



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:57 AM UTC

PDB ID : 8HW1 / pdb_00008hw1
EMDB ID : EMD-35080
Title : Far-red light-harvesting complex of Antarctic alga *Prasiola crista*
Authors : Kosugi, M.; Kawasaki, M.; Shibata, Y.; Moriya, T.; Adachi, N.; Senda, T.
Deposited on : 2022-12-28
Resolution : 3.13 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

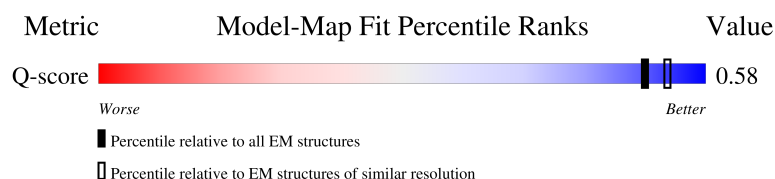
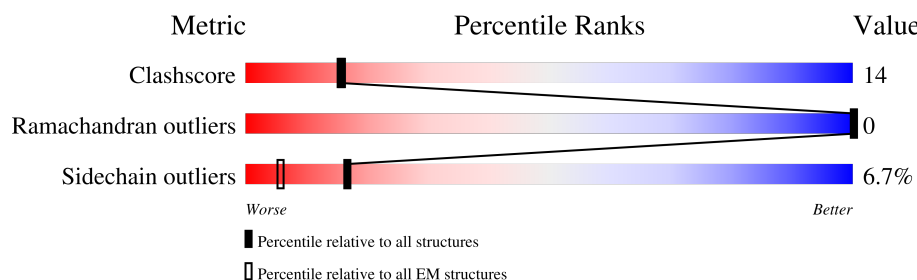
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.13 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	14478 (2.63 - 3.63)

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	307	
1	B	307	
1	C	307	
1	D	307	

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Mol	Chain	Length	Quality of chain
1	E	307	
1	F	307	
1	G	307	
1	H	307	
1	I	307	
1	J	307	
1	K	307	

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
2	CLA	A	601	X	-	-	-
2	CLA	A	602	X	-	-	-
2	CLA	A	603	X	-	-	-
2	CLA	A	604	X	-	-	-
2	CLA	A	605	X	-	-	-
2	CLA	A	606	X	-	-	-
2	CLA	A	607	X	-	-	-
2	CLA	A	608	X	-	-	-
2	CLA	A	609	X	-	-	-
2	CLA	A	610	X	-	-	-
2	CLA	A	611	X	-	-	-
2	CLA	B	601	X	-	-	-
2	CLA	B	602	X	-	-	-
2	CLA	B	603	X	-	-	-
2	CLA	B	604	X	-	-	-
2	CLA	B	605	X	-	-	-
2	CLA	B	606	X	-	-	-
2	CLA	B	607	X	-	-	-
2	CLA	B	608	X	-	-	-
2	CLA	B	609	X	-	-	-
2	CLA	B	610	X	-	-	-
2	CLA	B	611	X	-	-	-
2	CLA	C	601	X	-	-	-
2	CLA	C	602	X	-	-	-
2	CLA	C	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CLA	C	604	X	-	-	-
2	CLA	C	605	X	-	-	-
2	CLA	C	606	X	-	-	-
2	CLA	C	607	X	-	-	-
2	CLA	C	608	X	-	-	-
2	CLA	C	609	X	-	-	-
2	CLA	C	610	X	-	-	-
2	CLA	C	611	X	-	-	-
2	CLA	D	601	X	-	-	-
2	CLA	D	602	X	-	-	-
2	CLA	D	603	X	-	-	-
2	CLA	D	604	X	-	-	-
2	CLA	D	605	X	-	-	-
2	CLA	D	606	X	-	-	-
2	CLA	D	607	X	-	-	-
2	CLA	D	608	X	-	-	-
2	CLA	D	609	X	-	-	-
2	CLA	D	610	X	-	-	-
2	CLA	D	611	X	-	-	-
2	CLA	E	601	X	-	-	-
2	CLA	E	602	X	-	-	-
2	CLA	E	603	X	-	-	-
2	CLA	E	604	X	-	-	-
2	CLA	E	605	X	-	-	-
2	CLA	E	606	X	-	-	-
2	CLA	E	607	X	-	-	-
2	CLA	E	608	X	-	-	-
2	CLA	E	609	X	-	-	-
2	CLA	E	610	X	-	-	-
2	CLA	E	611	X	-	-	-
2	CLA	F	601	X	-	-	-
2	CLA	F	602	X	-	-	-
2	CLA	F	603	X	-	-	-
2	CLA	F	604	X	-	-	-
2	CLA	F	605	X	-	-	-
2	CLA	F	606	X	-	-	-
2	CLA	F	607	X	-	-	-
2	CLA	F	608	X	-	-	-
2	CLA	F	609	X	-	-	-
2	CLA	F	610	X	-	-	-
2	CLA	F	611	X	-	-	-
2	CLA	G	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CLA	G	602	X	-	-	-
2	CLA	G	603	X	-	-	-
2	CLA	G	604	X	-	-	-
2	CLA	G	605	X	-	-	-
2	CLA	G	606	X	-	-	-
2	CLA	G	607	X	-	-	-
2	CLA	G	608	X	-	-	-
2	CLA	G	609	X	-	-	-
2	CLA	G	610	X	-	-	-
2	CLA	G	611	X	-	-	-
2	CLA	H	601	X	-	-	-
2	CLA	H	602	X	-	-	-
2	CLA	H	603	X	-	-	-
2	CLA	H	604	X	-	-	-
2	CLA	H	605	X	-	-	-
2	CLA	H	606	X	-	-	-
2	CLA	H	607	X	-	-	-
2	CLA	H	608	X	-	-	-
2	CLA	H	609	X	-	-	-
2	CLA	H	610	X	-	-	-
2	CLA	H	611	X	-	-	-
2	CLA	I	601	X	-	-	-
2	CLA	I	602	X	-	-	-
2	CLA	I	603	X	-	-	-
2	CLA	I	604	X	-	-	-
2	CLA	I	605	X	-	-	-
2	CLA	I	606	X	-	-	-
2	CLA	I	607	X	-	-	-
2	CLA	I	608	X	-	-	-
2	CLA	I	609	X	-	-	-
2	CLA	I	610	X	-	-	-
2	CLA	I	611	X	-	-	-
2	CLA	J	601	X	-	-	-
2	CLA	J	602	X	-	-	-
2	CLA	J	603	X	-	-	-
2	CLA	J	604	X	-	-	-
2	CLA	J	605	X	-	-	-
2	CLA	J	606	X	-	-	-
2	CLA	J	607	X	-	-	-
2	CLA	J	608	X	-	-	-
2	CLA	J	609	X	-	-	-
2	CLA	J	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CLA	J	611	X	-	-	-
2	CLA	K	601	X	-	-	-
2	CLA	K	602	X	-	-	-
2	CLA	K	603	X	-	-	-
2	CLA	K	604	X	-	-	-
2	CLA	K	605	X	-	-	-
2	CLA	K	606	X	-	-	-
2	CLA	K	607	X	-	-	-
2	CLA	K	608	X	-	-	-
2	CLA	K	609	X	-	-	-
2	CLA	K	610	X	-	-	-
2	CLA	K	611	X	-	-	-

2 Entry composition

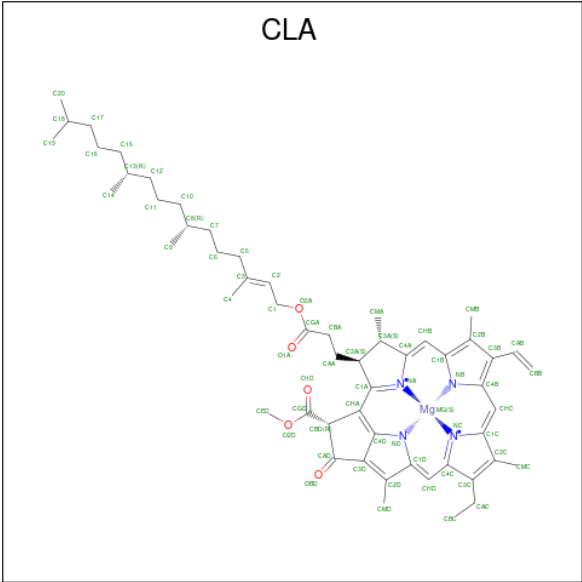
There are 4 unique types of molecules in this entry. The entry contains 29271 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Far-red light-harvesting complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	241	Total	C	N	O	S	0	0
			1886	1214	321	346	5		
1	B	241	Total	C	N	O	S	0	0
			1886	1214	321	346	5		
1	C	241	Total	C	N	O	S	0	0
			1886	1214	321	346	5		
1	D	241	Total	C	N	O	S	0	0
			1886	1214	321	346	5		
1	E	241	Total	C	N	O	S	0	0
			1886	1214	321	346	5		
1	F	241	Total	C	N	O	S	0	0
			1886	1214	321	346	5		
1	G	241	Total	C	N	O	S	0	0
			1886	1214	321	346	5		
1	H	241	Total	C	N	O	S	0	0
			1886	1214	321	346	5		
1	I	241	Total	C	N	O	S	0	0
			1886	1214	321	346	5		
1	J	241	Total	C	N	O	S	0	0
			1886	1214	321	346	5		
1	K	241	Total	C	N	O	S	0	0
			1886	1214	321	346	5		

- Molecule 2 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	C	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	C	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	C	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
2	D	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	D	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	E	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	E	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	E	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
2	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	F	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	F	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	F	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	G	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	G	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	G	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
2	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	H	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	H	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	H	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	I	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	I	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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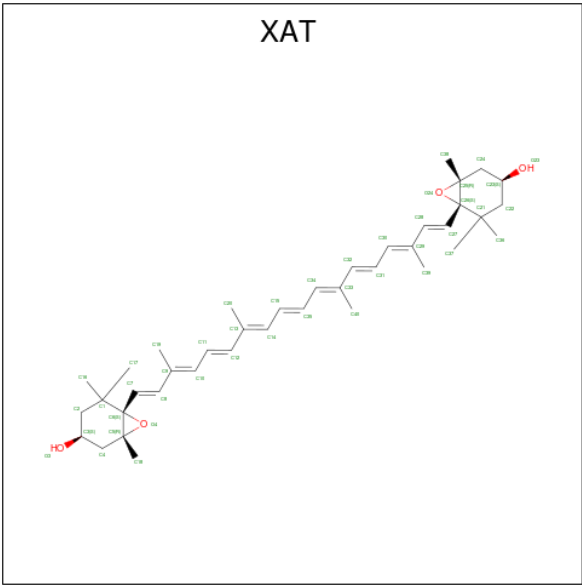
Mol	Chain	Residues	Atoms					AltConf
2	I	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	J	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	J	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	K	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	K	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
2	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
2	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
2	K	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

- Molecule 3 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) (labeled as "Ligand of Interest" by depositor).



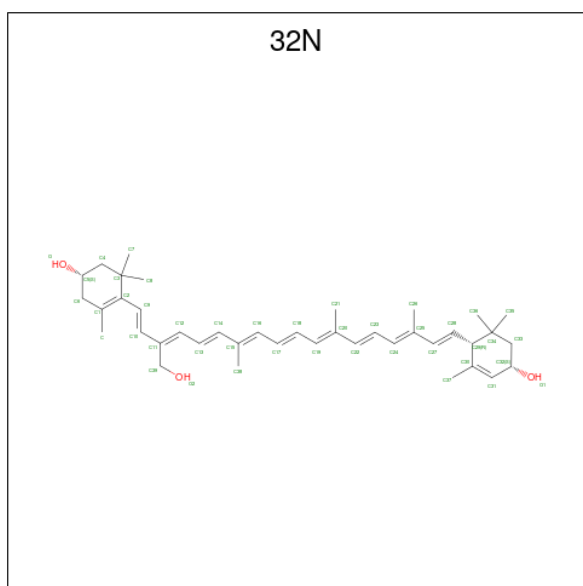
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			44	40	4	
3	B	1	Total	C	O	0
			44	40	4	
3	C	1	Total	C	O	0
			44	40	4	
3	D	1	Total	C	O	0
			44	40	4	
3	E	1	Total	C	O	0
			44	40	4	
3	F	1	Total	C	O	0
			44	40	4	
3	G	1	Total	C	O	0
			44	40	4	
3	H	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
3	I	1	Total	C	O	0
			44	40	4	
3	J	1	Total	C	O	0
			44	40	4	
3	K	1	Total	C	O	0
			44	40	4	

- Molecule 4 is (1S)-4-[(1E,3Z,5E,7E,9E,11E,13E,15E,17E)-3-(hydroxymethyl)-7,12,16-trimethyl-18-[(1R,4S)-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]-3,5,5-trimethyl-cyclohex-3-en-1-ol (CCD ID: 32N) (formula: C₄₀H₅₆O₃) (labeled as "Ligand of Interest" by depositor).

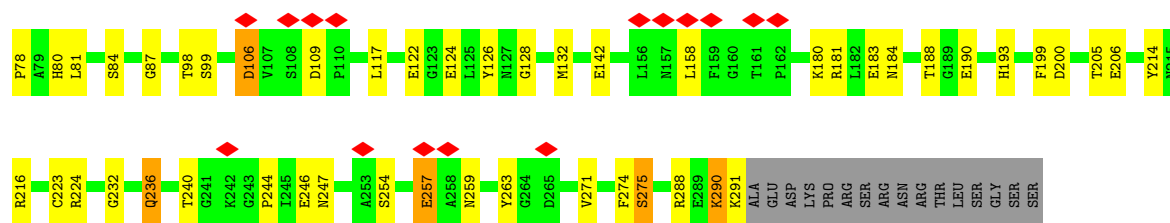


Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			43	40	3	
4	B	1	Total	C	O	0
			43	40	3	
4	C	1	Total	C	O	0
			43	40	3	
4	D	1	Total	C	O	0
			43	40	3	
4	E	1	Total	C	O	0
			43	40	3	
4	F	1	Total	C	O	0
			43	40	3	
4	G	1	Total	C	O	0
			43	40	3	

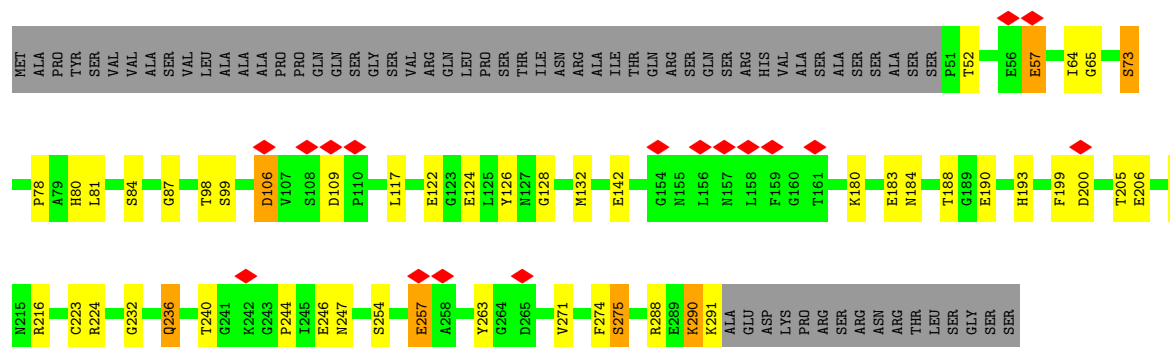
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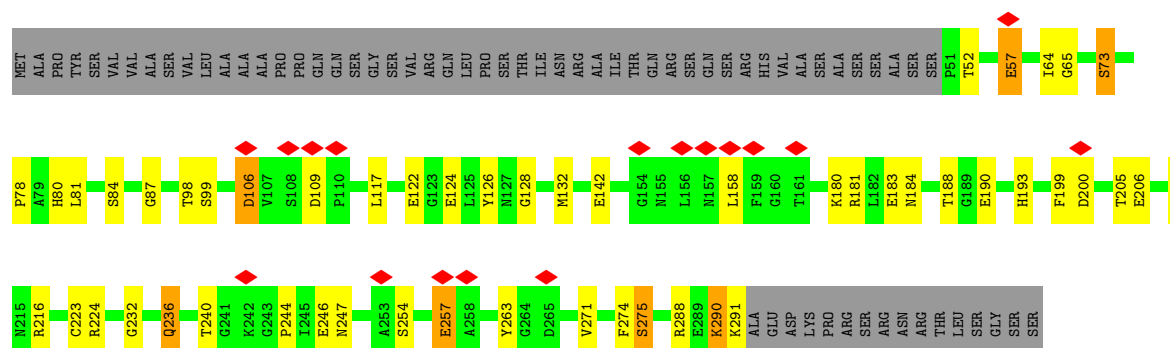
Mol	Chain	Residues	Atoms			AltConf
4	H	1	Total 43	C 40	O 3	0
4	I	1	Total 43	C 40	O 3	0
4	J	1	Total 43	C 40	O 3	0
4	K	1	Total 43	C 40	O 3	0



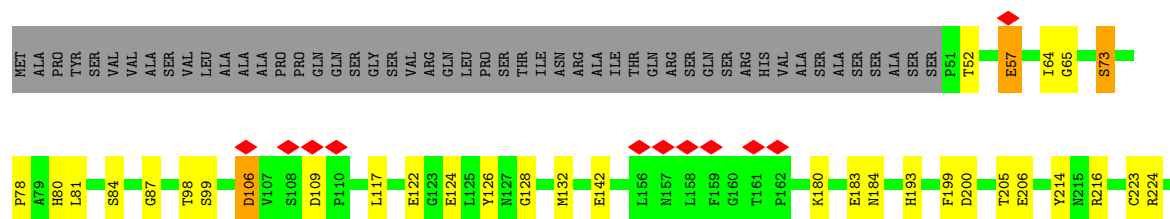
• Molecule 1: Far-red light-harvesting complex

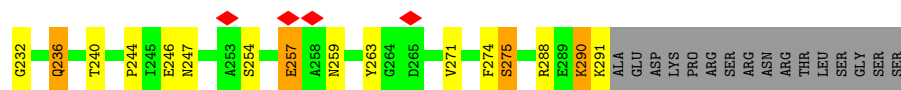


• Molecule 1: Far-red light-harvesting complex

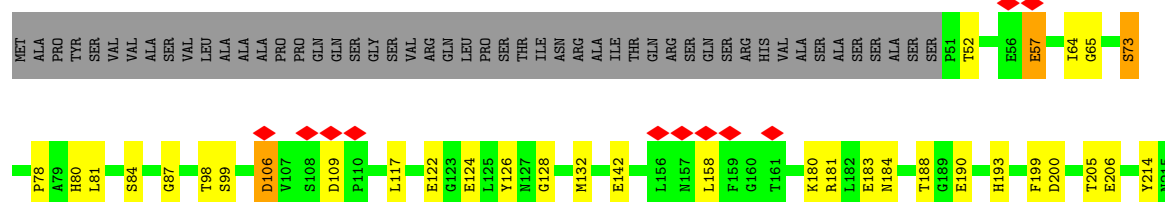


• Molecule 1: Far-red light-harvesting complex

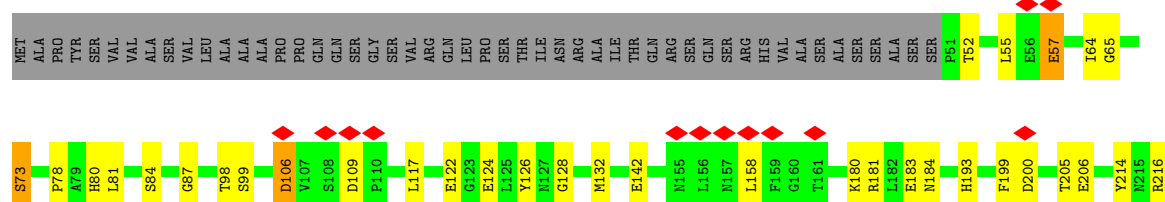




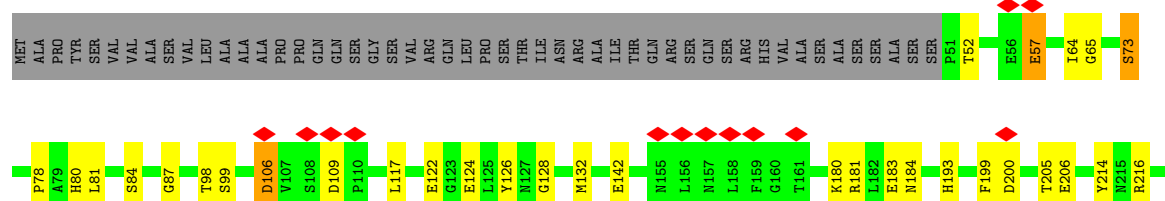
• Molecule 1: Far-red light-harvesting complex



• Molecule 1: Far-red light-harvesting complex



• Molecule 1: Far-red light-harvesting complex



• Molecule 1: Far-red light-harvesting complex

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C11	Depositor
Number of particles used	99510	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS TALOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	92000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.415	Depositor
Minimum map value	-0.229	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	282.5, 282.5, 282.5	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.13, 1.13, 1.13	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, XAT, 32N

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	0.39	0/1944	0.60	1/2650 (0.0%)
1	B	0.39	0/1944	0.60	1/2650 (0.0%)
1	C	0.38	0/1944	0.60	1/2650 (0.0%)
1	D	0.39	0/1944	0.60	1/2650 (0.0%)
1	E	0.39	0/1944	0.60	1/2650 (0.0%)
1	F	0.39	0/1944	0.60	1/2650 (0.0%)
1	G	0.39	0/1944	0.60	1/2650 (0.0%)
1	H	0.38	0/1944	0.60	1/2650 (0.0%)
1	I	0.39	0/1944	0.60	1/2650 (0.0%)
1	J	0.38	0/1944	0.60	1/2650 (0.0%)
1	K	0.39	0/1944	0.60	1/2650 (0.0%)
All	All	0.39	0/21384	0.60	11/29150 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	G	199	PHE	N-CA-C	5.78	118.24	111.02
1	C	199	PHE	N-CA-C	5.76	118.22	111.02
1	E	199	PHE	N-CA-C	5.76	118.22	111.02
1	A	199	PHE	N-CA-C	5.76	118.22	111.02
1	F	199	PHE	N-CA-C	5.76	118.22	111.02
1	D	199	PHE	N-CA-C	5.75	118.21	111.02
1	I	199	PHE	N-CA-C	5.75	118.21	111.02
1	H	199	PHE	N-CA-C	5.75	118.21	111.02
1	J	199	PHE	N-CA-C	5.74	118.20	111.02
1	K	199	PHE	N-CA-C	5.74	118.19	111.02
1	B	199	PHE	N-CA-C	5.73	118.18	111.02

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	1886	0	1811	47	0
1	B	1886	0	1811	48	0
1	C	1886	0	1811	49	0
1	D	1886	0	1811	46	0
1	E	1886	0	1811	48	0
1	F	1886	0	1811	47	0
1	G	1886	0	1811	50	0
1	H	1886	0	1811	49	0
1	I	1886	0	1811	47	0
1	J	1886	0	1811	49	0
1	K	1886	0	1811	48	0
2	A	688	0	729	43	0
2	B	688	0	729	40	0
2	C	688	0	729	40	0
2	D	688	0	729	40	0
2	E	688	0	729	40	0
2	F	688	0	729	40	0
2	G	688	0	729	41	0
2	H	688	0	729	40	0
2	I	688	0	729	43	0
2	J	688	0	729	43	0
2	K	688	0	729	39	0
3	A	44	0	56	4	0
3	B	44	0	56	4	0
3	C	44	0	56	4	0
3	D	44	0	56	4	0
3	E	44	0	56	4	0
3	F	44	0	56	4	0
3	G	44	0	56	4	0
3	H	44	0	56	4	0
3	I	44	0	56	4	0
3	J	44	0	56	4	0
3	K	44	0	56	4	0
4	A	43	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	43	0	0	0	0
4	C	43	0	0	0	0
4	D	43	0	0	0	0
4	E	43	0	0	0	0
4	F	43	0	0	0	0
4	G	43	0	0	0	0
4	H	43	0	0	0	0
4	I	43	0	0	0	0
4	J	43	0	0	0	0
4	K	43	0	0	0	0
All	All	29271	0	28556	837	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 14.

