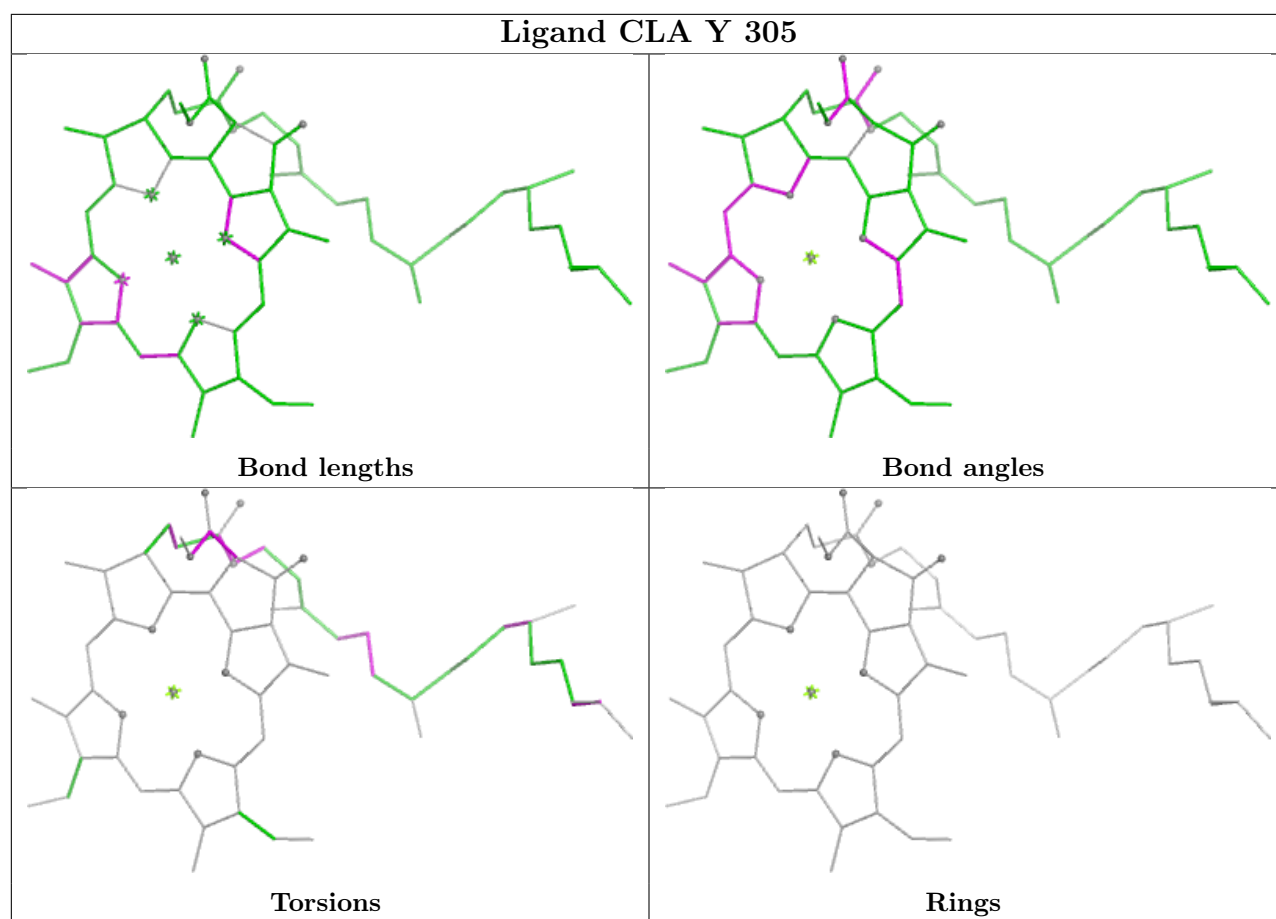
Bond angles



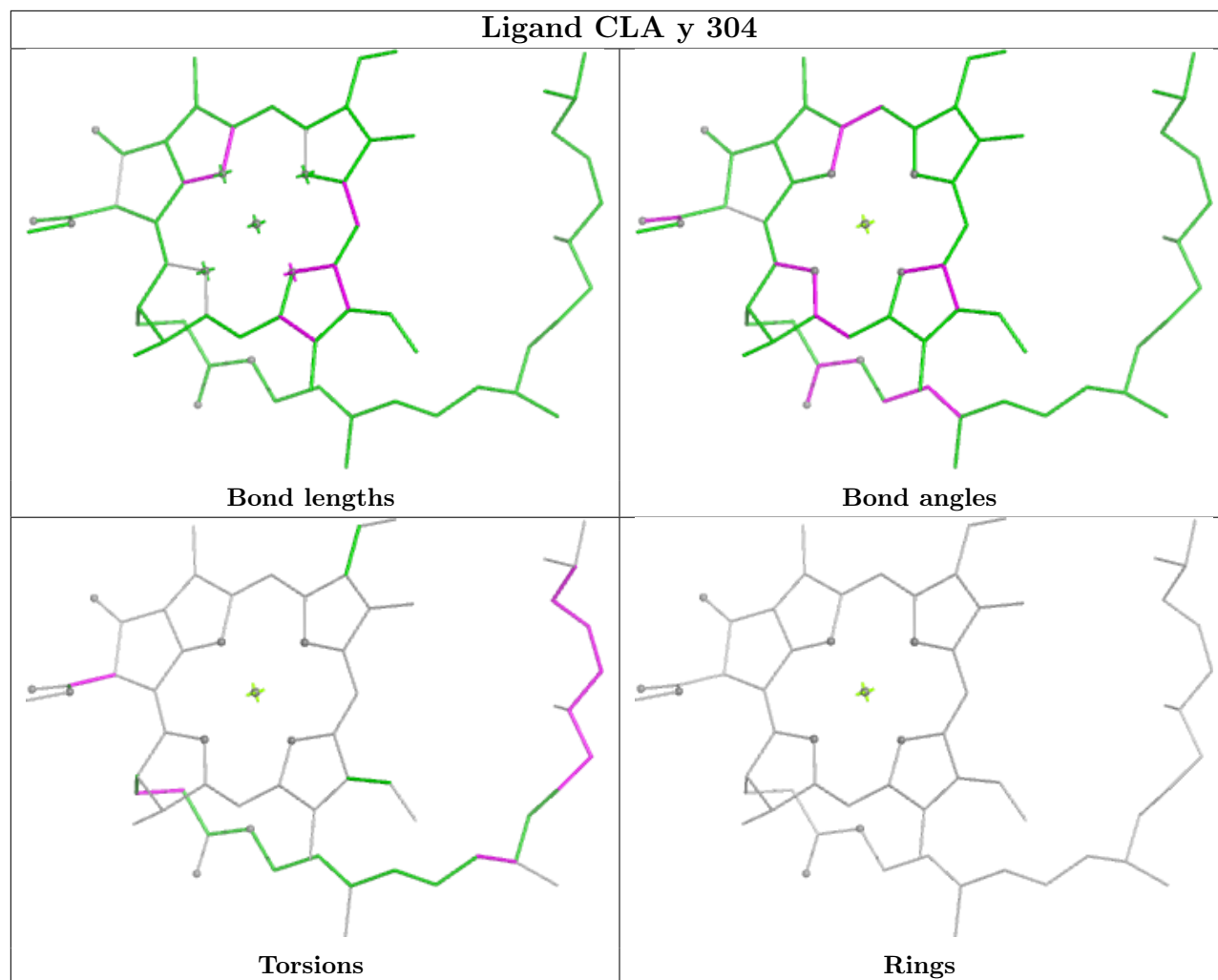
Torsions



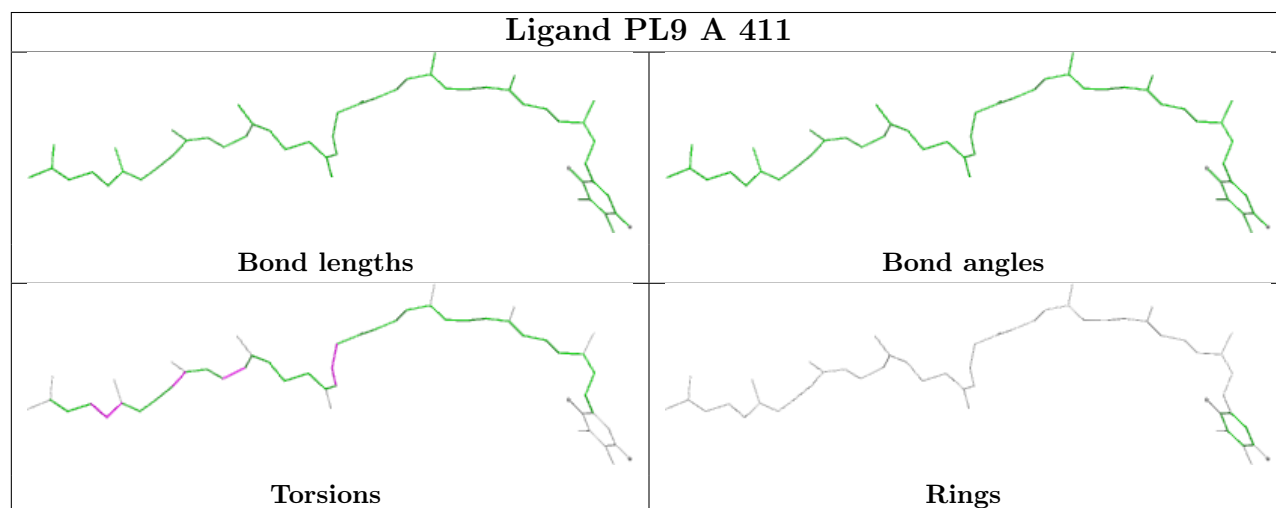
Rings

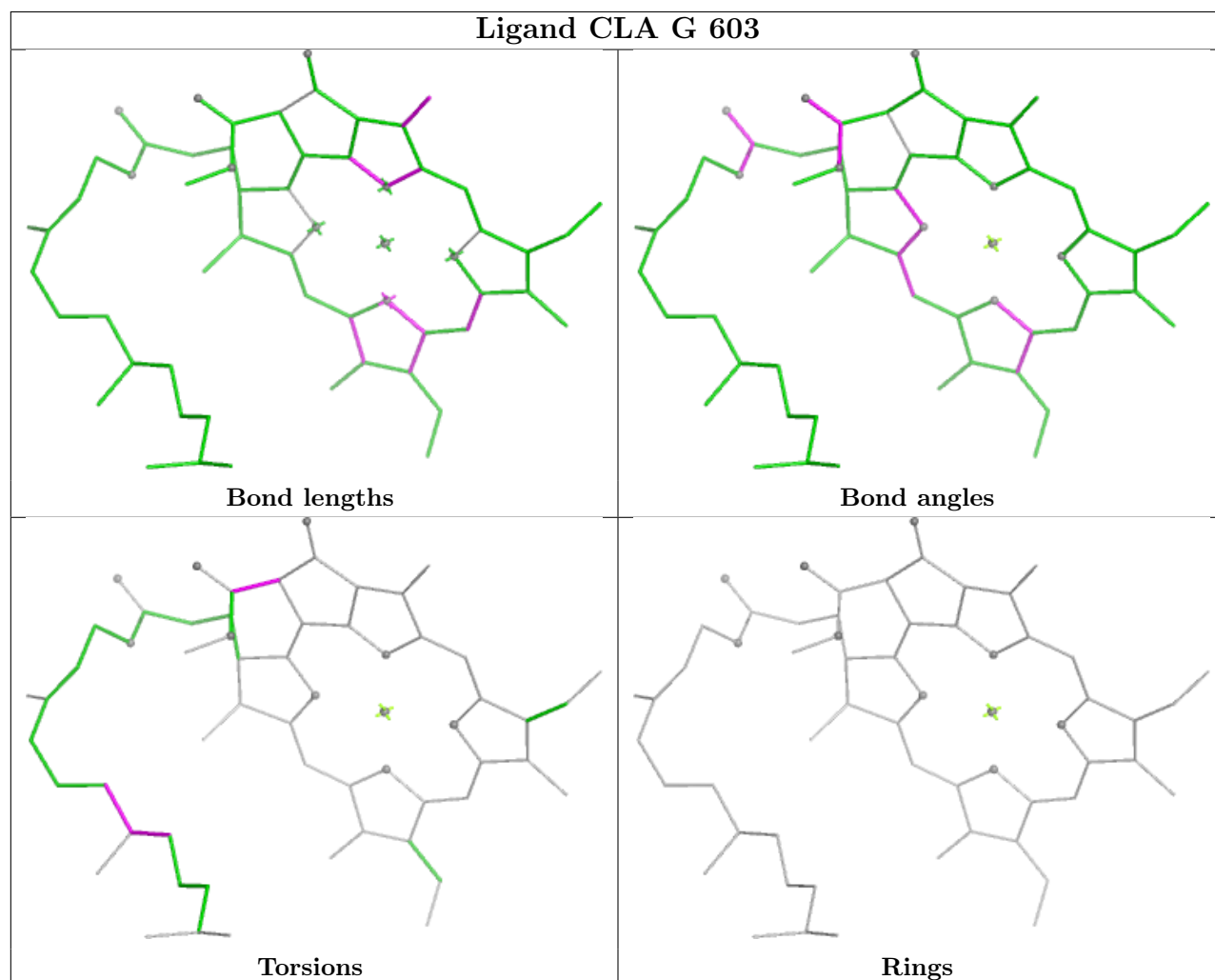
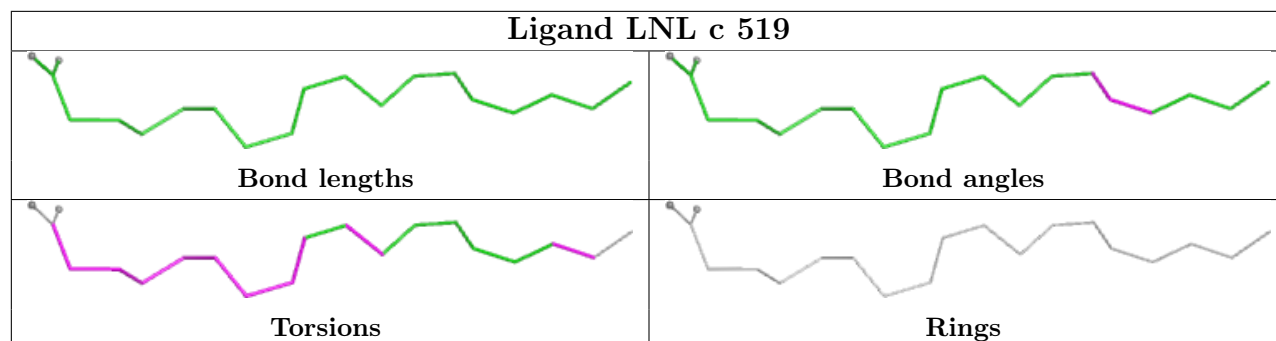