All (837) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:601:CLA:H141	2:A:601:CLA:H171	1.15	1.14
2:B:601:CLA:H141	2:B:601:CLA:H171	1.15	1.14
2:K:601:CLA:H141	2:K:601:CLA:H171	1.15	1.13
2:C:601:CLA:H141	2:C:601:CLA:H171	1.15	1.13
2:J:601:CLA:H141	2:J:601:CLA:H171	1.15	1.11
2:D:601:CLA:H171	2:D:601:CLA:H141	1.15	1.11
2:I:601:CLA:H171	2:I:601:CLA:H141	1.15	1.10
2:E:601:CLA:H141	2:E:601:CLA:H171	1.15	1.09
2:H:601:CLA:H141	2:H:601:CLA:H171	1.15	1.09
2:F:601:CLA:H141	2:F:601:CLA:H171	1.15	1.09
2:G:601:CLA:H141	2:G:601:CLA:H171	1.15	1.09
2:C:607:CLA:H142	2:C:607:CLA:H91	1.45	0.98
2:D:607:CLA:H91	2:D:607:CLA:H142	1.45	0.98
2:B:607:CLA:H91	2:B:607:CLA:H142	1.45	0.98
2:A:607:CLA:H142	2:A:607:CLA:H91	1.45	0.98
2:E:607:CLA:H91	2:E:607:CLA:H142	1.45	0.97
2:K:607:CLA:H142	2:K:607:CLA:H91	1.45	0.97
2:J:607:CLA:H91	2:J:607:CLA:H142	1.45	0.96
2:F:607:CLA:H142	2:F:607:CLA:H91	1.45	0.96
2:I:607:CLA:H91	2:I:607:CLA:H142	1.45	0.95
2:G:607:CLA:H91	2:G:607:CLA:H142	1.45	0.95
2:C:607:CLA:H91	2:C:607:CLA:C14	1.97	0.95
2:H:607:CLA:H142	2:H:607:CLA:H91	1.45	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:607:CLA:H91	2:G:607:CLA:C14	1.97	0.94
2:E:607:CLA:H91	2:E:607:CLA:C14	1.97	0.94
2:B:607:CLA:H91	2:B:607:CLA:C14	1.97	0.94
2:F:607:CLA:H91	2:F:607:CLA:C14	1.97	0.94
2:H:607:CLA:H91	2:H:607:CLA:C14	1.97	0.94
2:D:607:CLA:H91	2:D:607:CLA:C14	1.97	0.94
2:A:607:CLA:H91	2:A:607:CLA:C14	1.97	0.94
2:I:607:CLA:H91	2:I:607:CLA:C14	1.97	0.94
2:J:607:CLA:H91	2:J:607:CLA:C14	1.97	0.93
2:K:607:CLA:H91	2:K:607:CLA:C14	1.97	0.93
2:G:607:CLA:H91	2:G:607:CLA:H121	1.51	0.93
2:I:607:CLA:H91	2:I:607:CLA:H121	1.51	0.92
2:J:607:CLA:H91	2:J:607:CLA:H121	1.51	0.92
2:E:607:CLA:H91	2:E:607:CLA:H121	1.51	0.91
2:E:601:CLA:H171	2:E:601:CLA:C14	2.00	0.91
2:H:607:CLA:H91	2:H:607:CLA:H121	1.51	0.91
2:C:601:CLA:H171	2:C:601:CLA:C14	2.00	0.91
2:G:601:CLA:H171	2:G:601:CLA:C14	2.00	0.91
2:A:607:CLA:H91	2:A:607:CLA:H121	1.51	0.90
2:K:607:CLA:H91	2:K:607:CLA:H121	1.51	0.90
2:C:607:CLA:H91	2:C:607:CLA:H121	1.51	0.90
2:B:607:CLA:H91	2:B:607:CLA:H121	1.51	0.89
2:F:607:CLA:H91	2:F:607:CLA:H121	1.51	0.89
2:I:601:CLA:H171	2:I:601:CLA:C14	2.00	0.89
2:D:607:CLA:H91	2:D:607:CLA:H121	1.51	0.88
2:D:601:CLA:H171	2:D:601:CLA:C14	2.00	0.87
2:K:601:CLA:H171	2:K:601:CLA:C14	2.00	0.87
2:B:601:CLA:H171	2:B:601:CLA:C14	2.00	0.87
2:F:601:CLA:H171	2:F:601:CLA:C14	2.00	0.87
2:H:601:CLA:H171	2:H:601:CLA:C14	2.00	0.85
2:J:601:CLA:H171	2:J:601:CLA:C14	2.00	0.84
2:A:601:CLA:H171	2:A:601:CLA:C14	2.00	0.80
2:K:607:CLA:H91	2:K:607:CLA:C12	2.12	0.80
2:E:607:CLA:H91	2:E:607:CLA:C12	2.12	0.80
2:H:607:CLA:H91	2:H:607:CLA:C12	2.12	0.80
2:A:607:CLA:H91	2:A:607:CLA:C12	2.12	0.80
2:D:607:CLA:H91	2:D:607:CLA:C12	2.12	0.80
2:G:607:CLA:H91	2:G:607:CLA:C12	2.12	0.79
2:I:607:CLA:H91	2:I:607:CLA:C12	2.12	0.79
2:F:607:CLA:H91	2:F:607:CLA:C12	2.12	0.79
2:C:607:CLA:H91	2:C:607:CLA:C12	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:607:CLA:H91	2:J:607:CLA:C12	2.12	0.79
2:B:607:CLA:H91	2:B:607:CLA:C12	2.12	0.78
1:I:78:PRO:HG3	1:I:288:ARG:HH12	1.49	0.78
1:K:78:PRO:HG3	1:K:288:ARG:HH12	1.48	0.78
1:A:78:PRO:HG3	1:A:288:ARG:HH12	1.48	0.78
1:G:78:PRO:HG3	1:G:288:ARG:HH12	1.49	0.78
2:J:601:CLA:H72	2:J:601:CLA:C12	2.14	0.78
2:K:601:CLA:H72	2:K:601:CLA:C12	2.14	0.77
1:H:78:PRO:HG3	1:H:288:ARG:HH12	1.49	0.77
1:B:78:PRO:HG3	1:B:288:ARG:HH12	1.49	0.77
1:C:78:PRO:HG3	1:C:288:ARG:HH12	1.48	0.77
1:J:78:PRO:HG3	1:J:288:ARG:HH12	1.49	0.77
2:I:601:CLA:H72	2:I:601:CLA:C12	2.14	0.76
2:G:601:CLA:H72	2:G:601:CLA:C12	2.14	0.76
1:E:78:PRO:HG3	1:E:288:ARG:HH12	1.49	0.76
1:F:78:PRO:HG3	1:F:288:ARG:HH12	1.49	0.76
2:B:607:CLA:H142	2:B:607:CLA:C9	2.15	0.76
2:C:601:CLA:H72	2:C:601:CLA:C12	2.14	0.76
2:D:601:CLA:H72	2:D:601:CLA:C12	2.14	0.76
2:H:601:CLA:H72	2:H:601:CLA:C12	2.14	0.76
2:D:607:CLA:H142	2:D:607:CLA:C9	2.15	0.76
2:B:601:CLA:H72	2:B:601:CLA:C12	2.14	0.76
2:F:601:CLA:H72	2:F:601:CLA:C12	2.14	0.75
2:H:607:CLA:H142	2:H:607:CLA:C9	2.15	0.75
2:A:601:CLA:H72	2:A:601:CLA:C12	2.14	0.75
1:D:78:PRO:HG3	1:D:288:ARG:HH12	1.49	0.75
2:E:607:CLA:H142	2:E:607:CLA:C9	2.15	0.75
2:A:607:CLA:H142	2:A:607:CLA:C9	2.15	0.75
2:C:607:CLA:H142	2:C:607:CLA:C9	2.15	0.75
2:K:607:CLA:H142	2:K:607:CLA:C9	2.15	0.75
2:E:601:CLA:H72	2:E:601:CLA:C12	2.14	0.74
2:I:607:CLA:H142	2:I:607:CLA:C9	2.15	0.74
2:F:607:CLA:H142	2:F:607:CLA:C9	2.15	0.74
2:J:607:CLA:H142	2:J:607:CLA:C9	2.15	0.74
2:G:607:CLA:H142	2:G:607:CLA:C9	2.15	0.74
2:C:607:CLA:H121	2:C:607:CLA:C9	2.17	0.74
2:D:607:CLA:H121	2:D:607:CLA:C9	2.17	0.74
2:G:607:CLA:H121	2:G:607:CLA:C9	2.17	0.73
2:F:607:CLA:H121	2:F:607:CLA:C9	2.17	0.73
2:H:607:CLA:H121	2:H:607:CLA:C9	2.17	0.73
2:I:607:CLA:H121	2:I:607:CLA:C9	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:607:CLA:H121	2:B:607:CLA:C9	2.17	0.73
2:J:607:CLA:H121	2:J:607:CLA:C9	2.17	0.73
2:A:607:CLA:H121	2:A:607:CLA:C9	2.17	0.73
2:E:607:CLA:H121	2:E:607:CLA:C9	2.17	0.73
2:K:607:CLA:H121	2:K:607:CLA:C9	2.17	0.72
2:A:608:CLA:HBB2	2:A:609:CLA:H201	1.73	0.71
2:H:608:CLA:HBB2	2:H:609:CLA:H201	1.73	0.71
2:I:608:CLA:HBB2	2:I:609:CLA:H201	1.73	0.71
2:K:608:CLA:HBB2	2:K:609:CLA:H201	1.73	0.71
2:B:608:CLA:HBB2	2:B:609:CLA:H201	1.73	0.71
2:G:608:CLA:HBB2	2:G:609:CLA:H201	1.73	0.71
2:J:608:CLA:HBB2	2:J:609:CLA:H201	1.73	0.71
2:D:608:CLA:HBB2	2:D:609:CLA:H201	1.73	0.70
2:C:608:CLA:HBB2	2:C:609:CLA:H201	1.73	0.70
2:E:608:CLA:HBB2	2:E:609:CLA:H201	1.73	0.70
2:F:608:CLA:HBB2	2:F:609:CLA:H201	1.73	0.70
1:E:126:TYR:OH	1:E:193:HIS:NE2	2.26	0.69
1:C:126:TYR:OH	1:C:193:HIS:NE2	2.26	0.69
1:D:126:TYR:OH	1:D:193:HIS:NE2	2.26	0.69
1:F:126:TYR:OH	1:F:193:HIS:NE2	2.26	0.69
1:G:126:TYR:OH	1:G:193:HIS:NE2	2.26	0.69
1:H:126:TYR:OH	1:H:193:HIS:NE2	2.26	0.69
1:B:126:TYR:OH	1:B:193:HIS:NE2	2.26	0.68
1:I:126:TYR:OH	1:I:193:HIS:NE2	2.26	0.68
1:J:126:TYR:OH	1:J:193:HIS:NE2	2.26	0.68
1:K:126:TYR:OH	1:K:193:HIS:NE2	2.26	0.68
2:E:603:CLA:HBB1	2:E:603:CLA:HMB3	1.77	0.67
2:F:603:CLA:HBB1	2:F:603:CLA:HMB3	1.77	0.67
2:G:603:CLA:HMB3	2:G:603:CLA:HBB1	1.77	0.67
2:D:603:CLA:HBB1	2:D:603:CLA:HMB3	1.77	0.67
2:H:603:CLA:HBB1	2:H:603:CLA:HMB3	1.77	0.67
2:C:603:CLA:HBB1	2:C:603:CLA:HMB3	1.76	0.67
1:A:126:TYR:OH	1:A:193:HIS:NE2	2.26	0.66
1:I:271:VAL:O	1:I:275:SER:OG	2.14	0.66
1:K:271:VAL:O	1:K:275:SER:OG	2.14	0.66
2:B:603:CLA:HMB3	2:B:603:CLA:HBB1	1.76	0.66
2:I:603:CLA:HBB1	2:I:603:CLA:HMB3	1.77	0.66
2:J:603:CLA:HBB1	2:J:603:CLA:HMB3	1.76	0.66
1:G:271:VAL:O	1:G:275:SER:OG	2.14	0.66
2:A:603:CLA:HBB1	2:A:603:CLA:HMB3	1.76	0.66
2:K:603:CLA:HBB1	2:K:603:CLA:HMB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:607:CLA:HBB1	2:G:607:CLA:HMB1	1.79	0.65
1:H:271:VAL:O	1:H:275:SER:OG	2.14	0.65
1:B:271:VAL:O	1:B:275:SER:OG	2.14	0.65
1:J:271:VAL:O	1:J:275:SER:OG	2.14	0.65
1:A:78:PRO:HG3	1:A:288:ARG:NH1	2.12	0.65
1:C:271:VAL:O	1:C:275:SER:OG	2.14	0.65
2:C:603:CLA:HBC2	2:C:603:CLA:HHD	1.79	0.65
1:E:271:VAL:O	1:E:275:SER:OG	2.14	0.65
1:I:78:PRO:HG3	1:I:288:ARG:NH1	2.12	0.65
1:A:271:VAL:O	1:A:275:SER:OG	2.14	0.65
2:E:607:CLA:HBB1	2:E:607:CLA:HMB1	1.79	0.65
2:I:603:CLA:HBC2	2:I:603:CLA:HHD	1.79	0.65
2:K:603:CLA:HBC2	2:K:603:CLA:HHD	1.79	0.65
2:A:603:CLA:HBC2	2:A:603:CLA:HHD	1.79	0.64
2:B:603:CLA:HBC2	2:B:603:CLA:HHD	1.79	0.64
1:D:271:VAL:O	1:D:275:SER:OG	2.14	0.64
2:H:603:CLA:HHD	2:H:603:CLA:HBC2	1.79	0.64
1:J:78:PRO:HG3	1:J:288:ARG:NH1	2.12	0.64
2:J:603:CLA:HBC2	2:J:603:CLA:HHD	1.80	0.64
2:E:603:CLA:HBC2	2:E:603:CLA:HHD	1.79	0.64
1:F:271:VAL:O	1:F:275:SER:OG	2.14	0.64
2:G:603:CLA:HBC2	2:G:603:CLA:HHD	1.79	0.64
1:K:78:PRO:HG3	1:K:288:ARG:NH1	2.12	0.64
1:C:78:PRO:HG3	1:C:288:ARG:NH1	2.12	0.64
2:D:603:CLA:HBC2	2:D:603:CLA:HHD	1.80	0.64
2:F:603:CLA:HBC2	2:F:603:CLA:HHD	1.79	0.64
1:G:78:PRO:HG3	1:G:288:ARG:NH1	2.12	0.64
1:D:78:PRO:HG3	1:D:288:ARG:NH1	2.12	0.64
1:A:126:TYR:HH	1:A:193:HIS:CD2	2.16	0.63
1:F:78:PRO:HG3	1:F:288:ARG:NH1	2.12	0.63
2:A:606:CLA:HAB	3:A:612:XAT:H32	1.81	0.63
2:B:606:CLA:HAB	3:B:612:XAT:H32	1.81	0.63
1:H:78:PRO:HG3	1:H:288:ARG:NH1	2.12	0.63
2:K:607:CLA:HBB1	2:K:607:CLA:HMB3	1.81	0.63
2:C:606:CLA:HAB	3:C:612:XAT:H32	1.81	0.63
2:I:607:CLA:HBB1	2:I:607:CLA:HMB3	1.81	0.63
2:K:606:CLA:HAB	3:K:612:XAT:H32	1.81	0.63
2:G:606:CLA:HAB	3:G:612:XAT:H32	1.81	0.63
2:A:607:CLA:HBB1	2:A:607:CLA:HMB3	1.81	0.63
1:D:180:LYS:HE3	1:D:184:ASN:HD21	1.64	0.63
2:H:606:CLA:HAB	3:H:612:XAT:H32	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:607:CLA:HBB1	2:B:607:CLA:HMB3	1.81	0.63
2:D:606:CLA:HAB	3:D:612:XAT:H32	1.81	0.63
2:F:606:CLA:HAB	3:F:612:XAT:H32	1.81	0.63
1:A:246:GLU:OE1	1:A:246:GLU:N	2.32	0.62
1:B:246:GLU:N	1:B:246:GLU:OE1	2.32	0.62
2:E:606:CLA:HAB	3:E:612:XAT:H32	1.81	0.62
2:J:607:CLA:HMB3	2:J:607:CLA:HBB1	1.81	0.62
1:C:246:GLU:N	1:C:246:GLU:OE1	2.32	0.62
1:G:128:GLY:HA3	1:G:223:CYS:HB2	1.81	0.62
2:H:607:CLA:HBB1	2:H:607:CLA:HMB3	1.81	0.62
1:K:246:GLU:OE1	1:K:246:GLU:N	2.32	0.62
1:D:246:GLU:OE1	1:D:246:GLU:N	2.32	0.62
1:E:246:GLU:N	1:E:246:GLU:OE1	2.32	0.62
2:I:606:CLA:HAB	3:I:612:XAT:H32	1.81	0.62
1:B:180:LYS:HE3	1:B:184:ASN:HD21	1.64	0.62
1:F:180:LYS:HE3	1:F:184:ASN:HD21	1.64	0.62
1:F:246:GLU:OE1	1:F:246:GLU:N	2.32	0.62
1:A:180:LYS:HE3	1:A:184:ASN:HD21	1.64	0.62
1:B:78:PRO:HG3	1:B:288:ARG:NH1	2.12	0.62
1:G:246:GLU:N	1:G:246:GLU:OE1	2.32	0.62
1:I:128:GLY:HA3	1:I:223:CYS:HB2	1.82	0.62
2:J:606:CLA:HAB	3:J:612:XAT:H32	1.81	0.62
1:E:78:PRO:HG3	1:E:288:ARG:NH1	2.12	0.62
1:H:180:LYS:HE3	1:H:184:ASN:HD21	1.64	0.62
1:J:246:GLU:N	1:J:246:GLU:OE1	2.32	0.62
1:C:180:LYS:HE3	1:C:184:ASN:HD21	1.64	0.62
2:C:607:CLA:HBB1	2:C:607:CLA:HMB3	1.81	0.62
2:D:607:CLA:HBB1	2:D:607:CLA:HMB3	1.81	0.62
1:F:128:GLY:HA3	1:F:223:CYS:HB2	1.81	0.62
1:H:246:GLU:N	1:H:246:GLU:OE1	2.32	0.62
1:I:246:GLU:OE1	1:I:246:GLU:N	2.32	0.62
1:E:128:GLY:HA3	1:E:223:CYS:HB2	1.81	0.61
1:E:180:LYS:HE3	1:E:184:ASN:HD21	1.64	0.61
2:F:607:CLA:HBB1	2:F:607:CLA:HMB3	1.81	0.61
1:D:132:MET:HE2	2:D:606:CLA:HMC3	1.83	0.61
1:C:132:MET:HE2	2:C:606:CLA:HMC3	1.83	0.61
1:D:128:GLY:HA3	1:D:223:CYS:HB2	1.81	0.61
1:I:180:LYS:HE3	1:I:184:ASN:HD21	1.64	0.61
1:B:132:MET:HE2	2:B:606:CLA:HMC3	1.83	0.61
1:G:132:MET:HE2	2:G:606:CLA:HMC3	1.83	0.61
1:G:180:LYS:HE3	1:G:184:ASN:HD21	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:132:MET:HE2	2:F:606:CLA:HMC3	1.83	0.61
1:E:132:MET:HE2	2:E:606:CLA:HMC3	1.83	0.61
1:K:180:LYS:HE3	1:K:184:ASN:HD21	1.64	0.61
1:B:128:GLY:HA3	1:B:223:CYS:HB2	1.81	0.61
1:H:128:GLY:HA3	1:H:223:CYS:HB2	1.81	0.61
1:K:128:GLY:HA3	1:K:223:CYS:HB2	1.81	0.61
1:A:128:GLY:HA3	1:A:223:CYS:HB2	1.81	0.61
1:J:180:LYS:HE3	1:J:184:ASN:HD21	1.64	0.61
1:A:132:MET:HE2	2:A:606:CLA:HMC3	1.83	0.60
1:H:132:MET:HE2	2:H:606:CLA:HMC3	1.83	0.60
1:K:132:MET:HE2	2:K:606:CLA:HMC3	1.83	0.60
1:C:128:GLY:HA3	1:C:223:CYS:HB2	1.81	0.60
1:J:132:MET:HE2	2:J:606:CLA:HMC3	1.83	0.60
1:J:128:GLY:HA3	1:J:223:CYS:HB2	1.81	0.60
1:I:132:MET:HE2	2:I:606:CLA:HMC3	1.83	0.60
2:A:601:CLA:H122	2:A:601:CLA:C7	2.32	0.60
2:I:601:CLA:C7	2:I:601:CLA:H122	2.32	0.60
1:J:142:GLU:CD	1:J:244:PRO:HD2	2.27	0.59
1:A:142:GLU:CD	1:A:244:PRO:HD2	2.27	0.59
1:K:142:GLU:CD	1:K:244:PRO:HD2	2.28	0.59
2:F:601:CLA:H122	2:F:601:CLA:C7	2.32	0.59
2:J:601:CLA:H122	2:J:601:CLA:C7	2.32	0.59
2:B:601:CLA:C7	2:B:601:CLA:H122	2.32	0.59
1:C:142:GLU:CD	1:C:244:PRO:HD2	2.28	0.59
1:D:142:GLU:CD	1:D:244:PRO:HD2	2.28	0.59
2:D:601:CLA:C7	2:D:601:CLA:H122	2.32	0.59
2:G:601:CLA:C7	2:G:601:CLA:H122	2.32	0.59
1:B:142:GLU:CD	1:B:244:PRO:HD2	2.27	0.59
1:G:142:GLU:CD	1:G:244:PRO:HD2	2.27	0.59
1:I:142:GLU:CD	1:I:244:PRO:HD2	2.28	0.59
2:C:601:CLA:H122	2:C:601:CLA:C7	2.32	0.59
1:H:142:GLU:CD	1:H:244:PRO:HD2	2.27	0.59
1:B:57:GLU:OE1	1:B:57:GLU:HA	2.03	0.58
1:E:142:GLU:CD	1:E:244:PRO:HD2	2.27	0.58
2:E:601:CLA:H122	2:E:601:CLA:C7	2.32	0.58
1:F:142:GLU:CD	1:F:244:PRO:HD2	2.28	0.58
2:H:601:CLA:H122	2:H:601:CLA:C7	2.32	0.58
2:K:601:CLA:H122	2:K:601:CLA:C7	2.32	0.58
1:H:80:HIS:CD2	1:H:98:THR:HG23	2.39	0.58
1:E:57:GLU:OE1	1:E:57:GLU:HA	2.03	0.58
1:K:57:GLU:HA	1:K:57:GLU:OE1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:80:HIS:CD2	1:I:98:THR:HG23	2.39	0.58
1:F:80:HIS:CD2	1:F:98:THR:HG23	2.39	0.57
1:G:80:HIS:CD2	1:G:98:THR:HG23	2.39	0.57
1:D:57:GLU:OE1	1:D:57:GLU:HA	2.03	0.57
1:A:80:HIS:CD2	1:A:98:THR:HG23	2.39	0.57
2:K:601:CLA:H72	2:K:601:CLA:H122	1.87	0.57
1:C:80:HIS:CD2	1:C:98:THR:HG23	2.39	0.57
1:J:80:HIS:CD2	1:J:98:THR:HG23	2.39	0.57
1:B:80:HIS:CD2	1:B:98:THR:HG23	2.39	0.57
1:G:126:TYR:HH	1:G:193:HIS:HE2	1.51	0.57
1:D:80:HIS:CD2	1:D:98:THR:HG23	2.39	0.56
1:A:57:GLU:HA	1:A:57:GLU:OE1	2.03	0.56
1:E:80:HIS:CD2	1:E:98:THR:HG23	2.39	0.56
1:G:57:GLU:OE1	1:G:57:GLU:HA	2.03	0.56
2:H:601:CLA:H72	2:H:601:CLA:H122	1.87	0.56
1:I:57:GLU:OE1	1:I:57:GLU:HA	2.03	0.56
1:K:80:HIS:CD2	1:K:98:THR:HG23	2.39	0.56
2:B:601:CLA:H72	2:B:601:CLA:H122	1.87	0.56
1:E:132:MET:HE1	2:E:606:CLA:HHC	1.88	0.56
1:J:57:GLU:OE1	1:J:57:GLU:HA	2.03	0.56
2:J:601:CLA:H72	2:J:601:CLA:H122	1.87	0.56
1:G:132:MET:HE1	2:G:606:CLA:HHC	1.88	0.56
1:C:132:MET:HE1	2:C:606:CLA:HHC	1.88	0.56
2:C:601:CLA:H72	2:C:601:CLA:H122	1.87	0.56
1:B:132:MET:HE1	2:B:606:CLA:HHC	1.88	0.55
1:D:132:MET:HE1	2:D:606:CLA:HHC	1.88	0.55
1:H:57:GLU:HA	1:H:57:GLU:OE1	2.03	0.55
1:F:57:GLU:HA	1:F:57:GLU:OE1	2.03	0.55
1:A:65:GLY:HA3	2:A:601:CLA:HED3	1.89	0.55
1:C:65:GLY:HA3	2:C:601:CLA:HED3	1.89	0.55
2:E:601:CLA:H72	2:E:601:CLA:H122	1.87	0.55
2:F:601:CLA:H72	2:F:601:CLA:H122	1.87	0.55
1:I:132:MET:HE1	2:I:606:CLA:HHC	1.88	0.55
1:D:126:TYR:HH	1:D:193:HIS:HE2	1.55	0.55
1:K:132:MET:HE1	2:K:606:CLA:HHC	1.88	0.55
1:J:193:HIS:O	1:J:193:HIS:ND1	2.40	0.54
1:A:132:MET:HE1	2:A:606:CLA:HHC	1.88	0.54
1:E:65:GLY:HA3	2:E:601:CLA:HED3	1.89	0.54
1:F:132:MET:HE1	2:F:606:CLA:HHC	1.88	0.54
2:G:601:CLA:H72	2:G:601:CLA:H122	1.87	0.54
1:I:193:HIS:O	1:I:193:HIS:ND1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:65:GLY:HA3	2:J:601:CLA:HED3	1.89	0.54
2:J:601:CLA:C12	2:J:601:CLA:C7	2.85	0.54
1:K:193:HIS:O	1:K:193:HIS:ND1	2.40	0.54
1:D:193:HIS:O	1:D:193:HIS:ND1	2.40	0.54
1:G:87:GLY:HA3	1:G:224:ARG:NH2	2.23	0.54
1:C:57:GLU:HA	1:C:57:GLU:OE1	2.03	0.54
1:C:193:HIS:O	1:C:193:HIS:ND1	2.40	0.54
1:C:52:THR:O	1:C:216:ARG:NH2	2.40	0.54
1:H:87:GLY:HA3	1:H:224:ARG:NH2	2.23	0.54
1:H:126:TYR:HH	1:H:193:HIS:HE2	1.52	0.54
1:H:132:MET:HE1	2:H:606:CLA:HHC	1.88	0.54
1:H:193:HIS:O	1:H:193:HIS:ND1	2.40	0.54
1:A:87:GLY:HA3	1:A:224:ARG:NH2	2.23	0.54
1:A:193:HIS:O	1:A:193:HIS:ND1	2.40	0.54
1:B:193:HIS:O	1:B:193:HIS:ND1	2.40	0.54
1:D:87:GLY:HA3	1:D:224:ARG:NH2	2.23	0.54
2:G:601:CLA:C12	2:G:601:CLA:C7	2.85	0.54
1:J:132:MET:HE1	2:J:606:CLA:HHC	1.88	0.54
2:A:601:CLA:C12	2:A:601:CLA:C7	2.85	0.54
1:C:87:GLY:HA3	1:C:224:ARG:NH2	2.23	0.54
1:D:52:THR:O	1:D:216:ARG:NH2	2.40	0.54
1:E:193:HIS:O	1:E:193:HIS:ND1	2.40	0.54
1:J:254:SER:OG	1:J:257:GLU:OE2	2.25	0.54
2:D:601:CLA:H72	2:D:601:CLA:H122	1.87	0.53
1:F:87:GLY:HA3	1:F:224:ARG:NH2	2.23	0.53
2:F:601:CLA:C12	2:F:601:CLA:C7	2.85	0.53
1:G:193:HIS:O	1:G:193:HIS:ND1	2.40	0.53
1:I:254:SER:OG	1:I:257:GLU:OE2	2.25	0.53
1:J:87:GLY:HA3	1:J:224:ARG:NH2	2.23	0.53
1:B:65:GLY:HA3	2:B:601:CLA:HED3	1.89	0.53
1:D:65:GLY:HA3	2:D:601:CLA:HED3	1.89	0.53
1:H:65:GLY:HA3	2:H:601:CLA:HED3	1.89	0.53
1:E:87:GLY:HA3	1:E:224:ARG:NH2	2.23	0.53
1:F:193:HIS:O	1:F:193:HIS:ND1	2.40	0.53
1:K:52:THR:O	1:K:216:ARG:NH2	2.40	0.53
1:K:254:SER:OG	1:K:257:GLU:OE2	2.25	0.53
1:G:65:GLY:HA3	2:G:601:CLA:HED3	1.89	0.53
1:H:254:SER:OG	1:H:257:GLU:OE2	2.25	0.53
1:K:65:GLY:HA3	2:K:601:CLA:HED3	1.89	0.53
1:K:87:GLY:HA3	1:K:224:ARG:NH2	2.23	0.53
1:B:126:TYR:HH	1:B:193:HIS:HE2	1.52	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:601:CLA:C12	2:B:601:CLA:C7	2.85	0.53
1:F:65:GLY:HA3	2:F:601:CLA:HED3	1.89	0.53
1:E:52:THR:O	1:E:216:ARG:NH2	2.40	0.53
1:I:65:GLY:HA3	2:I:601:CLA:HED3	1.89	0.53
1:B:87:GLY:HA3	1:B:224:ARG:NH2	2.23	0.53
1:J:180:LYS:HE3	1:J:184:ASN:ND2	2.25	0.52
1:K:106:ASP:OD2	1:K:106:ASP:N	2.41	0.52
1:H:180:LYS:HE3	1:H:184:ASN:ND2	2.25	0.52
1:I:87:GLY:HA3	1:I:224:ARG:NH2	2.23	0.52
1:A:254:SER:OG	1:A:257:GLU:OE2	2.25	0.52
1:D:240:THR:HG21	1:D:247:ASN:HD21	1.75	0.52
1:H:240:THR:HG21	1:H:247:ASN:HD21	1.75	0.52
1:B:180:LYS:HE3	1:B:184:ASN:ND2	2.25	0.52
1:E:106:ASP:OD2	1:E:106:ASP:N	2.41	0.52
1:G:240:THR:HG21	1:G:247:ASN:HD21	1.75	0.52
1:K:180:LYS:HE3	1:K:184:ASN:ND2	2.25	0.52
1:G:180:LYS:HE3	1:G:184:ASN:ND2	2.25	0.52
1:G:254:SER:OG	1:G:257:GLU:OE2	2.25	0.52
1:J:240:THR:HG21	1:J:247:ASN:HD21	1.75	0.52
1:A:240:THR:HG21	1:A:247:ASN:HD21	1.75	0.52
1:E:180:LYS:HE3	1:E:184:ASN:ND2	2.25	0.52
1:K:240:THR:HG21	1:K:247:ASN:HD21	1.75	0.52
2:A:605:CLA:O1A	1:B:64:ILE:O	2.28	0.52
1:B:240:THR:HG21	1:B:247:ASN:HD21	1.75	0.52
1:C:106:ASP:OD2	1:C:106:ASP:N	2.41	0.52
1:D:87:GLY:HA3	1:D:224:ARG:HH22	1.75	0.52
1:C:87:GLY:HA3	1:C:224:ARG:HH22	1.75	0.52
1:E:87:GLY:HA3	1:E:224:ARG:HH22	1.75	0.52
1:B:254:SER:OG	1:B:257:GLU:OE2	2.25	0.52
1:C:240:THR:HG21	1:C:247:ASN:HD21	1.75	0.52
2:C:605:CLA:O1A	1:D:64:ILE:O	2.28	0.52
1:F:52:THR:O	1:F:216:ARG:NH2	2.40	0.52
1:G:106:ASP:OD2	1:G:106:ASP:N	2.41	0.52
1:G:236:GLN:OE1	2:G:609:CLA:ND	2.43	0.52
1:I:240:THR:HG21	1:I:247:ASN:HD21	1.75	0.52
1:A:180:LYS:HE3	1:A:184:ASN:ND2	2.25	0.52
1:D:236:GLN:OE1	2:D:609:CLA:ND	2.43	0.52
1:E:240:THR:HG21	1:E:247:ASN:HD21	1.75	0.52
1:B:87:GLY:HA3	1:B:224:ARG:HH22	1.75	0.51
1:F:87:GLY:HA3	1:F:224:ARG:HH22	1.75	0.51
1:A:236:GLN:OE1	2:A:609:CLA:ND	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:180:LYS:HE3	1:F:184:ASN:ND2	2.24	0.51
1:I:106:ASP:OD2	1:I:106:ASP:N	2.41	0.51
1:B:236:GLN:OE1	2:B:609:CLA:ND	2.43	0.51
2:E:611:CLA:H102	2:F:607:CLA:H8	1.93	0.51
2:H:605:CLA:O1A	1:I:64:ILE:O	2.28	0.51
1:K:236:GLN:OE1	2:K:609:CLA:ND	2.43	0.51
1:A:52:THR:O	1:A:216:ARG:NH2	2.40	0.51
1:C:180:LYS:HE3	1:C:184:ASN:ND2	2.25	0.51
1:D:180:LYS:HE3	1:D:184:ASN:ND2	2.25	0.51
1:F:254:SER:OG	1:F:257:GLU:OE2	2.25	0.51
1:G:87:GLY:HA3	1:G:224:ARG:HH22	1.75	0.51
1:I:236:GLN:OE1	2:I:609:CLA:ND	2.43	0.51
1:J:236:GLN:OE1	2:J:609:CLA:ND	2.43	0.51
2:J:605:CLA:O1A	1:K:64:ILE:O	2.27	0.51
1:C:236:GLN:OE1	2:C:609:CLA:ND	2.43	0.51
1:C:254:SER:OG	1:C:257:GLU:OE2	2.25	0.51
1:H:236:GLN:OE1	2:H:609:CLA:ND	2.43	0.51
1:A:87:GLY:HA3	1:A:224:ARG:HH22	1.75	0.51
1:D:254:SER:OG	1:D:257:GLU:OE2	2.25	0.51
1:I:180:LYS:HE3	1:I:184:ASN:ND2	2.25	0.51
1:E:236:GLN:OE1	2:E:609:CLA:ND	2.43	0.51
1:F:236:GLN:OE1	2:F:609:CLA:ND	2.43	0.51
1:H:87:GLY:HA3	1:H:224:ARG:HH22	1.75	0.51
1:I:87:GLY:HA3	1:I:224:ARG:HH22	1.75	0.51
1:K:87:GLY:HA3	1:K:224:ARG:HH22	1.75	0.51
1:J:87:GLY:HA3	1:J:224:ARG:HH22	1.75	0.51
2:A:607:CLA:H91	2:A:607:CLA:C13	2.41	0.51
2:B:607:CLA:H91	2:B:607:CLA:C13	2.41	0.51
1:F:80:HIS:ND1	1:F:81:LEU:HG	2.26	0.51
1:K:80:HIS:ND1	1:K:81:LEU:HG	2.26	0.51
1:C:80:HIS:ND1	1:C:81:LEU:HG	2.26	0.51
2:C:607:CLA:H91	2:C:607:CLA:C13	2.41	0.51
2:D:607:CLA:H91	2:D:607:CLA:C13	2.41	0.51
1:E:254:SER:OG	1:E:257:GLU:OE2	2.25	0.51
2:E:607:CLA:H91	2:E:607:CLA:C13	2.41	0.51
1:F:240:THR:HG21	1:F:247:ASN:HD21	1.75	0.51
2:F:607:CLA:H91	2:F:607:CLA:C13	2.41	0.51
1:I:80:HIS:ND1	1:I:81:LEU:HG	2.26	0.51
2:K:607:CLA:H91	2:K:607:CLA:C13	2.41	0.51
2:E:605:CLA:O1A	1:F:64:ILE:O	2.29	0.50
2:F:605:CLA:O1A	1:G:64:ILE:O	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:80:HIS:ND1	1:G:81:LEU:HG	2.26	0.50
2:G:605:CLA:O1A	1:H:64:ILE:O	2.28	0.50
1:B:80:HIS:ND1	1:B:81:LEU:HG	2.26	0.50
2:D:605:CLA:O1A	1:E:64:ILE:O	2.29	0.50
2:J:607:CLA:H91	2:J:607:CLA:C13	2.41	0.50
1:E:80:HIS:ND1	1:E:81:LEU:HG	2.26	0.50
1:G:52:THR:O	1:G:216:ARG:NH2	2.40	0.50
2:H:611:CLA:H102	2:I:607:CLA:H8	1.94	0.50
2:I:605:CLA:O1A	1:J:64:ILE:O	2.29	0.50
2:G:607:CLA:H91	2:G:607:CLA:C13	2.41	0.50
2:I:601:CLA:H141	2:I:601:CLA:C17	2.10	0.50
1:A:64:ILE:O	2:K:605:CLA:O1A	2.29	0.50
1:A:80:HIS:ND1	1:A:81:LEU:HG	2.26	0.50
1:J:80:HIS:ND1	1:J:81:LEU:HG	2.26	0.50
2:A:611:CLA:H102	2:B:607:CLA:H8	1.93	0.50
1:H:52:THR:O	1:H:216:ARG:NH2	2.40	0.50
2:I:607:CLA:H91	2:I:607:CLA:C13	2.41	0.50
1:D:80:HIS:ND1	1:D:81:LEU:HG	2.26	0.50
1:A:106:ASP:OD2	1:A:106:ASP:N	2.41	0.50
1:H:80:HIS:HD2	1:H:98:THR:HG23	1.77	0.50
1:H:80:HIS:ND1	1:H:81:LEU:HG	2.26	0.49
2:A:607:CLA:H8	2:K:611:CLA:H102	1.94	0.49
1:B:214:TYR:CE1	2:B:607:CLA:HED1	2.48	0.49
2:H:607:CLA:H91	2:H:607:CLA:C13	2.41	0.49
1:B:126:TYR:HD1	1:B:126:TYR:O	1.96	0.49
2:B:605:CLA:O1A	1:C:64:ILE:O	2.31	0.49
1:F:214:TYR:CE1	2:F:607:CLA:HED1	2.48	0.49
1:I:52:THR:O	1:I:216:ARG:NH2	2.40	0.49
1:K:126:TYR:O	1:K:126:TYR:HD1	1.96	0.49
2:C:611:CLA:H102	2:D:607:CLA:H8	1.95	0.49
1:D:214:TYR:CE1	2:D:607:CLA:HED1	2.48	0.49
1:J:80:HIS:HD2	1:J:98:THR:HG23	1.77	0.49
1:J:126:TYR:HD1	1:J:126:TYR:O	1.96	0.49
1:J:214:TYR:CE1	2:J:607:CLA:HED1	2.48	0.49
1:C:214:TYR:CE1	2:C:607:CLA:HED1	2.48	0.49
1:F:80:HIS:HD2	1:F:98:THR:HG23	1.77	0.49
1:I:126:TYR:HD1	1:I:126:TYR:O	1.96	0.49
1:I:214:TYR:CE1	2:I:607:CLA:HED1	2.48	0.49
1:A:126:TYR:HD1	1:A:126:TYR:O	1.96	0.49
1:C:126:TYR:HD1	1:C:126:TYR:O	1.96	0.49
1:D:126:TYR:OH	1:D:193:HIS:CD2	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:126:TYR:OH	1:F:193:HIS:CD2	2.66	0.49
1:G:214:TYR:CE1	2:G:607:CLA:HED1	2.48	0.49
2:G:611:CLA:H102	2:H:607:CLA:H8	1.95	0.49
1:H:99:SER:HA	1:I:73:SER:HB3	1.95	0.49
1:H:126:TYR:HD1	1:H:126:TYR:O	1.96	0.49
2:J:611:CLA:H102	2:K:607:CLA:H8	1.94	0.49
1:K:214:TYR:CE1	2:K:607:CLA:HED1	2.48	0.49
1:F:126:TYR:HD1	1:F:126:TYR:O	1.96	0.49
1:G:126:TYR:HD1	1:G:126:TYR:O	1.96	0.49
1:H:126:TYR:OH	1:H:193:HIS:CD2	2.66	0.49
1:H:214:TYR:CE1	2:H:607:CLA:HED1	2.48	0.49
1:I:126:TYR:HH	1:I:193:HIS:HE2	1.55	0.49
2:I:611:CLA:H102	2:J:607:CLA:H8	1.95	0.49
1:K:126:TYR:OH	1:K:193:HIS:CD2	2.66	0.49
1:F:99:SER:HA	1:G:73:SER:HB3	1.95	0.49
1:J:99:SER:HA	1:K:73:SER:HB3	1.95	0.49
1:B:52:THR:O	1:B:216:ARG:NH2	2.40	0.48
1:E:126:TYR:HD1	1:E:126:TYR:O	1.96	0.48
1:E:214:TYR:CE1	2:E:607:CLA:HED1	2.48	0.48
1:J:126:TYR:OH	1:J:193:HIS:CD2	2.66	0.48
2:F:611:CLA:H102	2:G:607:CLA:H8	1.95	0.48
1:G:99:SER:HA	1:H:73:SER:HB3	1.96	0.48
1:G:126:TYR:OH	1:G:193:HIS:CD2	2.66	0.48
1:A:214:TYR:CE1	2:A:607:CLA:HED1	2.48	0.48
1:E:80:HIS:HD2	1:E:98:THR:HG23	1.77	0.48
2:G:603:CLA:HBB1	2:G:603:CLA:CMB	2.43	0.48
2:H:603:CLA:HBB1	2:H:603:CLA:CMB	2.43	0.48
1:B:126:TYR:OH	1:B:193:HIS:CD2	2.66	0.48
2:B:611:CLA:H102	2:C:607:CLA:H8	1.95	0.48
1:E:126:TYR:OH	1:E:193:HIS:CD2	2.66	0.48
1:G:80:HIS:HD2	1:G:98:THR:HG23	1.77	0.48
1:I:99:SER:HA	1:J:73:SER:HB3	1.96	0.48
2:I:603:CLA:HBB1	2:I:603:CLA:CMB	2.43	0.48
1:A:80:HIS:HD2	1:A:98:THR:HG23	1.77	0.48
1:A:274:PHE:CE2	2:A:602:CLA:H191	2.49	0.48
1:D:80:HIS:HD2	1:D:98:THR:HG23	1.77	0.48
1:D:126:TYR:HD1	1:D:126:TYR:O	1.96	0.48
1:H:274:PHE:CE2	2:H:602:CLA:H191	2.49	0.48
1:I:274:PHE:CE2	2:I:602:CLA:H191	2.49	0.48
1:K:80:HIS:HD2	1:K:98:THR:HG23	1.77	0.48
1:E:99:SER:HA	1:F:73:SER:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:274:PHE:CE2	2:G:602:CLA:H191	2.49	0.48
1:I:80:HIS:HD2	1:I:98:THR:HG23	1.77	0.48
2:J:603:CLA:HBB1	2:J:603:CLA:CMB	2.43	0.48
2:A:606:CLA:HAA1	3:A:612:XAT:H363	1.96	0.48
1:C:126:TYR:OH	1:C:193:HIS:CD2	2.66	0.48
1:D:274:PHE:CE2	2:D:602:CLA:H191	2.49	0.48
2:F:603:CLA:HBB1	2:F:603:CLA:CMB	2.43	0.48
1:J:274:PHE:CE2	2:J:602:CLA:H191	2.49	0.48
1:D:106:ASP:OD2	1:D:106:ASP:N	2.41	0.48
1:D:126:TYR:CZ	1:D:193:HIS:CD2	3.02	0.48
2:E:606:CLA:HAA1	3:E:612:XAT:H363	1.96	0.48
2:K:606:CLA:HAA1	3:K:612:XAT:H363	1.96	0.48
1:A:99:SER:HA	1:B:73:SER:HB3	1.95	0.47
1:A:124:GLU:OE1	2:A:602:CLA:NB	2.47	0.47
1:A:126:TYR:OH	1:A:193:HIS:CD2	2.66	0.47
1:B:124:GLU:OE1	2:B:602:CLA:NB	2.47	0.47
2:B:606:CLA:HAA1	3:B:612:XAT:H363	1.96	0.47
1:C:240:THR:HG21	1:C:247:ASN:ND2	2.29	0.47
2:D:606:CLA:HAA1	3:D:612:XAT:H363	1.96	0.47
1:F:274:PHE:CE2	2:F:602:CLA:H191	2.49	0.47
2:F:606:CLA:HAA1	3:F:612:XAT:H363	1.96	0.47
1:G:126:TYR:CZ	1:G:193:HIS:CD2	3.02	0.47
1:I:126:TYR:OH	1:I:193:HIS:CD2	2.66	0.47
1:J:52:THR:O	1:J:216:ARG:NH2	2.40	0.47
2:J:606:CLA:HAA1	3:J:612:XAT:H363	1.96	0.47
1:K:124:GLU:OE1	2:K:602:CLA:NB	2.47	0.47
1:B:274:PHE:CE2	2:B:602:CLA:H191	2.49	0.47
1:C:124:GLU:OE1	2:C:602:CLA:NB	2.47	0.47
2:C:606:CLA:HAA1	3:C:612:XAT:H363	1.96	0.47
1:E:240:THR:HG21	1:E:247:ASN:ND2	2.30	0.47
1:J:106:ASP:OD2	1:J:106:ASP:N	2.41	0.47
2:K:603:CLA:HBB1	2:K:603:CLA:CMB	2.43	0.47
1:B:80:HIS:HD2	1:B:98:THR:HG23	1.77	0.47
1:C:80:HIS:HD2	1:C:98:THR:HG23	1.77	0.47
1:E:274:PHE:CE2	2:E:602:CLA:H191	2.49	0.47
1:J:124:GLU:OE1	2:J:602:CLA:NB	2.47	0.47
1:J:240:THR:HG21	1:J:247:ASN:ND2	2.30	0.47
2:D:605:CLA:H62	2:D:605:CLA:H41	1.38	0.47
1:F:124:GLU:OE1	2:F:602:CLA:NB	2.47	0.47
1:F:126:TYR:CZ	1:F:193:HIS:CD2	3.02	0.47
1:G:124:GLU:OE1	2:G:602:CLA:NB	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:SER:HB3	1:K:99:SER:HA	1.96	0.47
1:C:126:TYR:CZ	1:C:193:HIS:CD2	3.02	0.47
1:E:126:TYR:CZ	1:E:193:HIS:CD2	3.02	0.47
2:E:603:CLA:HBB1	2:E:603:CLA:CMB	2.43	0.47
1:F:106:ASP:OD2	1:F:106:ASP:N	2.41	0.47
2:G:606:CLA:HAA1	3:G:612:XAT:H363	1.96	0.47
2:A:603:CLA:HBB1	2:A:603:CLA:CMB	2.43	0.47
1:C:99:SER:HA	1:D:73:SER:HB3	1.95	0.47
2:C:606:CLA:H61	2:C:606:CLA:H41	1.65	0.47
1:D:124:GLU:OE1	2:D:602:CLA:NB	2.47	0.47
2:D:611:CLA:H102	2:E:607:CLA:H8	1.97	0.47
1:G:240:THR:HG21	1:G:247:ASN:ND2	2.29	0.47
1:G:240:THR:HG22	1:G:263:TYR:CE1	2.50	0.47
1:I:124:GLU:OE1	2:I:602:CLA:NB	2.47	0.47
1:I:240:THR:HG21	1:I:247:ASN:ND2	2.30	0.47
2:A:601:CLA:H72	2:A:601:CLA:H122	1.87	0.47
1:B:240:THR:HG21	1:B:247:ASN:ND2	2.30	0.47
1:B:240:THR:HG22	1:B:263:TYR:CE1	2.50	0.47
1:C:274:PHE:CE2	2:C:602:CLA:H191	2.49	0.47
1:D:99:SER:HA	1:E:73:SER:HB3	1.96	0.47
1:E:124:GLU:OE1	2:E:602:CLA:NB	2.47	0.47
2:E:605:CLA:H62	2:E:605:CLA:H41	1.39	0.47
1:H:240:THR:HG21	1:H:247:ASN:ND2	2.30	0.47
1:H:240:THR:HG22	1:H:263:TYR:CE1	2.50	0.47
2:I:601:CLA:H72	2:I:601:CLA:H122	1.87	0.47
2:I:606:CLA:HAA1	3:I:612:XAT:H363	1.96	0.47
1:K:274:PHE:CE2	2:K:602:CLA:H191	2.49	0.47
2:A:606:CLA:H3A	2:A:606:CLA:HBA2	1.69	0.47
1:F:240:THR:HG21	1:F:247:ASN:ND2	2.30	0.47
1:H:124:GLU:OE1	2:H:602:CLA:NB	2.47	0.47
1:I:205:THR:HG23	1:I:206:GLU:HG3	1.97	0.47
1:K:240:THR:HG22	1:K:263:TYR:CE1	2.50	0.47
1:A:240:THR:HG22	1:A:263:TYR:CE1	2.50	0.47
2:C:605:CLA:H62	2:C:605:CLA:H41	1.38	0.47
1:H:106:ASP:OD2	1:H:106:ASP:N	2.41	0.47
1:H:126:TYR:CZ	1:H:193:HIS:CD2	3.02	0.47
1:J:126:TYR:CZ	1:J:193:HIS:CD2	3.02	0.47
1:A:126:TYR:CZ	1:A:193:HIS:CD2	3.02	0.47
1:B:126:TYR:CZ	1:B:193:HIS:CD2	3.02	0.47
2:B:603:CLA:HBB1	2:B:603:CLA:CMB	2.43	0.47
1:C:240:THR:HG22	1:C:263:TYR:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:205:THR:HG23	1:F:206:GLU:HG3	1.97	0.47
1:F:240:THR:HG22	1:F:263:TYR:CE1	2.50	0.47
1:G:205:THR:HG23	1:G:206:GLU:HG3	1.97	0.47
1:H:78:PRO:HG2	1:H:81:LEU:HD12	1.97	0.47
1:I:78:PRO:HG2	1:I:81:LEU:HD12	1.97	0.47
1:K:78:PRO:HG2	1:K:81:LEU:HD12	1.97	0.47
1:K:126:TYR:CZ	1:K:193:HIS:CD2	3.02	0.47
1:H:205:THR:HG23	1:H:206:GLU:HG3	1.97	0.46
1:I:126:TYR:CZ	1:I:193:HIS:CD2	3.02	0.46
1:A:78:PRO:HG2	1:A:81:LEU:HD12	1.97	0.46
1:C:232:GLY:O	1:C:236:GLN:HB2	2.15	0.46
1:I:232:GLY:O	1:I:236:GLN:HB2	2.15	0.46
1:I:240:THR:HG22	1:I:263:TYR:CE1	2.49	0.46
1:J:78:PRO:HG2	1:J:81:LEU:HD12	1.97	0.46
1:J:205:THR:HG23	1:J:206:GLU:HG3	1.97	0.46
1:J:240:THR:HG22	1:J:263:TYR:CE1	2.50	0.46
1:D:232:GLY:O	1:D:236:GLN:HB2	2.15	0.46
2:H:606:CLA:HAA1	3:H:612:XAT:H363	1.96	0.46
1:A:240:THR:HG21	1:A:247:ASN:ND2	2.30	0.46
1:B:232:GLY:O	1:B:236:GLN:HB2	2.15	0.46
1:D:240:THR:HG21	1:D:247:ASN:ND2	2.30	0.46
2:D:603:CLA:HBB1	2:D:603:CLA:CMB	2.43	0.46
1:E:205:THR:HG23	1:E:206:GLU:HG3	1.97	0.46
1:E:232:GLY:O	1:E:236:GLN:HB2	2.15	0.46
1:H:232:GLY:O	1:H:236:GLN:HB2	2.15	0.46
2:I:605:CLA:H41	2:I:605:CLA:H62	1.38	0.46
1:J:126:TYR:HH	1:J:193:HIS:HE2	1.54	0.46
1:J:232:GLY:O	1:J:236:GLN:HB2	2.15	0.46
1:B:78:PRO:HG2	1:B:81:LEU:HD12	1.97	0.46
1:D:240:THR:HG22	1:D:263:TYR:CE1	2.50	0.46
1:F:232:GLY:O	1:F:236:GLN:HB2	2.15	0.46
1:I:78:PRO:CG	1:I:288:ARG:HH12	2.24	0.46
2:J:606:CLA:HBA2	2:J:606:CLA:H3A	1.69	0.46
1:A:232:GLY:O	1:A:236:GLN:HB2	2.15	0.46
1:B:106:ASP:OD2	1:B:106:ASP:N	2.41	0.46
2:C:603:CLA:HBB1	2:C:603:CLA:CMB	2.43	0.46
1:G:78:PRO:HG2	1:G:81:LEU:HD12	1.97	0.46
1:G:232:GLY:O	1:G:236:GLN:HB2	2.15	0.46
2:A:605:CLA:H41	2:A:605:CLA:H62	1.38	0.46
1:K:240:THR:HG21	1:K:247:ASN:ND2	2.30	0.46
1:K:205:THR:HG23	1:K:206:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:SER:OG	1:A:254:SER:O	2.34	0.46
1:D:205:THR:HG23	1:D:206:GLU:HG3	1.97	0.46
2:A:601:CLA:H141	2:A:601:CLA:C17	2.10	0.46
1:C:78:PRO:HG2	1:C:81:LEU:HD12	1.97	0.45
1:E:240:THR:HG22	1:E:263:TYR:CE1	2.49	0.45
1:F:78:PRO:HG2	1:F:81:LEU:HD12	1.97	0.45
1:K:232:GLY:O	1:K:236:GLN:HB2	2.15	0.45
1:K:254:SER:OG	1:K:254:SER:O	2.34	0.45
1:E:78:PRO:HG2	1:E:81:LEU:HD12	1.97	0.45
2:H:606:CLA:HBA2	2:H:606:CLA:H3A	1.69	0.45
1:I:254:SER:OG	1:I:254:SER:O	2.34	0.45
1:A:205:THR:HG23	1:A:206:GLU:HG3	1.97	0.45
1:C:254:SER:OG	1:C:254:SER:O	2.34	0.45
2:F:605:CLA:H62	2:F:605:CLA:H41	1.39	0.45
1:B:205:THR:HG23	1:B:206:GLU:HG3	1.97	0.45
1:C:205:THR:HG23	1:C:206:GLU:HG3	1.97	0.45
1:D:78:PRO:HG2	1:D:81:LEU:HD12	1.97	0.45
1:F:126:TYR:HH	1:F:193:HIS:CD2	2.33	0.45
2:A:607:CLA:H193	2:A:607:CLA:H161	1.83	0.45
2:C:606:CLA:H151	3:C:612:XAT:H403	1.99	0.45
2:D:603:CLA:H92	2:D:603:CLA:H62	1.81	0.45
2:E:606:CLA:H151	3:E:612:XAT:H403	1.99	0.45
2:G:606:CLA:H151	3:G:612:XAT:H403	1.99	0.45
2:J:605:CLA:H41	2:J:605:CLA:H62	1.39	0.45
1:B:99:SER:HA	1:C:73:SER:HB3	1.97	0.45
1:I:291:LYS:HD3	1:I:291:LYS:N	2.32	0.45
2:A:606:CLA:H151	3:A:612:XAT:H403	1.99	0.45
2:F:607:CLA:H193	2:F:607:CLA:H161	1.83	0.45
1:A:291:LYS:N	1:A:291:LYS:HD3	2.32	0.45
2:B:606:CLA:H61	2:B:606:CLA:H41	1.65	0.45
2:K:605:CLA:H41	2:K:605:CLA:H62	1.38	0.45
2:B:606:CLA:H151	3:B:612:XAT:H403	1.99	0.45
1:C:291:LYS:N	1:C:291:LYS:HD3	2.32	0.45
2:D:606:CLA:H151	3:D:612:XAT:H403	1.99	0.45
2:F:606:CLA:H151	3:F:612:XAT:H403	1.99	0.45
2:H:606:CLA:H151	3:H:612:XAT:H403	1.99	0.45
2:I:606:CLA:H151	3:I:612:XAT:H403	1.99	0.45
1:K:291:LYS:HD3	1:K:291:LYS:N	2.32	0.45
1:J:254:SER:OG	1:J:254:SER:O	2.34	0.44
2:J:601:CLA:H141	2:J:601:CLA:C17	2.10	0.44
1:D:224:ARG:HH11	2:D:602:CLA:C1D	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:254:SER:OG	1:G:254:SER:O	2.34	0.44
2:H:602:CLA:HBA2	2:H:602:CLA:H3A	1.80	0.44
2:J:606:CLA:H151	3:J:612:XAT:H403	1.99	0.44
1:K:126:TYR:HH	1:K:193:HIS:CD2	2.35	0.44
2:K:606:CLA:H151	3:K:612:XAT:H403	1.99	0.44
2:B:605:CLA:H41	2:B:605:CLA:H62	1.39	0.44
1:G:224:ARG:HH11	2:G:602:CLA:C1D	2.31	0.44
1:J:224:ARG:HH11	2:J:602:CLA:C1D	2.31	0.44
1:B:224:ARG:HH11	2:B:602:CLA:C1D	2.31	0.44
1:G:291:LYS:HD3	1:G:291:LYS:N	2.32	0.44
1:K:224:ARG:HH11	2:K:602:CLA:C1D	2.31	0.44
1:C:224:ARG:HH11	2:C:602:CLA:C1D	2.31	0.44
2:G:601:CLA:H141	2:G:601:CLA:C17	2.10	0.44
1:H:224:ARG:HH11	2:H:602:CLA:C1D	2.31	0.44
1:B:254:SER:OG	1:B:254:SER:O	2.34	0.44
1:E:291:LYS:HD3	1:E:291:LYS:N	2.32	0.44
1:J:291:LYS:HD3	1:J:291:LYS:N	2.32	0.44
1:D:290:LYS:HB2	1:D:290:LYS:HE3	1.84	0.44
1:A:224:ARG:HH11	2:A:602:CLA:C1D	2.31	0.44
2:H:605:CLA:H41	2:H:605:CLA:H62	1.38	0.43
2:C:607:CLA:H193	2:C:607:CLA:H161	1.83	0.43
1:E:188:THR:O	1:E:190:GLU:N	2.48	0.43
1:E:224:ARG:HH11	2:E:602:CLA:C1D	2.31	0.43
1:E:290:LYS:HB2	1:E:290:LYS:HE3	1.84	0.43
2:E:606:CLA:H3A	2:E:606:CLA:HBA2	1.69	0.43
2:E:606:CLA:H61	2:E:606:CLA:H41	1.65	0.43
2:I:607:CLA:H193	2:I:607:CLA:H161	1.83	0.43
1:A:188:THR:O	1:A:190:GLU:N	2.48	0.43
1:D:291:LYS:N	1:D:291:LYS:HD3	2.32	0.43
1:F:224:ARG:HH11	2:F:602:CLA:C1D	2.31	0.43
1:H:291:LYS:HD3	1:H:291:LYS:N	2.32	0.43
1:I:224:ARG:HH11	2:I:602:CLA:C1D	2.31	0.43
1:B:291:LYS:HD3	1:B:291:LYS:N	2.32	0.43
1:C:290:LYS:HB2	1:C:290:LYS:HE3	1.84	0.43
1:D:254:SER:OG	1:D:254:SER:O	2.34	0.43
2:D:606:CLA:H61	2:D:606:CLA:H41	1.65	0.43
1:E:158:LEU:HD12	1:E:158:LEU:HA	1.92	0.43
1:J:78:PRO:CG	1:J:288:ARG:HH12	2.24	0.43
1:J:218:ALA:O	1:J:222:ASN:ND2	2.40	0.43
2:I:606:CLA:H41	2:I:606:CLA:H61	1.65	0.43
2:B:607:CLA:H193	2:B:607:CLA:H161	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:PRO:CG	1:D:288:ARG:HH12	2.24	0.43
2:H:606:CLA:H61	2:H:606:CLA:H41	1.65	0.43
2:D:606:CLA:H3A	2:D:606:CLA:HBA2	1.69	0.43
2:K:602:CLA:HBA2	2:K:602:CLA:H3A	1.80	0.43
2:A:601:CLA:C14	2:A:601:CLA:C17	2.85	0.43
2:B:606:CLA:H3A	2:B:606:CLA:HBA2	1.69	0.43
1:E:78:PRO:CG	1:E:288:ARG:HH12	2.24	0.43
2:G:607:CLA:H193	2:G:607:CLA:H161	1.83	0.43
2:F:606:CLA:H3A	2:F:606:CLA:HBA2	1.69	0.42
2:F:606:CLA:H41	2:F:606:CLA:H61	1.65	0.42
1:H:254:SER:OG	1:H:254:SER:O	2.34	0.42
2:I:603:CLA:H92	2:I:603:CLA:H62	1.81	0.42
2:I:610:CLA:H162	2:I:610:CLA:H141	1.85	0.42
2:A:607:CLA:CAD	2:A:608:CLA:HMA3	2.50	0.42
2:B:607:CLA:CAD	2:B:608:CLA:HMA3	2.50	0.42
1:C:78:PRO:CG	1:C:288:ARG:HH12	2.24	0.42
1:F:291:LYS:N	1:F:291:LYS:HD3	2.32	0.42
1:B:188:THR:O	1:B:190:GLU:N	2.48	0.42
1:F:290:LYS:HB2	1:F:290:LYS:HE3	1.84	0.42
2:G:605:CLA:H62	2:G:605:CLA:H41	1.38	0.42
1:D:188:THR:O	1:D:190:GLU:N	2.48	0.42
2:G:606:CLA:H41	2:G:606:CLA:H61	1.65	0.42
2:J:607:CLA:CAD	2:J:608:CLA:HMA3	2.50	0.42
2:K:609:CLA:C3B	3:K:612:XAT:H183	2.50	0.42
1:F:254:SER:OG	1:F:254:SER:O	2.34	0.42
1:B:290:LYS:HB2	1:B:290:LYS:HE3	1.84	0.42
2:B:603:CLA:HBC2	2:B:603:CLA:CHD	2.49	0.42
2:D:607:CLA:CAD	2:D:608:CLA:HMA3	2.50	0.42
2:H:609:CLA:C3B	3:H:612:XAT:H183	2.50	0.42
2:J:603:CLA:HBC2	2:J:603:CLA:CHD	2.49	0.42
1:C:158:LEU:HD12	1:C:158:LEU:HA	1.92	0.42
2:I:607:CLA:CAD	2:I:608:CLA:HMA3	2.50	0.42
2:D:601:CLA:H2	2:D:601:CLA:H62	1.83	0.42
1:F:78:PRO:CG	1:F:288:ARG:HH12	2.24	0.42
2:J:606:CLA:H61	2:J:606:CLA:H41	1.65	0.42
1:K:224:ARG:NH1	2:K:602:CLA:C2D	2.83	0.42
2:K:607:CLA:CAD	2:K:608:CLA:HMA3	2.50	0.42
1:C:188:THR:O	1:C:190:GLU:N	2.48	0.41
2:F:603:CLA:HBC2	2:F:603:CLA:CHD	2.49	0.41
2:G:609:CLA:C3B	3:G:612:XAT:H183	2.50	0.41
1:G:188:THR:O	1:G:190:GLU:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:607:CLA:CAD	2:G:608:CLA:HMA3	2.50	0.41
2:J:609:CLA:C3B	3:J:612:XAT:H183	2.50	0.41
1:K:259:ASN:OD1	1:K:259:ASN:C	2.64	0.41
2:A:609:CLA:C3B	3:A:612:XAT:H183	2.50	0.41
2:C:607:CLA:CAD	2:C:608:CLA:HMA3	2.50	0.41
2:E:607:CLA:CAD	2:E:608:CLA:HMA3	2.50	0.41
1:G:78:PRO:CG	1:G:288:ARG:HH12	2.24	0.41
2:H:607:CLA:CAD	2:H:608:CLA:HMA3	2.50	0.41
1:I:224:ARG:NH1	2:I:602:CLA:C2D	2.83	0.41
1:J:55:LEU:HD23	1:J:55:LEU:HA	1.91	0.41
1:J:259:ASN:OD1	1:J:259:ASN:C	2.64	0.41
1:A:224:ARG:NH1	2:A:602:CLA:C2D	2.83	0.41
1:A:259:ASN:OD1	1:A:259:ASN:C	2.64	0.41
2:C:609:CLA:C3B	3:C:612:XAT:H183	2.50	0.41
2:D:609:CLA:C3B	3:D:612:XAT:H183	2.50	0.41
1:E:224:ARG:NH1	2:E:602:CLA:C2D	2.83	0.41
1:F:224:ARG:NH1	2:F:602:CLA:C2D	2.83	0.41
1:I:181:ARG:HH22	2:I:605:CLA:HED1	1.86	0.41
1:I:259:ASN:C	1:I:259:ASN:OD1	2.64	0.41
2:I:609:CLA:C3B	3:I:612:XAT:H183	2.50	0.41
1:J:224:ARG:NH1	2:J:602:CLA:C2D	2.83	0.41
1:B:224:ARG:NH1	2:B:602:CLA:C2D	2.83	0.41
2:E:610:CLA:H162	2:E:610:CLA:H141	1.85	0.41
1:G:181:ARG:HH22	2:G:605:CLA:HED1	1.86	0.41
1:H:158:LEU:HD12	1:H:158:LEU:HA	1.92	0.41
1:H:259:ASN:OD1	1:H:259:ASN:C	2.64	0.41
1:I:240:THR:HG22	1:I:263:TYR:CD1	2.56	0.41
1:J:240:THR:HG22	1:J:263:TYR:CD1	2.56	0.41
2:J:601:CLA:H2	2:J:601:CLA:H62	1.83	0.41
1:F:240:THR:HG22	1:F:263:TYR:CD1	2.56	0.41
1:G:240:THR:HG22	1:G:263:TYR:CD1	2.56	0.41
1:H:181:ARG:HH22	2:H:605:CLA:HED1	1.86	0.41
2:J:610:CLA:H162	2:J:610:CLA:H141	1.85	0.41
1:A:181:ARG:HH22	2:A:605:CLA:HED1	1.86	0.41
1:B:240:THR:HG22	1:B:263:TYR:CD1	2.56	0.41
2:C:602:CLA:HBA2	2:C:602:CLA:H3A	1.80	0.41
1:K:240:THR:HG22	1:K:263:TYR:CD1	2.56	0.41
1:B:259:ASN:OD1	1:B:259:ASN:C	2.64	0.41
2:E:609:CLA:C3B	3:E:612:XAT:H183	2.50	0.41
1:G:259:ASN:OD1	1:G:259:ASN:C	2.64	0.41
1:J:181:ARG:HH22	2:J:605:CLA:HED1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:609:CLA:C3B	3:B:612:XAT:H183	2.50	0.41
1:C:224:ARG:NH1	2:C:602:CLA:C2D	2.83	0.41
1:C:240:THR:HG22	1:C:263:TYR:CD1	2.56	0.41
2:C:606:CLA:H3A	2:C:606:CLA:HBA2	1.69	0.41
1:E:254:SER:OG	1:E:254:SER:O	2.34	0.41
2:F:607:CLA:CAD	2:F:608:CLA:HMA3	2.50	0.41
2:G:606:CLA:H3A	2:G:606:CLA:HBA2	1.69	0.41
1:H:224:ARG:NH1	2:H:602:CLA:C2D	2.83	0.41
1:K:181:ARG:HH22	2:K:605:CLA:HED1	1.86	0.41
2:K:606:CLA:H41	2:K:606:CLA:H61	1.65	0.41
2:K:607:CLA:H193	2:K:607:CLA:H161	1.83	0.41
1:B:78:PRO:CG	1:B:288:ARG:HH12	2.24	0.41
1:E:240:THR:HG22	1:E:263:TYR:CD1	2.56	0.41
1:G:290:LYS:HB2	1:G:290:LYS:HE3	1.84	0.41
1:H:240:THR:HG22	1:H:263:TYR:CD1	2.56	0.41
2:H:607:CLA:H193	2:H:607:CLA:H161	1.83	0.41
1:K:218:ALA:O	1:K:222:ASN:ND2	2.40	0.40
1:E:181:ARG:HH22	2:E:605:CLA:HED1	1.86	0.40
1:G:158:LEU:HD12	1:G:158:LEU:HA	1.92	0.40
1:G:224:ARG:NH1	2:G:602:CLA:C2D	2.83	0.40
2:I:603:CLA:HBC2	2:I:603:CLA:CHD	2.49	0.40
2:I:606:CLA:H3A	2:I:606:CLA:HBA2	1.69	0.40
1:K:188:THR:O	1:K:190:GLU:N	2.48	0.40
1:C:259:ASN:OD1	1:C:259:ASN:C	2.64	0.40
1:D:224:ARG:NH1	2:D:602:CLA:C2D	2.83	0.40
2:E:603:CLA:HBC2	2:E:603:CLA:CHD	2.49	0.40
1:H:55:LEU:HD23	1:H:55:LEU:HA	1.91	0.40
1:H:78:PRO:CG	1:H:288:ARG:HH12	2.24	0.40
1:A:240:THR:HG22	1:A:263:TYR:CD1	2.56	0.40
2:A:603:CLA:HBC2	2:A:603:CLA:CHD	2.49	0.40
1:C:181:ARG:HH22	2:C:605:CLA:HED1	1.86	0.40
1:F:259:ASN:OD1	1:F:259:ASN:C	2.64	0.40
2:F:609:CLA:C3B	3:F:612:XAT:H183	2.50	0.40
2:A:607:CLA:HBB1	2:A:607:CLA:CMB	2.50	0.40
2:D:607:CLA:H193	2:D:607:CLA:H161	1.83	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	239/307 (78%)	212 (89%)	27 (11%)	0	100	100
1	B	239/307 (78%)	212 (89%)	27 (11%)	0	100	100
1	C	239/307 (78%)	212 (89%)	27 (11%)	0	100	100
1	D	239/307 (78%)	212 (89%)	27 (11%)	0	100	100
1	E	239/307 (78%)	212 (89%)	27 (11%)	0	100	100
1	F	239/307 (78%)	212 (89%)	27 (11%)	0	100	100
1	G	239/307 (78%)	212 (89%)	27 (11%)	0	100	100
1	H	239/307 (78%)	212 (89%)	27 (11%)	0	100	100
1	I	239/307 (78%)	212 (89%)	27 (11%)	0	100	100
1	J	239/307 (78%)	212 (89%)	27 (11%)	0	100	100
1	K	239/307 (78%)	212 (89%)	27 (11%)	0	100	100
All	All	2629/3377 (78%)	2332 (89%)	297 (11%)	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	193/247 (78%)	180 (93%)	13 (7%)	15	39
1	B	193/247 (78%)	180 (93%)	13 (7%)	15	39
1	C	193/247 (78%)	180 (93%)	13 (7%)	15	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	193/247 (78%)	180 (93%)	13 (7%)	15	39
1	E	193/247 (78%)	180 (93%)	13 (7%)	15	39
1	F	193/247 (78%)	180 (93%)	13 (7%)	15	39
1	G	193/247 (78%)	180 (93%)	13 (7%)	15	39
1	H	193/247 (78%)	180 (93%)	13 (7%)	15	39
1	I	193/247 (78%)	180 (93%)	13 (7%)	15	39
1	J	193/247 (78%)	180 (93%)	13 (7%)	15	39
1	K	193/247 (78%)	180 (93%)	13 (7%)	15	39
All	All	2123/2717 (78%)	1980 (93%)	143 (7%)	17	39