Ligand CLA y 304

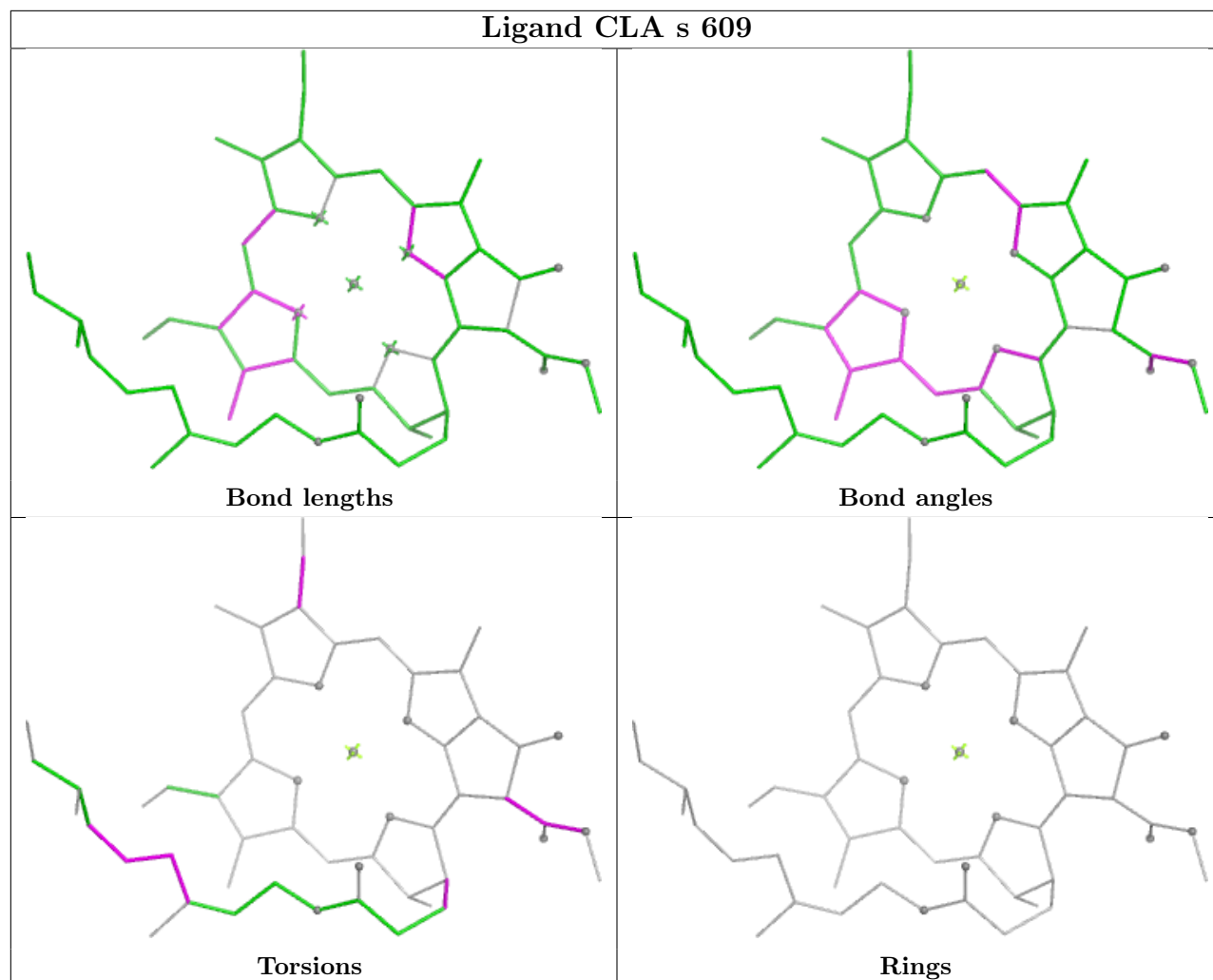


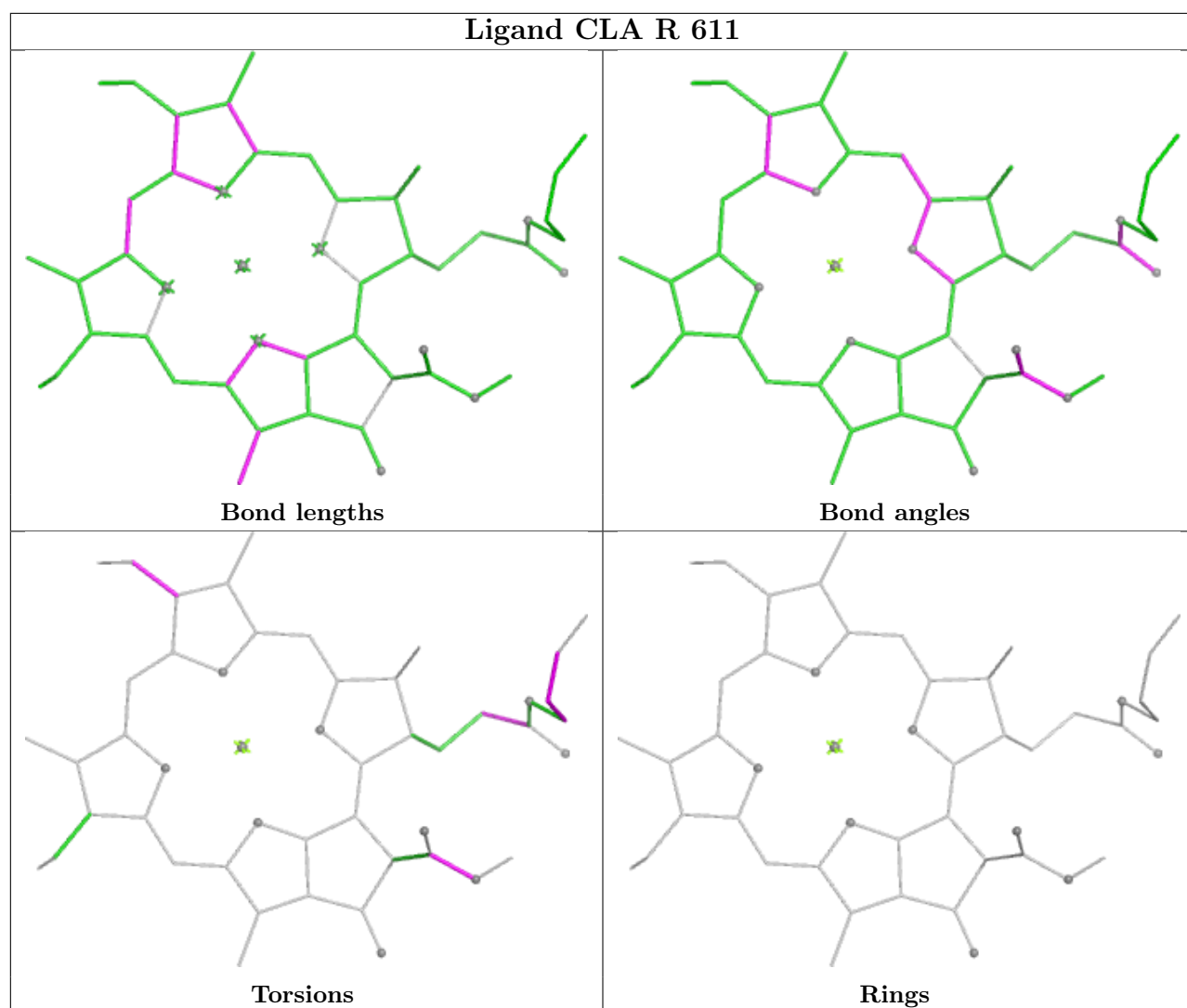
Ligand PL9 A 411

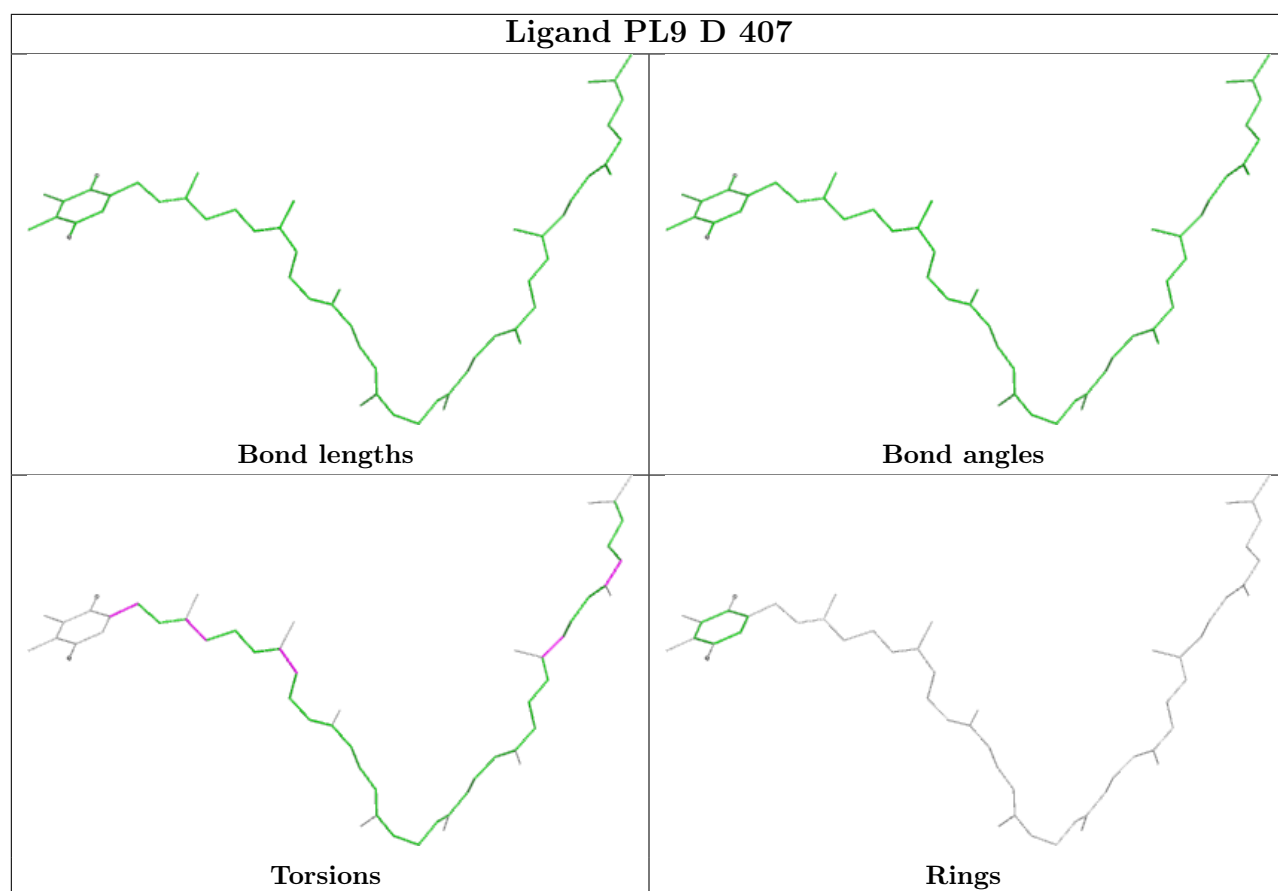


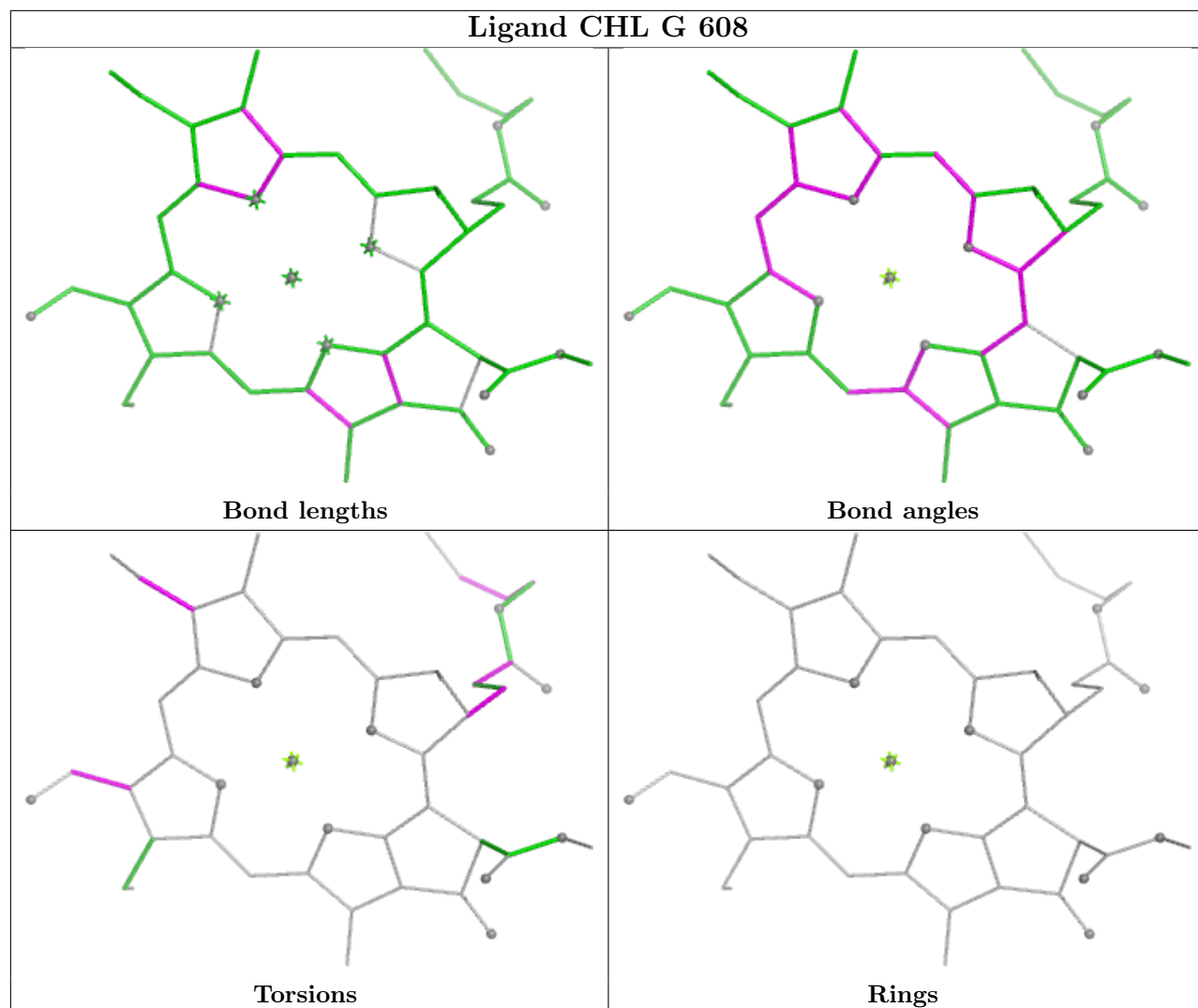


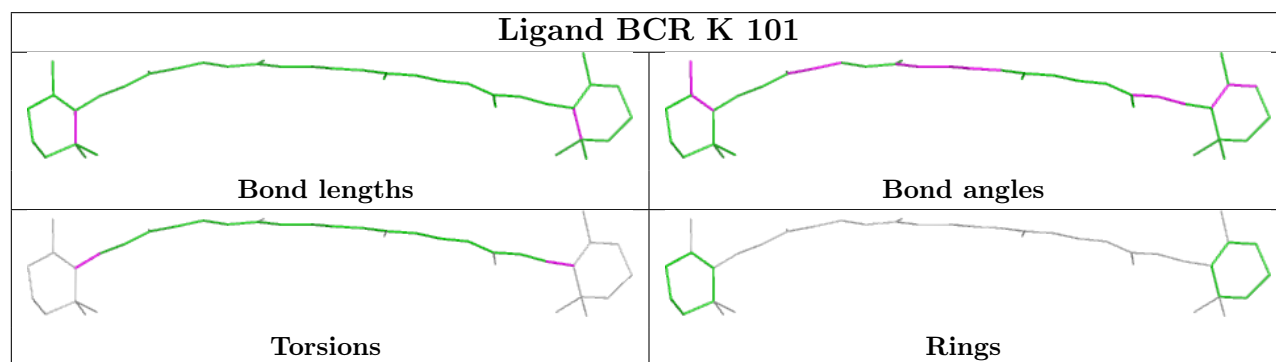
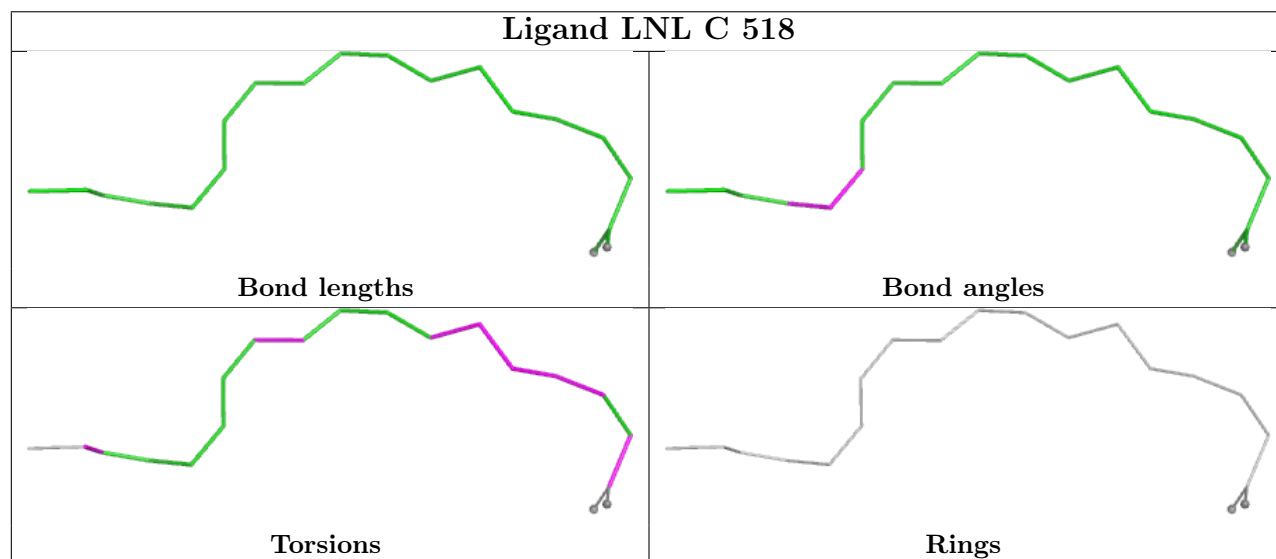
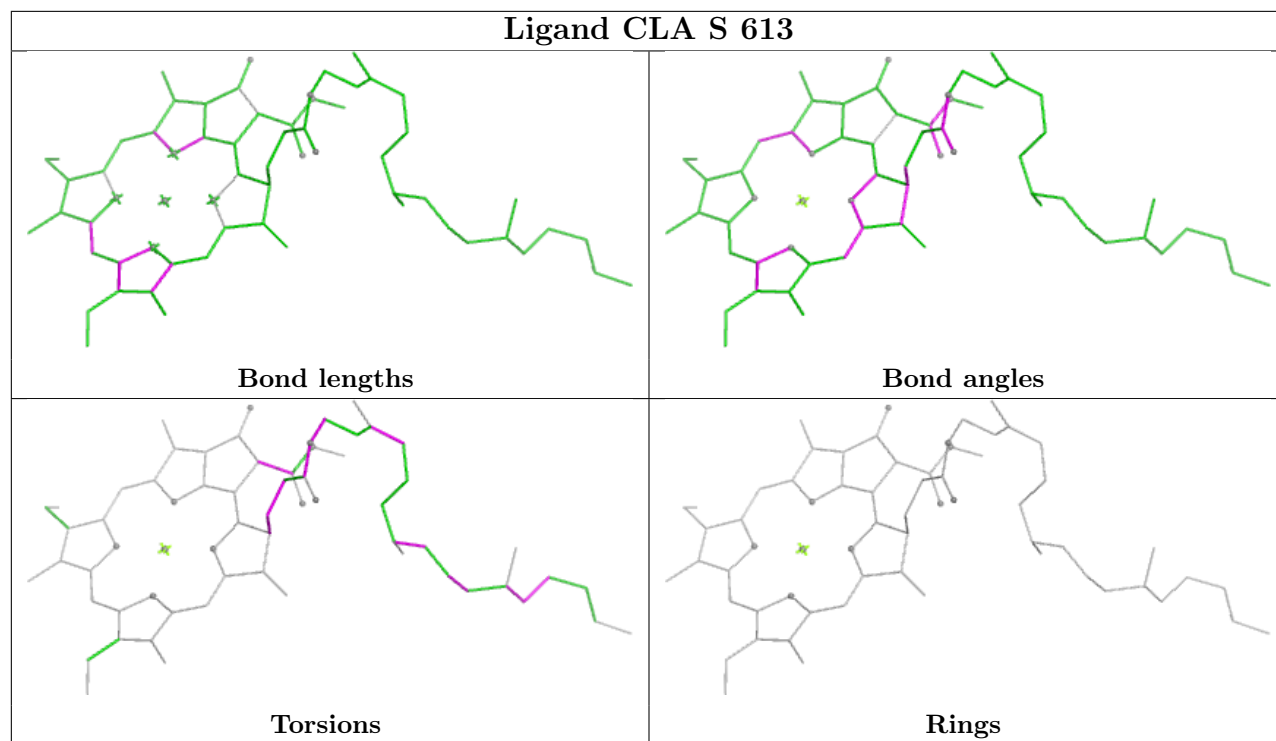
Ligand CLA s 609