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	GLU
1	A	73	SER
1	A	84	SER
1	A	106	ASP
1	A	109	ASP
1	A	117	LEU
1	A	122	GLU
1	A	183	GLU
1	A	200	ASP
1	A	236	GLN
1	A	257	GLU
1	A	275	SER
1	A	290	LYS
1	B	57	GLU
1	B	73	SER
1	B	84	SER
1	B	106	ASP
1	B	109	ASP
1	B	117	LEU
1	B	122	GLU
1	B	183	GLU
1	B	200	ASP
1	B	236	GLN
1	B	257	GLU
1	B	275	SER
1	B	290	LYS

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Mol	Chain	Res	Type
1	C	57	GLU
1	C	73	SER
1	C	84	SER
1	C	106	ASP
1	C	109	ASP
1	C	117	LEU
1	C	122	GLU
1	C	183	GLU
1	C	200	ASP
1	C	236	GLN
1	C	257	GLU
1	C	275	SER
1	C	290	LYS
1	D	57	GLU
1	D	73	SER
1	D	84	SER
1	D	106	ASP
1	D	109	ASP
1	D	117	LEU
1	D	122	GLU
1	D	183	GLU
1	D	200	ASP
1	D	236	GLN
1	D	257	GLU
1	D	275	SER
1	D	290	LYS
1	E	57	GLU
1	E	73	SER
1	E	84	SER
1	E	106	ASP
1	E	109	ASP
1	E	117	LEU
1	E	122	GLU
1	E	183	GLU
1	E	200	ASP
1	E	236	GLN
1	E	257	GLU
1	E	275	SER
1	E	290	LYS
1	F	57	GLU
1	F	73	SER
1	F	84	SER

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Mol	Chain	Res	Type
1	F	106	ASP
1	F	109	ASP
1	F	117	LEU
1	F	122	GLU
1	F	183	GLU
1	F	200	ASP
1	F	236	GLN
1	F	257	GLU
1	F	275	SER
1	F	290	LYS
1	G	57	GLU
1	G	73	SER
1	G	84	SER
1	G	106	ASP
1	G	109	ASP
1	G	117	LEU
1	G	122	GLU
1	G	183	GLU
1	G	200	ASP
1	G	236	GLN
1	G	257	GLU
1	G	275	SER
1	G	290	LYS
1	H	57	GLU
1	H	73	SER
1	H	84	SER
1	H	106	ASP
1	H	109	ASP
1	H	117	LEU
1	H	122	GLU
1	H	183	GLU
1	H	200	ASP
1	H	236	GLN
1	H	257	GLU
1	H	275	SER
1	H	290	LYS
1	I	57	GLU
1	I	73	SER
1	I	84	SER
1	I	106	ASP
1	I	109	ASP
1	I	117	LEU

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Mol	Chain	Res	Type
1	I	122	GLU
1	I	183	GLU
1	I	200	ASP
1	I	236	GLN
1	I	257	GLU
1	I	275	SER
1	I	290	LYS
1	J	57	GLU
1	J	73	SER
1	J	84	SER
1	J	106	ASP
1	J	109	ASP
1	J	117	LEU
1	J	122	GLU
1	J	183	GLU
1	J	200	ASP
1	J	236	GLN
1	J	257	GLU
1	J	275	SER
1	J	290	LYS
1	K	57	GLU
1	K	73	SER
1	K	84	SER
1	K	106	ASP
1	K	109	ASP
1	K	117	LEU
1	K	122	GLU
1	K	183	GLU
1	K	200	ASP
1	K	236	GLN
1	K	257	GLU
1	K	275	SER
1	K	290	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