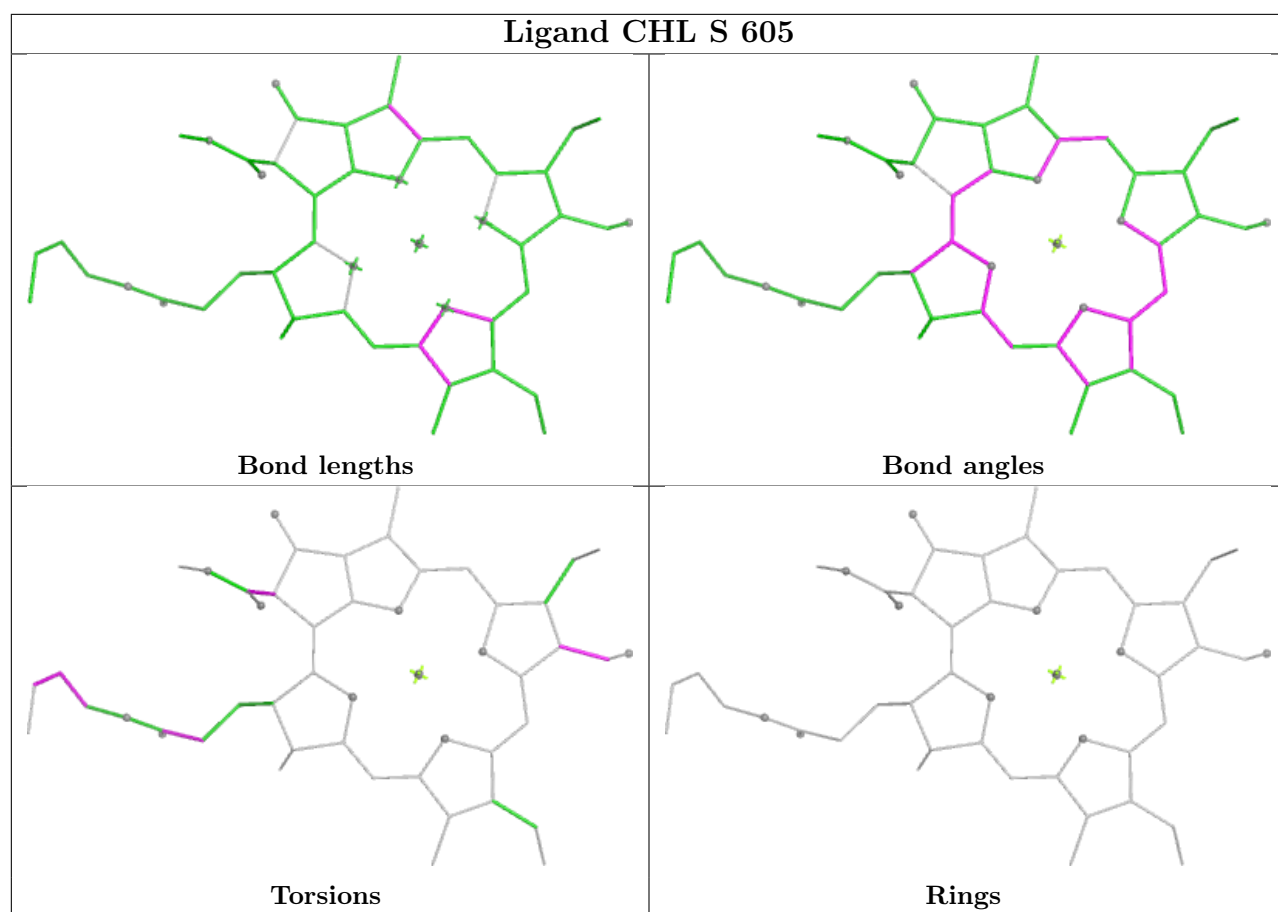


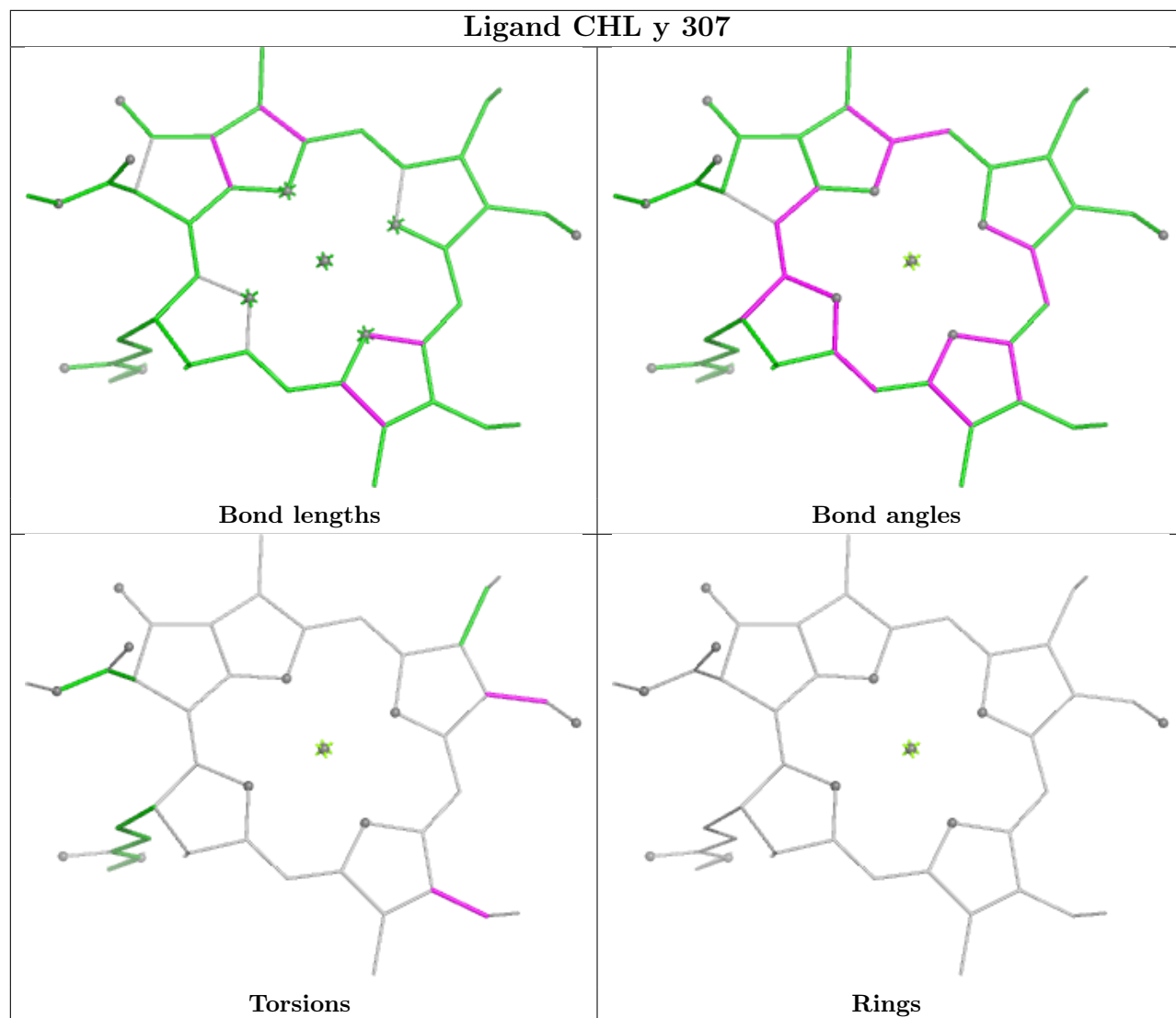


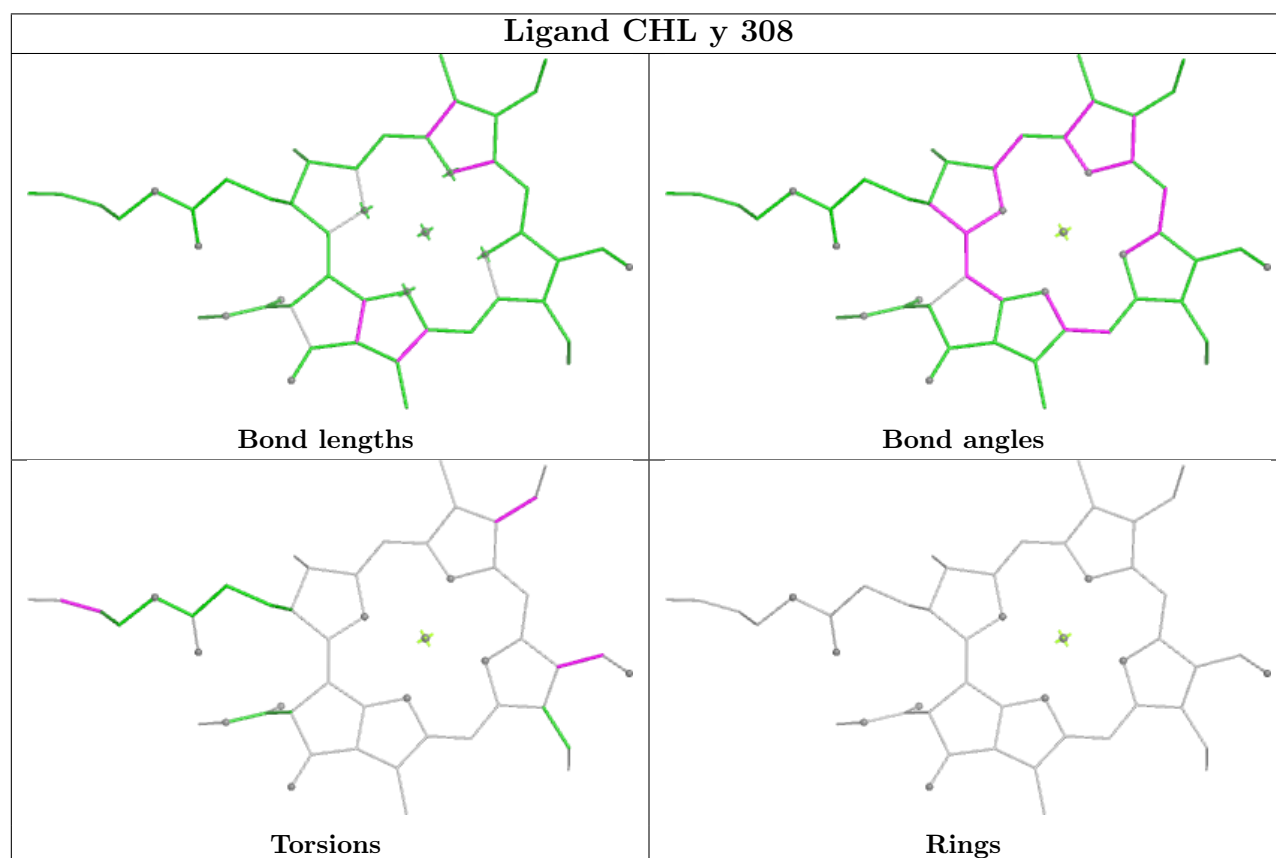
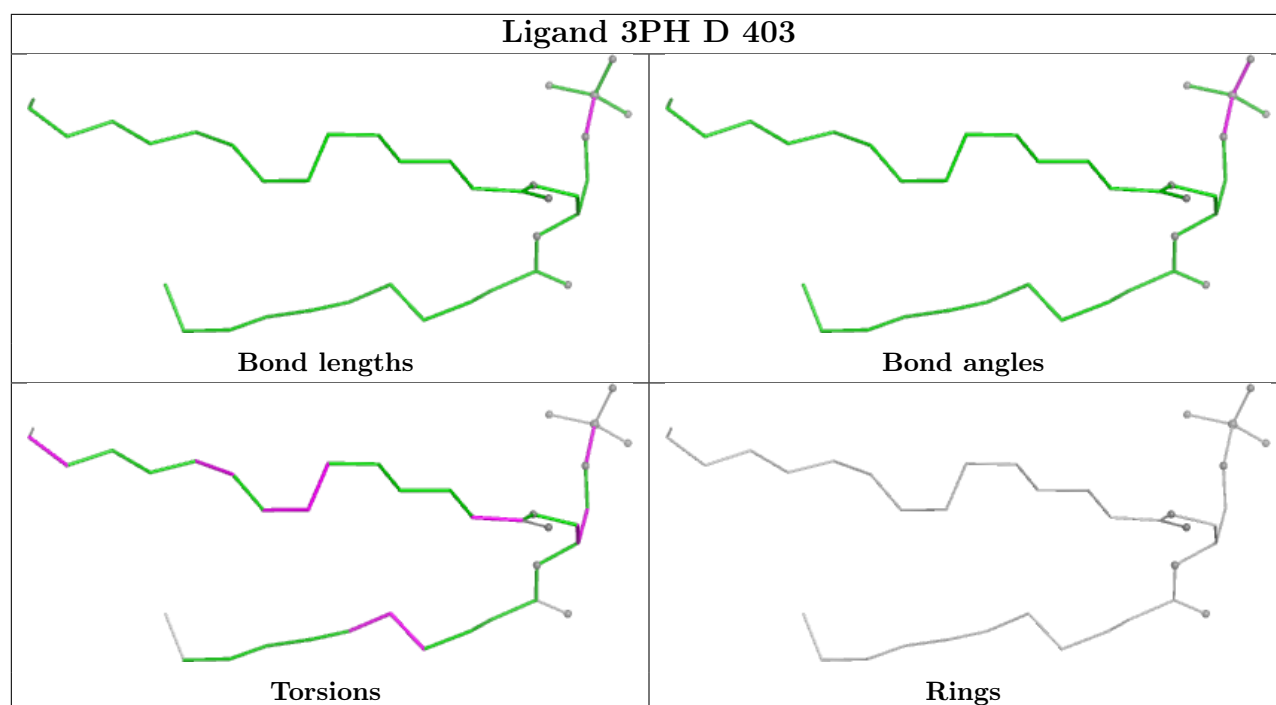


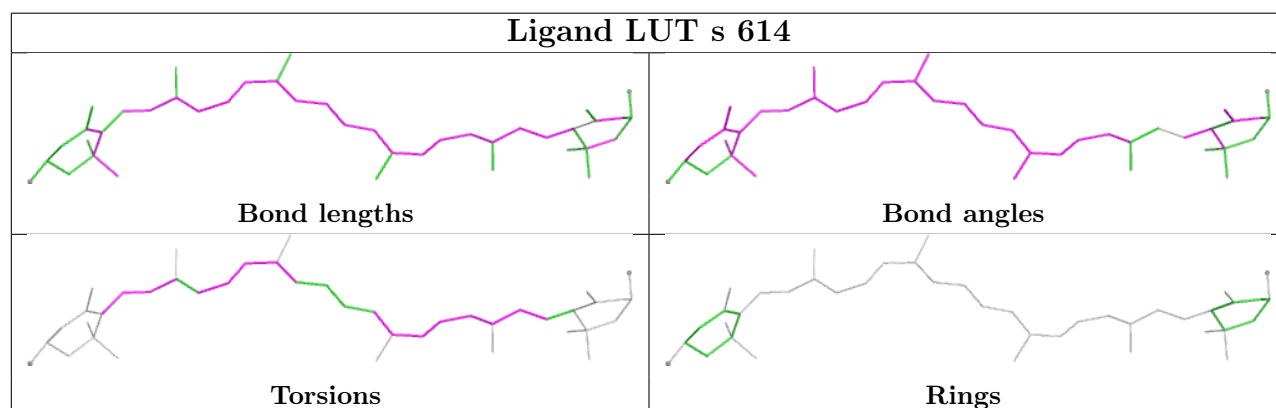
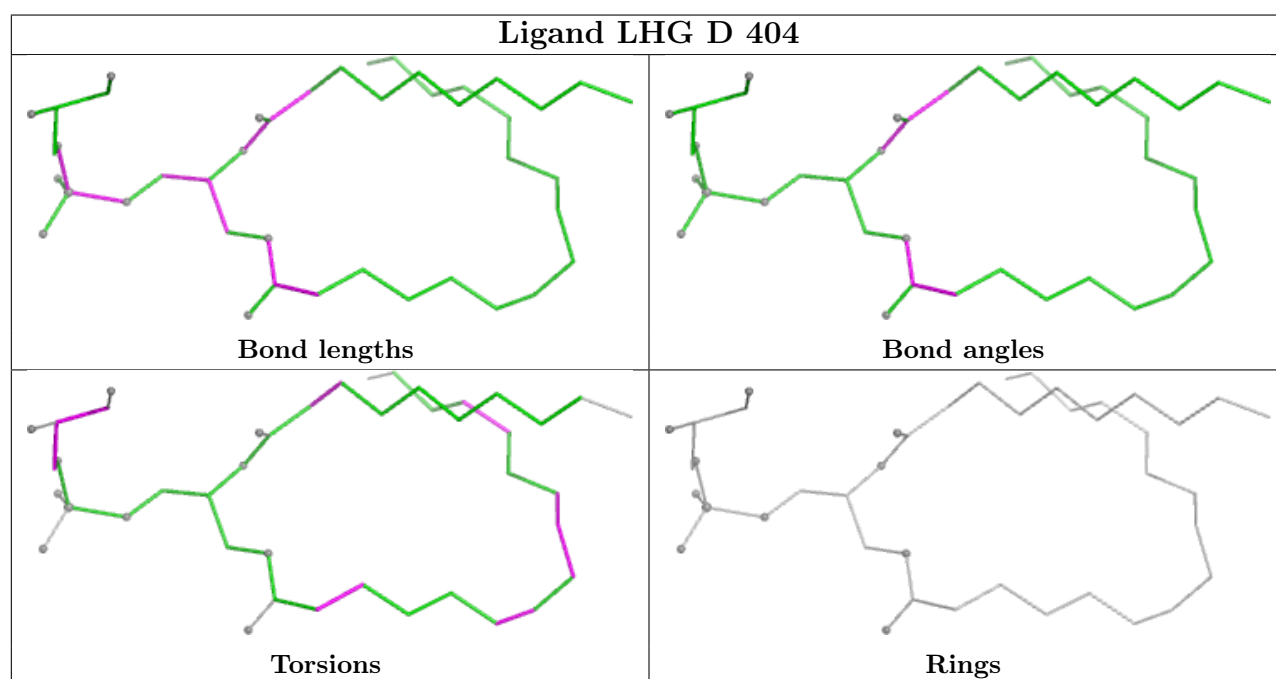
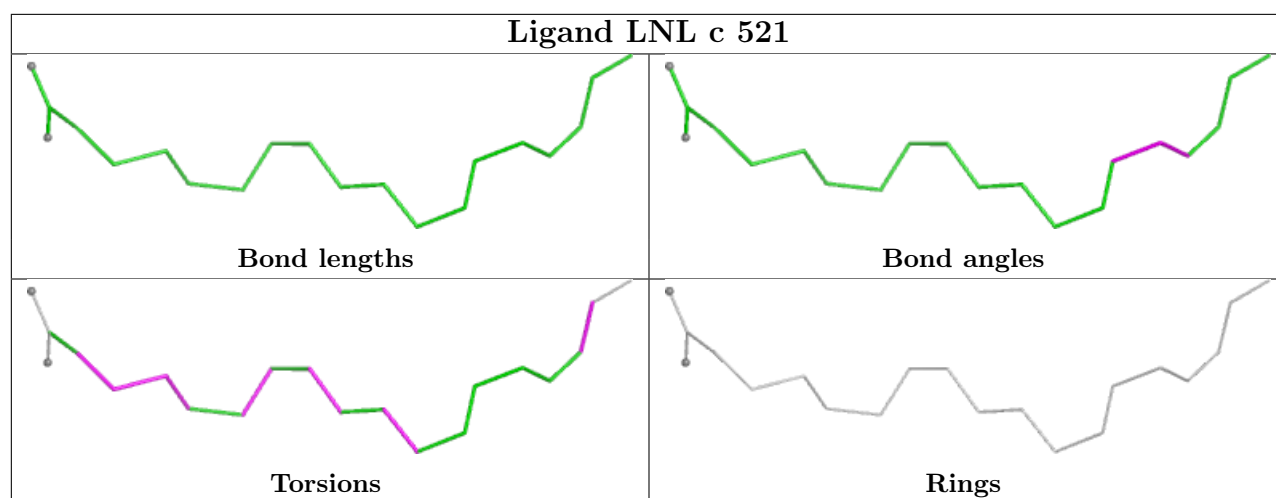


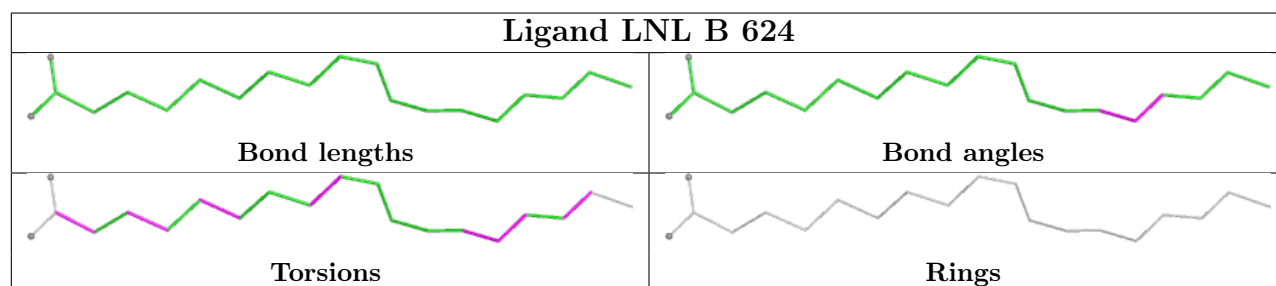
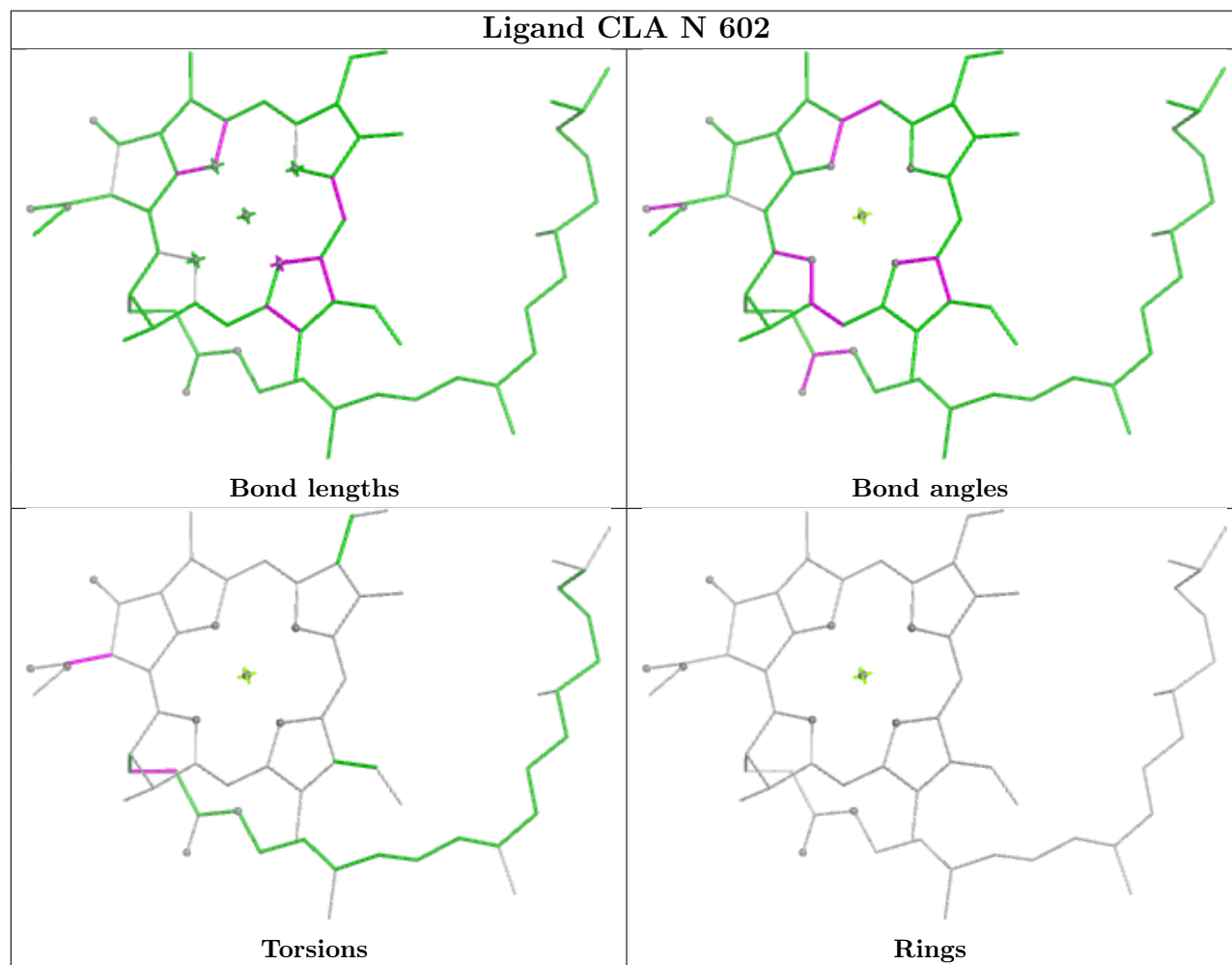
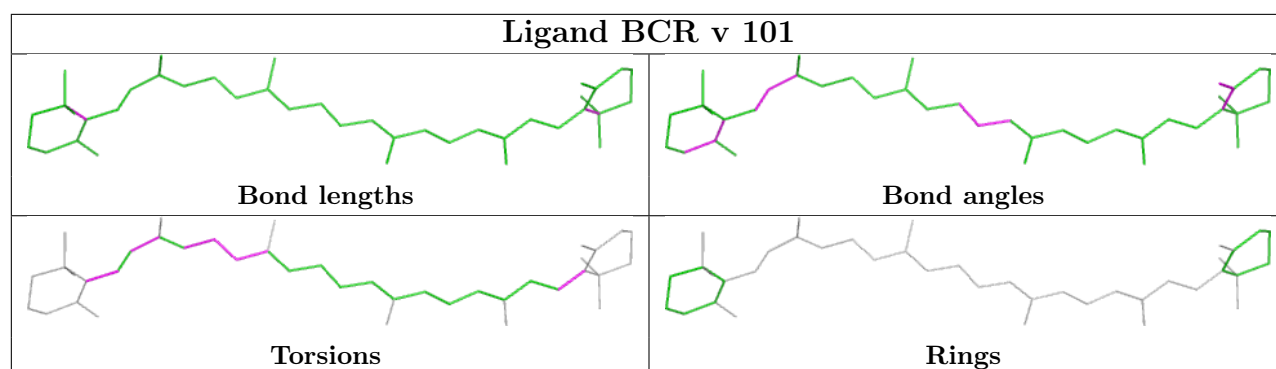


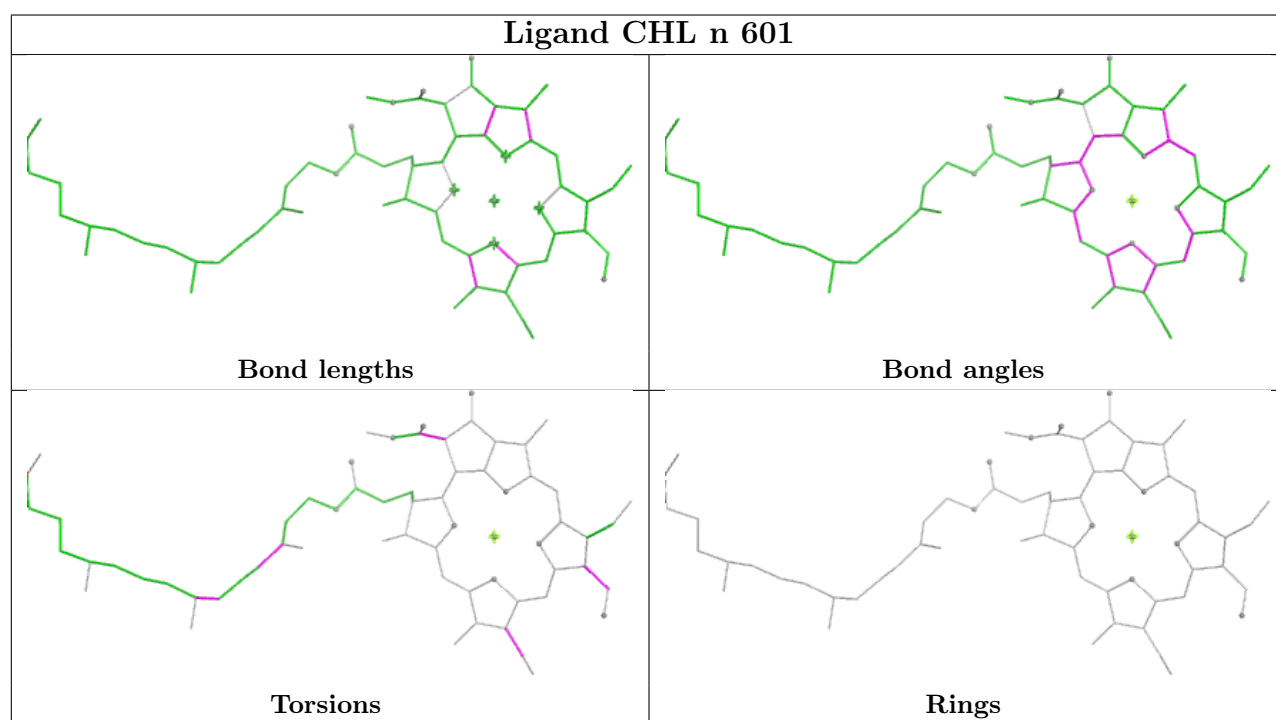
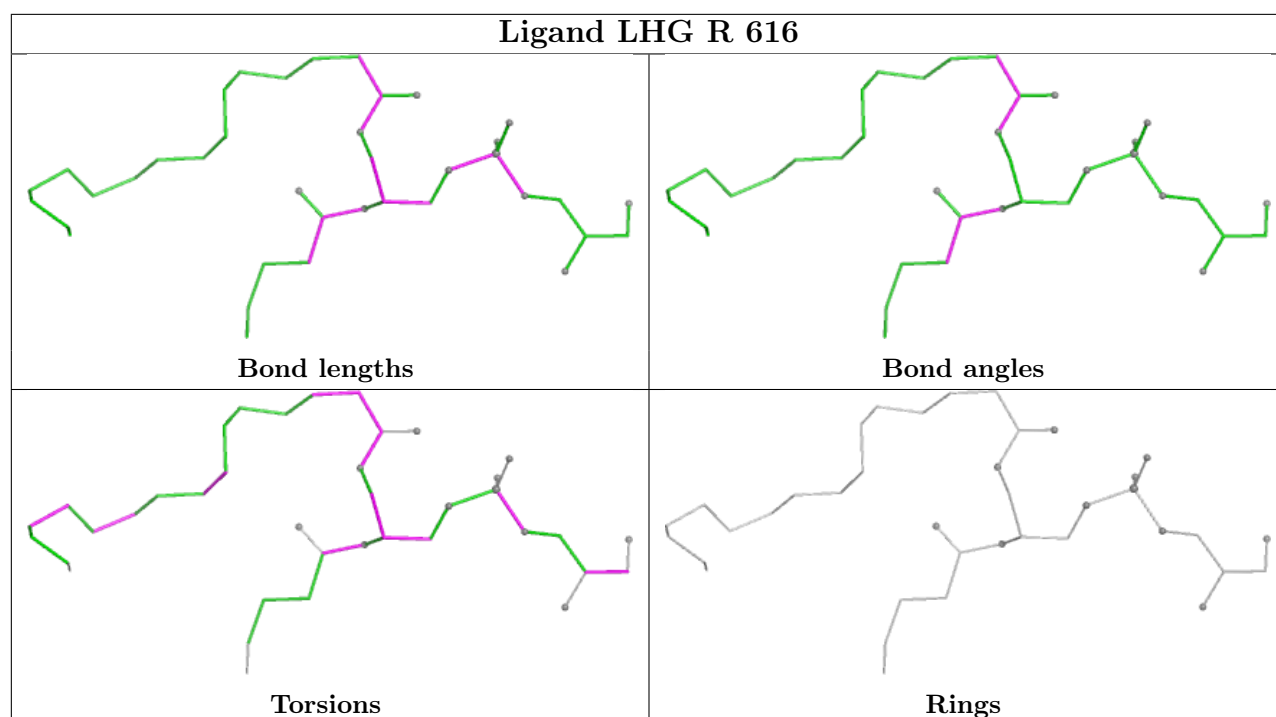


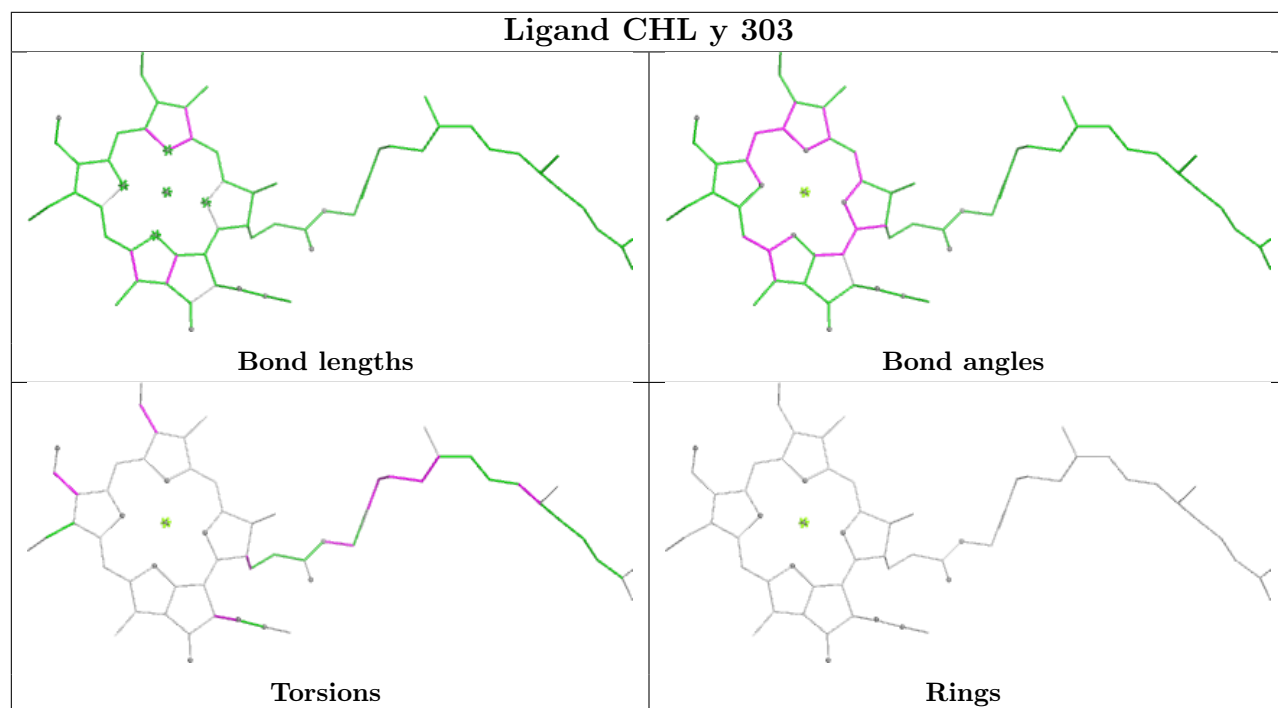
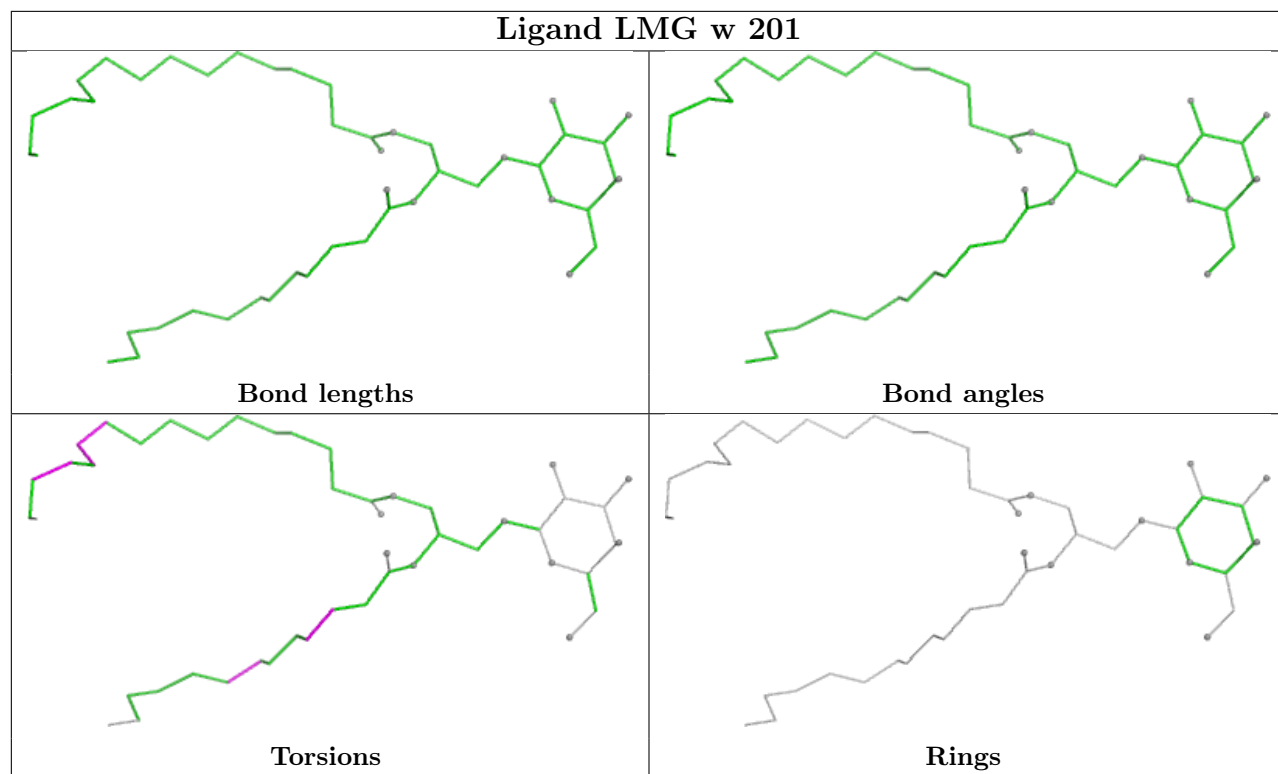