143 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CLA	F	607	1	69,73,73	1.55	9 (13%)	82,113,113	1.12	7 (8%)
2	CLA	D	608	-	60,64,73	1.82	11 (18%)	71,102,113	1.39	9 (12%)
2	CLA	E	601	-	69,73,73	1.60	10 (14%)	82,113,113	1.12	8 (9%)
2	CLA	B	601	-	69,73,73	1.60	10 (14%)	82,113,113	1.11	8 (9%)
2	CLA	D	610	-	69,73,73	1.67	10 (14%)	82,113,113	1.31	8 (9%)
2	CLA	G	605	1	69,73,73	1.58	10 (14%)	82,113,113	1.28	8 (9%)
2	CLA	J	604	-	69,73,73	1.60	9 (13%)	82,113,113	1.10	8 (9%)
2	CLA	D	611	-	60,64,73	1.67	9 (15%)	71,102,113	1.24	9 (12%)
2	CLA	H	603	1	60,64,73	1.76	9 (15%)	71,102,113	1.33	8 (11%)
2	CLA	A	608	-	60,64,73	1.82	11 (18%)	71,102,113	1.39	9 (12%)
2	CLA	I	602	1	69,73,73	1.59	9 (13%)	82,113,113	1.24	9 (10%)
4	32N	K	613	-	42,44,44	0.30	0	50,61,61	0.75	3 (6%)
2	CLA	E	608	-	60,64,73	1.83	11 (18%)	71,102,113	1.40	9 (12%)
4	32N	B	613	-	42,44,44	0.31	0	50,61,61	0.75	3 (6%)
4	32N	A	613	-	42,44,44	0.30	0	50,61,61	0.75	3 (6%)
2	CLA	B	607	1	69,73,73	1.55	9 (13%)	82,113,113	1.13	7 (8%)
2	CLA	F	601	-	69,73,73	1.60	10 (14%)	82,113,113	1.11	8 (9%)
2	CLA	J	611	-	60,64,73	1.67	9 (15%)	71,102,113	1.23	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CLA	A	609	1	69,73,73	1.63	9 (13%)	82,113,113	1.19	7 (8%)
3	XAT	I	612	-	41,47,47	0.24	0	54,74,74	1.00	4 (7%)
2	CLA	K	608	-	60,64,73	1.83	11 (18%)	71,102,113	1.39	9 (12%)
2	CLA	K	602	1	69,73,73	1.59	9 (13%)	82,113,113	1.24	9 (10%)
2	CLA	G	601	-	69,73,73	1.60	10 (14%)	82,113,113	1.11	8 (9%)
2	CLA	K	611	-	60,64,73	1.66	9 (15%)	71,102,113	1.23	9 (12%)
3	XAT	K	612	-	41,47,47	0.24	0	54,74,74	1.00	4 (7%)
2	CLA	J	609	1	69,73,73	1.63	9 (13%)	82,113,113	1.18	7 (8%)
2	CLA	A	606	-	69,73,73	1.65	10 (14%)	82,113,113	1.30	9 (10%)
3	XAT	A	612	-	41,47,47	0.24	0	54,74,74	1.00	4 (7%)
2	CLA	H	609	1	69,73,73	1.63	9 (13%)	82,113,113	1.19	8 (9%)
2	CLA	K	610	-	69,73,73	1.68	10 (14%)	82,113,113	1.32	8 (9%)
2	CLA	B	610	-	69,73,73	1.67	10 (14%)	82,113,113	1.32	8 (9%)
2	CLA	B	605	1	69,73,73	1.59	10 (14%)	82,113,113	1.29	8 (9%)
2	CLA	E	605	1	69,73,73	1.59	10 (14%)	82,113,113	1.29	8 (9%)
2	CLA	D	601	-	69,73,73	1.60	10 (14%)	82,113,113	1.11	8 (9%)
2	CLA	I	605	1	69,73,73	1.60	10 (14%)	82,113,113	1.29	8 (9%)
3	XAT	D	612	-	41,47,47	0.24	0	54,74,74	1.00	4 (7%)
2	CLA	E	610	-	69,73,73	1.67	10 (14%)	82,113,113	1.32	8 (9%)
2	CLA	K	609	1	69,73,73	1.63	9 (13%)	82,113,113	1.19	8 (9%)
2	CLA	G	608	-	60,64,73	1.83	11 (18%)	71,102,113	1.40	9 (12%)
4	32N	I	613	-	42,44,44	0.30	0	50,61,61	0.75	3 (6%)
3	XAT	C	612	-	41,47,47	0.23	0	54,74,74	1.00	4 (7%)
2	CLA	F	606	-	69,73,73	1.65	10 (14%)	82,113,113	1.30	9 (10%)
2	CLA	E	611	-	60,64,73	1.67	9 (15%)	71,102,113	1.23	9 (12%)
2	CLA	A	605	1	69,73,73	1.59	10 (14%)	82,113,113	1.29	8 (9%)
2	CLA	F	602	1	69,73,73	1.59	9 (13%)	82,113,113	1.24	9 (10%)
2	CLA	I	604	-	69,73,73	1.59	9 (13%)	82,113,113	1.10	8 (9%)
2	CLA	C	605	1	69,73,73	1.59	10 (14%)	82,113,113	1.29	8 (9%)
2	CLA	A	610	-	69,73,73	1.67	10 (14%)	82,113,113	1.32	8 (9%)
2	CLA	A	604	-	69,73,73	1.59	9 (13%)	82,113,113	1.10	8 (9%)
3	XAT	J	612	-	41,47,47	0.24	0	54,74,74	1.00	4 (7%)
2	CLA	E	606	-	69,73,73	1.65	10 (14%)	82,113,113	1.30	9 (10%)
2	CLA	I	606	-	69,73,73	1.66	10 (14%)	82,113,113	1.30	9 (10%)
2	CLA	F	605	1	69,73,73	1.59	10 (14%)	82,113,113	1.29	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CLA	D	607	1	69,73,73	1.55	9 (13%)	82,113,113	1.13	7 (8%)
2	CLA	B	606	-	69,73,73	1.66	10 (14%)	82,113,113	1.30	9 (10%)
2	CLA	J	603	1	60,64,73	1.76	9 (15%)	71,102,113	1.33	8 (11%)
2	CLA	G	602	1	69,73,73	1.59	9 (13%)	82,113,113	1.24	9 (10%)
4	32N	G	613	-	42,44,44	0.29	0	50,61,61	0.75	3 (6%)
2	CLA	G	611	-	60,64,73	1.66	9 (15%)	71,102,113	1.23	9 (12%)
2	CLA	H	602	1	69,73,73	1.59	9 (13%)	82,113,113	1.24	9 (10%)
2	CLA	E	607	1	69,73,73	1.56	9 (13%)	82,113,113	1.13	7 (8%)
2	CLA	F	610	-	69,73,73	1.67	10 (14%)	82,113,113	1.31	8 (9%)
2	CLA	H	606	-	69,73,73	1.65	10 (14%)	82,113,113	1.30	9 (10%)
2	CLA	C	606	-	69,73,73	1.65	10 (14%)	82,113,113	1.30	9 (10%)
2	CLA	I	607	1	69,73,73	1.56	9 (13%)	82,113,113	1.13	7 (8%)
2	CLA	C	604	-	69,73,73	1.59	9 (13%)	82,113,113	1.10	8 (9%)
2	CLA	K	603	1	60,64,73	1.76	9 (15%)	71,102,113	1.33	8 (11%)
3	XAT	B	612	-	41,47,47	0.24	0	54,74,74	1.00	4 (7%)
3	XAT	E	612	-	41,47,47	0.24	0	54,74,74	1.00	4 (7%)
2	CLA	F	604	-	69,73,73	1.59	9 (13%)	82,113,113	1.10	8 (9%)
2	CLA	D	602	1	69,73,73	1.59	9 (13%)	82,113,113	1.24	9 (10%)
2	CLA	J	607	1	69,73,73	1.56	9 (13%)	82,113,113	1.13	7 (8%)
2	CLA	D	605	1	69,73,73	1.59	10 (14%)	82,113,113	1.29	8 (9%)
2	CLA	C	603	1	60,64,73	1.76	9 (15%)	71,102,113	1.33	8 (11%)
2	CLA	J	605	1	69,73,73	1.59	10 (14%)	82,113,113	1.29	8 (9%)
2	CLA	B	602	1	69,73,73	1.59	9 (13%)	82,113,113	1.24	9 (10%)
2	CLA	G	603	1	60,64,73	1.76	9 (15%)	71,102,113	1.33	8 (11%)
2	CLA	C	601	-	69,73,73	1.60	10 (14%)	82,113,113	1.11	8 (9%)
2	CLA	B	604	-	69,73,73	1.59	9 (13%)	82,113,113	1.11	8 (9%)
2	CLA	G	607	1	69,73,73	1.55	9 (13%)	82,113,113	1.12	7 (8%)
2	CLA	J	606	-	69,73,73	1.65	10 (14%)	82,113,113	1.30	9 (10%)
2	CLA	C	602	1	69,73,73	1.59	9 (13%)	82,113,113	1.24	9 (10%)
4	32N	F	613	-	42,44,44	0.30	0	50,61,61	0.75	3 (6%)
2	CLA	C	608	-	60,64,73	1.83	11 (18%)	71,102,113	1.39	9 (12%)
2	CLA	F	608	-	60,64,73	1.83	11 (18%)	71,102,113	1.39	9 (12%)
2	CLA	E	609	1	69,73,73	1.63	9 (13%)	82,113,113	1.19	8 (9%)
2	CLA	H	604	-	69,73,73	1.59	9 (13%)	82,113,113	1.10	8 (9%)
4	32N	D	613	-	42,44,44	0.30	0	50,61,61	0.75	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CLA	H	601	-	69,73,73	1.60	10 (14%)	82,113,113	1.11	8 (9%)
2	CLA	D	606	-	69,73,73	1.65	10 (14%)	82,113,113	1.30	9 (10%)
2	CLA	D	604	-	69,73,73	1.60	9 (13%)	82,113,113	1.11	8 (9%)
2	CLA	E	603	1	60,64,73	1.76	9 (15%)	71,102,113	1.33	8 (11%)
4	32N	E	613	-	42,44,44	0.29	0	50,61,61	0.75	3 (6%)
2	CLA	I	601	-	69,73,73	1.60	10 (14%)	82,113,113	1.11	8 (9%)
2	CLA	I	611	-	60,64,73	1.66	9 (15%)	71,102,113	1.23	9 (12%)
2	CLA	H	610	-	69,73,73	1.67	10 (14%)	82,113,113	1.32	8 (9%)
2	CLA	I	608	-	60,64,73	1.82	11 (18%)	71,102,113	1.39	9 (12%)
4	32N	J	613	-	42,44,44	0.30	0	50,61,61	0.75	3 (6%)
4	32N	H	613	-	42,44,44	0.30	0	50,61,61	0.75	3 (6%)
4	32N	C	613	-	42,44,44	0.30	0	50,61,61	0.75	3 (6%)
2	CLA	B	603	1	60,64,73	1.76	9 (15%)	71,102,113	1.33	8 (11%)
2	CLA	J	608	-	60,64,73	1.82	11 (18%)	71,102,113	1.40	9 (12%)
2	CLA	K	601	-	69,73,73	1.60	10 (14%)	82,113,113	1.11	8 (9%)
2	CLA	A	602	1	69,73,73	1.59	9 (13%)	82,113,113	1.24	9 (10%)
2	CLA	K	605	1	69,73,73	1.60	10 (14%)	82,113,113	1.29	8 (9%)
2	CLA	A	611	-	60,64,73	1.66	9 (15%)	71,102,113	1.23	9 (12%)
2	CLA	F	603	1	60,64,73	1.76	9 (15%)	71,102,113	1.33	8 (11%)
2	CLA	H	611	-	60,64,73	1.66	9 (15%)	71,102,113	1.23	9 (12%)
2	CLA	I	603	1	60,64,73	1.76	9 (15%)	71,102,113	1.33	8 (11%)
3	XAT	H	612	-	41,47,47	0.24	0	54,74,74	1.00	4 (7%)
2	CLA	B	608	-	60,64,73	1.82	11 (18%)	71,102,113	1.40	9 (12%)
2	CLA	B	609	1	69,73,73	1.63	9 (13%)	82,113,113	1.19	7 (8%)
2	CLA	G	610	-	69,73,73	1.67	10 (14%)	82,113,113	1.32	8 (9%)
2	CLA	A	607	1	69,73,73	1.56	9 (13%)	82,113,113	1.13	7 (8%)
2	CLA	C	610	-	69,73,73	1.66	10 (14%)	82,113,113	1.31	8 (9%)
2	CLA	A	601	-	69,73,73	1.60	10 (14%)	82,113,113	1.11	8 (9%)
2	CLA	G	604	-	69,73,73	1.59	9 (13%)	82,113,113	1.10	8 (9%)
2	CLA	J	602	1	69,73,73	1.59	9 (13%)	82,113,113	1.24	9 (10%)
2	CLA	C	611	-	60,64,73	1.66	9 (15%)	71,102,113	1.23	9 (12%)
2	CLA	G	609	1	69,73,73	1.63	9 (13%)	82,113,113	1.18	8 (9%)
2	CLA	D	609	1	69,73,73	1.63	9 (13%)	82,113,113	1.19	7 (8%)
2	CLA	F	611	-	60,64,73	1.67	9 (15%)	71,102,113	1.23	9 (12%)
3	XAT	F	612	-	41,47,47	0.24	0	54,74,74	1.00	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CLA	K	607	1	69,73,73	1.55	9 (13%)	82,113,113	1.13	7 (8%)
2	CLA	A	603	1	60,64,73	1.76	9 (15%)	71,102,113	1.33	8 (11%)
2	CLA	H	608	-	60,64,73	1.82	11 (18%)	71,102,113	1.40	9 (12%)
2	CLA	K	606	-	69,73,73	1.65	10 (14%)	82,113,113	1.30	9 (10%)
2	CLA	H	607	1	69,73,73	1.56	9 (13%)	82,113,113	1.13	7 (8%)
2	CLA	C	607	1	69,73,73	1.56	9 (13%)	82,113,113	1.13	7 (8%)
2	CLA	E	602	1	69,73,73	1.59	9 (13%)	82,113,113	1.24	9 (10%)
2	CLA	G	606	-	69,73,73	1.65	10 (14%)	82,113,113	1.30	9 (10%)
2	CLA	J	601	-	69,73,73	1.60	10 (14%)	82,113,113	1.12	9 (10%)
3	XAT	G	612	-	41,47,47	0.24	0	54,74,74	1.00	4 (7%)
2	CLA	I	610	-	69,73,73	1.67	10 (14%)	82,113,113	1.32	8 (9%)
2	CLA	E	604	-	69,73,73	1.59	9 (13%)	82,113,113	1.10	8 (9%)
2	CLA	D	603	1	60,64,73	1.76	9 (15%)	71,102,113	1.33	8 (11%)
2	CLA	H	605	1	69,73,73	1.59	10 (14%)	82,113,113	1.28	8 (9%)
2	CLA	C	609	1	69,73,73	1.63	9 (13%)	82,113,113	1.19	8 (9%)
2	CLA	B	611	-	60,64,73	1.66	9 (15%)	71,102,113	1.23	9 (12%)
2	CLA	J	610	-	69,73,73	1.67	10 (14%)	82,113,113	1.32	8 (9%)
2	CLA	F	609	1	69,73,73	1.63	9 (13%)	82,113,113	1.19	8 (9%)
2	CLA	I	609	1	69,73,73	1.63	9 (13%)	82,113,113	1.18	8 (9%)
2	CLA	K	604	-	69,73,73	1.59	9 (13%)	82,113,113	1.10	8 (9%)

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
2	CLA	F	607	1	1/1/15/20	14/39/115/115	-
2	CLA	D	608	-	1/1/13/20	4/29/105/115	-
2	CLA	E	601	-	1/1/15/20	13/39/115/115	-
2	CLA	B	601	-	1/1/15/20	13/39/115/115	-
2	CLA	D	610	-	1/1/15/20	11/39/115/115	-
2	CLA	G	605	1	1/1/15/20	17/39/115/115	-
2	CLA	J	604	-	1/1/15/20	7/39/115/115	-
2	CLA	D	611	-	1/1/13/20	7/29/105/115	-
2	CLA	H	603	1	1/1/13/20	12/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CLA	A	608	-	1/1/13/20	4/29/105/115	-
2	CLA	I	602	1	1/1/15/20	8/39/115/115	-
4	32N	K	613	-	-	3/31/69/69	0/2/2/2
2	CLA	E	608	-	1/1/13/20	4/29/105/115	-
4	32N	B	613	-	-	3/31/69/69	0/2/2/2
4	32N	A	613	-	-	3/31/69/69	0/2/2/2
2	CLA	B	607	1	1/1/15/20	14/39/115/115	-
2	CLA	F	601	-	1/1/15/20	13/39/115/115	-
2	CLA	J	611	-	1/1/13/20	7/29/105/115	-
2	CLA	A	609	1	1/1/15/20	3/39/115/115	-
3	XAT	I	612	-	-	0/31/93/93	0/4/4/4
2	CLA	K	608	-	1/1/13/20	4/29/105/115	-
2	CLA	K	602	1	1/1/15/20	8/39/115/115	-
2	CLA	G	601	-	1/1/15/20	13/39/115/115	-
2	CLA	K	611	-	1/1/13/20	7/29/105/115	-
3	XAT	K	612	-	-	0/31/93/93	0/4/4/4
2	CLA	J	609	1	1/1/15/20	3/39/115/115	-
2	CLA	A	606	-	1/1/15/20	10/39/115/115	-
3	XAT	A	612	-	-	0/31/93/93	0/4/4/4
2	CLA	H	609	1	1/1/15/20	3/39/115/115	-
2	CLA	K	610	-	1/1/15/20	11/39/115/115	-
2	CLA	B	610	-	1/1/15/20	11/39/115/115	-
2	CLA	B	605	1	1/1/15/20	17/39/115/115	-
2	CLA	E	605	1	1/1/15/20	17/39/115/115	-
2	CLA	D	601	-	1/1/15/20	13/39/115/115	-
2	CLA	I	605	1	1/1/15/20	17/39/115/115	-
3	XAT	D	612	-	-	0/31/93/93	0/4/4/4
2	CLA	E	610	-	1/1/15/20	11/39/115/115	-
2	CLA	K	609	1	1/1/15/20	3/39/115/115	-
2	CLA	G	608	-	1/1/13/20	4/29/105/115	-
4	32N	I	613	-	-	3/31/69/69	0/2/2/2
3	XAT	C	612	-	-	0/31/93/93	0/4/4/4
2	CLA	F	606	-	1/1/15/20	10/39/115/115	-
2	CLA	E	611	-	1/1/13/20	7/29/105/115	-
2	CLA	A	605	1	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CLA	F	602	1	1/1/15/20	8/39/115/115	-
2	CLA	I	604	-	1/1/15/20	7/39/115/115	-
2	CLA	C	605	1	1/1/15/20	17/39/115/115	-
2	CLA	A	610	-	1/1/15/20	11/39/115/115	-
2	CLA	A	604	-	1/1/15/20	7/39/115/115	-
3	XAT	J	612	-	-	0/31/93/93	0/4/4/4
2	CLA	E	606	-	1/1/15/20	10/39/115/115	-
2	CLA	I	606	-	1/1/15/20	10/39/115/115	-
2	CLA	F	605	1	1/1/15/20	17/39/115/115	-
2	CLA	D	607	1	1/1/15/20	14/39/115/115	-
2	CLA	B	606	-	1/1/15/20	10/39/115/115	-
2	CLA	J	603	1	1/1/13/20	12/29/105/115	-
2	CLA	G	602	1	1/1/15/20	8/39/115/115	-
4	32N	G	613	-	-	3/31/69/69	0/2/2/2
2	CLA	G	611	-	1/1/13/20	7/29/105/115	-
2	CLA	H	602	1	1/1/15/20	8/39/115/115	-
2	CLA	E	607	1	1/1/15/20	14/39/115/115	-
2	CLA	F	610	-	1/1/15/20	11/39/115/115	-
2	CLA	H	606	-	1/1/15/20	10/39/115/115	-
2	CLA	C	606	-	1/1/15/20	10/39/115/115	-
2	CLA	I	607	1	1/1/15/20	14/39/115/115	-
2	CLA	C	604	-	1/1/15/20	7/39/115/115	-
2	CLA	K	603	1	1/1/13/20	12/29/105/115	-
3	XAT	B	612	-	-	0/31/93/93	0/4/4/4
3	XAT	E	612	-	-	0/31/93/93	0/4/4/4
2	CLA	F	604	-	1/1/15/20	7/39/115/115	-
2	CLA	D	602	1	1/1/15/20	8/39/115/115	-
2	CLA	J	607	1	1/1/15/20	14/39/115/115	-
2	CLA	D	605	1	1/1/15/20	17/39/115/115	-
2	CLA	C	603	1	1/1/13/20	12/29/105/115	-
2	CLA	J	605	1	1/1/15/20	17/39/115/115	-
2	CLA	B	602	1	1/1/15/20	8/39/115/115	-
2	CLA	G	603	1	1/1/13/20	12/29/105/115	-
2	CLA	C	601	-	1/1/15/20	13/39/115/115	-
2	CLA	B	604	-	1/1/15/20	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CLA	G	607	1	1/1/15/20	14/39/115/115	-
2	CLA	J	606	-	1/1/15/20	10/39/115/115	-
2	CLA	C	602	1	1/1/15/20	8/39/115/115	-
4	32N	F	613	-	-	3/31/69/69	0/2/2/2
2	CLA	C	608	-	1/1/13/20	4/29/105/115	-
2	CLA	F	608	-	1/1/13/20	4/29/105/115	-
2	CLA	E	609	1	1/1/15/20	3/39/115/115	-
2	CLA	H	604	-	1/1/15/20	7/39/115/115	-
4	32N	D	613	-	-	3/31/69/69	0/2/2/2
2	CLA	H	601	-	1/1/15/20	13/39/115/115	-
2	CLA	D	606	-	1/1/15/20	10/39/115/115	-
2	CLA	D	604	-	1/1/15/20	6/39/115/115	-
2	CLA	E	603	1	1/1/13/20	12/29/105/115	-
4	32N	E	613	-	-	3/31/69/69	0/2/2/2
2	CLA	I	601	-	1/1/15/20	13/39/115/115	-
2	CLA	I	611	-	1/1/13/20	7/29/105/115	-
2	CLA	H	610	-	1/1/15/20	11/39/115/115	-
2	CLA	I	608	-	1/1/13/20	4/29/105/115	-
4	32N	J	613	-	-	3/31/69/69	0/2/2/2
4	32N	H	613	-	-	3/31/69/69	0/2/2/2
4	32N	C	613	-	-	3/31/69/69	0/2/2/2
2	CLA	B	603	1	1/1/13/20	12/29/105/115	-
2	CLA	J	608	-	1/1/13/20	4/29/105/115	-
2	CLA	K	601	-	1/1/15/20	13/39/115/115	-
2	CLA	A	602	1	1/1/15/20	8/39/115/115	-
2	CLA	K	605	1	1/1/15/20	17/39/115/115	-
2	CLA	A	611	-	1/1/13/20	7/29/105/115	-
2	CLA	F	603	1	1/1/13/20	12/29/105/115	-
2	CLA	H	611	-	1/1/13/20	7/29/105/115	-
2	CLA	I	603	1	1/1/13/20	12/29/105/115	-
3	XAT	H	612	-	-	0/31/93/93	0/4/4/4
2	CLA	B	608	-	1/1/13/20	4/29/105/115	-
2	CLA	B	609	1	1/1/15/20	3/39/115/115	-
2	CLA	G	610	-	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CLA	A	607	1	1/1/15/20	14/39/115/115	-
2	CLA	C	610	-	1/1/15/20	11/39/115/115	-
2	CLA	A	601	-	1/1/15/20	13/39/115/115	-
2	CLA	G	604	-	1/1/15/20	7/39/115/115	-
2	CLA	J	602	1	1/1/15/20	8/39/115/115	-
2	CLA	C	611	-	1/1/13/20	7/29/105/115	-
2	CLA	G	609	1	1/1/15/20	3/39/115/115	-
2	CLA	D	609	1	1/1/15/20	3/39/115/115	-
2	CLA	F	611	-	1/1/13/20	7/29/105/115	-
3	XAT	F	612	-	-	0/31/93/93	0/4/4/4
2	CLA	K	607	1	1/1/15/20	14/39/115/115	-
2	CLA	A	603	1	1/1/13/20	12/29/105/115	-
2	CLA	H	608	-	1/1/13/20	4/29/105/115	-
2	CLA	K	606	-	1/1/15/20	10/39/115/115	-
2	CLA	H	607	1	1/1/15/20	14/39/115/115	-
2	CLA	C	607	1	1/1/15/20	14/39/115/115	-
2	CLA	E	602	1	1/1/15/20	8/39/115/115	-
2	CLA	G	606	-	1/1/15/20	10/39/115/115	-
2	CLA	J	601	-	1/1/15/20	13/39/115/115	-
3	XAT	G	612	-	-	0/31/93/93	0/4/4/4
2	CLA	I	610	-	1/1/15/20	11/39/115/115	-
2	CLA	E	604	-	1/1/15/20	7/39/115/115	-
2	CLA	D	603	1	1/1/13/20	12/29/105/115	-
2	CLA	H	605	1	1/1/15/20	17/39/115/115	-
2	CLA	C	609	1	1/1/15/20	3/39/115/115	-
2	CLA	B	611	-	1/1/13/20	7/29/105/115	-
2	CLA	J	610	-	1/1/15/20	11/39/115/115	-
2	CLA	F	609	1	1/1/15/20	3/39/115/115	-
2	CLA	I	609	1	1/1/15/20	3/39/115/115	-
2	CLA	K	604	-	1/1/15/20	7/39/115/115	-