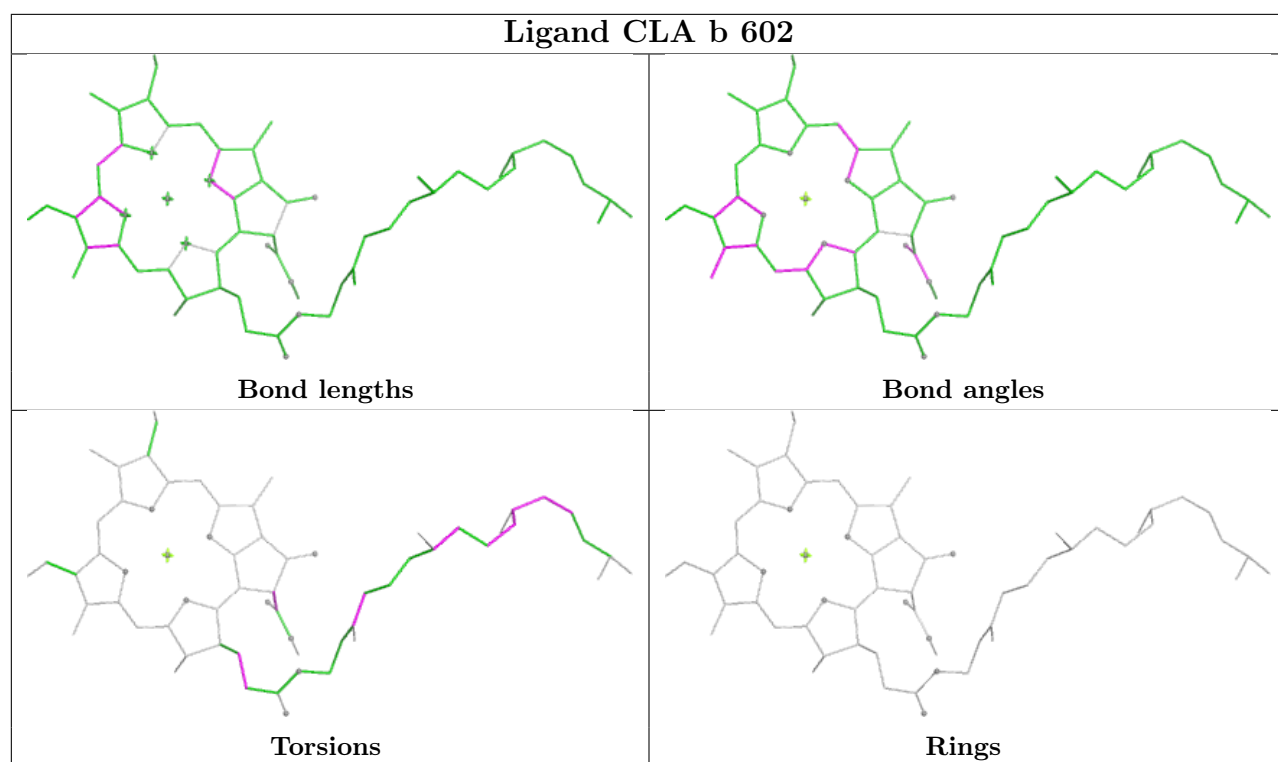


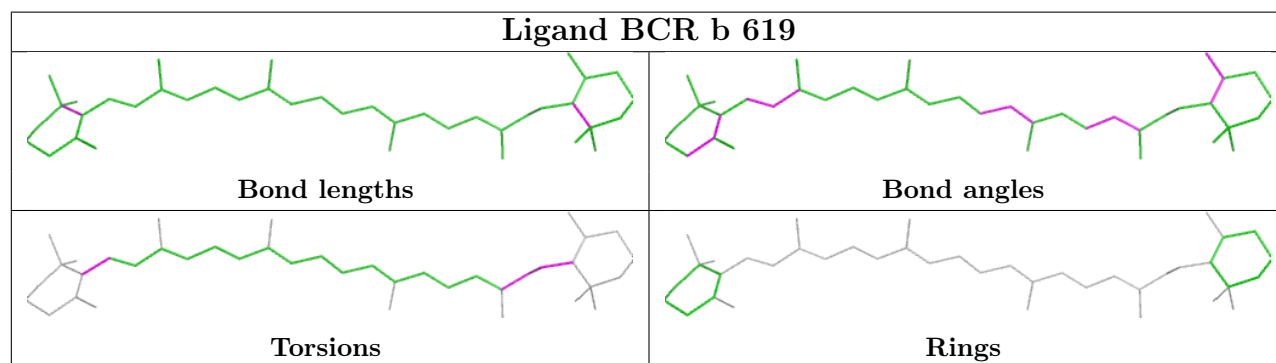
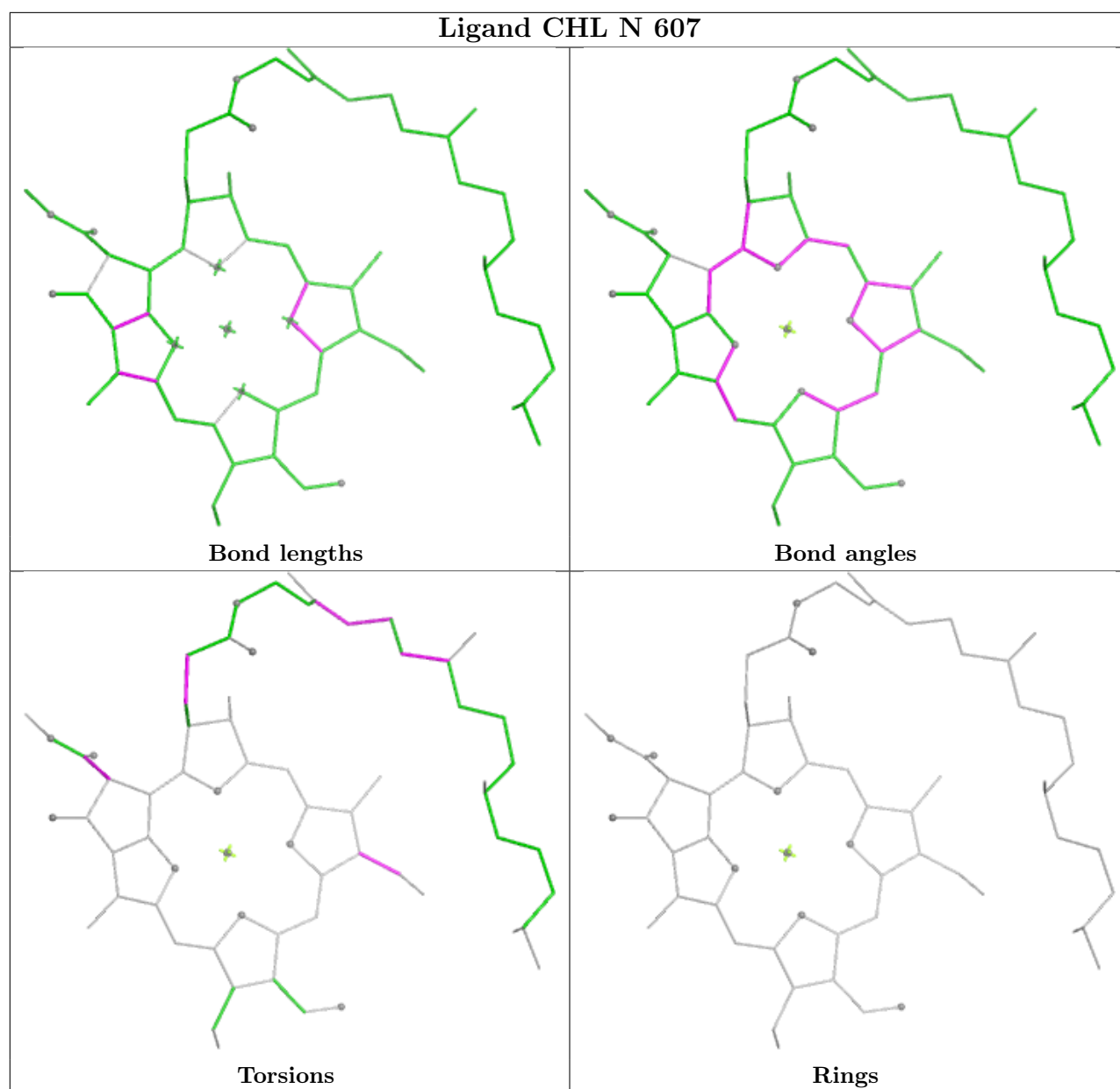


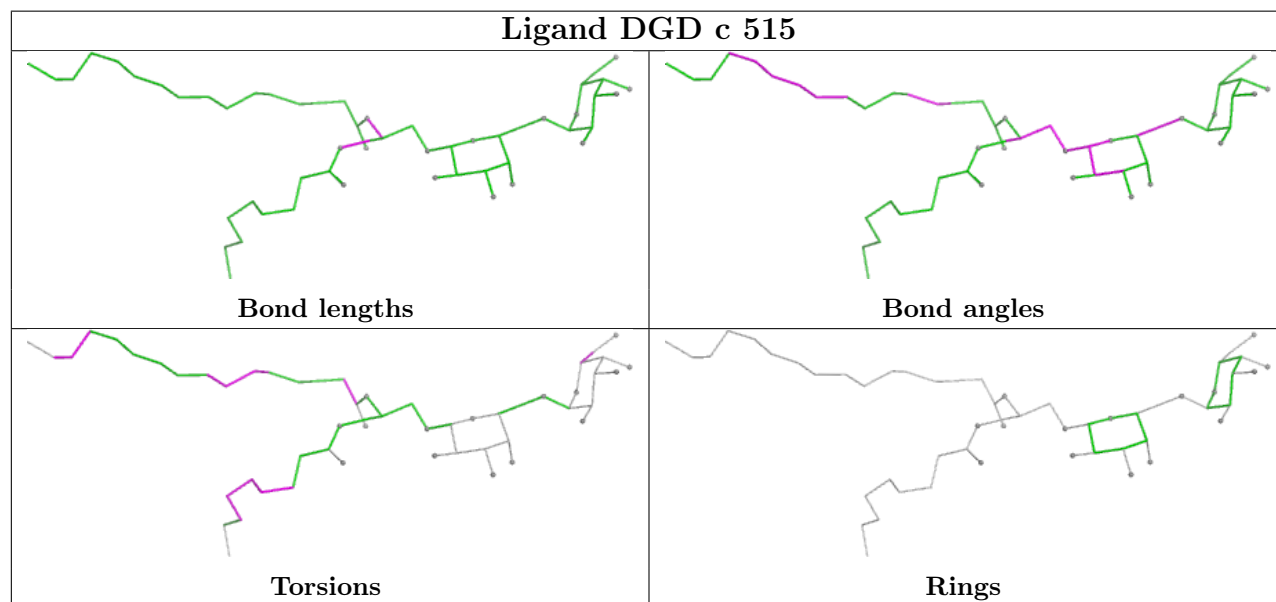
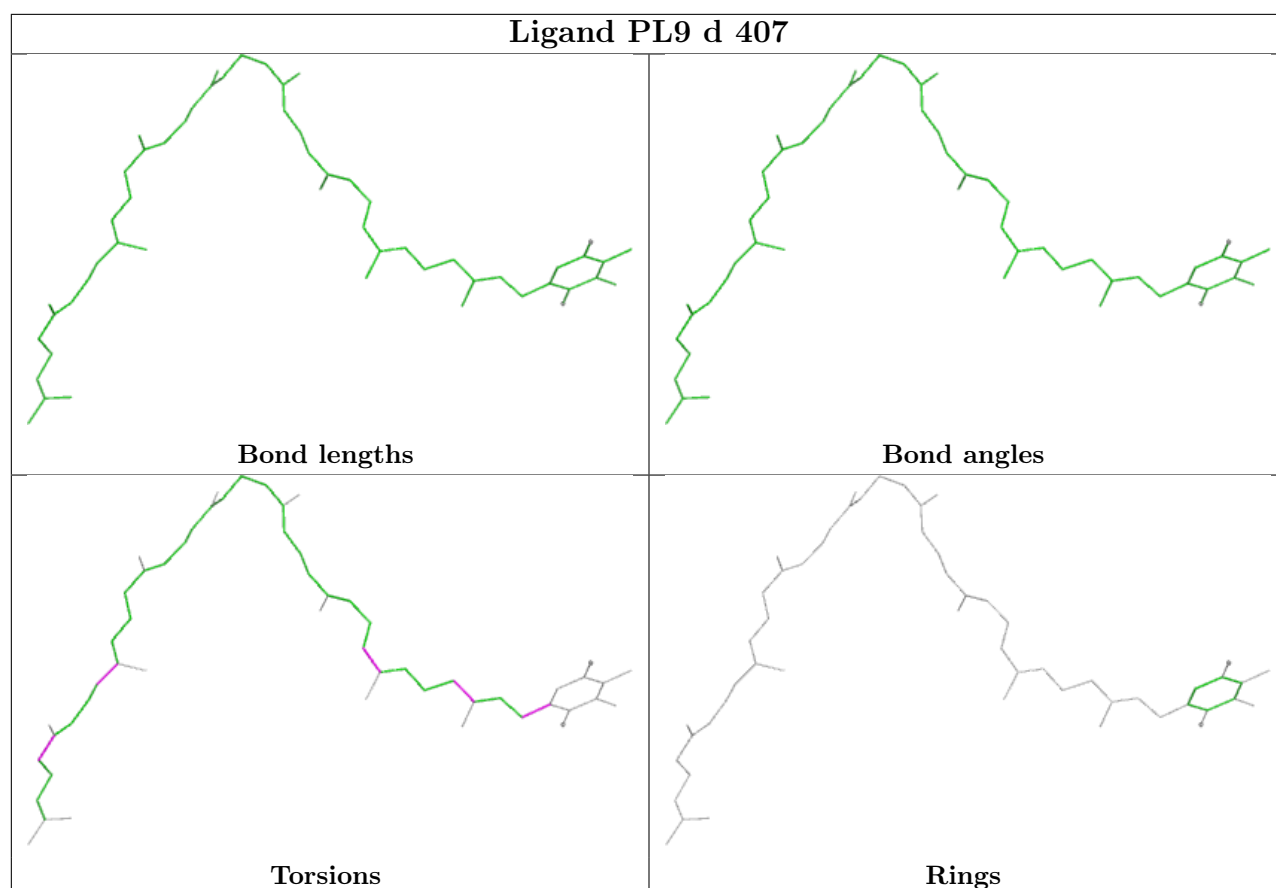


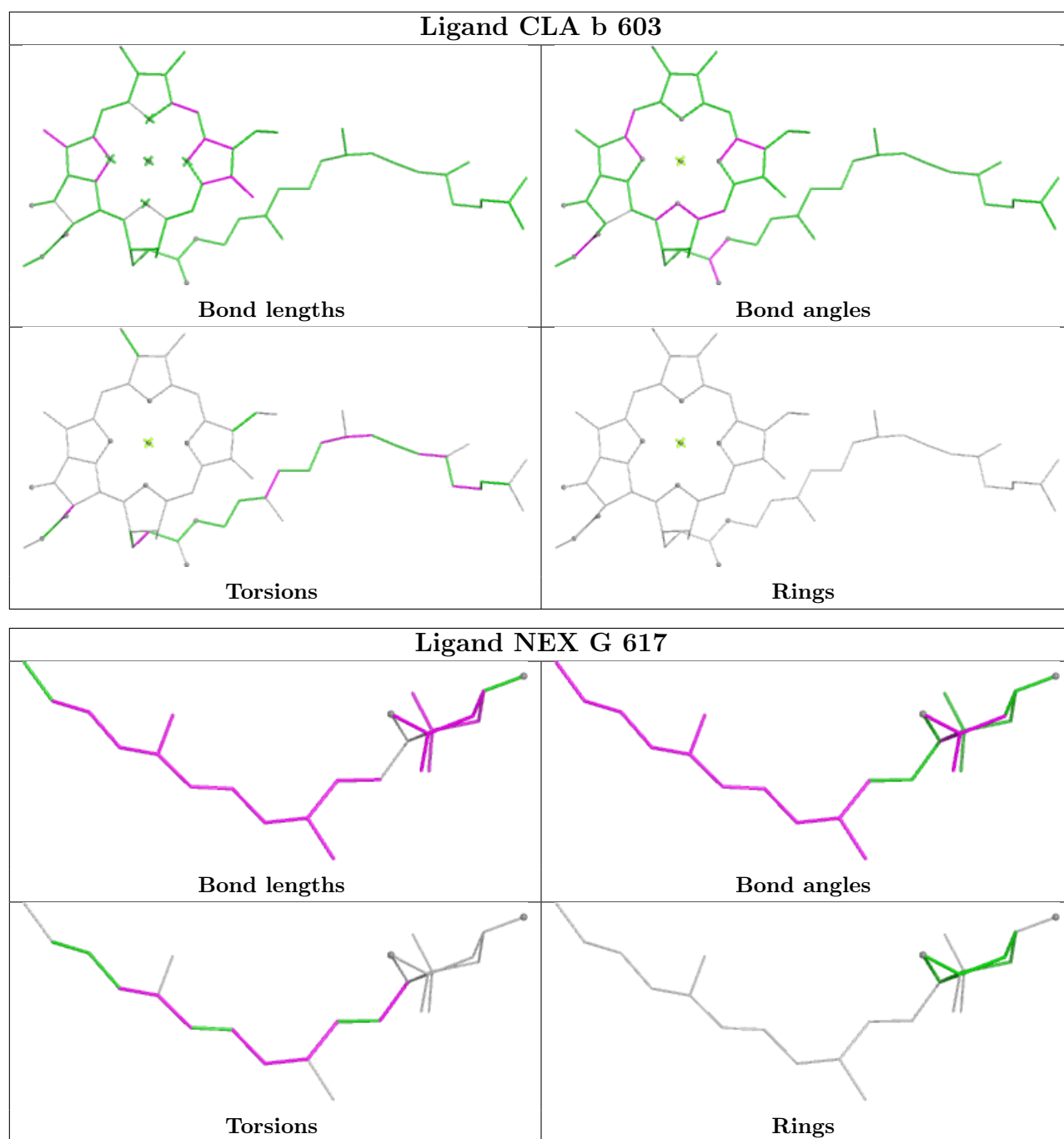


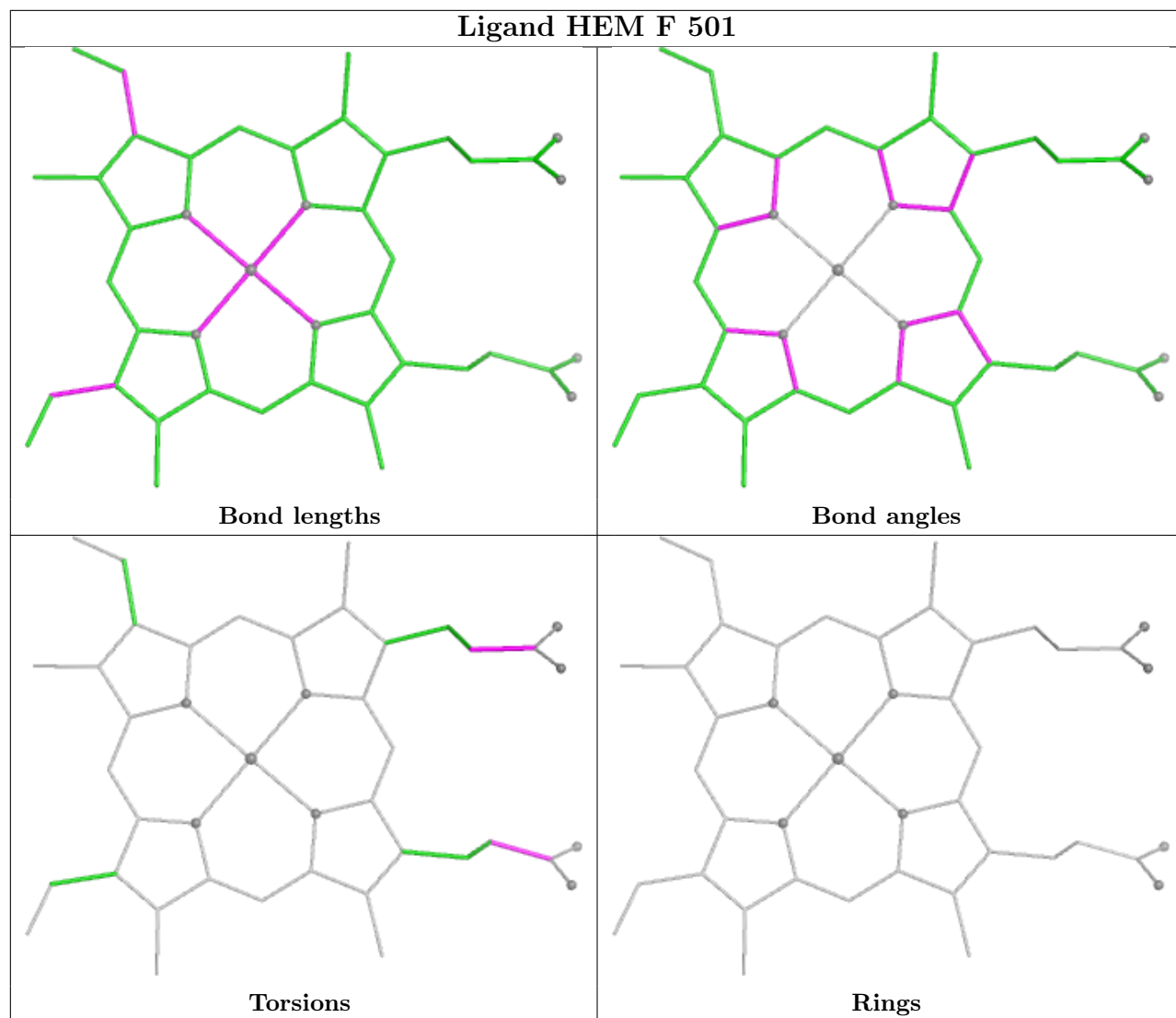




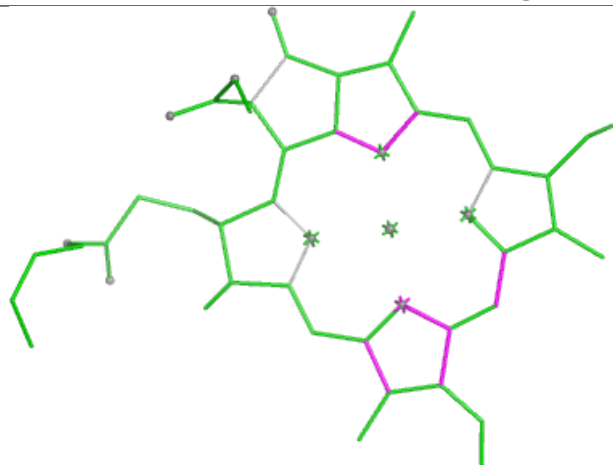




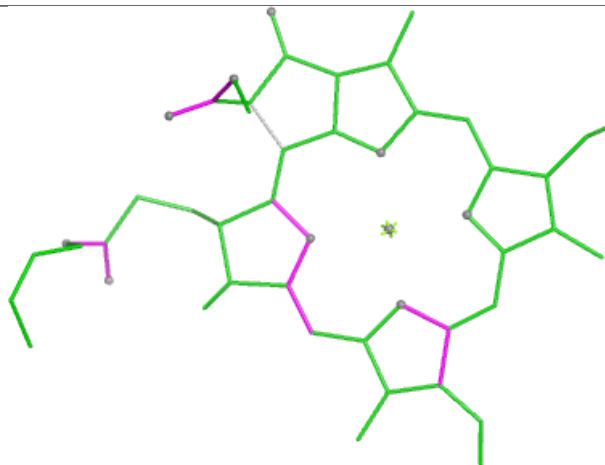




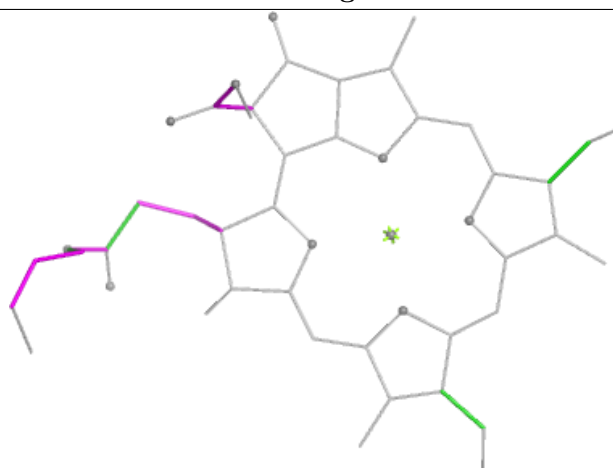
Ligand CLA S 603



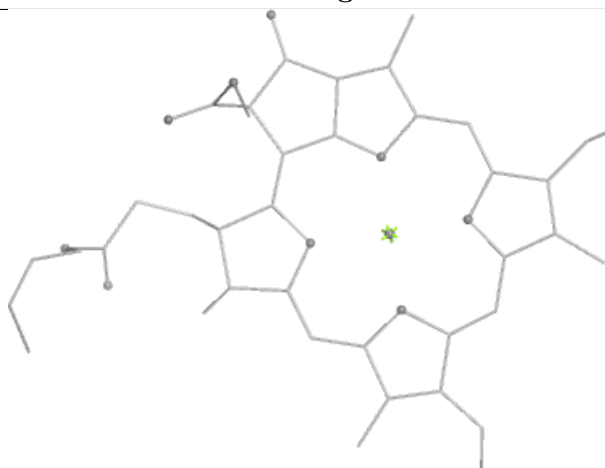
Bond lengths



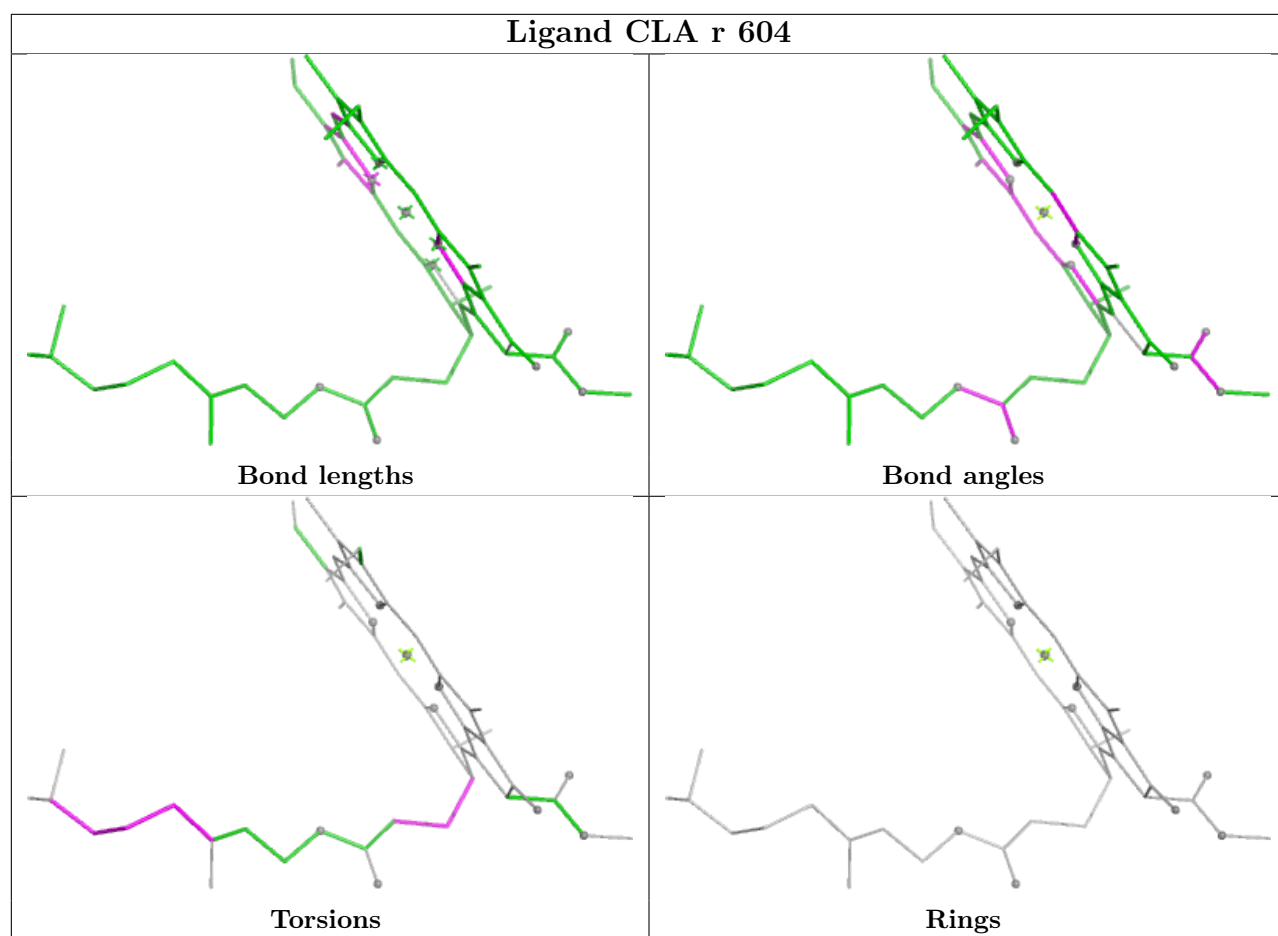
Bond angles



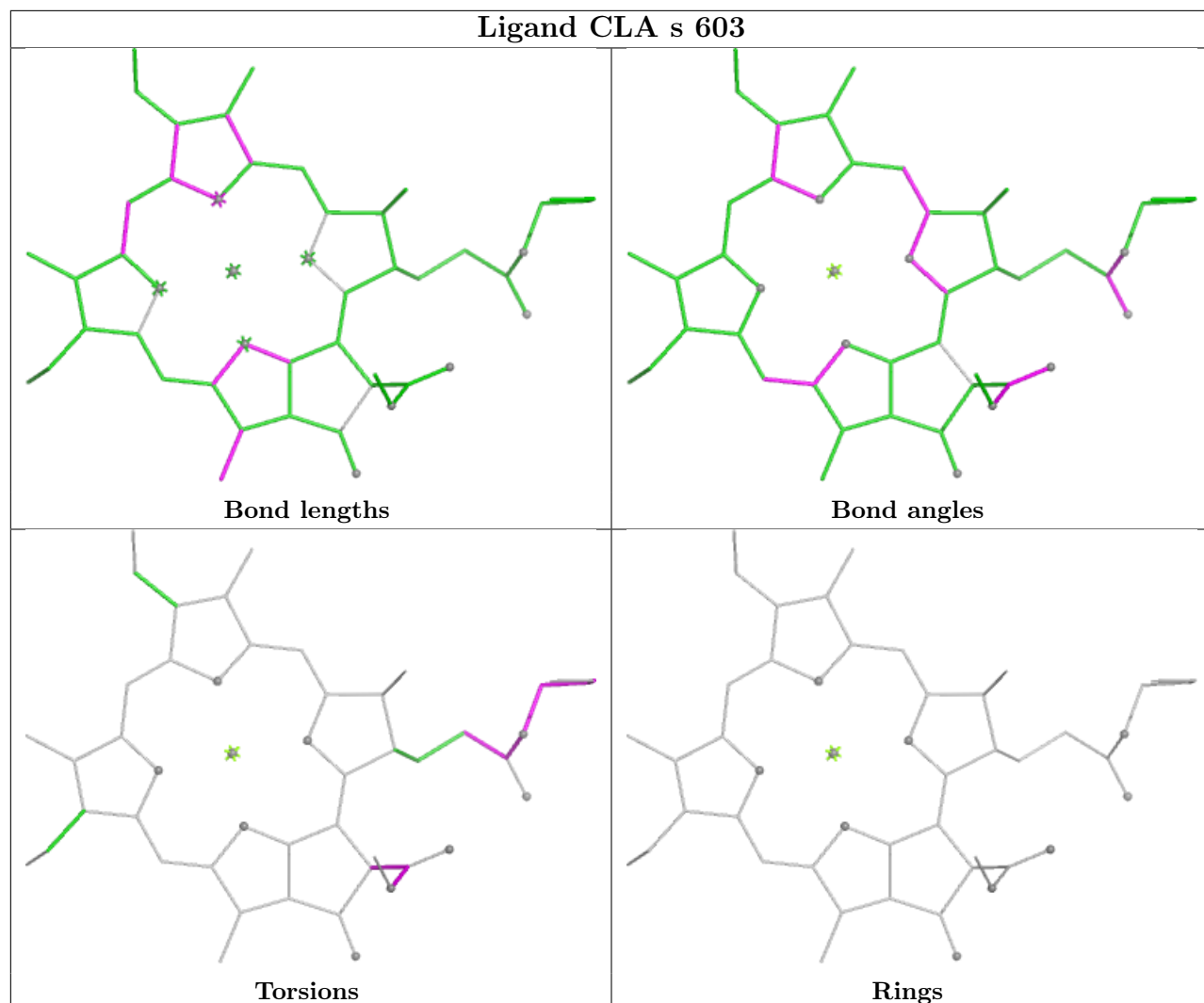
Torsions



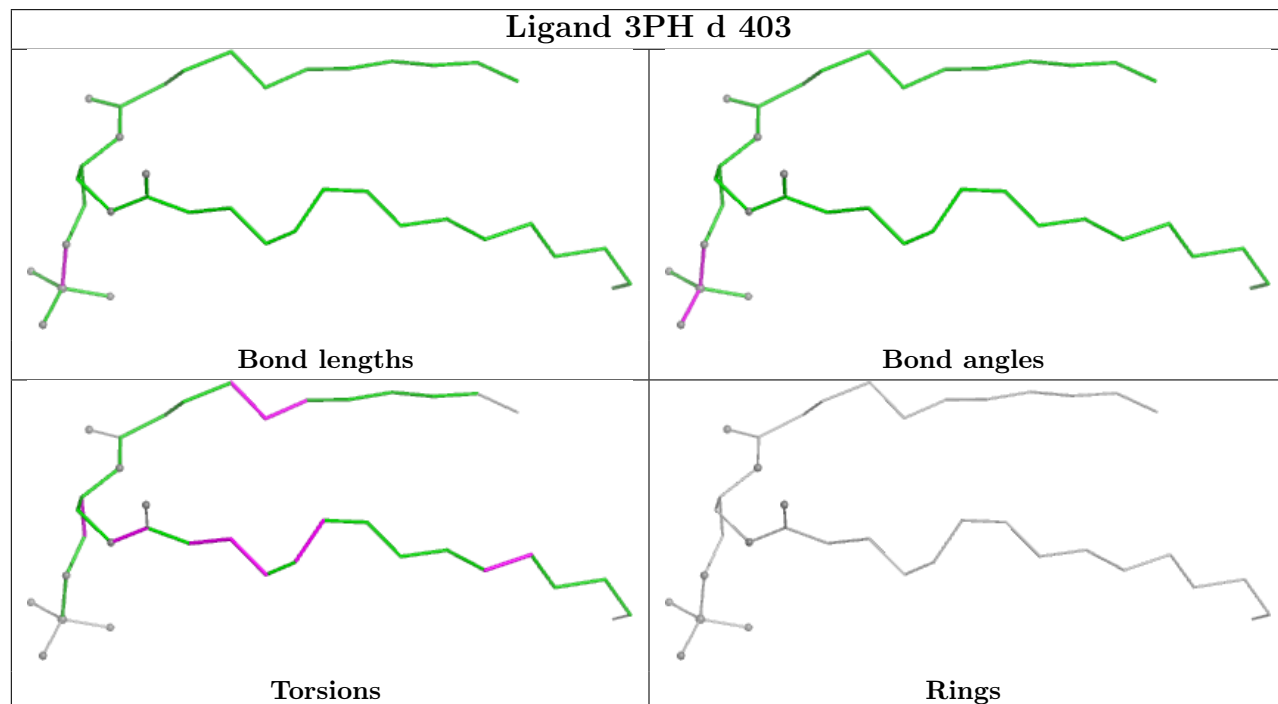
Rings

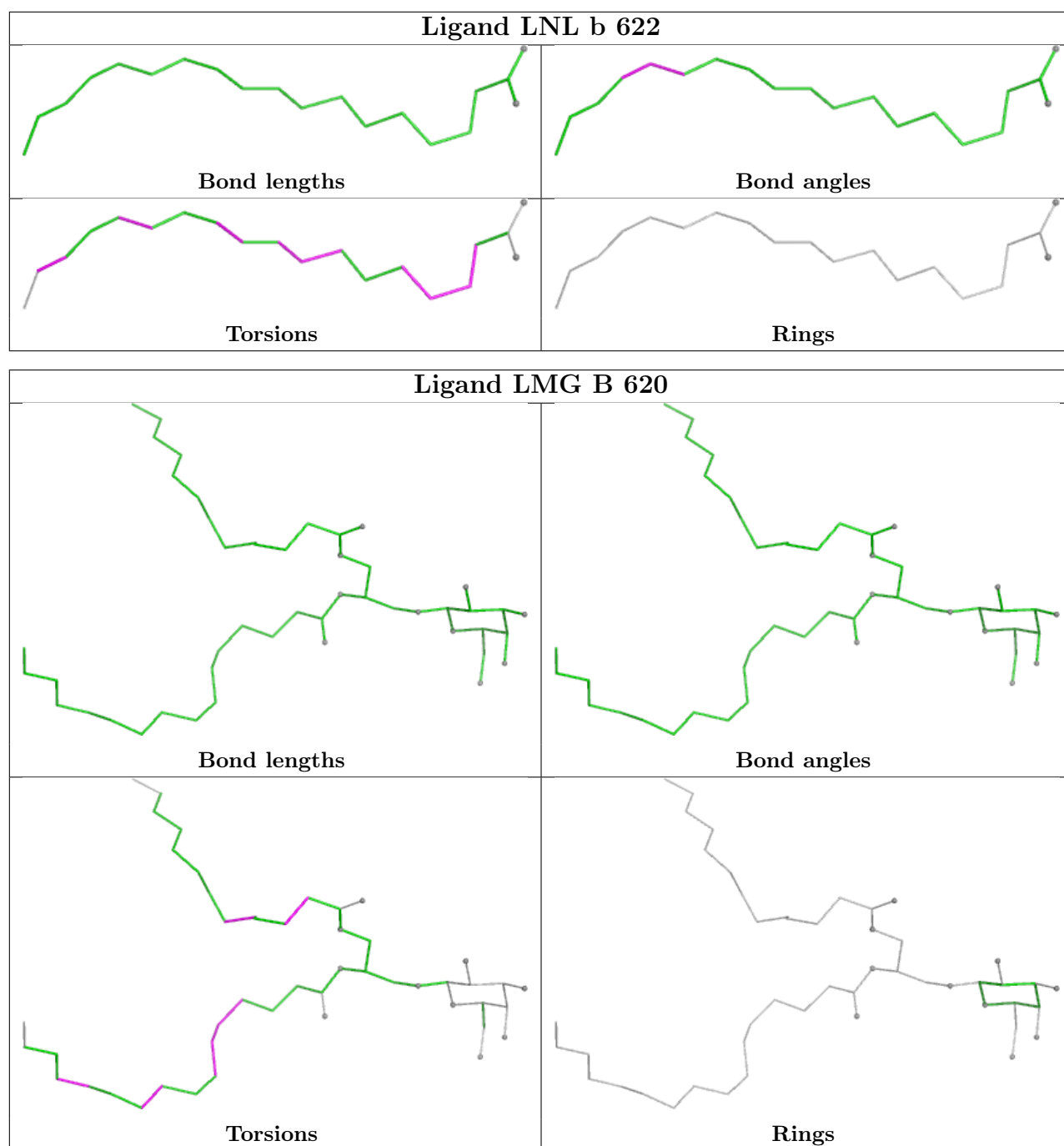


Ligand CLA s 603



Ligand 3PH d 403





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.

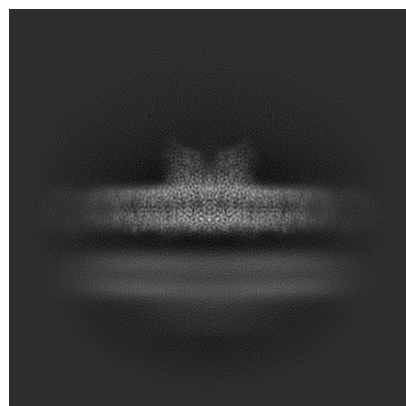
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16389. These allow visual inspection of the internal detail of the map and identification of artifacts.

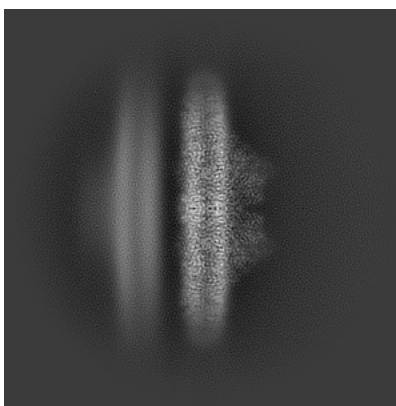
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

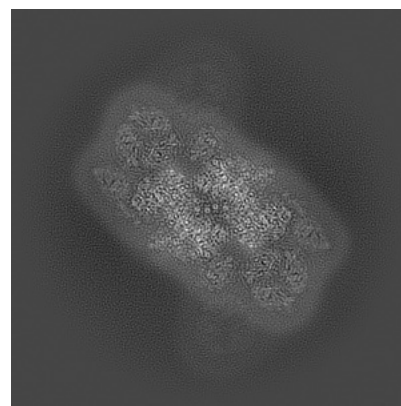
6.1.1 Primary map



X

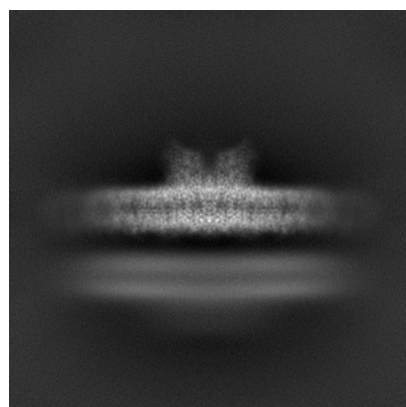


Y

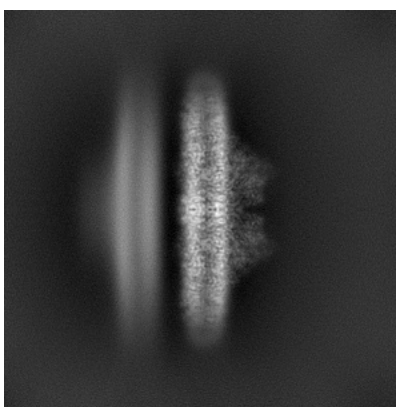


Z

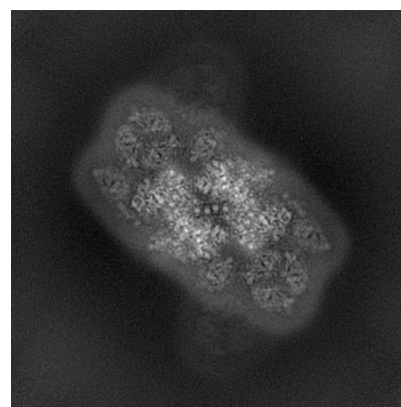
6.1.2 Raw map



X



Y

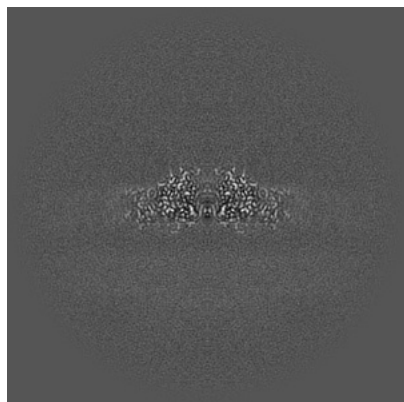


Z

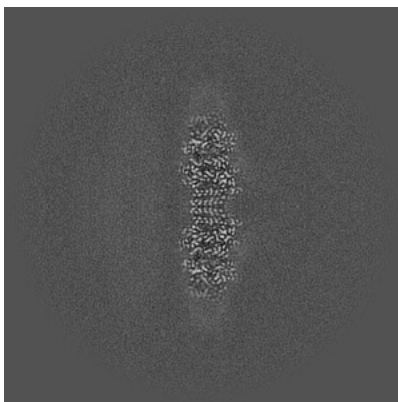
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