All (1155) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	609	CLA	C4B-NB	7.02	1.47	1.37
2	K	609	CLA	C4B-NB	7.01	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	609	CLA	C4B-NB	7.00	1.47	1.37
2	E	609	CLA	C4B-NB	7.00	1.47	1.37
2	G	609	CLA	C4B-NB	7.00	1.47	1.37
2	A	609	CLA	C4B-NB	6.99	1.47	1.37
2	F	609	CLA	C4B-NB	6.99	1.47	1.37
2	I	609	CLA	C4B-NB	6.99	1.47	1.37
2	H	609	CLA	C4B-NB	6.99	1.47	1.37
2	C	609	CLA	C4B-NB	6.98	1.47	1.37
2	J	609	CLA	C4B-NB	6.97	1.47	1.37
2	J	604	CLA	C4B-NB	6.96	1.47	1.37
2	F	604	CLA	C4B-NB	6.95	1.47	1.37
2	C	604	CLA	C4B-NB	6.94	1.47	1.37
2	A	604	CLA	C4B-NB	6.94	1.47	1.37
2	B	604	CLA	C4B-NB	6.93	1.47	1.37
2	G	604	CLA	C4B-NB	6.93	1.47	1.37
2	H	604	CLA	C4B-NB	6.93	1.47	1.37
2	I	604	CLA	C4B-NB	6.92	1.47	1.37
2	K	604	CLA	C4B-NB	6.92	1.47	1.37
2	E	604	CLA	C4B-NB	6.92	1.46	1.37
2	D	604	CLA	C4B-NB	6.91	1.46	1.37
2	B	605	CLA	C4B-NB	6.56	1.46	1.37
2	K	605	CLA	C4B-NB	6.56	1.46	1.37
2	I	605	CLA	C4B-NB	6.54	1.46	1.37
2	D	605	CLA	C4B-NB	6.54	1.46	1.37
2	E	605	CLA	C4B-NB	6.53	1.46	1.37
2	J	605	CLA	C4B-NB	6.53	1.46	1.37
2	A	605	CLA	C4B-NB	6.52	1.46	1.37
2	F	611	CLA	C4B-NB	6.52	1.46	1.37
2	H	605	CLA	C4B-NB	6.51	1.46	1.37
2	C	605	CLA	C4B-NB	6.50	1.46	1.37
2	G	605	CLA	C4B-NB	6.50	1.46	1.37
2	F	605	CLA	C4B-NB	6.49	1.46	1.37
2	D	611	CLA	C4B-NB	6.48	1.46	1.37
2	E	611	CLA	C4B-NB	6.47	1.46	1.37
2	A	611	CLA	C4B-NB	6.46	1.46	1.37
2	K	611	CLA	C4B-NB	6.46	1.46	1.37
2	C	611	CLA	C4B-NB	6.45	1.46	1.37
2	D	601	CLA	C4B-NB	6.45	1.46	1.37
2	B	611	CLA	C4B-NB	6.45	1.46	1.37
2	G	611	CLA	C4B-NB	6.45	1.46	1.37
2	J	611	CLA	C4B-NB	6.45	1.46	1.37
2	K	601	CLA	C4B-NB	6.44	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	611	CLA	C4B-NB	6.43	1.46	1.37
2	B	601	CLA	C4B-NB	6.43	1.46	1.37
2	F	601	CLA	C4B-NB	6.43	1.46	1.37
2	J	601	CLA	C4B-NB	6.42	1.46	1.37
2	H	611	CLA	C4B-NB	6.42	1.46	1.37
2	G	601	CLA	C4B-NB	6.41	1.46	1.37
2	A	601	CLA	C4B-NB	6.40	1.46	1.37
2	C	601	CLA	C4B-NB	6.39	1.46	1.37
2	I	601	CLA	C4B-NB	6.38	1.46	1.37
2	H	601	CLA	C4B-NB	6.38	1.46	1.37
2	K	610	CLA	C4B-NB	6.38	1.46	1.37
2	H	610	CLA	C4B-NB	6.38	1.46	1.37
2	E	601	CLA	C4B-NB	6.37	1.46	1.37
2	C	602	CLA	C4B-NB	6.37	1.46	1.37
2	G	602	CLA	C4B-NB	6.37	1.46	1.37
2	K	602	CLA	C4B-NB	6.37	1.46	1.37
2	F	602	CLA	C4B-NB	6.36	1.46	1.37
2	I	602	CLA	C4B-NB	6.36	1.46	1.37
2	H	602	CLA	C4B-NB	6.35	1.46	1.37
2	A	602	CLA	C4B-NB	6.35	1.46	1.37
2	E	602	CLA	C4B-NB	6.35	1.46	1.37
2	B	602	CLA	C4B-NB	6.35	1.46	1.37
2	B	610	CLA	C4B-NB	6.34	1.46	1.37
2	D	602	CLA	C4B-NB	6.34	1.46	1.37
2	J	602	CLA	C4B-NB	6.34	1.46	1.37
2	I	610	CLA	C4B-NB	6.34	1.46	1.37
2	G	610	CLA	C4B-NB	6.33	1.46	1.37
2	C	608	CLA	C4B-NB	6.33	1.46	1.37
2	G	608	CLA	C4B-NB	6.32	1.46	1.37
2	J	610	CLA	C4B-NB	6.32	1.46	1.37
2	D	608	CLA	C4B-NB	6.32	1.46	1.37
2	D	610	CLA	C4B-NB	6.32	1.46	1.37
2	F	608	CLA	C4B-NB	6.31	1.46	1.37
2	A	610	CLA	C4B-NB	6.31	1.46	1.37
2	J	608	CLA	C4B-NB	6.31	1.46	1.37
2	A	608	CLA	C4B-NB	6.31	1.46	1.37
2	K	608	CLA	C4B-NB	6.31	1.46	1.37
2	B	608	CLA	C4B-NB	6.30	1.46	1.37
2	E	610	CLA	C4B-NB	6.30	1.46	1.37
2	F	610	CLA	C4B-NB	6.30	1.46	1.37
2	H	608	CLA	C4B-NB	6.30	1.46	1.37
2	I	608	CLA	C4B-NB	6.29	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	608	CLA	C4B-NB	6.28	1.46	1.37
2	C	610	CLA	C4B-NB	6.27	1.46	1.37
2	K	610	CLA	MG-NB	-6.17	1.93	2.05
2	I	606	CLA	MG-NB	-6.16	1.93	2.05
2	E	610	CLA	MG-NB	-6.15	1.93	2.05
2	K	606	CLA	MG-NB	-6.15	1.93	2.05
2	I	610	CLA	MG-NB	-6.14	1.93	2.05
2	J	610	CLA	MG-NB	-6.14	1.93	2.05
2	D	610	CLA	MG-NB	-6.13	1.93	2.05
2	B	606	CLA	MG-NB	-6.13	1.93	2.05
2	A	610	CLA	MG-NB	-6.12	1.93	2.05
2	G	606	CLA	MG-NB	-6.12	1.93	2.05
2	A	606	CLA	MG-NB	-6.12	1.93	2.05
2	F	610	CLA	MG-NB	-6.12	1.93	2.05
2	C	606	CLA	MG-NB	-6.11	1.93	2.05
2	J	606	CLA	MG-NB	-6.11	1.93	2.05
2	H	610	CLA	MG-NB	-6.11	1.93	2.05
2	F	606	CLA	MG-NB	-6.11	1.93	2.05
2	G	610	CLA	MG-NB	-6.11	1.93	2.05
2	G	603	CLA	MG-NB	-6.10	1.93	2.05
2	E	603	CLA	MG-NB	-6.10	1.93	2.05
2	I	603	CLA	MG-NB	-6.10	1.93	2.05
2	B	610	CLA	MG-NB	-6.10	1.93	2.05
2	F	603	CLA	MG-NB	-6.09	1.93	2.05
2	H	606	CLA	MG-NB	-6.09	1.93	2.05
2	D	606	CLA	MG-NB	-6.09	1.93	2.05
2	C	610	CLA	MG-NB	-6.09	1.93	2.05
2	D	603	CLA	MG-NB	-6.09	1.93	2.05
2	A	603	CLA	MG-NB	-6.08	1.93	2.05
2	E	606	CLA	MG-NB	-6.08	1.93	2.05
2	J	606	CLA	C4B-NB	6.08	1.45	1.37
2	F	606	CLA	C4B-NB	6.08	1.45	1.37
2	I	606	CLA	C4B-NB	6.08	1.45	1.37
2	C	603	CLA	MG-NB	-6.08	1.93	2.05
2	C	606	CLA	C4B-NB	6.08	1.45	1.37
2	K	606	CLA	C4B-NB	6.08	1.45	1.37
2	G	606	CLA	C4B-NB	6.08	1.45	1.37
2	B	606	CLA	C4B-NB	6.08	1.45	1.37
2	H	606	CLA	C4B-NB	6.08	1.45	1.37
2	B	603	CLA	MG-NB	-6.07	1.93	2.05
2	A	606	CLA	C4B-NB	6.07	1.45	1.37
2	K	603	CLA	MG-NB	-6.07	1.93	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	603	CLA	MG-NB	-6.07	1.93	2.05
2	D	606	CLA	C4B-NB	6.07	1.45	1.37
2	H	603	CLA	MG-NB	-6.06	1.93	2.05
2	E	606	CLA	C4B-NB	6.05	1.45	1.37
2	E	608	CLA	MG-ND	-6.02	1.93	2.05
2	K	608	CLA	MG-ND	-6.01	1.93	2.05
2	F	608	CLA	MG-ND	-5.99	1.93	2.05
2	B	608	CLA	MG-ND	-5.99	1.93	2.05
2	G	608	CLA	MG-ND	-5.98	1.93	2.05
2	D	608	CLA	MG-ND	-5.98	1.93	2.05
2	A	608	CLA	MG-ND	-5.98	1.93	2.05
2	C	608	CLA	MG-ND	-5.98	1.93	2.05
2	J	608	CLA	MG-ND	-5.97	1.93	2.05
2	I	608	CLA	MG-ND	-5.97	1.93	2.05
2	H	608	CLA	MG-ND	-5.96	1.94	2.05
2	C	608	CLA	MG-NB	-5.95	1.94	2.05
2	G	608	CLA	MG-NB	-5.95	1.94	2.05
2	J	608	CLA	MG-NB	-5.94	1.94	2.05
2	D	608	CLA	MG-NB	-5.93	1.94	2.05
2	I	608	CLA	MG-NB	-5.93	1.94	2.05
2	K	608	CLA	MG-NB	-5.93	1.94	2.05
2	A	608	CLA	MG-NB	-5.93	1.94	2.05
2	F	608	CLA	MG-NB	-5.93	1.94	2.05
2	H	608	CLA	MG-NB	-5.91	1.94	2.05
2	E	608	CLA	MG-NB	-5.91	1.94	2.05
2	B	608	CLA	MG-NB	-5.90	1.94	2.05
2	G	610	CLA	MG-ND	-5.85	1.94	2.05
2	B	610	CLA	MG-ND	-5.84	1.94	2.05
2	H	610	CLA	MG-ND	-5.84	1.94	2.05
2	I	610	CLA	MG-ND	-5.83	1.94	2.05
2	A	610	CLA	MG-ND	-5.83	1.94	2.05
2	F	610	CLA	MG-ND	-5.82	1.94	2.05
2	C	610	CLA	MG-ND	-5.82	1.94	2.05
2	J	610	CLA	MG-ND	-5.82	1.94	2.05
2	K	610	CLA	MG-ND	-5.82	1.94	2.05
2	D	610	CLA	MG-ND	-5.81	1.94	2.05
2	E	610	CLA	MG-ND	-5.80	1.94	2.05
2	H	607	CLA	MG-NB	-5.78	1.94	2.05
2	C	603	CLA	C4B-NB	5.78	1.45	1.37
2	B	603	CLA	C4B-NB	5.78	1.45	1.37
2	G	603	CLA	C4B-NB	5.78	1.45	1.37
2	C	607	CLA	MG-NB	-5.78	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	607	CLA	MG-NB	-5.77	1.94	2.05
2	F	603	CLA	C4B-NB	5.77	1.45	1.37
2	D	603	CLA	C4B-NB	5.77	1.45	1.37
2	E	603	CLA	C4B-NB	5.77	1.45	1.37
2	I	603	CLA	C4B-NB	5.77	1.45	1.37
2	D	607	CLA	MG-NB	-5.77	1.94	2.05
2	K	603	CLA	C4B-NB	5.77	1.45	1.37
2	J	607	CLA	MG-NB	-5.77	1.94	2.05
2	A	603	CLA	C4B-NB	5.77	1.45	1.37
2	J	603	CLA	C4B-NB	5.76	1.45	1.37
2	E	602	CLA	MG-NB	-5.76	1.94	2.05
2	G	607	CLA	MG-NB	-5.76	1.94	2.05
2	K	602	CLA	MG-NB	-5.76	1.94	2.05
2	E	607	CLA	MG-NB	-5.76	1.94	2.05
2	H	603	CLA	C4B-NB	5.75	1.45	1.37
2	A	607	CLA	MG-NB	-5.75	1.94	2.05
2	B	602	CLA	MG-NB	-5.75	1.94	2.05
2	G	601	CLA	MG-NB	-5.74	1.94	2.05
2	K	601	CLA	MG-NB	-5.74	1.94	2.05
2	J	601	CLA	MG-NB	-5.74	1.94	2.05
2	F	607	CLA	MG-NB	-5.74	1.94	2.05
2	I	602	CLA	MG-NB	-5.74	1.94	2.05
2	A	602	CLA	MG-NB	-5.73	1.94	2.05
2	C	602	CLA	MG-NB	-5.73	1.94	2.05
2	D	602	CLA	MG-NB	-5.73	1.94	2.05
2	E	601	CLA	MG-NB	-5.73	1.94	2.05
2	B	607	CLA	MG-NB	-5.73	1.94	2.05
2	F	602	CLA	MG-NB	-5.73	1.94	2.05
2	H	602	CLA	MG-NB	-5.73	1.94	2.05
2	G	602	CLA	MG-NB	-5.73	1.94	2.05
2	F	601	CLA	MG-NB	-5.73	1.94	2.05
2	I	607	CLA	MG-NB	-5.72	1.94	2.05
2	A	601	CLA	MG-NB	-5.72	1.94	2.05
2	B	601	CLA	MG-NB	-5.72	1.94	2.05
2	H	601	CLA	MG-NB	-5.71	1.94	2.05
2	I	601	CLA	MG-NB	-5.71	1.94	2.05
2	C	601	CLA	MG-NB	-5.71	1.94	2.05
2	D	601	CLA	MG-NB	-5.71	1.94	2.05
2	J	602	CLA	MG-NB	-5.69	1.94	2.05
2	E	609	CLA	MG-NB	-5.66	1.94	2.05
2	G	609	CLA	MG-NB	-5.66	1.94	2.05
2	K	609	CLA	MG-NB	-5.66	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	609	CLA	MG-NB	-5.66	1.94	2.05
2	D	609	CLA	MG-NB	-5.65	1.94	2.05
2	A	609	CLA	MG-NB	-5.64	1.94	2.05
2	C	609	CLA	MG-NB	-5.64	1.94	2.05
2	H	609	CLA	MG-NB	-5.64	1.94	2.05
2	B	609	CLA	MG-NB	-5.63	1.94	2.05
2	I	609	CLA	MG-NB	-5.63	1.94	2.05
2	F	609	CLA	MG-NB	-5.62	1.94	2.05
2	K	605	CLA	MG-ND	-5.59	1.94	2.05
2	J	605	CLA	MG-ND	-5.58	1.94	2.05
2	E	605	CLA	MG-ND	-5.57	1.94	2.05
2	I	605	CLA	MG-ND	-5.57	1.94	2.05
2	C	605	CLA	MG-ND	-5.56	1.94	2.05
2	A	605	CLA	MG-ND	-5.56	1.94	2.05
2	D	605	CLA	MG-ND	-5.56	1.94	2.05
2	B	605	CLA	MG-ND	-5.55	1.94	2.05
2	F	605	CLA	MG-ND	-5.54	1.94	2.05
2	G	605	CLA	MG-ND	-5.53	1.94	2.05
2	H	605	CLA	MG-ND	-5.53	1.94	2.05
2	I	607	CLA	MG-ND	-5.52	1.94	2.05
2	C	604	CLA	MG-NB	-5.51	1.94	2.05
2	E	607	CLA	MG-ND	-5.51	1.94	2.05
2	J	604	CLA	MG-NB	-5.51	1.94	2.05
2	H	604	CLA	MG-NB	-5.50	1.94	2.05
2	K	604	CLA	MG-NB	-5.49	1.94	2.05
2	B	606	CLA	MG-ND	-5.49	1.94	2.05
2	G	604	CLA	MG-NB	-5.49	1.94	2.05
2	A	604	CLA	MG-NB	-5.49	1.94	2.05
2	J	607	CLA	MG-ND	-5.49	1.94	2.05
2	A	607	CLA	MG-ND	-5.48	1.94	2.05
2	E	604	CLA	MG-NB	-5.48	1.94	2.05
2	F	607	CLA	MG-ND	-5.48	1.94	2.05
2	I	604	CLA	MG-NB	-5.48	1.94	2.05
2	B	607	CLA	MG-ND	-5.48	1.94	2.05
2	D	604	CLA	MG-NB	-5.48	1.94	2.05
2	F	604	CLA	MG-NB	-5.48	1.94	2.05
2	B	604	CLA	MG-NB	-5.47	1.94	2.05
2	E	606	CLA	MG-ND	-5.47	1.94	2.05
2	H	607	CLA	MG-ND	-5.47	1.94	2.05
2	F	606	CLA	MG-ND	-5.47	1.95	2.05
2	C	606	CLA	MG-ND	-5.46	1.95	2.05
2	D	607	CLA	MG-ND	-5.46	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	607	CLA	MG-ND	-5.46	1.95	2.05
2	H	606	CLA	MG-ND	-5.46	1.95	2.05
2	G	607	CLA	MG-ND	-5.46	1.95	2.05
2	C	607	CLA	C4B-NB	5.46	1.45	1.37
2	J	607	CLA	C4B-NB	5.45	1.45	1.37
2	A	606	CLA	MG-ND	-5.45	1.95	2.05
2	A	607	CLA	C4B-NB	5.45	1.45	1.37
2	B	605	CLA	MG-NB	-5.45	1.95	2.05
2	E	607	CLA	C4B-NB	5.45	1.45	1.37
2	G	607	CLA	C4B-NB	5.45	1.45	1.37
2	I	605	CLA	MG-NB	-5.45	1.95	2.05
2	J	606	CLA	MG-ND	-5.45	1.95	2.05
2	I	607	CLA	C4B-NB	5.45	1.45	1.37
2	C	607	CLA	MG-ND	-5.45	1.95	2.05
2	D	606	CLA	MG-ND	-5.45	1.95	2.05
2	I	606	CLA	MG-ND	-5.44	1.95	2.05
2	C	605	CLA	MG-NB	-5.44	1.95	2.05
2	B	607	CLA	C4B-NB	5.44	1.45	1.37
2	G	606	CLA	MG-ND	-5.43	1.95	2.05
2	K	605	CLA	MG-NB	-5.43	1.95	2.05
2	K	606	CLA	MG-ND	-5.43	1.95	2.05
2	D	607	CLA	C4B-NB	5.43	1.45	1.37
2	K	607	CLA	C4B-NB	5.43	1.45	1.37
2	H	607	CLA	C4B-NB	5.42	1.45	1.37
2	D	605	CLA	MG-NB	-5.42	1.95	2.05
2	A	605	CLA	MG-NB	-5.42	1.95	2.05
2	F	607	CLA	C4B-NB	5.42	1.45	1.37
2	J	605	CLA	MG-NB	-5.42	1.95	2.05
2	E	605	CLA	MG-NB	-5.41	1.95	2.05
2	G	605	CLA	MG-NB	-5.41	1.95	2.05
2	F	605	CLA	MG-NB	-5.41	1.95	2.05
2	H	605	CLA	MG-NB	-5.40	1.95	2.05
2	B	611	CLA	MG-NB	-5.38	1.95	2.05
2	F	611	CLA	MG-NB	-5.38	1.95	2.05
2	J	611	CLA	MG-NB	-5.38	1.95	2.05
2	K	611	CLA	MG-NB	-5.38	1.95	2.05
2	A	611	CLA	MG-NB	-5.38	1.95	2.05
2	I	611	CLA	MG-NB	-5.37	1.95	2.05
2	D	611	CLA	MG-NB	-5.37	1.95	2.05
2	E	611	CLA	MG-NB	-5.37	1.95	2.05
2	C	611	CLA	MG-NB	-5.37	1.95	2.05
2	G	611	CLA	MG-NB	-5.37	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	611	CLA	MG-NB	-5.36	1.95	2.05
2	K	603	CLA	MG-ND	-5.24	1.95	2.05
2	F	603	CLA	MG-ND	-5.24	1.95	2.05
2	D	609	CLA	MG-ND	-5.22	1.95	2.05
2	H	609	CLA	MG-ND	-5.22	1.95	2.05
2	K	609	CLA	MG-ND	-5.22	1.95	2.05
2	A	609	CLA	MG-ND	-5.21	1.95	2.05
2	H	603	CLA	MG-ND	-5.21	1.95	2.05
2	B	609	CLA	MG-ND	-5.21	1.95	2.05
2	C	609	CLA	MG-ND	-5.21	1.95	2.05
2	G	609	CLA	MG-ND	-5.20	1.95	2.05
2	A	603	CLA	MG-ND	-5.20	1.95	2.05
2	F	609	CLA	MG-ND	-5.20	1.95	2.05
2	I	609	CLA	MG-ND	-5.20	1.95	2.05
2	E	603	CLA	MG-ND	-5.20	1.95	2.05
2	C	603	CLA	MG-ND	-5.20	1.95	2.05
2	J	603	CLA	MG-ND	-5.20	1.95	2.05
2	B	603	CLA	MG-ND	-5.20	1.95	2.05
2	G	603	CLA	MG-ND	-5.20	1.95	2.05
2	E	609	CLA	MG-ND	-5.19	1.95	2.05
2	I	603	CLA	MG-ND	-5.19	1.95	2.05
2	J	602	CLA	MG-ND	-5.19	1.95	2.05
2	D	603	CLA	MG-ND	-5.19	1.95	2.05
2	J	609	CLA	MG-ND	-5.18	1.95	2.05
2	H	602	CLA	MG-ND	-5.18	1.95	2.05
2	G	602	CLA	MG-ND	-5.18	1.95	2.05
2	B	602	CLA	MG-ND	-5.17	1.95	2.05
2	F	602	CLA	MG-ND	-5.17	1.95	2.05
2	E	602	CLA	MG-ND	-5.17	1.95	2.05
2	A	602	CLA	MG-ND	-5.16	1.95	2.05
2	D	602	CLA	MG-ND	-5.16	1.95	2.05
2	I	602	CLA	MG-ND	-5.15	1.95	2.05
2	D	604	CLA	MG-ND	-5.15	1.95	2.05
2	F	604	CLA	MG-ND	-5.14	1.95	2.05
2	C	602	CLA	MG-ND	-5.14	1.95	2.05
2	K	602	CLA	MG-ND	-5.14	1.95	2.05
2	B	604	CLA	MG-ND	-5.13	1.95	2.05
2	A	604	CLA	MG-ND	-5.13	1.95	2.05
2	E	604	CLA	MG-ND	-5.13	1.95	2.05
2	I	604	CLA	MG-ND	-5.13	1.95	2.05
2	H	604	CLA	MG-ND	-5.13	1.95	2.05
2	J	604	CLA	MG-ND	-5.12	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	604	CLA	MG-ND	-5.11	1.95	2.05
2	C	604	CLA	MG-ND	-5.11	1.95	2.05
2	K	604	CLA	MG-ND	-5.09	1.95	2.05
2	H	601	CLA	MG-ND	-5.02	1.95	2.05
2	I	601	CLA	MG-ND	-5.01	1.95	2.05
2	B	601	CLA	MG-ND	-5.01	1.95	2.05
2	E	601	CLA	MG-ND	-5.00	1.95	2.05
2	F	601	CLA	MG-ND	-5.00	1.95	2.05
2	A	601	CLA	MG-ND	-5.00	1.95	2.05
2	J	601	CLA	MG-ND	-5.00	1.95	2.05
2	D	601	CLA	MG-ND	-5.00	1.95	2.05
2	C	601	CLA	MG-ND	-4.99	1.95	2.05
2	K	601	CLA	MG-ND	-4.99	1.95	2.05
2	G	601	CLA	MG-ND	-4.98	1.95	2.05
2	C	611	CLA	MG-ND	-4.91	1.96	2.05
2	D	611	CLA	MG-ND	-4.91	1.96	2.05
2	E	611	CLA	MG-ND	-4.91	1.96	2.05
2	G	611	CLA	MG-ND	-4.91	1.96	2.05
2	K	611	CLA	MG-ND	-4.91	1.96	2.05
2	A	611	CLA	MG-ND	-4.91	1.96	2.05
2	H	611	CLA	MG-ND	-4.91	1.96	2.05
2	J	611	CLA	MG-ND	-4.91	1.96	2.05
2	B	611	CLA	MG-ND	-4.91	1.96	2.05
2	F	611	CLA	MG-ND	-4.91	1.96	2.05
2	I	611	CLA	MG-ND	-4.91	1.96	2.05
2	I	606	CLA	MG-NA	-4.64	1.95	2.06
2	K	606	CLA	MG-NA	-4.64	1.95	2.06
2	G	606	CLA	MG-NA	-4.64	1.95	2.06
2	C	606	CLA	MG-NA	-4.63	1.95	2.06
2	D	606	CLA	MG-NA	-4.63	1.95	2.06
2	F	606	CLA	MG-NA	-4.63	1.95	2.06
2	A	606	CLA	MG-NA	-4.63	1.95	2.06
2	J	606	CLA	MG-NA	-4.63	1.95	2.06
2	H	606	CLA	MG-NA	-4.63	1.95	2.06
2	E	606	CLA	MG-NA	-4.63	1.95	2.06
2	B	606	CLA	MG-NA	-4.62	1.95	2.06
2	H	608	CLA	MG-NA	-4.59	1.95	2.06
2	G	608	CLA	MG-NA	-4.58	1.95	2.06
2	B	608	CLA	MG-NA	-4.58	1.95	2.06
2	E	608	CLA	MG-NA	-4.58	1.95	2.06
2	A	608	CLA	MG-NA	-4.58	1.95	2.06
2	C	608	CLA	MG-NA	-4.58	1.95	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	608	CLA	MG-NA	-4.57	1.95	2.06
2	J	608	CLA	MG-NA	-4.57	1.95	2.06
2	D	608	CLA	MG-NA	-4.57	1.95	2.06
2	F	608	CLA	MG-NA	-4.57	1.95	2.06
2	K	608	CLA	MG-NA	-4.57	1.95	2.06
2	E	601	CLA	MG-NA	-4.55	1.95	2.06
2	J	601	CLA	MG-NA	-4.55	1.95	2.06
2	C	601	CLA	MG-NA	-4.54	1.95	2.06
2	I	601	CLA	MG-NA	-4.54	1.95	2.06
2	B	601	CLA	MG-NA	-4.53	1.95	2.06
2	G	601	CLA	MG-NA	-4.53	1.95	2.06
2	A	601	CLA	MG-NA	-4.52	1.95	2.06
2	D	601	CLA	MG-NA	-4.52	1.95	2.06
2	H	601	CLA	MG-NA	-4.51	1.95	2.06
2	F	601	CLA	MG-NA	-4.50	1.95	2.06
2	K	601	CLA	MG-NA	-4.49	1.95	2.06
2	E	609	CLA	MG-NA	-4.33	1.96	2.06
2	K	609	CLA	MG-NA	-4.33	1.96	2.06
2	K	602	CLA	MG-NA	-4.33	1.96	2.06
2	E	602	CLA	MG-NA	-4.32	1.96	2.06
2	B	609	CLA	MG-NA	-4.32	1.96	2.06
2	A	602	CLA	MG-NA	-4.32	1.96	2.06
2	I	602	CLA	MG-NA	-4.32	1.96	2.06
2	J	602	CLA	MG-NA	-4.32	1.96	2.06
2	D	602	CLA	MG-NA	-4.32	1.96	2.06
2	B	602	CLA	MG-NA	-4.31	1.96	2.06
2	F	602	CLA	MG-NA	-4.31	1.96	2.06
2	F	609	CLA	MG-NA	-4.31	1.96	2.06
2	H	602	CLA	MG-NA	-4.31	1.96	2.06
2	D	609	CLA	MG-NA	-4.31	1.96	2.06
2	G	602	CLA	MG-NA	-4.31	1.96	2.06
2	C	602	CLA	MG-NA	-4.31	1.96	2.06
2	G	609	CLA	MG-NA	-4.31	1.96	2.06
2	C	609	CLA	MG-NA	-4.30	1.96	2.06
2	A	609	CLA	MG-NA	-4.30	1.96	2.06
2	H	609	CLA	MG-NA	-4.30	1.96	2.06
2	J	609	CLA	MG-NA	-4.30	1.96	2.06
2	I	609	CLA	MG-NA	-4.29	1.96	2.06
2	I	607	CLA	MG-NA	-4.11	1.96	2.06
2	E	607	CLA	MG-NA	-4.11	1.96	2.06
2	B	607	CLA	MG-NA	-4.11	1.96	2.06
2	C	607	CLA	MG-NA	-4.11	1.96	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	607	CLA	MG-NA	-4.10	1.96	2.06
2	A	607	CLA	MG-NA	-4.10	1.96	2.06
2	F	607	CLA	MG-NA	-4.10	1.96	2.06
2	G	607	CLA	MG-NA	-4.10	1.96	2.06
2	J	607	CLA	MG-NA	-4.10	1.96	2.06
2	H	603	CLA	MG-NA	-4.10	1.96	2.06
2	H	607	CLA	MG-NA	-4.10	1.96	2.06
2	D	603	CLA	MG-NA	-4.09	1.96	2.06
2	D	607	CLA	MG-NA	-4.09	1.96	2.06
2	G	603	CLA	MG-NA	-4.09	1.96	2.06
2	I	603	CLA	MG-NA	-4.09	1.96	2.06
2	A	603	CLA	MG-NA	-4.08	1.96	2.06
2	B	610	CLA	MG-NA	-4.08	1.96	2.06
2	H	610	CLA	MG-NA	-4.08	1.96	2.06
2	F	603	CLA	MG-NA	-4.07	1.96	2.06
2	C	603	CLA	MG-NA	-4.07	1.96	2.06
2	C	610	CLA	MG-NA	-4.07	1.96	2.06
2	K	603	CLA	MG-NA	-4.07	1.96	2.06
2	E	610	CLA	MG-NA	-4.06	1.96	2.06
2	D	610	CLA	MG-NA	-4.06	1.96	2.06
2	A	610	CLA	MG-NA	-4.06	1.96	2.06
2	E	603	CLA	MG-NA	-4.06	1.96	2.06
2	B	603	CLA	MG-NA	-4.06	1.96	2.06
2	I	610	CLA	MG-NA	-4.06	1.96	2.06
2	K	610	CLA	MG-NA	-4.06	1.96	2.06
2	J	603	CLA	MG-NA	-4.05	1.96	2.06
2	G	610	CLA	MG-NA	-4.05	1.96	2.06
2	F	610	CLA	MG-NA	-4.05	1.96	2.06
2	J	610	CLA	MG-NA	-4.05	1.96	2.06
2	G	604	CLA	MG-NA	-3.94	1.96	2.06
2	K	604	CLA	MG-NA	-3.94	1.96	2.06
2	H	604	CLA	MG-NA	-3.93	1.96	2.06
2	C	604	CLA	MG-NA	-3.93	1.96	2.06
2	B	604	CLA	MG-NA	-3.92	1.97	2.06
2	D	604	CLA	MG-NA	-3.92	1.97	2.06
2	A	604	CLA	MG-NA	-3.92	1.97	2.06
2	J	604	CLA	MG-NA	-3.91	1.97	2.06
2	E	604	CLA	MG-NA	-3.90	1.97	2.06
2	F	604	CLA	MG-NA	-3.90	1.97	2.06
2	I	604	CLA	MG-NA	-3.90	1.97	2.06
2	E	611	CLA	MG-NA	-3.82	1.97	2.06
2	C	611	CLA	MG-NA	-3.81	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	611	CLA	MG-NA	-3.81	1.97	2.06
2	A	611	CLA	MG-NA	-3.79	1.97	2.06
2	H	611	CLA	MG-NA	-3.79	1.97	2.06
2	J	611	CLA	MG-NA	-3.79	1.97	2.06
2	K	611	CLA	MG-NA	-3.78	1.97	2.06
2	F	611	CLA	MG-NA	-3.77	1.97	2.06
2	G	611	CLA	MG-NA	-3.77	1.97	2.06
2	I	611	CLA	MG-NA	-3.76	1.97	2.06
2	B	611	CLA	MG-NA	-3.76	1.97	2.06
2	B	605	CLA	MG-NA	-3.75	1.97	2.06
2	F	605	CLA	MG-NA	-3.75	1.97	2.06
2	H	605	CLA	MG-NA	-3.75	1.97	2.06
2	A	605	CLA	MG-NA	-3.75	1.97	2.06
2	K	605	CLA	MG-NA	-3.75	1.97	2.06
2	G	605	CLA	MG-NA	-3.75	1.97	2.06
2	I	605	CLA	MG-NA	-3.75	1.97	2.06
2	C	605	CLA	MG-NA	-3.75	1.97	2.06
2	J	605	CLA	MG-NA	-3.74	1.97	2.06
2	E	605	CLA	MG-NA	-3.74	1.97	2.06
2	D	605	CLA	MG-NA	-3.74	1.97	2.06
2	J	606	CLA	MG-NC	-3.66	1.97	2.06
2	F	606	CLA	MG-NC	-3.66	1.97	2.06
2	B	606	CLA	MG-NC	-3.66	1.97	2.06
2	G	606	CLA	MG-NC	-3.66	1.97	2.06
2	E	606	CLA	MG-NC	-3.65	1.97	2.06
2	H	606	CLA	MG-NC	-3.65	1.97	2.06
2	A	606	CLA	MG-NC	-3.65	1.97	2.06
2	C	606	CLA	MG-NC	-3.65	1.97	2.06
2	D	606	CLA	MG-NC	-3.65	1.97	2.06
2	K	606	CLA	MG-NC	-3.65	1.97	2.06
2	I	606	CLA	MG-NC	-3.65	1.97	2.06
2	K	603	CLA	C3A-C2A	-3.46	1.45	1.54
2	I	603	CLA	C3A-C2A	-3.45	1.45	1.54
2	C	603	CLA	C3A-C2A	-3.43	1.45	1.54
2	H	609	CLA	MG-NC	-3.43	1.98	2.06
2	A	603	CLA	C3A-C2A	-3.43	1.45	1.54
2	K	603	CLA	MG-NC	-3.43	1.98	2.06
2	B	603	CLA	MG-NC	-3.42	1.98	2.06
2	G	603	CLA	C3A-C2A	-3.42	1.45	1.54
2	E	603	CLA	C3A-C2A	-3.42	1.45	1.54
2	J	603	CLA	MG-NC	-3.42	1.98	2.06
2	C	603	CLA	MG-NC	-3.42	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	603	CLA	C3A-C2A	-3.42	1.45	1.54
2	E	603	CLA	MG-NC	-3.42	1.98	2.06
2	B	603	CLA	C3A-C2A	-3.41	1.45	1.54
2	J	603	CLA	C3A-C2A	-3.41	1.45	1.54
2	A	603	CLA	MG-NC	-3.41	1.98	2.06
2	F	603	CLA	MG-NC	-3.41	1.98	2.06
2	F	609	CLA	MG-NC	-3.41	1.98	2.06
2	I	603	CLA	MG-NC	-3.40	1.98	2.06
2	I	609	CLA	MG-NC	-3.40	1.98	2.06
2	K	608	CLA	MG-NC	-3.40	1.98	2.06
2	K	609	CLA	MG-NC	-3.40	1.98	2.06
2	D	603	CLA	C3A-C2A	-3.40	1.45	1.54
2	H	603	CLA	MG-NC	-3.40	1.98	2.06
2	G	603	CLA	MG-NC	-3.40	1.98	2.06
2	H	603	CLA	C3A-C2A	-3.40	1.45	1.54
2	G	609	CLA	MG-NC	-3.40	1.98	2.06
2	D	603	CLA	MG-NC	-3.40	1.98	2.06
2	D	608	CLA	MG-NC	-3.40	1.98	2.06
2	A	609	CLA	MG-NC	-3.40	1.98	2.06
2	I	608	CLA	MG-NC	-3.40	1.98	2.06
2	E	609	CLA	MG-NC	-3.40	1.98	2.06
2	C	608	CLA	MG-NC	-3.39	1.98	2.06
2	E	608	CLA	MG-NC	-3.39	1.98	2.06
2	D	609	CLA	MG-NC	-3.39	1.98	2.06
2	J	609	CLA	MG-NC	-3.39	1.98	2.06
2	E	610	CLA	MG-NC	-3.39	1.98	2.06
2	C	609	CLA	MG-NC	-3.39	1.98	2.06
2	A	608	CLA	MG-NC	-3.38	1.98	2.06
2	F	610	CLA	MG-NC	-3.38	1.98	2.06
2	B	608	CLA	MG-NC	-3.38	1.98	2.06
2	B	610	CLA	MG-NC	-3.38	1.98	2.06
2	J	610	CLA	MG-NC	-3.38	1.98	2.06
2	H	608	CLA	MG-NC	-3.38	1.98	2.06
2	B	609	CLA	MG-NC	-3.38	1.98	2.06
2	F	608	CLA	MG-NC	-3.37	1.98	2.06
2	J	608	CLA	MG-NC	-3.37	1.98	2.06
2	G	608	CLA	MG-NC	-3.37	1.98	2.06
2	B	611	CLA	MG-NC	-3.37	1.98	2.06
2	K	611	CLA	MG-NC	-3.37	1.98	2.06
2	D	610	CLA	MG-NC	-3.37	1.98	2.06
2	A	610	CLA	MG-NC	-3.36	1.98	2.06
2	G	610	CLA	MG-NC	-3.36	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	610	CLA	MG-NC	-3.36	1.98	2.06
2	H	611	CLA	MG-NC	-3.35	1.98	2.06
2	G	611	CLA	MG-NC	-3.35	1.98	2.06
2	I	611	CLA	MG-NC	-3.34	1.98	2.06
2	C	610	CLA	MG-NC	-3.34	1.98	2.06
2	D	611	CLA	MG-NC	-3.34	1.98	2.06
2	F	611	CLA	MG-NC	-3.34	1.98	2.06
2	K	610	CLA	MG-NC	-3.34	1.98	2.06
2	H	610	CLA	MG-NC	-3.34	1.98	2.06
2	A	611	CLA	MG-NC	-3.34	1.98	2.06
2	E	611	CLA	MG-NC	-3.34	1.98	2.06
2	C	611	CLA	MG-NC	-3.33	1.98	2.06
2	H	610	CLA	CBD-CAD	-3.33	1.41	1.56
2	I	610	CLA	CBD-CAD	-3.33	1.41	1.56
2	B	610	CLA	CBD-CAD	-3.33	1.41	1.56
2	E	610	CLA	CBD-CAD	-3.33	1.41	1.56
2	K	610	CLA	CBD-CAD	-3.33	1.41	1.56
2	J	611	CLA	MG-NC	-3.32	1.98	2.06
2	A	610	CLA	CBD-CAD	-3.32	1.41	1.56
2	G	610	CLA	CBD-CAD	-3.32	1.41	1.56
2	C	610	CLA	CBD-CAD	-3.32	1.41	1.56
2	D	610	CLA	CBD-CAD	-3.32	1.41	1.56
2	F	610	CLA	CBD-CAD	-3.31	1.41	1.56
2	J	610	CLA	CBD-CAD	-3.31	1.41	1.56
2	J	604	CLA	MG-NC	-3.16	1.98	2.06
2	I	604	CLA	MG-NC	-3.15	1.98	2.06
2	B	604	CLA	MG-NC	-3.14	1.98	2.06
2	D	604	CLA	MG-NC	-3.14	1.98	2.06
2	F	604	CLA	MG-NC	-3.14	1.98	2.06
2	H	604	CLA	MG-NC	-3.14	1.98	2.06
2	E	604	CLA	MG-NC	-3.14	1.98	2.06
2	A	604	CLA	MG-NC	-3.13	1.98	2.06
2	K	604	CLA	MG-NC	-3.13	1.98	2.06
2	G	604	CLA	MG-NC	-3.13	1.98	2.06
2	C	604	CLA	MG-NC	-3.12	1.98	2.06
2	H	607	CLA	C3A-C2A	-3.10	1.46	1.54
2	D	607	CLA	C3A-C2A	-3.10	1.46	1.54
2	C	607	CLA	C3A-C2A	-3.09	1.46	1.54
2	I	604	CLA	C1D-ND	3.08	1.41	1.37
2	A	607	CLA	C3A-C2A	-3.08	1.46	1.54
2	B	607	CLA	C3A-C2A	-3.08	1.46	1.54
2	F	601	CLA	MG-NC	-3.08	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	604	CLA	C1D-ND	3.08	1.41	1.37
2	I	607	CLA	C3A-C2A	-3.08	1.46	1.54
2	J	607	CLA	C3A-C2A	-3.08	1.46	1.54
2	E	607	CLA	C3A-C2A	-3.07	1.46	1.54
2	K	607	CLA	C3A-C2A	-3.07	1.46	1.54
2	G	607	CLA	C3A-C2A	-3.07	1.46	1.54
2	F	607	CLA	C3A-C2A	-3.06	1.46	1.54
2	K	601	CLA	MG-NC	-3.06	1.99	2.06
2	B	601	CLA	MG-NC	-3.06	1.99	2.06
2	F	604	CLA	C1D-ND	3.06	1.41	1.37
2	G	601	CLA	MG-NC	-3.05	1.99	2.06
2	A	601	CLA	MG-NC	-3.05	1.99	2.06
2	A	604	CLA	C1D-ND	3.05	1.41	1.37
2	H	601	CLA	MG-NC	-3.04	1.99	2.06
2	C	604	CLA	C1D-ND	3.04	1.41	1.37
2	I	601	CLA	MG-NC	-3.04	1.99	2.06
2	D	601	CLA	MG-NC	-3.03	1.99	2.06
2	C	601	CLA	MG-NC	-3.03	1.99	2.06
2	E	601	CLA	MG-NC	-3.03	1.99	2.06
2	J	601	CLA	MG-NC	-3.03	1.99	2.06
2	E	604	CLA	C1D-ND	3.02	1.41	1.37
2	G	604	CLA	C1D-ND	3.00	1.41	1.37
2	K	604	CLA	C1D-ND	3.00	1.41	1.37
2	H	604	CLA	C1D-ND	3.00	1.41	1.37
2	E	608	CLA	C3A-C2A	-2.99	1.46	1.54
2	J	604	CLA	C1D-ND	2.99	1.41	1.37
2	G	608	CLA	C3A-C2A	-2.99	1.46	1.54
2	B	604	CLA	C1D-ND	2.99	1.41	1.37
2	I	608	CLA	C3A-C2A	-2.98	1.46	1.54
2	G	602	CLA	MG-NC	-2.98	1.99	2.06
2	H	602	CLA	MG-NC	-2.98	1.99	2.06
2	A	608	CLA	C3A-C2A	-2.98	1.46	1.54
2	K	608	CLA	C3A-C2A	-2.97	1.46	1.54
2	J	602	CLA	MG-NC	-2.97	1.99	2.06
2	J	608	CLA	C3A-C2A	-2.97	1.46	1.54
2	J	611	CLA	C1D-ND	2.97	1.41	1.37
2	D	608	CLA	C3A-C2A	-2.97	1.46	1.54
2	F	608	CLA	C3A-C2A	-2.97	1.46	1.54
2	B	608	CLA	C3A-C2A	-2.97	1.46	1.54
2	I	602	CLA	MG-NC	-2.97	1.99	2.06
2	F	602	CLA	MG-NC	-2.97	1.99	2.06
2	A	602	CLA	MG-NC	-2.97	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	608	CLA	C3A-C2A	-2.96	1.46	1.54
2	B	602	CLA	MG-NC	-2.96	1.99	2.06
2	C	602	CLA	MG-NC	-2.96	1.99	2.06
2	H	611	CLA	C1D-ND	2.96	1.41	1.37
2	D	602	CLA	MG-NC	-2.96	1.99	2.06
2	K	602	CLA	MG-NC	-2.96	1.99	2.06
2	F	611	CLA	C1D-ND	2.96	1.41	1.37
2	G	611	CLA	C1D-ND	2.95	1.41	1.37
2	C	608	CLA	C3A-C2A	-2.95	1.46	1.54
2	E	602	CLA	MG-NC	-2.95	1.99	2.06
2	D	611	CLA	C1D-ND	2.94	1.41	1.37
2	C	611	CLA	C1D-ND	2.94	1.41	1.37
2	A	611	CLA	C1D-ND	2.94	1.41	1.37
2	I	611	CLA	C1D-ND	2.93	1.41	1.37
2	B	611	CLA	C1D-ND	2.92	1.41	1.37
2	K	611	CLA	C1D-ND	2.90	1.41	1.37
2	E	611	CLA	C1D-ND	2.90	1.41	1.37
2	G	608	CLA	C1D-C2D	-2.89	1.39	1.45
2	I	608	CLA	C1D-C2D	-2.88	1.39	1.45
2	C	608	CLA	C1D-C2D	-2.88	1.39	1.45
2	K	608	CLA	C1D-C2D	-2.88	1.39	1.45
2	A	608	CLA	C1D-C2D	-2.88	1.39	1.45
2	H	608	CLA	C1D-C2D	-2.88	1.39	1.45
2	J	608	CLA	C1D-C2D	-2.88	1.39	1.45
2	E	608	CLA	C1D-C2D	-2.87	1.39	1.45
2	F	608	CLA	C1D-C2D	-2.87	1.39	1.45
2	D	607	CLA	MG-NC	-2.87	1.99	2.06
2	H	607	CLA	MG-NC	-2.87	1.99	2.06
2	J	607	CLA	MG-NC	-2.86	1.99	2.06
2	B	608	CLA	C1D-C2D	-2.86	1.39	1.45
2	G	607	CLA	MG-NC	-2.86	1.99	2.06
2	K	607	CLA	MG-NC	-2.86	1.99	2.06
2	B	607	CLA	MG-NC	-2.86	1.99	2.06
2	A	607	CLA	MG-NC	-2.86	1.99	2.06
2	F	607	CLA	MG-NC	-2.85	1.99	2.06
2	E	607	CLA	MG-NC	-2.85	1.99	2.06
2	C	607	CLA	MG-NC	-2.84	1.99	2.06
2	D	608	CLA	C1D-C2D	-2.84	1.39	1.45
2	I	607	CLA	MG-NC	-2.83	1.99	2.06
2	G	603	CLA	C1D-ND	2.80	1.41	1.37
2	F	603	CLA	C1D-ND	2.79	1.41	1.37
2	B	603	CLA	C1D-ND	2.79	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	605	CLA	MG-NC	-2.78	1.99	2.06
2	D	605	CLA	MG-NC	-2.78	1.99	2.06
2	I	603	CLA	C1D-ND	2.78	1.41	1.37
2	F	605	CLA	MG-NC	-2.77	1.99	2.06
2	H	603	CLA	C1D-ND	2.77	1.41	1.37
2	I	605	CLA	MG-NC	-2.77	1.99	2.06
2	J	605	CLA	MG-NC	-2.77	1.99	2.06
2	A	605	CLA	MG-NC	-2.77	1.99	2.06
2	E	605	CLA	MG-NC	-2.77	1.99	2.06
2	A	603	CLA	C1D-ND	2.77	1.41	1.37
2	D	603	CLA	C1D-ND	2.77	1.41	1.37
2	C	605	CLA	MG-NC	-2.76	1.99	2.06
2	B	605	CLA	MG-NC	-2.76	1.99	2.06
2	E	603	CLA	C1D-ND	2.75	1.41	1.37
2	H	605	CLA	MG-NC	-2.75	1.99	2.06
2	G	605	CLA	MG-NC	-2.75	1.99	2.06
2	J	603	CLA	C1D-ND	2.75	1.41	1.37
2	K	603	CLA	C1D-ND	2.74	1.41	1.37
2	C	603	CLA	C1D-ND	2.74	1.41	1.37
2	I	605	CLA	C3A-C2A	-2.70	1.47	1.54
2	B	605	CLA	C3A-C2A	-2.70	1.47	1.54
2	D	605	CLA	C3A-C2A	-2.69	1.47	1.54
2	H	605	CLA	C3A-C2A	-2.68	1.47	1.54
2	E	605	CLA	C3A-C2A	-2.68	1.47	1.54
2	A	605	CLA	C3A-C2A	-2.68	1.47	1.54
2	C	605	CLA	C3A-C2A	-2.67	1.47	1.54
2	G	605	CLA	C3A-C2A	-2.67	1.47	1.54
2	K	605	CLA	C3A-C2A	-2.67	1.47	1.54
2	J	605	CLA	C3A-C2A	-2.66	1.47	1.54
2	F	605	CLA	C3A-C2A	-2.65	1.47	1.54
2	D	605	CLA	C1D-C2D	-2.65	1.40	1.45
2	J	605	CLA	C1D-C2D	-2.64	1.40	1.45
2	F	605	CLA	C1D-C2D	-2.64	1.40	1.45
2	I	605	CLA	C1D-C2D	-2.64	1.40	1.45
2	K	605	CLA	C1D-C2D	-2.64	1.40	1.45
2	A	605	CLA	C1D-C2D	-2.61	1.40	1.45
2	E	605	CLA	C1D-C2D	-2.61	1.40	1.45
2	K	606	CLA	C1D-C2D	-2.61	1.40	1.45
2	C	605	CLA	C1D-C2D	-2.60	1.40	1.45
2	E	606	CLA	C1D-C2D	-2.60	1.40	1.45
2	H	605	CLA	C1D-C2D	-2.60	1.40	1.45
2	G	606	CLA	C1D-C2D	-2.59	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	606	CLA	C1D-C2D	-2.59	1.40	1.45
2	G	605	CLA	C1D-C2D	-2.59	1.40	1.45
2	B	605	CLA	C1D-C2D	-2.59	1.40	1.45
2	K	609	CLA	C1D-ND	2.59	1.41	1.37
2	H	602	CLA	C3A-C2A	-2.58	1.47	1.54
2	H	606	CLA	C1D-C2D	-2.58	1.40	1.45
2	C	606	CLA	C1D-C2D	-2.58	1.40	1.45
2	A	606	CLA	C1D-C2D	-2.58	1.40	1.45
2	I	606	CLA	C1D-C2D	-2.58	1.40	1.45
2	D	606	CLA	C1D-C2D	-2.57	1.40	1.45
2	F	602	CLA	C3A-C2A	-2.57	1.47	1.54
2	K	602	CLA	C3A-C2A	-2.57	1.47	1.54
2	B	606	CLA	C1D-C2D	-2.57	1.40	1.45
2	C	602	CLA	C3A-C2A	-2.57	1.47	1.54
2	G	602	CLA	C3A-C2A	-2.56	1.47	1.54
2	A	602	CLA	C3A-C2A	-2.56	1.47	1.54
2	J	602	CLA	C3A-C2A	-2.56	1.47	1.54
2	D	602	CLA	C3A-C2A	-2.55	1.47	1.54
2	D	609	CLA	C1D-ND	2.55	1.41	1.37
2	J	606	CLA	C1D-C2D	-2.55	1.40	1.45
2	E	602	CLA	C3A-C2A	-2.55	1.47	1.54
2	I	603	CLA	C3D-C4D	-2.55	1.38	1.44
2	E	601	CLA	C1D-C2D	-2.55	1.40	1.45
2	B	602	CLA	C3A-C2A	-2.55	1.47	1.54
2	I	602	CLA	C3A-C2A	-2.54	1.47	1.54
2	B	603	CLA	C3D-C4D	-2.54	1.38	1.44
2	G	609	CLA	C1D-ND	2.54	1.41	1.37
2	F	603	CLA	C3D-C4D	-2.54	1.38	1.44
2	K	601	CLA	C1D-C2D	-2.54	1.40	1.45
2	K	603	CLA	C3D-C4D	-2.53	1.38	1.44
2	J	603	CLA	C3D-C4D	-2.53	1.38	1.44
2	G	603	CLA	C3D-C4D	-2.53	1.38	1.44
2	A	601	CLA	C1D-C2D	-2.53	1.40	1.45
2	H	601	CLA	C1D-C2D	-2.53	1.40	1.45
2	I	601	CLA	C1D-C2D	-2.53	1.40	1.45
2	E	603	CLA	C3D-C4D	-2.53	1.38	1.44
2	H	609	CLA	C1D-ND	2.53	1.41	1.37
2	F	609	CLA	C1D-ND	2.53	1.41	1.37
2	A	609	CLA	C1D-ND	2.52	1.41	1.37
2	D	601	CLA	C1D-C2D	-2.52	1.40	1.45
2	J	601	CLA	C1D-C2D	-2.52	1.40	1.45
2	G	601	CLA	C1D-C2D	-2.52	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	603	CLA	C3D-C4D	-2.52	1.38	1.44
2	E	609	CLA	C1D-ND	2.51	1.41	1.37
2	I	605	CLA	C1D-ND	2.51	1.41	1.37
2	C	601	CLA	C1D-C2D	-2.51	1.40	1.45
2	C	609	CLA	C1D-ND	2.51	1.41	1.37
2	B	601	CLA	C1D-C2D	-2.51	1.40	1.45
2	F	601	CLA	C1D-C2D	-2.51	1.40	1.45
2	D	603	CLA	C3D-C4D	-2.51	1.38	1.44
2	C	603	CLA	C3D-C4D	-2.50	1.38	1.44
2	K	610	CLA	C1D-ND	2.50	1.41	1.37
2	J	605	CLA	C1D-ND	2.50	1.41	1.37
2	B	609	CLA	C1D-ND	2.50	1.41	1.37
2	D	605	CLA	C1D-ND	2.49	1.41	1.37
2	J	606	CLA	C3D-C4D	-2.49	1.38	1.44
2	D	607	CLA	C1D-C2D	-2.49	1.40	1.45
2	J	609	CLA	C1D-ND	2.49	1.41	1.37
2	J	601	CLA	C3D-C4D	-2.49	1.38	1.44
2	C	610	CLA	C1D-C2D	-2.49	1.40	1.45
2	E	610	CLA	C1D-ND	2.48	1.41	1.37
2	C	607	CLA	C1D-C2D	-2.48	1.40	1.45
2	H	603	CLA	C3D-C4D	-2.48	1.38	1.44
2	I	601	CLA	C3D-C4D	-2.48	1.38	1.44
2	E	610	CLA	C1D-C2D	-2.48	1.40	1.45
2	J	607	CLA	C1D-C2D	-2.48	1.40	1.45
2	J	610	CLA	C1D-ND	2.48	1.41	1.37
2	K	610	CLA	C1D-C2D	-2.48	1.40	1.45
2	E	607	CLA	C3D-C4D	-2.48	1.38	1.44
2	G	606	CLA	C3D-C4D	-2.48	1.38	1.44
2	G	606	CLA	C3A-C2A	-2.48	1.47	1.54
2	F	605	CLA	C1D-ND	2.48	1.41	1.37
2	B	610	CLA	C1D-C2D	-2.48	1.40	1.45
2	E	601	CLA	C3D-C4D	-2.48	1.38	1.44
2	D	607	CLA	C3D-C4D	-2.47	1.38	1.44
2	H	610	CLA	C1D-C2D	-2.47	1.40	1.45
2	B	610	CLA	C1D-ND	2.47	1.41	1.37
2	C	605	CLA	C1D-ND	2.47	1.41	1.37
2	G	601	CLA	C3D-C4D	-2.47	1.38	1.44
2	I	607	CLA	C1D-C2D	-2.47	1.40	1.45
2	B	605	CLA	C1D-ND	2.47	1.41	1.37
2	K	607	CLA	C3D-C4D	-2.47	1.38	1.44
2	J	606	CLA	C3A-C2A	-2.47	1.47	1.54
2	A	605	CLA	C1D-ND	2.47	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	609	CLA	C1D-ND	2.47	1.41	1.37
2	D	606	CLA	C3D-C4D	-2.47	1.38	1.44
2	B	606	CLA	C1D-ND	2.47	1.41	1.37
2	B	606	CLA	C3D-C4D	-2.47	1.38	1.44
2	A	601	CLA	C3D-C4D	-2.46	1.38	1.44
2	C	601	CLA	C3D-C4D	-2.46	1.38	1.44
2	J	607	CLA	C3D-C4D	-2.46	1.38	1.44
2	H	607	CLA	C1D-C2D	-2.46	1.40	1.45
2	H	606	CLA	C3D-C4D	-2.46	1.38	1.44
2	F	607	CLA	C1D-C2D	-2.46	1.40	1.45
2	F	601	CLA	C3D-C4D	-2.46	1.38	1.44
2	G	607	CLA	C3D-C4D	-2.46	1.38	1.44
2	G	607	CLA	C1D-C2D	-2.46	1.40	1.45
2	K	601	CLA	C3D-C4D	-2.46	1.38	1.44
2	A	606	CLA	C3D-C4D	-2.46	1.38	1.44
2	H	601	CLA	C3D-C4D	-2.46	1.38	1.44
2	A	607	CLA	C1D-C2D	-2.46	1.40	1.45
2	A	607	CLA	C3D-C4D	-2.46	1.38	1.44
2	E	606	CLA	C3D-C4D	-2.46	1.38	1.44
2	G	602	CLA	C3D-C4D	-2.46	1.38	1.44
2	H	610	CLA	C1D-ND	2.46	1.41	1.37
2	F	607	CLA	C3D-C4D	-2.46	1.38	1.44
2	B	602	CLA	C1D-C2D	-2.46	1.40	1.45
2	D	601	CLA	C3D-C4D	-2.46	1.38	1.44
2	K	605	CLA	C1D-ND	2.46	1.41	1.37
2	F	606	CLA	C3D-C4D	-2.46	1.38	1.44
2	D	610	CLA	C1D-C2D	-2.45	1.40	1.45
2	A	610	CLA	C1D-C2D	-2.45	1.40	1.45
2	A	606	CLA	C3A-C2A	-2.45	1.47	1.54
2	K	607	CLA	C1D-C2D	-2.45	1.40	1.45
2	D	601	CLA	C3A-C2A	-2.45	1.47	1.54
2	A	610	CLA	C1D-ND	2.45	1.41	1.37
2	I	606	CLA	C3D-C4D	-2.45	1.38	1.44
2	C	606	CLA	C3A-C2A	-2.45	1.47	1.54
2	G	610	CLA	C1D-ND	2.45	1.41	1.37
2	B	607	CLA	C3D-C4D	-2.45	1.38	1.44
2	C	607	CLA	C3D-C4D	-2.45	1.38	1.44
2	J	601	CLA	C3A-C2A	-2.45	1.47	1.54
2	I	610	CLA	C1D-ND	2.45	1.41	1.37
2	G	610	CLA	C1D-C2D	-2.45	1.40	1.45
2	C	601	CLA	C3A-C2A	-2.45	1.47	1.54
2	E	606	CLA	C3A-C2A	-2.45	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	CLA	C3D-C4D	-2.45	1.38	1.44
2	D	610	CLA	C1D-ND	2.45	1.41	1.37
2	H	607	CLA	C3D-C4D	-2.45	1.38	1.44
2	I	607	CLA	C3D-C4D	-2.45	1.38	1.44
2	C	606	CLA	C1D-ND	2.45	1.41	1.37
2	E	601	CLA	C3A-C2A	-2.44	1.47	1.54
2	I	606	CLA	C3A-C2A	-2.44	1.47	1.54
2	H	606	CLA	C3A-C2A	-2.44	1.47	1.54
2	I	610	CLA	C1D-C2D	-2.44	1.40	1.45
2	E	607	CLA	C1D-C2D	-2.44	1.40	1.45
2	F	602	CLA	C1D-C2D	-2.44	1.40	1.45
2	A	601	CLA	C3A-C2A	-2.44	1.47	1.54
2	K	601	CLA	C3A-C2A	-2.44	1.47	1.54
2	K	606	CLA	C3D-C4D	-2.44	1.38	1.44
2	D	602	CLA	C3D-C4D	-2.44	1.38	1.44
2	F	610	CLA	C1D-C2D	-2.44	1.40	1.45
2	B	607	CLA	C1D-C2D	-2.44	1.40	1.45
2	B	606	CLA	C3A-C2A	-2.44	1.47	1.54
2	D	602	CLA	C1D-C2D	-2.43	1.40	1.45
2	B	601	CLA	C3A-C2A	-2.43	1.47	1.54
2	I	601	CLA	C3A-C2A	-2.43	1.47	1.54
2	C	610	CLA	C1D-ND	2.43	1.41	1.37
2	E	606	CLA	C1D-ND	2.43	1.41	1.37
2	G	601	CLA	C3A-C2A	-2.43	1.47	1.54
2	H	601	CLA	C3A-C2A	-2.43	1.47	1.54
2	F	606	CLA	C3A-C2A	-2.43	1.47	1.54
2	D	606	CLA	C3A-C2A	-2.43	1.47	1.54
2	C	602	CLA	C1D-C2D	-2.43	1.40	1.45
2	C	606	CLA	C3D-C4D	-2.43	1.38	1.44
2	D	606	CLA	C1D-ND	2.43	1.41	1.37
2	I	602	CLA	C3D-C4D	-2.43	1.38	1.44
2	J	610	CLA	C1D-C2D	-2.43	1.40	1.45
2	K	602	CLA	C3D-C4D	-2.43	1.38	1.44
2	A	602	CLA	C3D-C4D	-2.43	1.38	1.44
2	E	605	CLA	C1D-ND	2.43	1.41	1.37
2	E	603	CLA	C1D-C2D	-2.42	1.40	1.45
2	G	606	CLA	C1D-ND	2.42	1.41	1.37
2	H	603	CLA	C1D-C2D	-2.42	1.40	1.45
2	A	602	CLA	C1D-C2D	-2.42	1.40	1.45
2	H	602	CLA	C3D-C4D	-2.42	1.38	1.44
2	H	605	CLA	C1D-ND	2.42	1.41	1.37
2	A	606	CLA	C1D-ND	2.42	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	606	CLA	C1D-ND	2.42	1.41	1.37
2	K	606	CLA	C3A-C2A	-2.42	1.47	1.54
2	F	606	CLA	C1D-ND	2.42	1.41	1.37
2	I	604	CLA	C1D-C2D	-2.42	1.40	1.45
2	I	606	CLA	C1D-ND	2.42	1.41	1.37
2	D	603	CLA	C1D-C2D	-2.42	1.40	1.45
2	I	602	CLA	C1D-C2D	-2.42	1.40	1.45
2	E	602	CLA	C3D-C4D	-2.42	1.38	1.44
2	F	601	CLA	C3A-C2A	-2.42	1.47	1.54
2	D	604	CLA	C1D-C2D	-2.41	1.40	1.45
2	K	602	CLA	C1D-C2D	-2.41	1.40	1.45
2	E	602	CLA	C1D-C2D	-2.41	1.40	1.45
2	B	603	CLA	C1D-C2D	-2.41	1.40	1.45
2	F	604	CLA	C1D-C2D	-2.41	1.40	1.45
2	G	602	CLA	C1D-C2D	-2.41	1.40	1.45
2	C	602	CLA	C3D-C4D	-2.41	1.38	1.44
2	I	603	CLA	C1D-C2D	-2.41	1.40	1.45
2	B	608	CLA	CBD-CAD	-2.41	1.45	1.56
2	F	608	CLA	CBD-CAD	-2.41	1.45	1.56
2	A	603	CLA	C1D-C2D	-2.41	1.40	1.45
2	G	604	CLA	C1D-C2D	-2.41	1.40	1.45
2	K	611	CLA	C1D-C2D	-2.41	1.40	1.45
2	C	604	CLA	C1D-C2D	-2.40	1.40	1.45
2	J	602	CLA	C1D-C2D	-2.40	1.40	1.45
2	F	610	CLA	C1D-ND	2.40	1.41	1.37
2	G	605	CLA	C1D-ND	2.40	1.41	1.37
2	A	604	CLA	C1D-C2D	-2.40	1.40	1.45
2	B	604	CLA	C1D-C2D	-2.40	1.40	1.45
2	E	608	CLA	CHD-C4C	-2.40	1.33	1.39
2	K	608	CLA	CBD-CAD	-2.40	1.45	1.56
2	B	602	CLA	C3D-C4D	-2.40	1.38	1.44
2	E	608	CLA	CBD-CAD	-2.40	1.45	1.56
2	K	604	CLA	C1D-C2D	-2.40	1.40	1.45
2	B	611	CLA	C1D-C2D	-2.40	1.40	1.45
2	H	602	CLA	C1D-C2D	-2.40	1.40	1.45
2	J	604	CLA	C1D-C2D	-2.40	1.40	1.45
2	I	605	CLA	C3D-C4D	-2.40	1.38	1.44
2	J	602	CLA	C3D-C4D	-2.40	1.38	1.44
2	E	611	CLA	C1D-C2D	-2.40	1.40	1.45
2	G	603	CLA	C1D-C2D	-2.40	1.40	1.45
2	I	608	CLA	CBD-CAD	-2.40	1.45	1.56
2	E	604	CLA	C1D-C2D	-2.40	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	608	CLA	CHD-C4C	-2.40	1.33	1.39
2	A	608	CLA	CBD-CAD	-2.40	1.45	1.56
2	J	603	CLA	C1D-C2D	-2.40	1.40	1.45
2	F	602	CLA	C3D-C4D	-2.40	1.38	1.44
2	F	603	CLA	C1D-C2D	-2.39	1.40	1.45
2	B	608	CLA	CHD-C4C	-2.39	1.33	1.39
2	A	611	CLA	C1D-C2D	-2.39	1.40	1.45
2	C	603	CLA	C1D-C2D	-2.39	1.40	1.45
2	C	608	CLA	CBD-CAD	-2.39	1.45	1.56
2	H	604	CLA	C1D-C2D	-2.39	1.40	1.45
2	J	608	CLA	CBD-CAD	-2.39	1.45	1.56
2	J	611	CLA	C1D-C2D	-2.39	1.40	1.45
2	G	608	CLA	CBD-CAD	-2.39	1.45	1.56
2	I	611	CLA	C1D-C2D	-2.39	1.40	1.45
2	K	603	CLA	C1D-C2D	-2.39	1.40	1.45
2	E	610	CLA	C3D-C4D	-2.38	1.38	1.44
2	E	605	CLA	C3D-C4D	-2.38	1.38	1.44
2	H	611	CLA	C1D-C2D	-2.38	1.40	1.45
2	C	611	CLA	C1D-C2D	-2.38	1.40	1.45
2	D	611	CLA	C1D-C2D	-2.38	1.40	1.45
2	D	608	CLA	CBD-CAD	-2.38	1.45	1.56
2	B	610	CLA	C3D-C4D	-2.38	1.38	1.44
2	D	608	CLA	CHD-C4C	-2.38	1.33	1.39
2	G	611	CLA	C1D-C2D	-2.38	1.40	1.45
2	J	608	CLA	CHD-C4C	-2.38	1.33	1.39
2	J	606	CLA	C1D-ND	2.38	1.41	1.37
2	H	606	CLA	C1D-ND	2.38	1.41	1.37
2	K	609	CLA	C1D-C2D	-2.38	1.40	1.45
2	F	611	CLA	C1D-C2D	-2.38	1.40	1.45
2	C	608	CLA	CHD-C4C	-2.38	1.33	1.39
2	H	609	CLA	C1D-C2D	-2.38	1.40	1.45
2	I	610	CLA	C3D-C4D	-2.38	1.38	1.44
2	G	608	CLA	CHD-C4C	-2.38	1.33	1.39
2	K	608	CLA	CHD-C4C	-2.38	1.33	1.39
2	A	608	CLA	CHD-C4C	-2.37	1.33	1.39
2	J	605	CLA	C3D-C4D	-2.37	1.38	1.44
2	H	608	CLA	CBD-CAD	-2.37	1.45	1.56
2	B	605	CLA	C3D-C4D	-2.37	1.38	1.44
2	H	608	CLA	CHD-C4C	-2.37	1.33	1.39
2	E	609	CLA	C1D-C2D	-2.37	1.40	1.45
2	I	609	CLA	C1D-C2D	-2.37	1.40	1.45
2	F	609	CLA	C1D-C2D	-2.37	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	CLA	C3D-C4D	-2.37	1.38	1.44
2	G	609	CLA	C1D-C2D	-2.37	1.40	1.45
2	F	605	CLA	C3D-C4D	-2.37	1.38	1.44
2	A	609	CLA	C1D-C2D	-2.37	1.40	1.45
2	I	608	CLA	CHD-C4C	-2.36	1.33	1.39
2	H	605	CLA	C3D-C4D	-2.36	1.38	1.44
2	J	610	CLA	C3D-C4D	-2.36	1.38	1.44
2	F	610	CLA	C3D-C4D	-2.36	1.38	1.44
2	K	605	CLA	C3D-C4D	-2.36	1.38	1.44
2	J	609	CLA	C1D-C2D	-2.36	1.40	1.45
2	C	609	CLA	C1D-C2D	-2.36	1.40	1.45
2	C	605	CLA	C3D-C4D	-2.36	1.38	1.44
2	D	609	CLA	C1D-C2D	-2.36	1.40	1.45
2	B	609	CLA	C1D-C2D	-2.35	1.40	1.45
2	G	605	CLA	C3D-C4D	-2.35	1.38	1.44
2	A	610	CLA	C3D-C4D	-2.35	1.38	1.44
2	K	610	CLA	C3D-C4D	-2.35	1.38	1.44
2	D	605	CLA	C3D-C4D	-2.35	1.38	1.44
2	G	610	CLA	C3D-C4D	-2.35	1.38	1.44
2	B	608	CLA	C3D-C4D	-2.35	1.38	1.44
2	I	608	CLA	C3D-C4D	-2.35	1.38	1.44
2	C	610	CLA	C3D-C4D	-2.35	1.38	1.44
2	H	610	CLA	C3D-C4D	-2.35	1.38	1.44
2	H	608	CLA	C3D-C4D	-2.34	1.38	1.44
2	J	608	CLA	C3D-C4D	-2.34	1.38	1.44
2	D	610	CLA	C3D-C4D	-2.34	1.38	1.44
2	E	609	CLA	C3D-C4D	-2.34	1.38	1.44
2	F	608	CLA	C3D-C4D	-2.34	1.38	1.44
2	B	609	CLA	C3D-C4D	-2.34	1.38	1.44
2	G	608	CLA	C3D-C4D	-2.34	1.38	1.44
2	D	608	CLA	C3D-C4D	-2.33	1.38	1.44
2	A	608	CLA	C3D-C4D	-2.33	1.38	1.44
2	K	609	CLA	C3D-C4D	-2.33	1.39	1.44
2	C	609	CLA	C3D-C4D	-2.33	1.39	1.44
2	F	609	CLA	C3D-C4D	-2.32	1.39	1.44
2	A	609	CLA	C3D-C4D	-2.32	1.39	1.44
2	E	608	CLA	C3D-C4D	-2.32	1.39	1.44
2	G	609	CLA	C3D-C4D	-2.31	1.39	1.44
2	K	608	CLA	C3D-C4D	-2.31	1.39	1.44
2	J	609	CLA	C3D-C4D	-2.31	1.39	1.44
2	I	609	CLA	C3D-C4D	-2.31	1.39	1.44
2	H	609	CLA	C3D-C4D	-2.30	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	609	CLA	C3D-C4D	-2.30	1.39	1.44
2	C	608	CLA	C3D-C4D	-2.30	1.39	1.44
2	D	605	CLA	CBD-CAD	-2.29	1.46	1.56
2	H	605	CLA	CBD-CAD	-2.29	1.46	1.56
2	F	605	CLA	CBD-CAD	-2.28	1.46	1.56
2	B	605	CLA	CBD-CAD	-2.28	1.46	1.56
2	G	605	CLA	CBD-CAD	-2.28	1.46	1.56
2	J	605	CLA	CBD-CAD	-2.28	1.46	1.56
2	A	605	CLA	CBD-CAD	-2.28	1.46	1.56
2	C	605	CLA	CBD-CAD	-2.27	1.46	1.56
2	I	605	CLA	CBD-CAD	-2.27	1.46	1.56
2	E	605	CLA	CBD-CAD	-2.27	1.46	1.56
2	K	605	CLA	CBD-CAD	-2.27	1.46	1.56
2	E	604	CLA	C3D-C4D	-2.26	1.39	1.44
2	G	604	CLA	C3D-C4D	-2.25	1.39	1.44
2	H	604	CLA	C1B-NB	2.25	1.40	1.37
2	J	601	CLA	C1D-ND	2.25	1.40	1.37
2	D	604	CLA	C1B-NB	2.25	1.40	1.37
2	B	604	CLA	C3D-C4D	-2.25	1.39	1.44
2	C	604	CLA	C1B-NB	2.24	1.40	1.37
2	A	604	CLA	C3D-C4D	-2.24	1.39	1.44
2	B	601	CLA	C1D-ND	2.24	1.40	1.37
2	E	601	CLA	C1D-ND	2.24	1.40	1.37
2	D	604	CLA	C3D-C4D	-2.23	1.39	1.44
2	J	604	CLA	C3D-C4D	-2.23	1.39	1.44
2	B	611	CLA	C3D-C4D	-2.23	1.39	1.44
2	E	611	CLA	C3D-C4D	-2.23	1.39	1.44
2	C	611	CLA	C3D-C4D	-2.23	1.39	1.44
2	J	611	CLA	C3D-C4D	-2.23	1.39	1.44
2	D	611	CLA	C3D-C4D	-2.23	1.39	1.44
2	I	604	CLA	C3D-C4D	-2.23	1.39	1.44
2	I	611	CLA	C3D-C4D	-2.23	1.39	1.44
2	K	611	CLA	C3D-C4D	-2.23	1.39	1.44
2	A	611	CLA	C3D-C4D	-2.23	1.39	1.44
2	H	611	CLA	C3D-C4D	-2.23	1.39	1.44
2	D	601	CLA	C1D-ND	2.23	1.40	1.37
2	C	604	CLA	C3D-C4D	-2.23	1.39	1.44
2	G	611	CLA	C3D-C4D	-2.23	1.39	1.44
2	K	604	CLA	C3D-C4D	-2.23	1.39	1.44
2	H	604	CLA	C3D-C4D	-2.23	1.39	1.44
2	I	601	CLA	C1D-ND	2.22	1.40	1.37
2	F	611	CLA	C3D-C4D	-2.22	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	CLA	C1D-ND	2.22	1.40	1.37
2	F	604	CLA	C3D-C4D	-2.21	1.39	1.44
2	I	604	CLA	C1B-NB	2.21	1.40	1.37
2	K	601	CLA	C1D-ND	2.20	1.40	1.37
2	C	601	CLA	C1D-ND	2.20	1.40	1.37
2	J	604	CLA	C1B-NB	2.19	1.40	1.37
2	G	601	CLA	C1D-ND	2.19	1.40	1.37
2	A	604	CLA	C1B-NB	2.19	1.40	1.37
2	F	604	CLA	C1B-NB	2.19	1.40	1.37
2	B	602	CLA	C1D-ND	2.19	1.40	1.37
2	G	604	CLA	C1B-NB	2.18	1.40	1.37
2	H	601	CLA	C1D-ND	2.18	1.40	1.37
2	E	604	CLA	C1B-NB	2.18	1.40	1.37
2	D	611	CLA	C3A-C2A	-2.17	1.48	1.54
2	E	610	CLA	CHD-C4C	-2.17	1.34	1.39
2	K	604	CLA	C1B-NB	2.17	1.40	1.37
2	B	604	CLA	C1B-NB	2.17	1.40	1.37
2	F	601	CLA	C1D-ND	2.17	1.40	1.37
2	I	611	CLA	C3A-C2A	-2.17	1.48	1.54
2	D	610	CLA	CHD-C4C	-2.17	1.34	1.39
2	K	611	CLA	C3A-C2A	-2.17	1.48	1.54
2	A	611	CLA	C3A-C2A	-2.17	1.48	1.54
2	C	611	CLA	C3A-C2A	-2.16	1.48	1.54
2	J	611	CLA	C3A-C2A	-2.16	1.48	1.54
2	C	601	CLA	C1B-NB	2.16	1.40	1.37
2	E	611	CLA	C3A-C2A	-2.16	1.48	1.54
2	H	611	CLA	C3A-C2A	-2.16	1.48	1.54
2	G	611	CLA	C3A-C2A	-2.16	1.48	1.54
2	B	611	CLA	C3A-C2A	-2.16	1.48	1.54
2	B	610	CLA	CHD-C4C	-2.16	1.34	1.39
2	F	611	CLA	C3A-C2A	-2.16	1.48	1.54
2	E	608	CLA	C1D-ND	2.15	1.40	1.37
2	K	601	CLA	C1B-NB	2.15	1.40	1.37
2	G	610	CLA	CHD-C4C	-2.15	1.34	1.39
2	A	610	CLA	CHD-C4C	-2.15	1.34	1.39
2	K	610	CLA	CHD-C4C	-2.15	1.34	1.39
2	H	610	CLA	CHD-C4C	-2.15	1.34	1.39
2	C	608	CLA	C1D-ND	2.15	1.40	1.37
2	C	610	CLA	CHD-C4C	-2.15	1.34	1.39
2	F	602	CLA	C1D-ND	2.14	1.40	1.37
2	F	608	CLA	C1D-ND	2.13	1.40	1.37
2	K	608	CLA	C1D-ND	2.13	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	CLA	C1B-NB	2.13	1.40	1.37
2	F	610	CLA	CHD-C4C	-2.13	1.34	1.39
2	G	608	CLA	C1D-ND	2.13	1.40	1.37
2	J	602	CLA	C1D-ND	2.13	1.40	1.37
2	J	601	CLA	C1B-NB	2.13	1.40	1.37
2	J	610	CLA	CHD-C4C	-2.13	1.34	1.39
2	I	610	CLA	CHD-C4C	-2.12	1.34	1.39
2	D	602	CLA	C1D-ND	2.12	1.40	1.37
2	A	602	CLA	C1D-ND	2.12	1.40	1.37
2	E	602	CLA	C1D-ND	2.12	1.40	1.37
2	G	601	CLA	C1B-NB	2.11	1.40	1.37
2	F	601	CLA	C1B-NB	2.11	1.40	1.37
2	A	601	CLA	C1B-NB	2.11	1.40	1.37
2	A	608	CLA	C1D-ND	2.11	1.40	1.37
2	I	602	CLA	C1D-ND	2.11	1.40	1.37
2	I	601	CLA	C1B-NB	2.11	1.40	1.37
2	H	601	CLA	C1B-NB	2.10	1.40	1.37
2	H	602	CLA	C1D-ND	2.10	1.40	1.37
2	H	608	CLA	C1D-ND	2.10	1.40	1.37
2	H	609	CLA	C3A-C2A	-2.10	1.48	1.54
2	B	609	CLA	C3A-C2A	-2.10	1.48	1.54
2	B	608	CLA	C1D-ND	2.09	1.40	1.37
2	K	602	CLA	C1D-ND	2.09	1.40	1.37
2	E	609	CLA	C3A-C2A	-2.09	1.48	1.54
2	G	609	CLA	C3A-C2A	-2.09	1.48	1.54
2	A	609	CLA	C3A-C2A	-2.09	1.48	1.54
2	J	608	CLA	C1D-ND	2.09	1.40	1.37
2	I	609	CLA	C3A-C2A	-2.08	1.48	1.54
2	D	609	CLA	C3A-C2A	-2.08	1.48	1.54
2	C	609	CLA	C3A-C2A	-2.08	1.48	1.54
2	B	606	CLA	CHD-C4C	-2.08	1.34	1.39
2	H	606	CLA	CHD-C4C	-2.08	1.34	1.39
2	I	608	CLA	C1D-ND	2.08	1.40	1.37
2	F	609	CLA	C3A-C2A	-2.08	1.48	1.54
2	D	608	CLA	C1D-ND	2.08	1.40	1.37
2	C	606	CLA	CHD-C4C	-2.08	1.34	1.39
2	J	609	CLA	C3A-C2A	-2.07	1.48	1.54
2	C	602	CLA	C1D-ND	2.07	1.40	1.37
2	K	609	CLA	C3A-C2A	-2.07	1.48	1.54
2	G	602	CLA	C1D-ND	2.07	1.40	1.37
2	D	601	CLA	C1B-NB	2.06	1.40	1.37
2	K	606	CLA	CHD-C4C	-2.05	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	606	CLA	CHD-C4C	-2.05	1.34	1.39
2	E	606	CLA	CHD-C4C	-2.05	1.34	1.39
2	A	606	CLA	CHD-C4C	-2.05	1.34	1.39
2	G	606	CLA	CHD-C4C	-2.05	1.34	1.39
2	D	606	CLA	CHD-C4C	-2.04	1.34	1.39
2	I	606	CLA	CHD-C4C	-2.04	1.34	1.39
2	B	601	CLA	C1B-NB	2.04	1.40	1.37
2	F	606	CLA	CHD-C4C	-2.03	1.34	1.39
2	J	607	CLA	CBD-CAD	-2.02	1.47	1.56
2	H	607	CLA	CBD-CAD	-2.02	1.47	1.56
2	E	607	CLA	CBD-CAD	-2.02	1.47	1.56
2	B	607	CLA	CBD-CAD	-2.02	1.47	1.56
2	F	607	CLA	CBD-CAD	-2.02	1.47	1.56
2	A	607	CLA	CBD-CAD	-2.02	1.47	1.56
2	G	607	CLA	CBD-CAD	-2.02	1.47	1.56
2	I	607	CLA	CBD-CAD	-2.01	1.47	1.56
2	K	607	CLA	CBD-CAD	-2.01	1.47	1.56
2	D	607	CLA	CBD-CAD	-2.01	1.47	1.56
2	C	607	CLA	CBD-CAD	-2.01	1.47	1.56