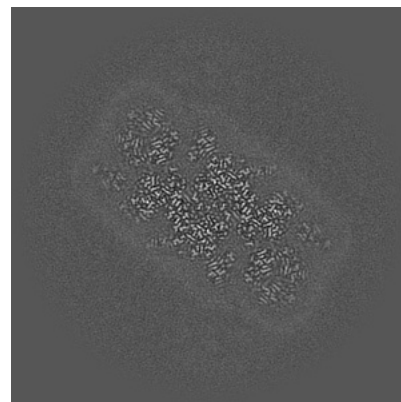
6.2.1 Primary map



X Index: 224

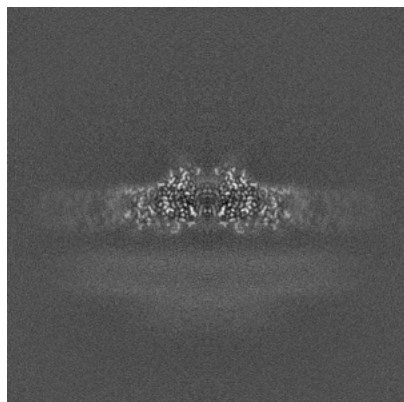


Y Index: 224

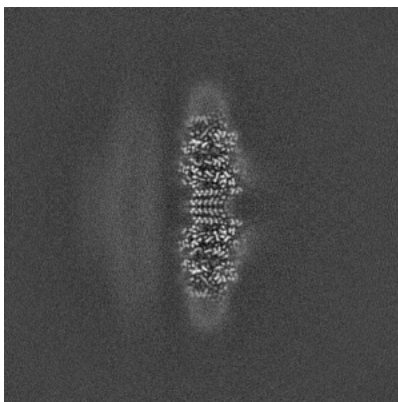


Z Index: 224

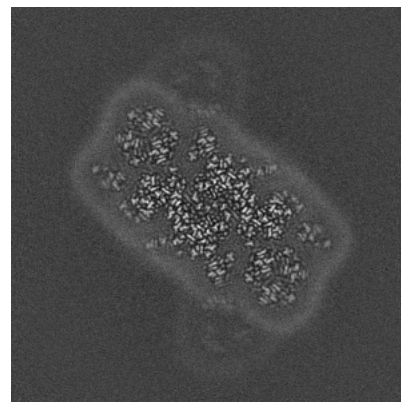
6.2.2 Raw map



X Index: 224



Y Index: 224

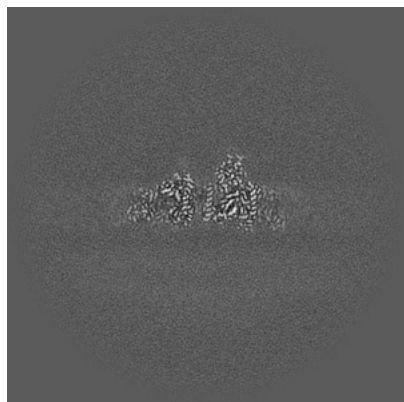


Z Index: 224

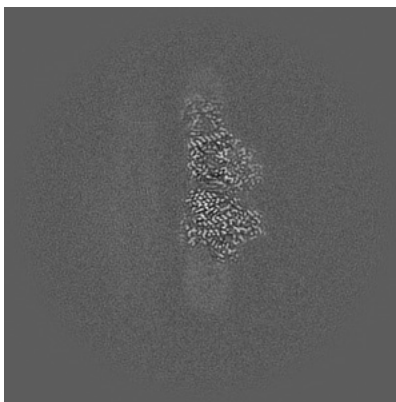
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

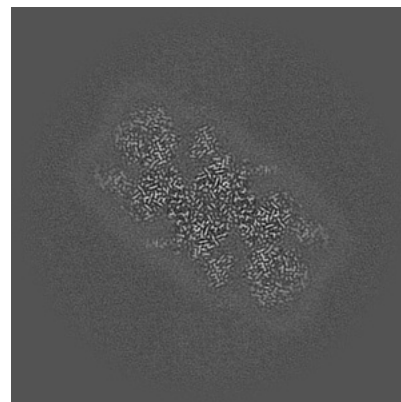
6.3.1 Primary map



X Index: 230

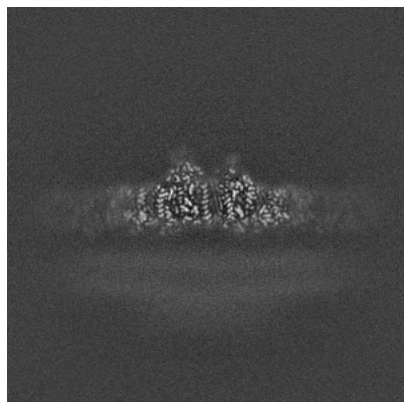


Y Index: 200

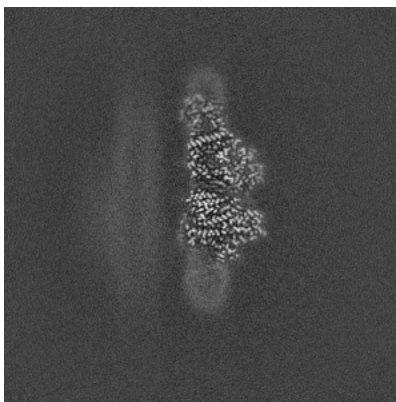


Z Index: 218

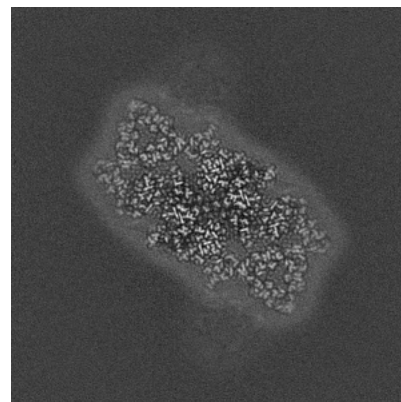
6.3.2 Raw map



X Index: 221



Y Index: 200

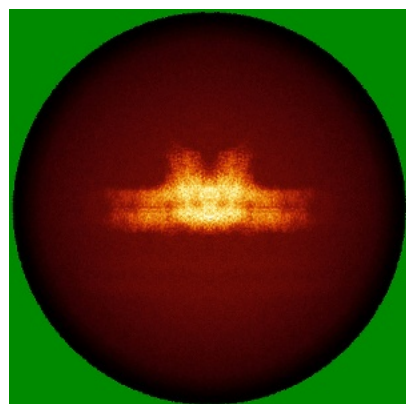


Z Index: 239

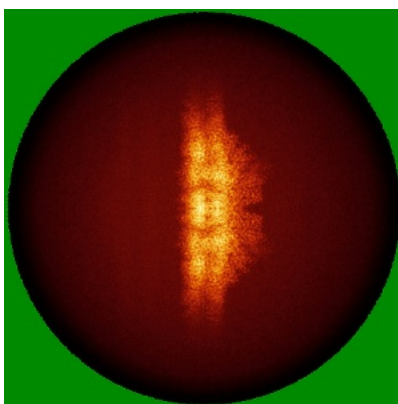
The images above show the largest variance slices of the map in three orthogonal directions.

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

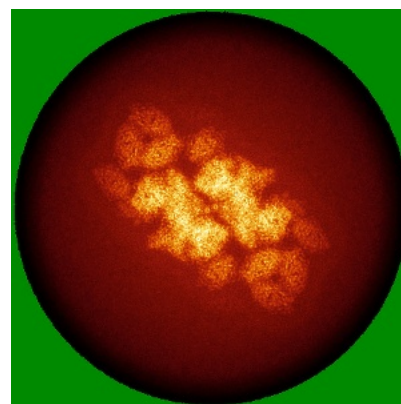
6.4.1 Primary map



X

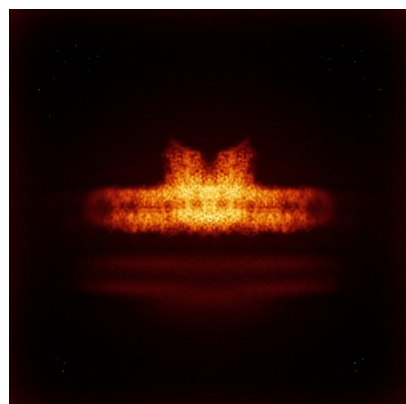


Y

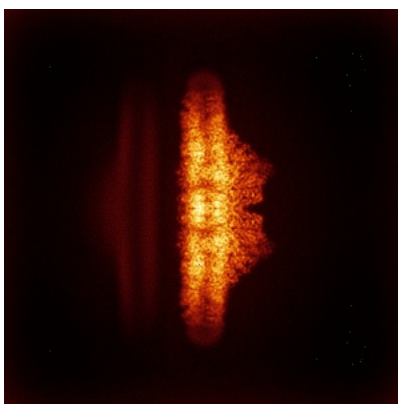


Z

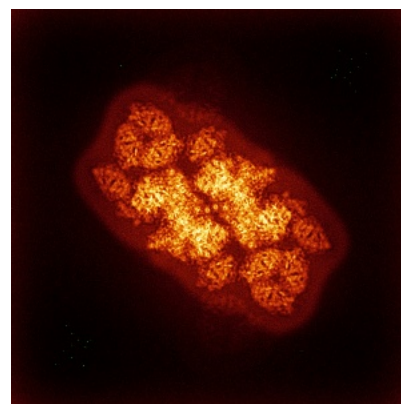
6.4.2 Raw map



X



Y

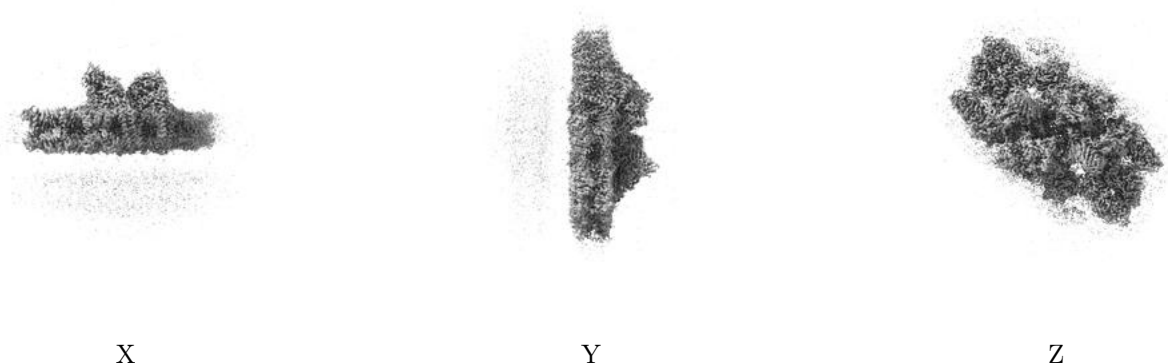


Z

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 0.886. 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.

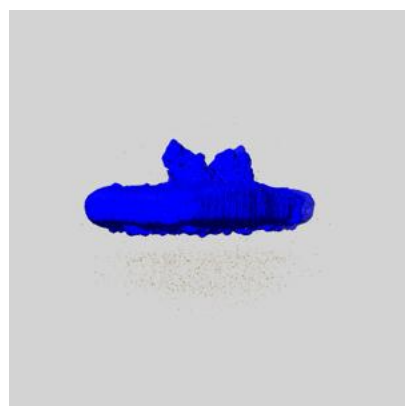
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

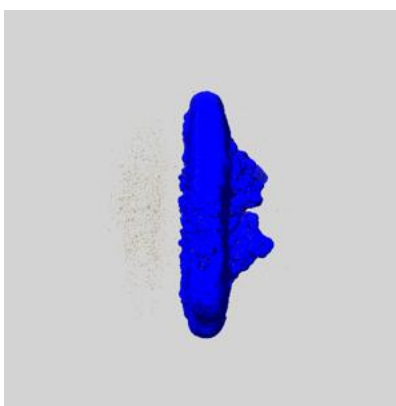
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

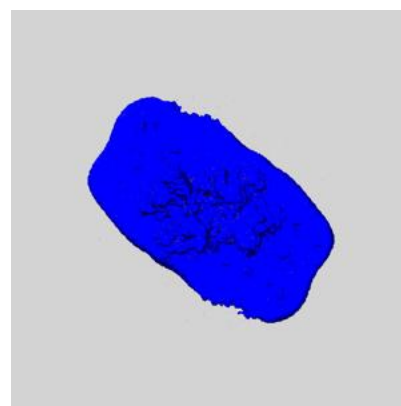
6.6.1 emd_16389_msk_1.map [i](#)



X



Y

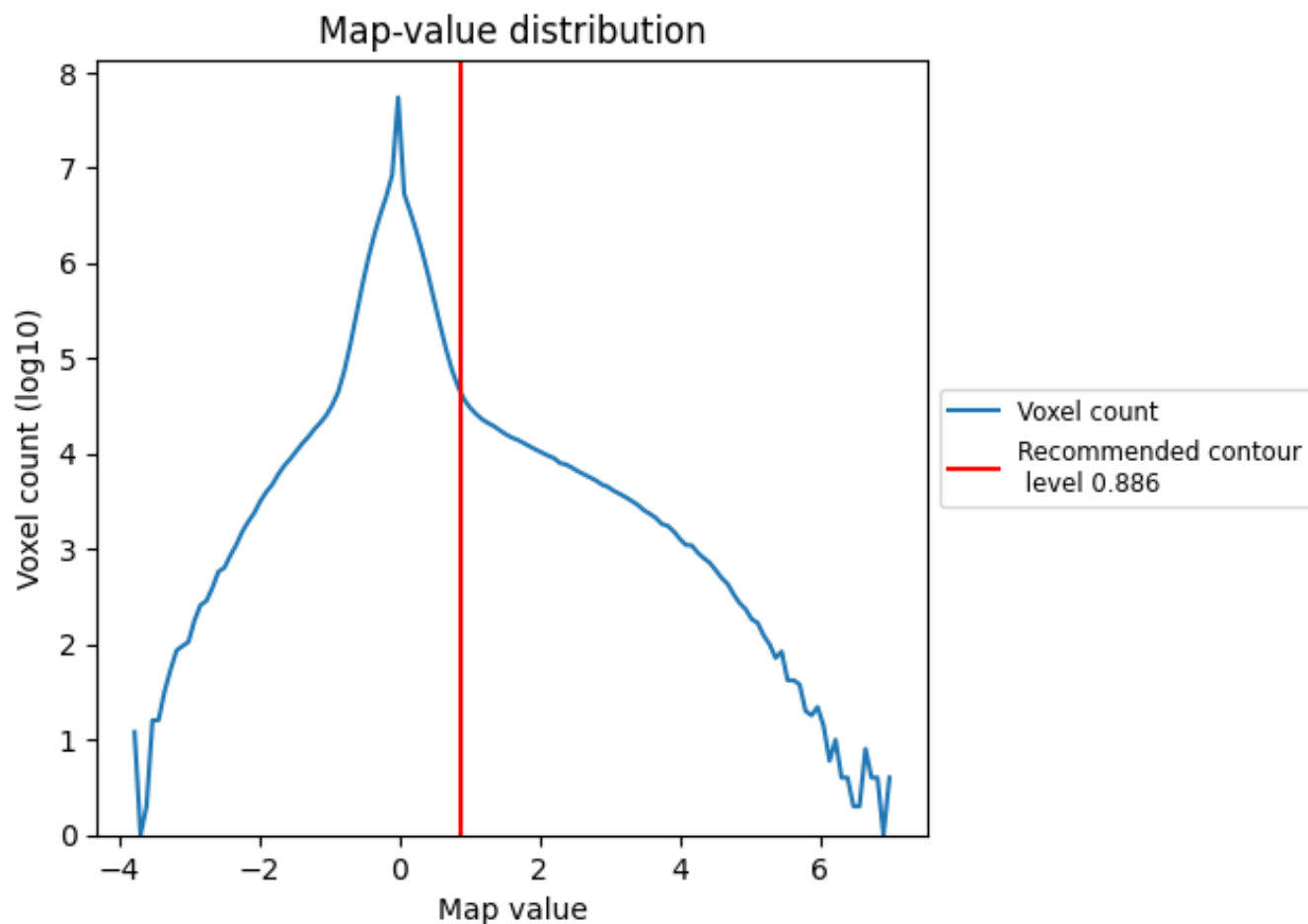


Z

7 Map analysis [i](#)

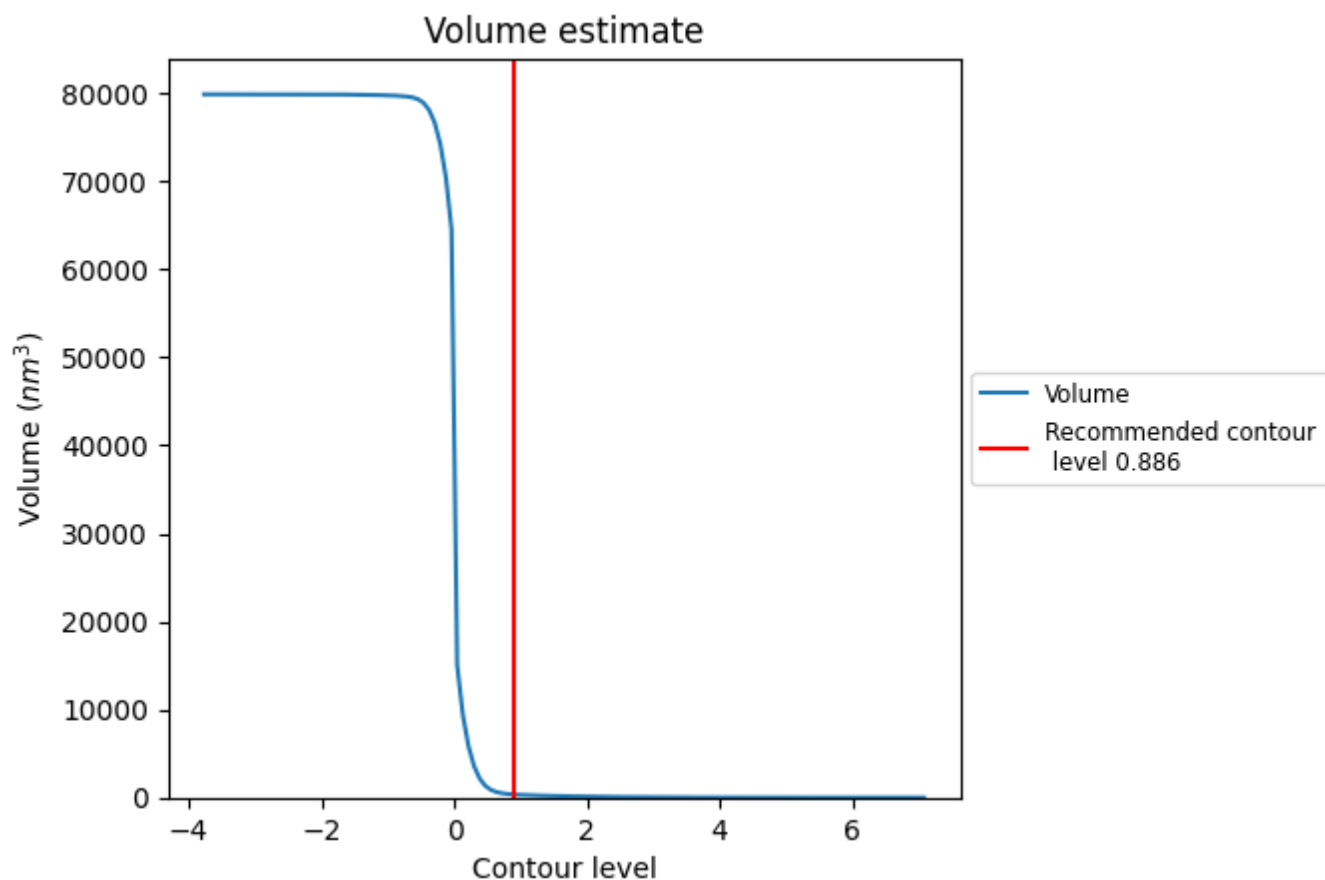
This section contains the results of statistical analysis of the map.