All (1075) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	606	CLA	C4A-NA-C1A	-6.42	103.75	106.68
2	D	606	CLA	C4A-NA-C1A	-6.38	103.77	106.68
2	G	606	CLA	C4A-NA-C1A	-6.38	103.77	106.68
2	I	606	CLA	C4A-NA-C1A	-6.37	103.77	106.68
2	F	606	CLA	C4A-NA-C1A	-6.37	103.78	106.68
2	A	606	CLA	C4A-NA-C1A	-6.36	103.78	106.68
2	B	606	CLA	C4A-NA-C1A	-6.36	103.78	106.68
2	C	606	CLA	C4A-NA-C1A	-6.35	103.78	106.68
2	E	606	CLA	C4A-NA-C1A	-6.33	103.79	106.68
2	J	606	CLA	C4A-NA-C1A	-6.33	103.79	106.68
2	H	606	CLA	C4A-NA-C1A	-6.31	103.80	106.68
2	C	603	CLA	C4A-NA-C1A	-6.26	103.82	106.68
2	H	603	CLA	C4A-NA-C1A	-6.21	103.84	106.68
2	F	603	CLA	C4A-NA-C1A	-6.21	103.85	106.68
2	D	603	CLA	C4A-NA-C1A	-6.21	103.85	106.68
2	I	603	CLA	C4A-NA-C1A	-6.20	103.85	106.68
2	J	603	CLA	C4A-NA-C1A	-6.20	103.85	106.68
2	K	603	CLA	C4A-NA-C1A	-6.19	103.85	106.68
2	A	603	CLA	C4A-NA-C1A	-6.19	103.86	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	603	CLA	C4A-NA-C1A	-6.17	103.86	106.68
2	B	603	CLA	C4A-NA-C1A	-6.15	103.88	106.68
2	E	603	CLA	C4A-NA-C1A	-6.15	103.88	106.68
2	F	605	CLA	C4A-NA-C1A	-6.00	103.94	106.68
2	I	605	CLA	C4A-NA-C1A	-5.96	103.96	106.68
2	A	605	CLA	C4A-NA-C1A	-5.94	103.97	106.68
2	C	605	CLA	C4A-NA-C1A	-5.94	103.97	106.68
2	B	605	CLA	C4A-NA-C1A	-5.93	103.97	106.68
2	H	605	CLA	C4A-NA-C1A	-5.93	103.97	106.68
2	J	605	CLA	C4A-NA-C1A	-5.93	103.97	106.68
2	K	605	CLA	C4A-NA-C1A	-5.92	103.98	106.68
2	D	605	CLA	C4A-NA-C1A	-5.92	103.98	106.68
2	E	605	CLA	C4A-NA-C1A	-5.92	103.98	106.68
2	G	605	CLA	C4A-NA-C1A	-5.88	104.00	106.68
2	H	607	CLA	C4A-NA-C1A	-5.79	104.04	106.68
2	I	607	CLA	C4A-NA-C1A	-5.76	104.05	106.68
2	A	607	CLA	C4A-NA-C1A	-5.76	104.05	106.68
2	B	607	CLA	C4A-NA-C1A	-5.75	104.05	106.68
2	K	607	CLA	C4A-NA-C1A	-5.75	104.06	106.68
2	D	607	CLA	C4A-NA-C1A	-5.75	104.06	106.68
2	C	607	CLA	C4A-NA-C1A	-5.74	104.06	106.68
2	E	607	CLA	C4A-NA-C1A	-5.74	104.06	106.68
2	J	607	CLA	C4A-NA-C1A	-5.73	104.06	106.68
2	F	607	CLA	C4A-NA-C1A	-5.71	104.08	106.68
2	G	607	CLA	C4A-NA-C1A	-5.68	104.09	106.68
2	E	602	CLA	C4A-NA-C1A	-5.45	104.19	106.68
2	I	602	CLA	C4A-NA-C1A	-5.44	104.20	106.68
2	G	602	CLA	C4A-NA-C1A	-5.44	104.20	106.68
2	J	602	CLA	C4A-NA-C1A	-5.42	104.21	106.68
2	F	602	CLA	C4A-NA-C1A	-5.41	104.21	106.68
2	A	602	CLA	C4A-NA-C1A	-5.41	104.21	106.68
2	D	602	CLA	C4A-NA-C1A	-5.40	104.22	106.68
2	K	602	CLA	C4A-NA-C1A	-5.40	104.22	106.68
2	H	602	CLA	C4A-NA-C1A	-5.39	104.22	106.68
2	C	602	CLA	C4A-NA-C1A	-5.38	104.22	106.68
2	B	602	CLA	C4A-NA-C1A	-5.38	104.23	106.68
2	J	610	CLA	CGD-CBD-CAD	-5.32	93.61	110.85
2	D	610	CLA	CGD-CBD-CAD	-5.32	93.61	110.85
2	F	610	CLA	CGD-CBD-CAD	-5.32	93.64	110.85
2	C	610	CLA	CGD-CBD-CAD	-5.31	93.64	110.85
2	A	610	CLA	CGD-CBD-CAD	-5.31	93.65	110.85
2	B	610	CLA	CGD-CBD-CAD	-5.31	93.65	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	610	CLA	CGD-CBD-CAD	-5.31	93.66	110.85
2	H	610	CLA	CGD-CBD-CAD	-5.31	93.66	110.85
2	K	610	CLA	CGD-CBD-CAD	-5.31	93.66	110.85
2	E	610	CLA	CGD-CBD-CAD	-5.31	93.66	110.85
2	G	610	CLA	CGD-CBD-CAD	-5.31	93.66	110.85
2	B	608	CLA	C4A-NA-C1A	-5.26	104.28	106.68
2	K	609	CLA	C4A-NA-C1A	-5.25	104.28	106.68
2	H	608	CLA	C4A-NA-C1A	-5.24	104.29	106.68
2	J	608	CLA	C4A-NA-C1A	-5.24	104.29	106.68
2	D	608	CLA	C4A-NA-C1A	-5.23	104.30	106.68
2	E	608	CLA	C4A-NA-C1A	-5.22	104.30	106.68
2	D	609	CLA	C4A-NA-C1A	-5.22	104.30	106.68
2	H	609	CLA	C4A-NA-C1A	-5.22	104.30	106.68
2	G	608	CLA	C4A-NA-C1A	-5.21	104.30	106.68
2	K	608	CLA	C4A-NA-C1A	-5.21	104.30	106.68
2	A	608	CLA	C4A-NA-C1A	-5.19	104.31	106.68
2	B	609	CLA	C4A-NA-C1A	-5.19	104.31	106.68
2	C	609	CLA	C4A-NA-C1A	-5.19	104.31	106.68
2	I	608	CLA	C4A-NA-C1A	-5.19	104.31	106.68
2	E	609	CLA	C4A-NA-C1A	-5.18	104.31	106.68
2	F	609	CLA	C4A-NA-C1A	-5.18	104.31	106.68
2	C	608	CLA	C4A-NA-C1A	-5.18	104.32	106.68
2	A	609	CLA	C4A-NA-C1A	-5.16	104.33	106.68
2	I	609	CLA	C4A-NA-C1A	-5.14	104.33	106.68
2	J	609	CLA	C4A-NA-C1A	-5.14	104.33	106.68
2	F	608	CLA	C4A-NA-C1A	-5.14	104.34	106.68
2	G	609	CLA	C4A-NA-C1A	-5.10	104.35	106.68
2	E	610	CLA	C4A-NA-C1A	-4.82	104.48	106.68
2	I	610	CLA	C4A-NA-C1A	-4.80	104.49	106.68
2	D	611	CLA	C4A-NA-C1A	-4.80	104.49	106.68
2	J	611	CLA	C4A-NA-C1A	-4.79	104.49	106.68
2	B	610	CLA	C4A-NA-C1A	-4.79	104.49	106.68
2	A	611	CLA	C4A-NA-C1A	-4.77	104.50	106.68
2	G	610	CLA	C4A-NA-C1A	-4.77	104.50	106.68
2	H	611	CLA	C4A-NA-C1A	-4.77	104.50	106.68
2	H	610	CLA	C4A-NA-C1A	-4.77	104.50	106.68
2	C	610	CLA	C4A-NA-C1A	-4.77	104.50	106.68
2	A	610	CLA	C4A-NA-C1A	-4.77	104.50	106.68
2	C	611	CLA	C4A-NA-C1A	-4.76	104.51	106.68
2	E	611	CLA	C4A-NA-C1A	-4.76	104.51	106.68
2	J	610	CLA	C4A-NA-C1A	-4.76	104.51	106.68
2	K	611	CLA	C4A-NA-C1A	-4.76	104.51	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	610	CLA	C4A-NA-C1A	-4.74	104.52	106.68
2	F	611	CLA	C4A-NA-C1A	-4.74	104.52	106.68
2	B	611	CLA	C4A-NA-C1A	-4.73	104.52	106.68
2	F	610	CLA	C4A-NA-C1A	-4.71	104.53	106.68
2	G	611	CLA	C4A-NA-C1A	-4.71	104.53	106.68
2	K	610	CLA	C4A-NA-C1A	-4.71	104.53	106.68
2	I	611	CLA	C4A-NA-C1A	-4.69	104.54	106.68
2	I	608	CLA	C2A-C1A-CHA	4.69	132.00	123.87
2	G	608	CLA	C2A-C1A-CHA	4.68	132.00	123.87
2	B	608	CLA	C2A-C1A-CHA	4.68	131.99	123.87
2	A	608	CLA	C2A-C1A-CHA	4.67	131.98	123.87
2	F	608	CLA	C2A-C1A-CHA	4.67	131.98	123.87
2	H	608	CLA	C2A-C1A-CHA	4.67	131.97	123.87
2	C	608	CLA	C2A-C1A-CHA	4.67	131.97	123.87
2	E	608	CLA	C2A-C1A-CHA	4.67	131.97	123.87
2	K	608	CLA	C2A-C1A-CHA	4.67	131.97	123.87
2	J	608	CLA	C2A-C1A-CHA	4.66	131.96	123.87
2	D	608	CLA	C2A-C1A-CHA	4.66	131.95	123.87
2	D	604	CLA	C4A-NA-C1A	-4.55	104.60	106.68
2	G	604	CLA	C4A-NA-C1A	-4.54	104.61	106.68
2	B	604	CLA	C4A-NA-C1A	-4.53	104.61	106.68
2	H	604	CLA	C4A-NA-C1A	-4.51	104.62	106.68
2	C	604	CLA	C4A-NA-C1A	-4.50	104.62	106.68
2	A	604	CLA	C4A-NA-C1A	-4.49	104.63	106.68
2	K	604	CLA	C4A-NA-C1A	-4.48	104.64	106.68
2	J	604	CLA	C4A-NA-C1A	-4.45	104.65	106.68
2	F	604	CLA	C4A-NA-C1A	-4.45	104.65	106.68
2	J	602	CLA	C1-C2-C3	-4.42	118.95	126.20
2	I	602	CLA	C1-C2-C3	-4.42	118.96	126.20
2	D	602	CLA	C1-C2-C3	-4.42	118.96	126.20
2	I	604	CLA	C4A-NA-C1A	-4.41	104.67	106.68
2	E	604	CLA	C4A-NA-C1A	-4.41	104.67	106.68
2	B	602	CLA	C1-C2-C3	-4.41	118.97	126.20
2	E	602	CLA	C1-C2-C3	-4.41	118.97	126.20
2	F	602	CLA	C1-C2-C3	-4.41	118.97	126.20
2	A	602	CLA	C1-C2-C3	-4.40	118.99	126.20
2	H	602	CLA	C1-C2-C3	-4.40	118.99	126.20
2	C	602	CLA	C1-C2-C3	-4.39	119.00	126.20
2	K	602	CLA	C1-C2-C3	-4.39	119.00	126.20
2	G	602	CLA	C1-C2-C3	-4.39	119.00	126.20
2	J	601	CLA	C4A-NA-C1A	-4.37	104.69	106.68
2	B	601	CLA	C4A-NA-C1A	-4.35	104.69	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	CLA	C4A-NA-C1A	-4.35	104.70	106.68
2	C	601	CLA	C4A-NA-C1A	-4.32	104.71	106.68
2	D	601	CLA	C4A-NA-C1A	-4.32	104.71	106.68
2	I	601	CLA	C4A-NA-C1A	-4.31	104.71	106.68
2	G	601	CLA	C4A-NA-C1A	-4.31	104.71	106.68
2	F	601	CLA	C4A-NA-C1A	-4.29	104.72	106.68
2	A	601	CLA	C4A-NA-C1A	-4.27	104.73	106.68
2	H	601	CLA	C4A-NA-C1A	-4.25	104.74	106.68
3	E	612	XAT	C27-C28-C29	-4.25	118.93	125.53
3	C	612	XAT	C27-C28-C29	-4.25	118.94	125.53
3	D	612	XAT	C27-C28-C29	-4.25	118.94	125.53
3	F	612	XAT	C27-C28-C29	-4.25	118.94	125.53
3	A	612	XAT	C27-C28-C29	-4.25	118.94	125.53
3	G	612	XAT	C27-C28-C29	-4.24	118.94	125.53
3	K	612	XAT	C27-C28-C29	-4.24	118.95	125.53
3	H	612	XAT	C27-C28-C29	-4.24	118.95	125.53
3	J	612	XAT	C27-C28-C29	-4.24	118.96	125.53
3	B	612	XAT	C27-C28-C29	-4.23	118.96	125.53
3	I	612	XAT	C27-C28-C29	-4.23	118.97	125.53
2	K	601	CLA	C4A-NA-C1A	-4.20	104.76	106.68
2	F	605	CLA	C1-C2-C3	-4.02	119.61	126.20
2	E	605	CLA	C1-C2-C3	-4.02	119.61	126.20
2	G	605	CLA	C1-C2-C3	-4.02	119.61	126.20
2	K	605	CLA	C1-C2-C3	-4.02	119.61	126.20
2	B	605	CLA	C1-C2-C3	-4.02	119.62	126.20
2	I	605	CLA	C1-C2-C3	-4.01	119.62	126.20
2	J	605	CLA	C1-C2-C3	-4.01	119.62	126.20
2	A	605	CLA	C1-C2-C3	-4.01	119.62	126.20
2	D	605	CLA	C1-C2-C3	-4.01	119.63	126.20
2	C	605	CLA	C1-C2-C3	-4.00	119.64	126.20
2	H	605	CLA	C1-C2-C3	-4.00	119.65	126.20
2	H	608	CLA	CHA-C1A-NA	-3.84	117.70	126.39
2	B	608	CLA	CHA-C1A-NA	-3.84	117.70	126.39
2	E	608	CLA	CHA-C1A-NA	-3.83	117.71	126.39
2	G	608	CLA	CHA-C1A-NA	-3.83	117.71	126.39
2	J	608	CLA	CHA-C1A-NA	-3.83	117.71	126.39
2	I	608	CLA	CHA-C1A-NA	-3.83	117.72	126.39
2	A	608	CLA	CHA-C1A-NA	-3.83	117.72	126.39
2	D	608	CLA	CHA-C1A-NA	-3.83	117.72	126.39
2	K	608	CLA	CHA-C1A-NA	-3.83	117.73	126.39
2	C	608	CLA	CHA-C1A-NA	-3.82	117.73	126.39
2	F	608	CLA	CHA-C1A-NA	-3.81	117.75	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	606	CLA	C1-C2-C3	-3.70	120.14	126.20
2	G	606	CLA	C1-C2-C3	-3.70	120.14	126.20
2	H	606	CLA	C1-C2-C3	-3.69	120.16	126.20
2	A	606	CLA	C1-C2-C3	-3.68	120.16	126.20
2	C	606	CLA	C1-C2-C3	-3.68	120.17	126.20
2	I	606	CLA	C1-C2-C3	-3.67	120.18	126.20
2	K	606	CLA	C1-C2-C3	-3.67	120.18	126.20
2	D	606	CLA	C1-C2-C3	-3.67	120.19	126.20
2	J	606	CLA	C1-C2-C3	-3.66	120.19	126.20
2	B	606	CLA	C1-C2-C3	-3.66	120.20	126.20
2	E	606	CLA	C1-C2-C3	-3.66	120.20	126.20
2	J	610	CLA	CHA-C1A-NA	-3.51	118.45	126.39
2	H	610	CLA	CHA-C1A-NA	-3.51	118.45	126.39
2	E	610	CLA	CHA-C1A-NA	-3.51	118.45	126.39
2	I	610	CLA	CHA-C1A-NA	-3.50	118.46	126.39
2	A	610	CLA	CHA-C1A-NA	-3.50	118.47	126.39
2	B	610	CLA	CHA-C1A-NA	-3.50	118.47	126.39
2	D	610	CLA	CHA-C1A-NA	-3.50	118.47	126.39
2	C	610	CLA	CHA-C1A-NA	-3.50	118.48	126.39
2	G	610	CLA	CHA-C1A-NA	-3.49	118.48	126.39
2	K	610	CLA	CHA-C1A-NA	-3.49	118.49	126.39
2	F	610	CLA	CHA-C1A-NA	-3.49	118.49	126.39
2	D	604	CLA	C1D-ND-C4D	-3.31	103.99	106.31
2	B	604	CLA	C1D-ND-C4D	-3.30	103.99	106.31
2	A	604	CLA	C1D-ND-C4D	-3.30	104.00	106.31
2	F	604	CLA	C1D-ND-C4D	-3.29	104.00	106.31
2	I	604	CLA	C1D-ND-C4D	-3.29	104.00	106.31
2	H	604	CLA	C1D-ND-C4D	-3.29	104.00	106.31
2	E	604	CLA	C1D-ND-C4D	-3.29	104.01	106.31
2	G	604	CLA	C1D-ND-C4D	-3.28	104.01	106.31
2	B	609	CLA	C1D-ND-C4D	-3.27	104.02	106.31
2	C	604	CLA	C1D-ND-C4D	-3.27	104.02	106.31
2	K	609	CLA	C1D-ND-C4D	-3.27	104.02	106.31
2	J	604	CLA	C1D-ND-C4D	-3.26	104.02	106.31
2	K	604	CLA	C1D-ND-C4D	-3.26	104.03	106.31
2	C	609	CLA	C1D-ND-C4D	-3.25	104.03	106.31
2	D	609	CLA	C1D-ND-C4D	-3.24	104.04	106.31
2	A	609	CLA	C1D-ND-C4D	-3.24	104.04	106.31
2	F	609	CLA	C1D-ND-C4D	-3.24	104.04	106.31
2	G	609	CLA	C1D-ND-C4D	-3.24	104.04	106.31
2	D	609	CLA	C1-C2-C3	-3.23	120.90	126.20
2	H	609	CLA	C1D-ND-C4D	-3.23	104.04	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	609	CLA	C1-C2-C3	-3.23	120.90	126.20
2	K	609	CLA	C1-C2-C3	-3.23	120.91	126.20
2	G	609	CLA	C1-C2-C3	-3.22	120.92	126.20
2	C	609	CLA	C1-C2-C3	-3.22	120.92	126.20
2	E	609	CLA	C1D-ND-C4D	-3.22	104.05	106.31
2	E	611	CLA	C1D-ND-C4D	-3.22	104.05	106.31
2	J	609	CLA	C1D-ND-C4D	-3.22	104.05	106.31
2	E	609	CLA	C1-C2-C3	-3.22	120.92	126.20
2	A	609	CLA	C1-C2-C3	-3.22	120.93	126.20
2	B	611	CLA	C1D-ND-C4D	-3.21	104.06	106.31
2	H	609	CLA	C1-C2-C3	-3.21	120.94	126.20
2	B	609	CLA	C1-C2-C3	-3.21	120.94	126.20
2	K	611	CLA	C1D-ND-C4D	-3.20	104.06	106.31
2	F	609	CLA	C1-C2-C3	-3.20	120.95	126.20
2	I	611	CLA	C1D-ND-C4D	-3.20	104.07	106.31
2	I	609	CLA	C1-C2-C3	-3.20	120.96	126.20
2	I	609	CLA	C1D-ND-C4D	-3.20	104.07	106.31
2	C	611	CLA	C1D-ND-C4D	-3.19	104.07	106.31
2	D	611	CLA	C1D-ND-C4D	-3.19	104.08	106.31
2	A	611	CLA	C1D-ND-C4D	-3.18	104.08	106.31
2	J	611	CLA	C1D-ND-C4D	-3.18	104.08	106.31
2	H	611	CLA	C1D-ND-C4D	-3.17	104.09	106.31
2	F	611	CLA	C1D-ND-C4D	-3.16	104.09	106.31
2	G	611	CLA	C1D-ND-C4D	-3.16	104.09	106.31
2	D	610	CLA	CHA-C4D-ND	3.16	139.07	132.55
2	J	610	CLA	CHA-C4D-ND	3.16	139.07	132.55
2	F	603	CLA	C1D-ND-C4D	-3.16	104.10	106.31
2	C	610	CLA	CHA-C4D-ND	3.15	139.05	132.55
2	H	610	CLA	CHA-C4D-ND	3.15	139.04	132.55
2	A	610	CLA	CHA-C4D-ND	3.15	139.04	132.55
2	I	603	CLA	C1D-ND-C4D	-3.14	104.11	106.31
2	F	610	CLA	CHA-C4D-ND	3.14	139.03	132.55
2	E	610	CLA	CHA-C4D-ND	3.14	139.02	132.55
2	G	610	CLA	CHA-C4D-ND	3.14	139.02	132.55
2	K	610	CLA	CHA-C4D-ND	3.13	139.01	132.55
2	B	610	CLA	CHA-C4D-ND	3.13	139.01	132.55
2	G	603	CLA	C1D-ND-C4D	-3.12	104.12	106.31
2	I	610	CLA	CHA-C4D-ND	3.11	138.97	132.55
2	E	603	CLA	C1D-ND-C4D	-3.11	104.13	106.31
2	B	603	CLA	C1D-ND-C4D	-3.10	104.14	106.31
2	H	603	CLA	C1D-ND-C4D	-3.09	104.14	106.31
2	K	603	CLA	C1D-ND-C4D	-3.09	104.14	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	603	CLA	C1D-ND-C4D	-3.09	104.15	106.31
2	A	603	CLA	C1D-ND-C4D	-3.08	104.15	106.31
2	J	603	CLA	C1D-ND-C4D	-3.07	104.16	106.31
2	B	606	CLA	C1D-ND-C4D	-3.06	104.16	106.31
2	F	606	CLA	C1D-ND-C4D	-3.05	104.17	106.31
2	C	606	CLA	C1D-ND-C4D	-3.04	104.18	106.31
2	C	603	CLA	C1D-ND-C4D	-3.04	104.18	106.31
2	G	606	CLA	C1D-ND-C4D	-3.03	104.18	106.31
2	A	606	CLA	C1D-ND-C4D	-3.03	104.19	106.31
2	I	606	CLA	C1D-ND-C4D	-3.03	104.19	106.31
2	J	606	CLA	C1D-ND-C4D	-3.02	104.19	106.31
2	E	606	CLA	C1D-ND-C4D	-3.02	104.19	106.31
2	D	606	CLA	C1D-ND-C4D	-3.02	104.20	106.31
2	H	606	CLA	C1D-ND-C4D	-3.01	104.20	106.31
2	K	606	CLA	C1D-ND-C4D	-2.98	104.22	106.31
2	E	605	CLA	CHA-C1A-NA	-2.97	119.68	126.39
2	D	605	CLA	CHA-C1A-NA	-2.96	119.69	126.39
2	J	605	CLA	CHA-C1A-NA	-2.96	119.69	126.39
2	K	605	CLA	CHA-C1A-NA	-2.96	119.69	126.39
2	I	605	CLA	CHA-C1A-NA	-2.96	119.69	126.39
2	A	605	CLA	CHA-C1A-NA	-2.96	119.70	126.39
2	F	605	CLA	CHA-C1A-NA	-2.95	119.70	126.39
2	H	605	CLA	CHA-C1A-NA	-2.95	119.71	126.39
2	G	605	CLA	CHA-C1A-NA	-2.95	119.71	126.39
2	B	605	CLA	CHA-C1A-NA	-2.95	119.72	126.39
2	C	605	CLA	CHA-C1A-NA	-2.95	119.72	126.39
2	H	610	CLA	C2A-C1A-CHA	2.94	128.97	123.87
2	A	610	CLA	C2A-C1A-CHA	2.94	128.96	123.87
2	C	610	CLA	C2A-C1A-CHA	2.93	128.96	123.87
2	D	610	CLA	C2A-C1A-CHA	2.93	128.96	123.87
2	G	610	CLA	C2A-C1A-CHA	2.93	128.96	123.87
2	E	610	CLA	C2A-C1A-CHA	2.93	128.96	123.87
2	B	610	CLA	C2A-C1A-CHA	2.93	128.95	123.87
2	I	610	CLA	C2A-C1A-CHA	2.93	128.95	123.87
2	F	610	CLA	C2A-C1A-CHA	2.93	128.95	123.87
2	K	610	CLA	C2A-C1A-CHA	2.93	128.95	123.87
2	J	610	CLA	C2A-C1A-CHA	2.92	128.93	123.87
2	K	605	CLA	C2A-C1A-CHA	2.89	128.88	123.87
2	K	603	CLA	C2C-C1C-NC	2.88	113.01	109.98
2	G	605	CLA	C2A-C1A-CHA	2.88	128.87	123.87
2	H	605	CLA	C2A-C1A-CHA	2.88	128.87	123.87
2	J	605	CLA	C2A-C1A-CHA	2.88	128.87	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	605	CLA	C2A-C1A-CHA	2.88	128.86	123.87
2	I	605	CLA	C2A-C1A-CHA	2.88	128.86	123.87
2	B	602	CLA	C1D-ND-C4D	-2.88	104.29	106.31
2	A	605	CLA	C2A-C1A-CHA	2.87	128.85	123.87
2	C	605	CLA	C2A-C1A-CHA	2.87	128.85	123.87
2	B	605	CLA	C2A-C1A-CHA	2.87	128.85	123.87
2	D	605	CLA	C2A-C1A-CHA	2.87	128.85	123.87
2	C	603	CLA	C2C-C1C-NC	2.87	112.99	109.98
2	F	603	CLA	C2C-C1C-NC	2.86	112.99	109.98
2	J	602	CLA	C1D-ND-C4D	-2.85	104.31	106.31
2	E	603	CLA	C2C-C1C-NC	2.85	112.98	109.98
2	F	605	CLA	C2A-C1A-CHA	2.85	128.82	123.87
2	F	602	CLA	C1D-ND-C4D	-2.85	104.31	106.31
2	D	602	CLA	C1D-ND-C4D	-2.85	104.31	106.31
2	B	603	CLA	C2C-C1C-NC	2.85	112.97	109.98
2	A	602	CLA	C1D-ND-C4D	-2.85	104.31	106.31
2	A	603	CLA	C2C-C1C-NC	2.84	112.97	109.98
2	E	602	CLA	C1D-ND-C4D	-2.84	104.32	106.31
2	I	610	CLA	C1D-ND-C4D	-2.84	104.32	106.31
2	J	603	CLA	C2C-C1C-NC	2.84	112.96	109.98
2	I	603	CLA	C2C-C1C-NC	2.83	112.95	109.98
2	I	602	CLA	C1D-ND-C4D	-2.83	104.33	106.31
2	G	602	CLA	C1D-ND-C4D	-2.83	104.33	106.31
2	G	606	CLA	CHA-C1A-NA	-2.82	120.00	126.39
2	K	606	CLA	CHA-C1A-NA	-2.82	120.00	126.39
2	F	606	CLA	CHA-C1A-NA	-2.82	120.00	126.39
2	D	606	CLA	CHA-C1A-NA	-2.82	120.00	126.39
2	C	606	CLA	CHA-C1A-NA	-2.82	120.01	126.39
2	H	603	CLA	C2C-C1C-NC	2.82	112.94	109.98
2	H	606	CLA	CHA-C1A-NA	-2.82	120.02	126.39
2	K	602	CLA	C1D-ND-C4D	-2.81	104.34	106.31
2	D	603	CLA	C2C-C1C-NC	2.81	112.94	109.98
2	A	606	CLA	CHA-C1A-NA	-2.81	120.02	126.39
2	H	602	CLA	C1D-ND-C4D	-2.81	104.34	106.31
2	E	606	CLA	CHA-C1A-NA	-2.81	120.02	126.39
2	G	603	CLA	C2C-C1C-NC	2.81	112.94	109.98
2	I	606	CLA	CHA-C1A-NA	-2.81	120.03	126.39
2	J	606	CLA	CHA-C1A-NA	-2.81	120.03	126.39
2	C	602	CLA	C1D-ND-C4D	-2.81	104.34	106.31
2	B	606	CLA	CHA-C1A-NA	-2.81	120.04	126.39
2	K	610	CLA	C1D-ND-C4D	-2.79	104.35	106.31
2	B	610	CLA	C1D-ND-C4D	-2.78	104.36	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	610	CLA	C1D-ND-C4D	-2.76	104.38	106.31
2	J	601	CLA	C1D-ND-C4D	-2.75	104.38	106.31
2	A	610	CLA	C1D-ND-C4D	-2.75	104.38	106.31
2	H	610	CLA	C1D-ND-C4D	-2.75	104.38	106.31
2	B	607	CLA	CAA-C2A-C1A	-2.75	102.98	111.97
2	I	607	CLA	CAA-C2A-C1A	-2.74	102.98	111.97
2	C	607	CLA	CAA-C2A-C1A	-2.74	102.98	111.97
2	E	601	CLA	C1D-ND-C4D	-2.74	104.39	106.31
2	E	607	CLA	CAA-C2A-C1A	-2.74	103.00	111.97
2	G	607	CLA	CAA-C2A-C1A	-2.74	103.00	111.97
2	A	607	CLA	CAA-C2A-C1A	-2.74	103.00	111.97
2	H	607	CLA	CAA-C2A-C1A	-2.74	103.00	111.97
2	K	607	CLA	CAA-C2A-C1A	-2.74	103.00	111.97
2	J	607	CLA	CAA-C2A-C1A	-2.74	103.01	111.97
2	D	607	CLA	CAA-C2A-C1A	-2.74	103.01	111.97
2	F	607	CLA	CAA-C2A-C1A	-2.73	103.02	111.97
2	C	610	CLA	C1D-ND-C4D	-2.72	104.40	106.31
2	E	610	CLA	C1D-ND-C4D	-2.72	104.40	106.31
2	F	601	CLA	C1D-ND-C4D	-2.72	104.41	106.31
2	H	601	CLA	C1D-ND-C4D	-2.72	104.41	106.31
2	I	601	CLA	C1D-ND-C4D	-2.72	104.41	106.31
2	B	604	CLA	CHA-C1A-NA	-2.72	120.24	126.39
2	D	604	CLA	CHA-C1A-NA	-2.71	120.25	126.39
2	A	601	CLA	C1D-ND-C4D	-2.71	104.41	106.31
2	G	604	CLA	CHA-C1A-NA	-2.71	120.26	126.39
2	D	610	CLA	C1D-ND-C4D	-2.71	104.41	106.31
2	H	604	CLA	CHA-C1A-NA	-2.70	120.27	126.39
2	A	604	CLA	CHA-C1A-NA	-2.70	120.27	126.39
2	C	604	CLA	CHA-C1A-NA	-2.70	120.27	126.39
2	J	610	CLA	C1D-ND-C4D	-2.70	104.42	106.31
2	F	610	CLA	C1D-ND-C4D	-2.70	104.42	106.31
2	J	604	CLA	CHA-C1A-NA	-2.69	120.29	126.39
2	K	604	CLA	CHA-C1A-NA	-2.69	120.29	126.39
2	K	610	CLA	CHD-C1D-ND	-2.69	121.02	124.80
2	F	604	CLA	CHA-C1A-NA	-2.69	120.30	126.39
2	B	610	CLA	CHD-C1D-ND	-2.69	121.02	124.80
2	I	604	CLA	CHA-C1A-NA	-2.69	120.30	126.39
2	C	601	CLA	C1D-ND-C4D	-2.69	104.42	106.31
2	G	601	CLA	C1D-ND-C4D	-2.69	104.42	106.31
2	B	601	CLA	C1D-ND-C4D	-2.69	104.43	106.31
2	E	604	CLA	CHA-C1A-NA	-2.69	120.31	126.39
2	K	601	CLA	C1D-ND-C4D	-2.68	104.43	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	CLA	C1D-ND-C4D	-2.67	104.44	106.31
2	H	610	CLA	CHD-C1D-ND	-2.67	121.04	124.80
2	I	610	CLA	CHD-C1D-ND	-2.66	121.05	124.80
2	E	610	CLA	CHD-C1D-ND	-2.66	121.06	124.80
2	J	602	CLA	CAA-C2A-C1A	-2.66	103.27	111.97
2	K	602	CLA	CAA-C2A-C1A	-2.66	103.27	111.97
2	C	602	CLA	CAA-C2A-C1A	-2.66	103.27	111.97
2	A	610	CLA	CHD-C1D-ND	-2.66	121.07	124.80
2	G	602	CLA	CAA-C2A-C1A	-2.65	103.28	111.97
2	H	602	CLA	CAA-C2A-C1A	-2.65	103.28	111.97
2	A	602	CLA	CAA-C2A-C1A	-2.65	103.28	111.97
2	B	602	CLA	CAA-C2A-C1A	-2.65	103.28	111.97
2	D	611	CLA	CHA-C1A-NA	-2.65	120.38	126.39
2	D	610	CLA	CHD-C1D-ND	-2.65	121.07	124.80
2	D	602	CLA	CAA-C2A-C1A	-2.65	103.29	111.97
2	C	610	CLA	CHD-C1D-ND	-2.65	121.07	124.80
2	E	602	CLA	CAA-C2A-C1A	-2.65	103.30	111.97
2	J	611	CLA	CHA-C1A-NA	-2.65	120.40	126.39
2	I	602	CLA	CAA-C2A-C1A	-2.64	103.32	111.97
2	A	611	CLA	CHA-C1A-NA	-2.64	120.41	126.39
2	F	602	CLA	CAA-C2A-C1A	-2.64	103.32	111.97
2	E	611	CLA	CHA-C1A-NA	-2.64	120.42	126.39
2	G	610	CLA	CHD-C1D-ND	-2.64	121.09	124.80
2	H	611	CLA	CHA-C1A-NA	-2.64	120.42	126.39
2	I	611	CLA	CHA-C1A-NA	-2.64	120.42	126.39
2	E	609	CLA	CHD-C1D-ND	-2.64	121.09	124.80
2	C	611	CLA	CHA-C1A-NA	-2.63	120.43	126.39
2	K	611	CLA	CHA-C1A-NA	-2.63	120.43	126.39
2	F	611	CLA	CHA-C1A-NA	-2.63	120.44	126.39
2	B	611	CLA	CHA-C1A-NA	-2.63	120.44	126.39
2	J	610	CLA	CHD-C1D-ND	-2.63	121.11	124.80
2	K	609	CLA	CHD-C1D-ND	-2.63	121.11	124.80
2	G	611	CLA	CHA-C1A-NA	-2.63	120.44	126.39
2	G	609	CLA	CHD-C1D-ND	-2.63	121.11	124.80
2	H	609	CLA	CHD-C1D-ND	-2.62	121.11	124.80
2	E	601	CLA	CHD-C1D-ND	-2.62	121.11	124.80
2	A	609	CLA	CHD-C1D-ND	-2.62	121.12	124.80
2	C	609	CLA	CHD-C1D-ND	-2.62	121.12	124.80
2	D	609	CLA	CHD-C1D-ND	-2.62	121.12	124.80
2	I	609	CLA	CHD-C1D-ND	-2.61	121.12	124.80
2	J	609	CLA	CHD-C1D-ND	-2.61	121.13	124.80
2	J	601	CLA	CHD-C1D-ND	-2.61	121.14	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	605	CLA	CHA-C4D-ND	2.61	137.93	132.55
2	F	605	CLA	CHA-C4D-ND	2.60	137.92	132.55
2	J	605	CLA	CHA-C4D-ND	2.60	137.92	132.55
2	F	609	CLA	CHD-C1D-ND	-2.60	121.14	124.80
2	F	610	CLA	CHD-C1D-ND	-2.60	121.14	124.80
2	G	605	CLA	CHA-C4D-ND	2.60	137.92	132.55
2	D	605	CLA	CHA-C4D-ND	2.60	137.91	132.55
2	A	601	CLA	CHD-C1D-ND	-2.60	121.15	124.80
2	B	609	CLA	CHD-C1D-ND	-2.60	121.15	124.80
2	F	601	CLA	CHD-C1D-ND	-2.59	121.15	124.80
2	C	601	CLA	CHD-C1D-ND	-2.59	121.16	124.80