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.

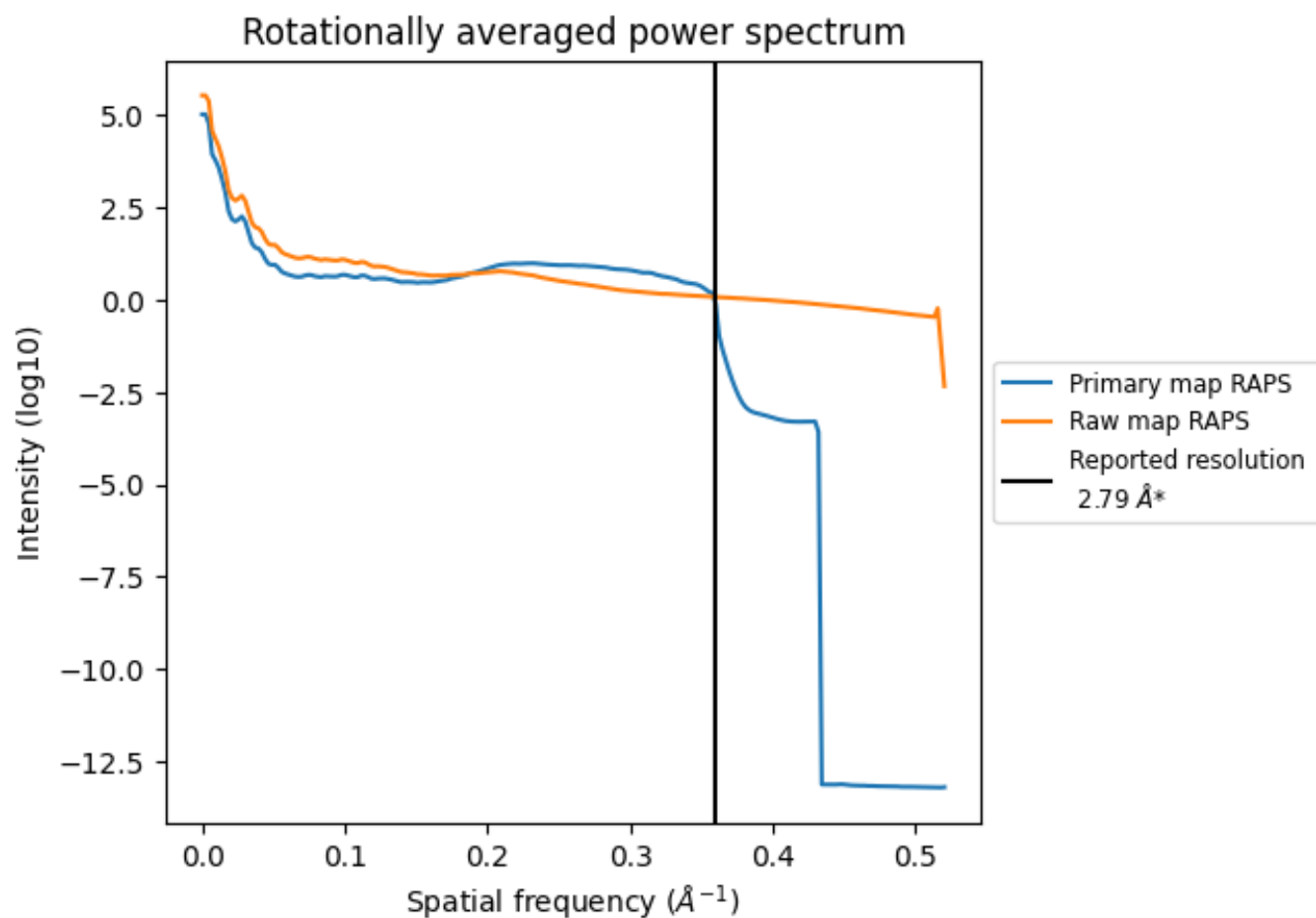
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 356 nm³; this corresponds to an approximate mass of 322 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 ⓘ

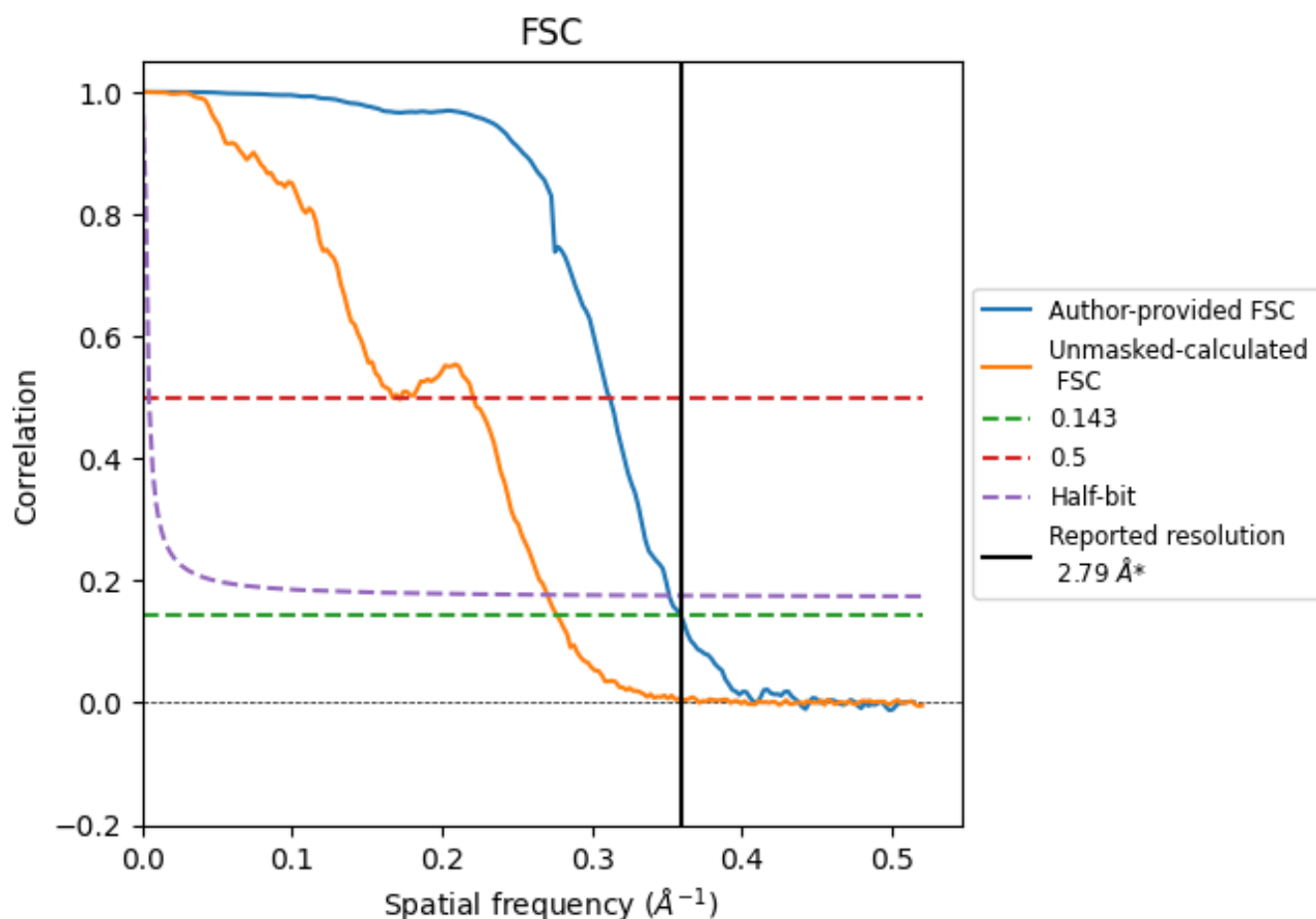


*Reported resolution corresponds to spatial frequency of 0.359 $\text{\AA}^{-1}$

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 0.359 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

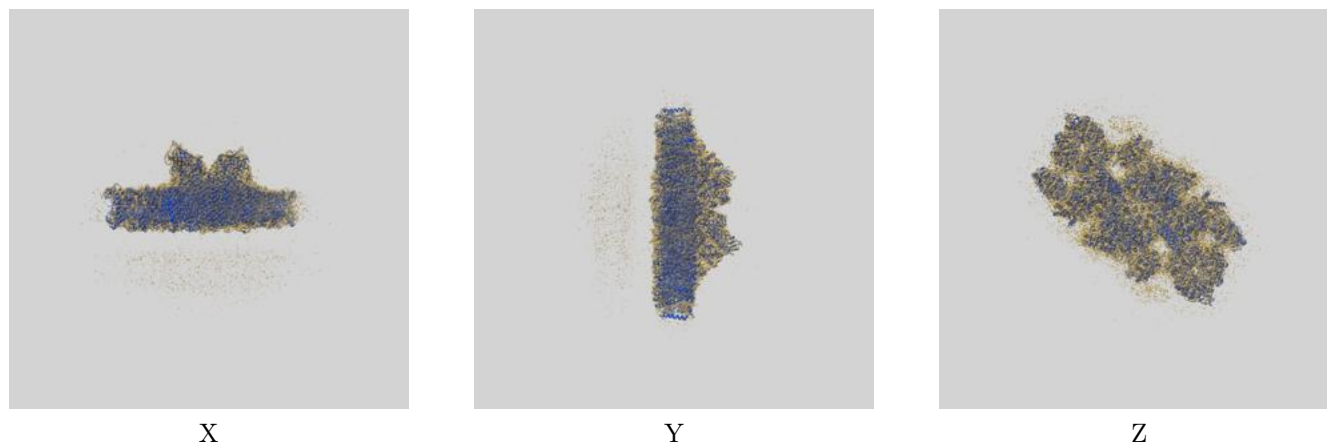
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.79	-	-
Author-provided FSC curve	2.79	3.21	2.84
Unmasked-calculated*	3.62	5.99	3.70

*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 3.62 differs from the reported value 2.785 by more than 10 %

9 Map-model fit [i](#)

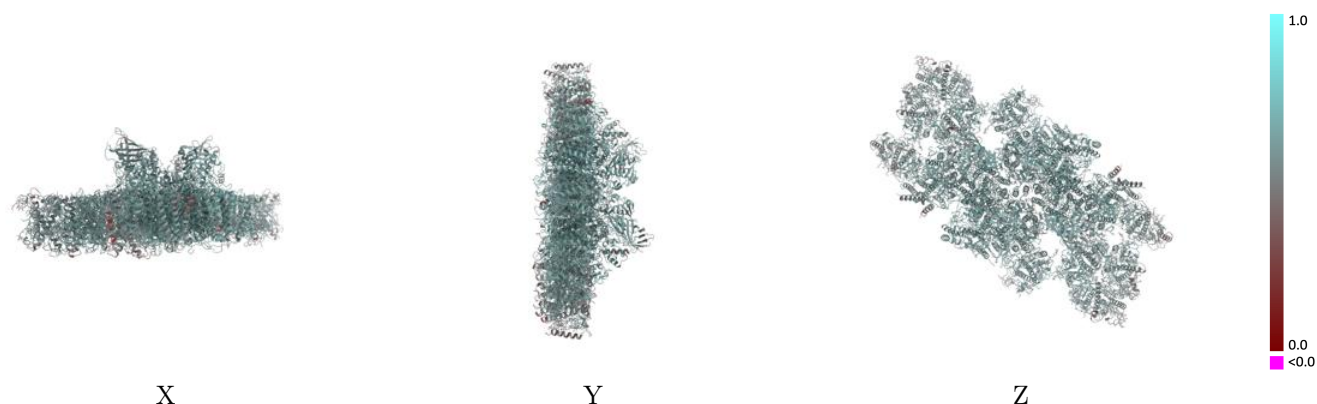
This section contains information regarding the fit between EMDB map EMD-16389 and PDB model 8C29. Per-residue inclusion information can be found in [section 3](#) on [page 40](#).

9.1 Map-model overlay [i](#)



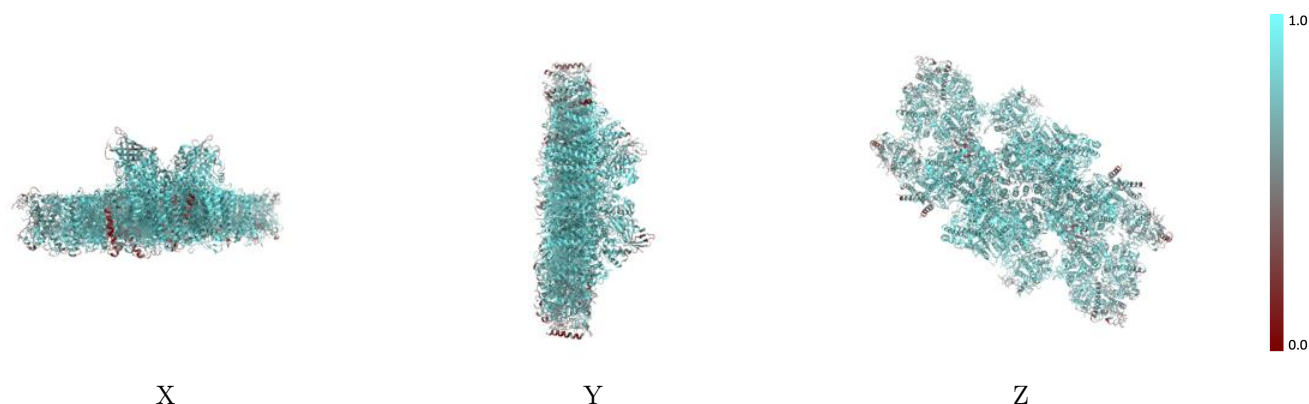
The images above show the 3D surface view of the map at the recommended contour level 0.886 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



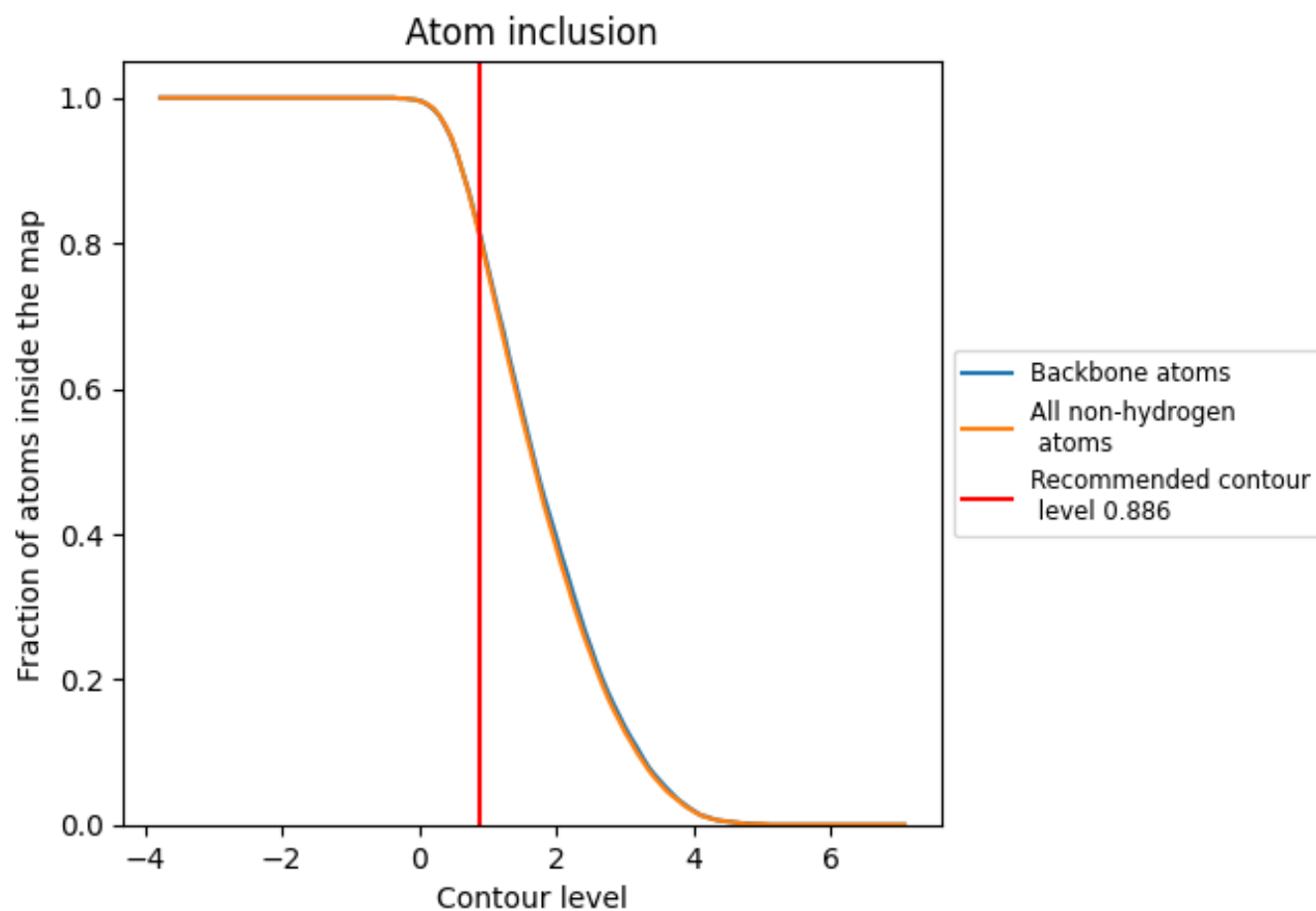
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.886).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% 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 (0.886) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8090	 0.5940
A	 0.8960	 0.6280
B	 0.9040	 0.6220
C	 0.8840	 0.6170
D	 0.8970	 0.6250
E	 0.7820	 0.5800
F	 0.7590	 0.5570
G	 0.6900	 0.5490
H	 0.8960	 0.6190
I	 0.8810	 0.6120
K	 0.8250	 0.5820
L	 0.8480	 0.6220
M	 0.8080	 0.5920
N	 0.7500	 0.5650
O	 0.6380	 0.5610
R	 0.7710	 0.5880
S	 0.6040	 0.5240
T	 0.7910	 0.6000
U	 0.6850	 0.5800
V	 0.4960	 0.5000
W	 0.7230	 0.5730
X	 0.7600	 0.5730
Y	 0.8680	 0.6120
Z	 0.6150	 0.5390
a	 0.8970	 0.6240
b	 0.9010	 0.6240
c	 0.8870	 0.6170
d	 0.8980	 0.6270
e	 0.7940	 0.5770
f	 0.7550	 0.5620
g	 0.6830	 0.5500
h	 0.8930	 0.6200
i	 0.8720	 0.6050
k	 0.8250	 0.5830
l	 0.8920	 0.6190



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Chain	Atom inclusion	Q-score
m	 0.8140	 0.6030
n	 0.7440	 0.5620
o	 0.6360	 0.5600
r	 0.7680	 0.5870
s	 0.6030	 0.5240
t	 0.8170	 0.6110
u	 0.7050	 0.5920
v	 0.5000	 0.5000
w	 0.7360	 0.5810
x	 0.7750	 0.5860
y	 0.8750	 0.6120
z	 0.6050	 0.5330