2	G	601	CLA	CHD-C1D-ND	-2.59	121.16	124.80
2	I	601	CLA	CHD-C1D-ND	-2.59	121.16	124.80
2	K	601	CLA	CHD-C1D-ND	-2.59	121.16	124.80
2	A	605	CLA	CHA-C4D-ND	2.59	137.89	132.55
2	K	605	CLA	CHA-C4D-ND	2.59	137.89	132.55
2	E	605	CLA	CHA-C4D-ND	2.59	137.89	132.55
2	H	605	CLA	CHA-C4D-ND	2.59	137.88	132.55
2	H	601	CLA	CHD-C1D-ND	-2.59	121.16	124.80
2	D	601	CLA	CHD-C1D-ND	-2.58	121.17	124.80
2	I	603	CLA	CHD-C1D-ND	-2.58	121.17	124.80
2	G	603	CLA	CHD-C1D-ND	-2.58	121.17	124.80
2	C	605	CLA	CHA-C4D-ND	2.58	137.87	132.55
2	B	603	CLA	CHD-C1D-ND	-2.58	121.18	124.80
2	B	601	CLA	CHD-C1D-ND	-2.57	121.18	124.80
3	D	612	XAT	O4-C5-C6	-2.57	56.89	58.93
2	E	603	CLA	CHD-C1D-ND	-2.56	121.20	124.80
2	F	603	CLA	CHD-C1D-ND	-2.55	121.21	124.80
2	A	603	CLA	CHD-C1D-ND	-2.55	121.21	124.80
2	H	603	CLA	CHD-C1D-ND	-2.55	121.21	124.80
2	I	605	CLA	CHA-C4D-ND	2.55	137.81	132.55
2	K	611	CLA	CHD-C1D-ND	-2.54	121.22	124.80
2	D	603	CLA	CHD-C1D-ND	-2.54	121.23	124.80
3	F	612	XAT	O4-C5-C6	-2.54	56.92	58.93
2	E	611	CLA	CHD-C1D-ND	-2.54	121.23	124.80
2	B	611	CLA	CHD-C1D-ND	-2.54	121.23	124.80
2	B	602	CLA	CHD-C1D-ND	-2.54	121.23	124.80
2	K	603	CLA	CHD-C1D-ND	-2.54	121.23	124.80
2	C	603	CLA	CHD-C1D-ND	-2.54	121.23	124.80
2	D	611	CLA	CHD-C1D-ND	-2.53	121.24	124.80
3	J	612	XAT	O4-C5-C6	-2.53	56.93	58.93
2	A	611	CLA	CHD-C1D-ND	-2.53	121.25	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	611	CLA	CHD-C1D-ND	-2.53	121.25	124.80
2	D	602	CLA	CHD-C1D-ND	-2.53	121.25	124.80
2	F	602	CLA	CHD-C1D-ND	-2.53	121.25	124.80
2	C	611	CLA	CHD-C1D-ND	-2.52	121.25	124.80
2	K	602	CLA	CHD-C1D-ND	-2.52	121.25	124.80
2	F	611	CLA	CHD-C1D-ND	-2.52	121.25	124.80
2	G	611	CLA	CHD-C1D-ND	-2.52	121.25	124.80
3	E	612	XAT	O4-C5-C6	-2.52	56.93	58.93
2	I	602	CLA	CHD-C1D-ND	-2.52	121.26	124.80
2	A	602	CLA	CHD-C1D-ND	-2.52	121.26	124.80
2	H	611	CLA	CHD-C1D-ND	-2.51	121.26	124.80
2	J	603	CLA	CHD-C1D-ND	-2.51	121.27	124.80
2	J	611	CLA	CHD-C1D-ND	-2.51	121.27	124.80
3	G	612	XAT	O4-C5-C6	-2.51	56.94	58.93
2	I	607	CLA	C2C-C1C-NC	2.51	112.62	109.98
2	G	607	CLA	C2C-C1C-NC	2.51	112.62	109.98
2	F	607	CLA	C2C-C1C-NC	2.51	112.62	109.98
2	K	607	CLA	C2C-C1C-NC	2.51	112.62	109.98
3	A	612	XAT	O4-C5-C6	-2.51	56.94	58.93
2	H	602	CLA	CHD-C1D-ND	-2.50	121.28	124.80
3	I	612	XAT	O4-C5-C6	-2.50	56.95	58.93
2	A	607	CLA	C2C-C1C-NC	2.50	112.61	109.98
2	E	602	CLA	CHD-C1D-ND	-2.50	121.28	124.80
2	C	607	CLA	C2C-C1C-NC	2.50	112.61	109.98
2	H	607	CLA	C2C-C1C-NC	2.50	112.60	109.98
2	C	602	CLA	CHD-C1D-ND	-2.49	121.29	124.80
2	F	603	CLA	CHC-C1C-C2C	-2.49	119.86	126.95
3	K	612	XAT	O4-C5-C6	-2.49	56.95	58.93
2	G	602	CLA	CHD-C1D-ND	-2.49	121.30	124.80
2	J	602	CLA	CHD-C1D-ND	-2.49	121.30	124.80
2	D	607	CLA	C2C-C1C-NC	2.49	112.60	109.98
2	J	607	CLA	C2C-C1C-NC	2.49	112.60	109.98
2	J	603	CLA	CHC-C1C-C2C	-2.49	119.88	126.95
2	C	603	CLA	CHC-C1C-C2C	-2.49	119.88	126.95
2	K	603	CLA	CHC-C1C-C2C	-2.49	119.88	126.95
3	H	612	XAT	O4-C5-C6	-2.49	56.96	58.93
2	D	603	CLA	CHC-C1C-C2C	-2.49	119.89	126.95
2	B	607	CLA	C2C-C1C-NC	2.48	112.59	109.98
2	A	603	CLA	CHC-C1C-C2C	-2.48	119.89	126.95
2	E	603	CLA	CHC-C1C-C2C	-2.48	119.89	126.95
2	H	603	CLA	CHC-C1C-C2C	-2.48	119.89	126.95
3	C	612	XAT	O4-C5-C6	-2.48	56.96	58.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	603	CLA	CHC-C1C-C2C	-2.48	119.89	126.95
2	B	603	CLA	CHC-C1C-C2C	-2.48	119.90	126.95
2	E	607	CLA	C2C-C1C-NC	2.48	112.58	109.98
2	I	603	CLA	CHC-C1C-C2C	-2.48	119.91	126.95
3	B	612	XAT	O4-C5-C6	-2.46	56.98	58.93
2	B	606	CLA	CHD-C1D-ND	-2.45	121.35	124.80
2	C	608	CLA	CHA-C4D-ND	2.44	137.59	132.55
2	C	606	CLA	CHD-C1D-ND	-2.44	121.37	124.80
2	K	606	CLA	CHD-C1D-ND	-2.44	121.37	124.80
2	G	606	CLA	CHD-C1D-ND	-2.43	121.38	124.80
2	F	608	CLA	CHA-C4D-ND	2.43	137.56	132.55
2	E	606	CLA	CHD-C1D-ND	-2.43	121.39	124.80
2	E	608	CLA	CHA-C4D-ND	2.43	137.55	132.55
2	I	606	CLA	CHD-C1D-ND	-2.42	121.39	124.80
2	B	608	CLA	CHA-C4D-ND	2.42	137.55	132.55
2	J	608	CLA	CHA-C4D-ND	2.42	137.55	132.55
2	K	608	CLA	CHA-C4D-ND	2.42	137.55	132.55
2	A	606	CLA	CHD-C1D-ND	-2.42	121.39	124.80
2	G	608	CLA	CHA-C4D-ND	2.42	137.54	132.55
2	C	607	CLA	CHD-C1D-ND	-2.42	121.40	124.80
2	A	608	CLA	CHA-C4D-ND	2.42	137.54	132.55
2	H	608	CLA	CHA-C4D-ND	2.42	137.53	132.55
2	D	606	CLA	CHD-C1D-ND	-2.42	121.40	124.80
2	H	606	CLA	CHD-C1D-ND	-2.41	121.40	124.80
2	K	607	CLA	CHD-C1D-ND	-2.41	121.41	124.80
2	D	608	CLA	CHA-C4D-ND	2.41	137.52	132.55
2	B	607	CLA	CHA-C1A-NA	-2.41	120.93	126.39
2	F	606	CLA	CHD-C1D-ND	-2.41	121.41	124.80
2	I	607	CLA	CHD-C1D-ND	-2.41	121.41	124.80
2	D	611	CLA	C1-C2-C3	-2.41	122.25	126.20
2	I	608	CLA	CHA-C4D-ND	2.41	137.51	132.55
2	G	607	CLA	CHD-C1D-ND	-2.40	121.42	124.80
2	I	604	CLA	CHD-C1D-ND	-2.40	121.42	124.80
2	J	607	CLA	CHD-C1D-ND	-2.40	121.42	124.80
2	C	607	CLA	CHA-C1A-NA	-2.40	120.95	126.39
2	I	607	CLA	CHA-C1A-NA	-2.40	120.95	126.39
2	A	607	CLA	CHD-C1D-ND	-2.40	121.42	124.80
2	J	606	CLA	CHD-C1D-ND	-2.40	121.42	124.80
2	G	605	CLA	CAA-C2A-C1A	-2.40	104.11	111.97
2	F	611	CLA	C1-C2-C3	-2.40	122.27	126.20
2	E	605	CLA	CAA-C2A-C1A	-2.40	104.11	111.97
2	I	605	CLA	CAA-C2A-C1A	-2.40	104.12	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	605	CLA	CAA-C2A-C1A	-2.40	104.12	111.97
2	K	605	CLA	CAA-C2A-C1A	-2.40	104.12	111.97
2	E	607	CLA	CHA-C1A-NA	-2.40	120.96	126.39
2	B	605	CLA	CAA-C2A-C1A	-2.40	104.12	111.97
2	D	605	CLA	CAA-C2A-C1A	-2.40	104.12	111.97
2	A	605	CLA	CAA-C2A-C1A	-2.40	104.12	111.97
2	J	607	CLA	CHA-C1A-NA	-2.39	120.97	126.39
2	D	607	CLA	CHD-C1D-ND	-2.39	121.44	124.80
2	A	607	CLA	CHA-C1A-NA	-2.39	120.97	126.39
2	H	607	CLA	CHA-C1A-NA	-2.39	120.97	126.39
2	F	605	CLA	CAA-C2A-C1A	-2.39	104.14	111.97
2	D	607	CLA	CHA-C1A-NA	-2.39	120.97	126.39
2	C	611	CLA	C1-C2-C3	-2.39	122.28	126.20
2	J	602	CLA	C2C-C1C-NC	2.39	112.49	109.98
2	C	605	CLA	CAA-C2A-C1A	-2.39	104.14	111.97
2	K	607	CLA	CHA-C1A-NA	-2.39	120.98	126.39
2	G	607	CLA	CHA-C1A-NA	-2.39	120.98	126.39
2	J	611	CLA	C1-C2-C3	-2.39	122.28	126.20
2	D	604	CLA	CHD-C1D-ND	-2.39	121.44	124.80
2	A	611	CLA	C1-C2-C3	-2.39	122.28	126.20
2	H	605	CLA	CAA-C2A-C1A	-2.39	104.15	111.97
2	G	611	CLA	C1-C2-C3	-2.39	122.29	126.20
2	E	607	CLA	CHD-C1D-ND	-2.39	121.44	124.80
2	F	607	CLA	CHA-C1A-NA	-2.39	120.99	126.39
2	I	611	CLA	C1-C2-C3	-2.38	122.29	126.20
2	H	607	CLA	CHD-C1D-ND	-2.38	121.45	124.80
2	A	604	CLA	CHD-C1D-ND	-2.38	121.45	124.80
2	B	611	CLA	C1-C2-C3	-2.38	122.29	126.20
2	J	604	CLA	CHD-C1D-ND	-2.38	121.45	124.80
2	K	604	CLA	CHD-C1D-ND	-2.38	121.45	124.80
2	K	611	CLA	C1-C2-C3	-2.38	122.30	126.20
2	E	611	CLA	C1-C2-C3	-2.38	122.30	126.20
2	C	602	CLA	C2C-C1C-NC	2.38	112.48	109.98
2	C	603	CLA	CHA-C1A-NA	-2.38	121.00	126.39
2	H	604	CLA	CHD-C1D-ND	-2.38	121.45	124.80
2	C	604	CLA	CHD-C1D-ND	-2.38	121.46	124.80
2	F	604	CLA	CHD-C1D-ND	-2.38	121.46	124.80
2	H	611	CLA	C1-C2-C3	-2.38	122.31	126.20
2	F	603	CLA	CHA-C1A-NA	-2.37	121.02	126.39
2	B	607	CLA	CHD-C1D-ND	-2.37	121.47	124.80
2	F	607	CLA	CHD-C1D-ND	-2.37	121.47	124.80
2	E	604	CLA	CHD-C1D-ND	-2.37	121.47	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	603	CLA	CHA-C1A-NA	-2.37	121.03	126.39
2	F	602	CLA	C2C-C1C-NC	2.37	112.47	109.98
2	K	603	CLA	CHA-C1A-NA	-2.37	121.03	126.39
2	H	609	CLA	CHA-C1A-NA	-2.37	121.03	126.39
2	B	603	CLA	CHA-C1A-NA	-2.36	121.04	126.39
2	A	603	CLA	CHA-C1A-NA	-2.36	121.04	126.39
2	D	603	CLA	CHA-C1A-NA	-2.36	121.04	126.39
2	I	603	CLA	CHA-C1A-NA	-2.36	121.04	126.39
2	B	602	CLA	C2C-C1C-NC	2.36	112.46	109.98
2	G	603	CLA	CHA-C1A-NA	-2.36	121.04	126.39
2	J	603	CLA	CHA-C1A-NA	-2.36	121.04	126.39
2	K	609	CLA	CHA-C1A-NA	-2.36	121.04	126.39
2	G	604	CLA	CHD-C1D-ND	-2.36	121.48	124.80
2	B	604	CLA	CHD-C1D-ND	-2.36	121.49	124.80
2	D	609	CLA	CHA-C1A-NA	-2.35	121.06	126.39
2	J	609	CLA	CHA-C1A-NA	-2.35	121.06	126.39
2	E	603	CLA	CHA-C1A-NA	-2.35	121.06	126.39
2	F	605	CLA	C4D-CHA-C1A	-2.35	118.44	121.24
2	I	602	CLA	C2C-C1C-NC	2.35	112.45	109.98
2	B	605	CLA	C4D-CHA-C1A	-2.35	118.44	121.24
2	B	609	CLA	CHA-C1A-NA	-2.35	121.07	126.39
2	C	609	CLA	CHA-C1A-NA	-2.35	121.07	126.39
2	I	609	CLA	CHA-C1A-NA	-2.35	121.07	126.39
2	G	602	CLA	C2C-C1C-NC	2.35	112.45	109.98
2	C	608	CLA	C4D-CHA-C1A	-2.35	118.44	121.24
2	E	602	CLA	C2C-C1C-NC	2.35	112.45	109.98
2	F	609	CLA	CHA-C1A-NA	-2.35	121.08	126.39
2	A	609	CLA	CHA-C1A-NA	-2.35	121.08	126.39
2	D	602	CLA	C2C-C1C-NC	2.34	112.44	109.98
2	E	608	CLA	C4D-CHA-C1A	-2.34	118.45	121.24
2	A	602	CLA	C2C-C1C-NC	2.34	112.44	109.98
2	E	609	CLA	CHA-C1A-NA	-2.34	121.08	126.39
2	F	608	CLA	C4D-CHA-C1A	-2.34	118.46	121.24
2	K	608	CLA	C4D-CHA-C1A	-2.34	118.46	121.24
2	G	609	CLA	CHA-C1A-NA	-2.33	121.11	126.39
2	D	605	CLA	C4D-CHA-C1A	-2.33	118.47	121.24
2	J	605	CLA	C4D-CHA-C1A	-2.33	118.47	121.24
2	H	602	CLA	C2C-C1C-NC	2.33	112.42	109.98
2	A	605	CLA	C4D-CHA-C1A	-2.32	118.47	121.24
2	G	608	CLA	C4D-CHA-C1A	-2.32	118.47	121.24
2	B	608	CLA	C4D-CHA-C1A	-2.32	118.47	121.24
2	K	602	CLA	C2C-C1C-NC	2.32	112.42	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	608	CLA	C4D-CHA-C1A	-2.32	118.48	121.24
2	C	605	CLA	C4D-CHA-C1A	-2.32	118.48	121.24
2	G	605	CLA	C4D-CHA-C1A	-2.32	118.48	121.24
2	G	606	CLA	CAA-C2A-C1A	-2.32	104.38	111.97
2	A	608	CLA	C4D-CHA-C1A	-2.32	118.48	121.24
4	J	613	32N	C34-C29-C28	2.31	115.48	112.83
2	J	608	CLA	C4D-CHA-C1A	-2.31	118.49	121.24
2	K	605	CLA	C4D-CHA-C1A	-2.31	118.49	121.24
2	J	606	CLA	CAA-C2A-C1A	-2.31	104.40	111.97
2	H	606	CLA	CAA-C2A-C1A	-2.31	104.40	111.97
2	C	606	CLA	CAA-C2A-C1A	-2.31	104.41	111.97
2	A	606	CLA	CAA-C2A-C1A	-2.31	104.41	111.97
2	E	605	CLA	C4D-CHA-C1A	-2.31	118.49	121.24
2	B	606	CLA	CAA-C2A-C1A	-2.31	104.42	111.97
2	E	606	CLA	CAA-C2A-C1A	-2.31	104.42	111.97
2	F	606	CLA	CAA-C2A-C1A	-2.30	104.43	111.97
2	H	605	CLA	C4D-CHA-C1A	-2.30	118.50	121.24
2	H	608	CLA	C4D-CHA-C1A	-2.30	118.50	121.24
2	D	606	CLA	CAA-C2A-C1A	-2.30	104.44	111.97
4	D	613	32N	C34-C29-C28	2.30	115.47	112.83
2	K	606	CLA	CAA-C2A-C1A	-2.30	104.44	111.97
4	I	613	32N	C34-C29-C28	2.30	115.47	112.83
2	B	601	CLA	CHC-C1C-C2C	-2.30	120.42	126.95
2	I	606	CLA	CAA-C2A-C1A	-2.30	104.44	111.97
2	I	608	CLA	C4D-CHA-C1A	-2.29	118.51	121.24
2	D	601	CLA	CHC-C1C-C2C	-2.29	120.44	126.95
2	I	605	CLA	C4D-CHA-C1A	-2.29	118.51	121.24
4	B	613	32N	C34-C29-C28	2.29	115.46	112.83
2	I	601	CLA	CHC-C1C-C2C	-2.29	120.44	126.95
2	H	601	CLA	CHC-C1C-C2C	-2.29	120.44	126.95
2	G	601	CLA	CHC-C1C-C2C	-2.29	120.45	126.95
2	E	601	CLA	CHC-C1C-C2C	-2.29	120.45	126.95
2	B	611	CLA	C2C-C1C-NC	2.29	112.38	109.98
2	F	601	CLA	CHC-C1C-C2C	-2.29	120.45	126.95
2	A	601	CLA	CHC-C1C-C2C	-2.28	120.46	126.95
2	J	601	CLA	CHC-C1C-C2C	-2.28	120.46	126.95
2	B	609	CLA	C3D-C4D-ND	2.28	113.70	109.99
2	K	609	CLA	C3D-C4D-ND	2.28	113.69	109.99
2	B	601	CLA	CHA-C1A-NA	-2.28	121.22	126.39
2	G	611	CLA	C2C-C1C-NC	2.28	112.38	109.98
2	K	601	CLA	CHC-C1C-C2C	-2.28	120.47	126.95
2	D	611	CLA	C2C-C1C-NC	2.28	112.38	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	613	32N	C34-C29-C28	2.28	115.44	112.83
2	J	601	CLA	CHA-C1A-NA	-2.28	121.23	126.39
2	G	601	CLA	CHA-C1A-NA	-2.28	121.24	126.39
2	F	604	CLA	C2C-C1C-NC	2.28	112.37	109.98
2	C	601	CLA	CHA-C1A-NA	-2.27	121.24	126.39
2	E	601	CLA	CHA-C1A-NA	-2.27	121.24	126.39
2	C	611	CLA	C2C-C1C-NC	2.27	112.37	109.98
2	D	608	CLA	CHC-C1C-C2C	-2.27	120.49	126.95
2	F	608	CLA	CHC-C1C-C2C	-2.27	120.49	126.95
2	E	608	CLA	CHC-C1C-C2C	-2.27	120.49	126.95
2	A	611	CLA	C2C-C1C-NC	2.27	112.37	109.98
2	C	601	CLA	CHC-C1C-C2C	-2.27	120.49	126.95
2	I	611	CLA	C2C-C1C-NC	2.27	112.37	109.98
2	G	608	CLA	CHC-C1C-C2C	-2.27	120.49	126.95
2	K	611	CLA	C2C-C1C-NC	2.27	112.37	109.98
2	H	611	CLA	C2C-C1C-NC	2.27	112.37	109.98
2	F	609	CLA	C3D-C4D-ND	2.27	113.67	109.99
2	C	608	CLA	CHC-C1C-C2C	-2.27	120.50	126.95
2	G	602	CLA	CHA-C1A-NA	-2.27	121.25	126.39
2	A	608	CLA	CHC-C1C-C2C	-2.27	120.50	126.95
2	J	602	CLA	CHA-C1A-NA	-2.27	121.26	126.39
2	I	608	CLA	CHC-C1C-C2C	-2.27	120.51	126.95
2	B	608	CLA	CHC-C1C-C2C	-2.27	120.51	126.95
2	H	608	CLA	CHC-C1C-C2C	-2.27	120.51	126.95
2	D	601	CLA	CHA-C1A-NA	-2.27	121.26	126.39
2	J	608	CLA	CHC-C1C-C2C	-2.26	120.51	126.95
2	I	602	CLA	CHA-C1A-NA	-2.26	121.26	126.39
2	E	611	CLA	C2C-C1C-NC	2.26	112.36	109.98
2	I	604	CLA	C2C-C1C-NC	2.26	112.36	109.98
2	K	602	CLA	CHA-C1A-NA	-2.26	121.27	126.39
2	E	602	CLA	CHA-C1A-NA	-2.26	121.27	126.39
2	A	601	CLA	CHA-C1A-NA	-2.26	121.27	126.39
2	C	609	CLA	C3D-C4D-ND	2.26	113.66	109.99
2	G	609	CLA	C3D-C4D-ND	2.26	113.66	109.99
2	K	608	CLA	CHC-C1C-C2C	-2.26	120.52	126.95
2	D	602	CLA	CHA-C1A-NA	-2.26	121.27	126.39
2	A	609	CLA	C3D-C4D-ND	2.26	113.66	109.99
4	E	613	32N	C34-C29-C28	2.26	115.42	112.83
2	A	602	CLA	CHA-C1A-NA	-2.26	121.28	126.39
2	D	609	CLA	C3D-C4D-ND	2.26	113.66	109.99
2	F	601	CLA	CHA-C1A-NA	-2.26	121.28	126.39
2	F	602	CLA	CHA-C1A-NA	-2.26	121.28	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	613	32N	C34-C29-C28	2.26	115.42	112.83
2	H	602	CLA	CHA-C1A-NA	-2.26	121.28	126.39
2	H	601	CLA	CHA-C1A-NA	-2.26	121.28	126.39
2	C	604	CLA	C2C-C1C-NC	2.26	112.35	109.98
4	G	613	32N	C34-C29-C28	2.26	115.42	112.83
2	I	601	CLA	CHA-C1A-NA	-2.25	121.28	126.39
2	J	611	CLA	C2C-C1C-NC	2.25	112.35	109.98
2	E	609	CLA	C3D-C4D-ND	2.25	113.65	109.99
2	F	611	CLA	C2C-C1C-NC	2.25	112.35	109.98
2	C	602	CLA	CHA-C1A-NA	-2.25	121.29	126.39
2	H	609	CLA	C3D-C4D-ND	2.25	113.65	109.99
2	J	611	CLA	CHC-C1C-C2C	-2.25	120.55	126.95
2	K	601	CLA	CHA-C1A-NA	-2.25	121.30	126.39
2	J	609	CLA	C3D-C4D-ND	2.25	113.64	109.99
2	B	602	CLA	CHA-C1A-NA	-2.25	121.30	126.39
2	D	611	CLA	CHC-C1C-C2C	-2.25	120.56	126.95
2	C	611	CLA	CHC-C1C-C2C	-2.25	120.56	126.95
2	F	611	CLA	CHC-C1C-C2C	-2.25	120.57	126.95
2	I	611	CLA	CHC-C1C-C2C	-2.25	120.57	126.95
2	E	601	CLA	C1-C2-C3	-2.24	122.52	126.20
2	D	604	CLA	C2C-C1C-NC	2.24	112.34	109.98
2	K	604	CLA	C2C-C1C-NC	2.24	112.34	109.98
2	A	604	CLA	C2C-C1C-NC	2.24	112.34	109.98
2	H	604	CLA	C2C-C1C-NC	2.24	112.34	109.98
4	H	613	32N	C34-C29-C28	2.24	115.40	112.83
2	H	608	CLA	CGD-CBD-CAD	-2.24	103.59	110.85
3	C	612	XAT	C18-C5-C4	-2.24	111.72	114.24
2	E	611	CLA	CHC-C1C-C2C	-2.24	120.58	126.95
2	H	606	CLA	C2A-C1A-CHA	2.24	127.75	123.87
2	G	611	CLA	CHC-C1C-C2C	-2.24	120.59	126.95
3	K	612	XAT	C18-C5-C4	-2.24	111.73	114.24
2	H	611	CLA	CHC-C1C-C2C	-2.24	120.59	126.95
2	G	606	CLA	C2A-C1A-CHA	2.24	127.75	123.87
2	A	611	CLA	CHC-C1C-C2C	-2.24	120.59	126.95
4	E	613	32N	C28-C27-C25	-2.24	121.51	126.32
4	F	613	32N	C28-C27-C25	-2.24	121.51	126.32
4	F	613	32N	C34-C29-C28	2.23	115.39	112.83
2	C	608	CLA	CGD-CBD-CAD	-2.23	103.61	110.85
2	C	606	CLA	C2A-C1A-CHA	2.23	127.74	123.87
2	J	608	CLA	CGD-CBD-CAD	-2.23	103.62	110.85
2	B	611	CLA	CHC-C1C-C2C	-2.23	120.60	126.95
4	G	613	32N	C28-C27-C25	-2.23	121.52	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	613	32N	C28-C27-C25	-2.23	121.52	126.32
2	E	606	CLA	C2A-C1A-CHA	2.23	127.74	123.87
2	K	611	CLA	CHC-C1C-C2C	-2.23	120.61	126.95
2	C	601	CLA	C1-C2-C3	-2.23	122.54	126.20
4	B	613	32N	C28-C27-C25	-2.23	121.53	126.32
2	D	608	CLA	CGD-CBD-CAD	-2.23	103.63	110.85
2	A	608	CLA	CGD-CBD-CAD	-2.23	103.64	110.85
2	J	610	CLA	C4D-CHA-C1A	-2.23	118.59	121.24
4	C	613	32N	C28-C27-C25	-2.23	121.54	126.32
2	J	604	CLA	C2C-C1C-NC	2.23	112.32	109.98
2	F	606	CLA	C2A-C1A-CHA	2.22	127.73	123.87
2	F	608	CLA	CGD-CBD-CAD	-2.22	103.64	110.85
2	J	606	CLA	C2A-C1A-CHA	2.22	127.73	123.87
2	I	609	CLA	C3D-C4D-ND	2.22	113.60	109.99
2	A	606	CLA	C2A-C1A-CHA	2.22	127.72	123.87
2	G	608	CLA	CGD-CBD-CAD	-2.22	103.65	110.85
2	K	608	CLA	CGD-CBD-CAD	-2.22	103.65	110.85
2	E	608	CLA	CGD-CBD-CAD	-2.22	103.66	110.85
4	H	613	32N	C28-C27-C25	-2.22	121.55	126.32
2	B	604	CLA	C2C-C1C-NC	2.22	112.31	109.98
2	I	608	CLA	CGD-CBD-CAD	-2.22	103.66	110.85
4	A	613	32N	C28-C27-C25	-2.22	121.55	126.32
2	G	604	CLA	C2C-C1C-NC	2.22	112.31	109.98
4	D	613	32N	C28-C27-C25	-2.22	121.55	126.32
4	J	613	32N	C28-C27-C25	-2.22	121.55	126.32
2	C	610	CLA	C4D-CHA-C1A	-2.22	118.60	121.24
2	D	610	CLA	C4D-CHA-C1A	-2.22	118.60	121.24
2	E	604	CLA	C2C-C1C-NC	2.22	112.31	109.98
4	K	613	32N	C28-C27-C25	-2.22	121.56	126.32
2	I	606	CLA	C2A-C1A-CHA	2.22	127.71	123.87
2	B	608	CLA	CGD-CBD-CAD	-2.22	103.67	110.85
2	K	601	CLA	C1-C2-C3	-2.21	122.57	126.20
3	J	612	XAT	C18-C5-C4	-2.21	111.75	114.24
4	C	613	32N	C34-C29-C28	2.21	115.37	112.83
2	I	601	CLA	C1-C2-C3	-2.21	122.57	126.20
2	A	610	CLA	C4D-CHA-C1A	-2.21	118.61	121.24
2	F	610	CLA	C4D-CHA-C1A	-2.21	118.61	121.24
3	H	612	XAT	C18-C5-C4	-2.21	111.76	114.24
2	B	606	CLA	C2A-C1A-CHA	2.21	127.70	123.87
2	K	606	CLA	C2A-C1A-CHA	2.21	127.70	123.87
3	D	612	XAT	C18-C5-C4	-2.21	111.76	114.24
2	K	603	CLA	CAA-C2A-C1A	-2.21	104.74	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	CLA	C1-C2-C3	-2.21	122.58	126.20
2	D	606	CLA	C2A-C1A-CHA	2.21	127.70	123.87
2	A	603	CLA	CAA-C2A-C1A	-2.21	104.75	111.97
2	F	603	CLA	CAA-C2A-C1A	-2.21	104.75	111.97
2	K	610	CLA	C4D-CHA-C1A	-2.20	118.61	121.24
2	B	601	CLA	C1-C2-C3	-2.20	122.58	126.20
2	B	603	CLA	CAA-C2A-C1A	-2.20	104.75	111.97
2	H	610	CLA	C4D-CHA-C1A	-2.20	118.61	121.24
2	J	601	CLA	C1-C2-C3	-2.20	122.59	126.20
2	E	603	CLA	CAA-C2A-C1A	-2.20	104.76	111.97
2	H	603	CLA	CAA-C2A-C1A	-2.20	104.76	111.97
3	A	612	XAT	C18-C5-C4	-2.20	111.77	114.24
2	G	601	CLA	C1-C2-C3	-2.20	122.59	126.20
2	I	603	CLA	CAA-C2A-C1A	-2.20	104.76	111.97
2	G	603	CLA	CAA-C2A-C1A	-2.20	104.77	111.97
2	G	610	CLA	C4D-CHA-C1A	-2.20	118.62	121.24
2	D	603	CLA	CAA-C2A-C1A	-2.20	104.77	111.97
2	B	610	CLA	C4D-CHA-C1A	-2.20	118.62	121.24
2	K	606	CLA	C4D-CHA-C1A	-2.19	118.63	121.24
2	J	603	CLA	CAA-C2A-C1A	-2.19	104.79	111.97
3	G	612	XAT	C18-C5-C4	-2.19	111.78	114.24
2	D	606	CLA	C4D-CHA-C1A	-2.19	118.63	121.24
2	F	609	CLA	CHC-C1C-C2C	-2.19	120.72	126.95
2	C	603	CLA	CAA-C2A-C1A	-2.19	104.79	111.97
2	D	601	CLA	C1-C2-C3	-2.19	122.61	126.20
2	E	609	CLA	CHC-C1C-C2C	-2.19	120.72	126.95
3	E	612	XAT	C18-C5-C4	-2.19	111.78	114.24
4	C	613	32N	C29-C28-C27	2.19	127.99	124.58
2	E	610	CLA	C4D-CHA-C1A	-2.19	118.63	121.24
2	H	601	CLA	C1-C2-C3	-2.19	122.61	126.20
2	H	609	CLA	CHC-C1C-C2C	-2.19	120.73	126.95
3	I	612	XAT	C18-C5-C4	-2.19	111.78	114.24
2	D	609	CLA	CHC-C1C-C2C	-2.19	120.74	126.95
2	B	609	CLA	CHC-C1C-C2C	-2.19	120.74	126.95
2	K	609	CLA	CHC-C1C-C2C	-2.19	120.74	126.95
2	I	610	CLA	C4D-CHA-C1A	-2.18	118.64	121.24
2	C	601	CLA	C2C-C1C-NC	2.18	112.28	109.98
2	A	609	CLA	CHC-C1C-C2C	-2.18	120.74	126.95
3	B	612	XAT	C18-C5-C4	-2.18	111.79	114.24
2	C	609	CLA	CHC-C1C-C2C	-2.18	120.75	126.95
2	G	609	CLA	CHC-C1C-C2C	-2.18	120.75	126.95
2	K	601	CLA	CAA-C2A-C1A	-2.18	104.83	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	613	32N	C29-C28-C27	2.18	127.97	124.58
4	F	613	32N	C29-C28-C27	2.18	127.97	124.58
2	G	601	CLA	CAA-C2A-C1A	-2.18	104.83	111.97
2	F	601	CLA	C1-C2-C3	-2.18	122.63	126.20
2	J	609	CLA	CHC-C1C-C2C	-2.18	120.76	126.95
3	F	612	XAT	C18-C5-C4	-2.18	111.80	114.24
2	D	601	CLA	CAA-C2A-C1A	-2.18	104.84	111.97
2	E	601	CLA	C2C-C1C-NC	2.18	112.27	109.98
4	J	613	32N	C29-C28-C27	2.18	127.97	124.58
2	A	601	CLA	CAA-C2A-C1A	-2.18	104.84	111.97
2	H	601	CLA	CAA-C2A-C1A	-2.17	104.85	111.97
4	H	613	32N	C29-C28-C27	2.17	127.96	124.58
2	I	609	CLA	CHC-C1C-C2C	-2.17	120.77	126.95
2	B	601	CLA	CAA-C2A-C1A	-2.17	104.85	111.97
2	C	606	CLA	C4D-CHA-C1A	-2.17	118.65	121.24
2	J	601	CLA	CAA-C2A-C1A	-2.17	104.86	111.97
4	G	613	32N	C29-C28-C27	2.17	127.96	124.58
2	J	606	CLA	C4D-CHA-C1A	-2.17	118.66	121.24
4	A	613	32N	C29-C28-C27	2.17	127.96	124.58
2	I	606	CLA	C4D-CHA-C1A	-2.17	118.66	121.24
2	C	601	CLA	CAA-C2A-C1A	-2.17	104.87	111.97
2	A	606	CLA	C4D-CHA-C1A	-2.17	118.66	121.24
2	I	601	CLA	CAA-C2A-C1A	-2.17	104.87	111.97
2	E	601	CLA	CAA-C2A-C1A	-2.17	104.87	111.97
4	D	613	32N	C29-C28-C27	2.17	127.95	124.58
2	B	601	CLA	C2C-C1C-NC	2.16	112.25	109.98
2	F	601	CLA	CAA-C2A-C1A	-2.16	104.89	111.97
4	E	613	32N	C29-C28-C27	2.16	127.94	124.58
2	B	606	CLA	C4D-CHA-C1A	-2.16	118.67	121.24
2	E	606	CLA	C4D-CHA-C1A	-2.16	118.67	121.24
2	G	606	CLA	C4D-CHA-C1A	-2.16	118.67	121.24
2	C	602	CLA	CHC-C1C-C2C	-2.16	120.82	126.95
2	F	601	CLA	C2C-C1C-NC	2.16	112.25	109.98
2	H	606	CLA	C4D-CHA-C1A	-2.16	118.67	121.24
2	K	601	CLA	C2C-C1C-NC	2.15	112.25	109.98
2	I	602	CLA	CHC-C1C-C2C	-2.15	120.83	126.95
4	I	613	32N	C29-C28-C27	2.15	127.93	124.58
2	F	606	CLA	C4D-CHA-C1A	-2.15	118.68	121.24
4	B	613	32N	C29-C28-C27	2.15	127.93	124.58
2	A	601	CLA	C2C-C1C-NC	2.15	112.24	109.98
2	E	608	CLA	C2C-C1C-NC	2.15	112.24	109.98
2	D	602	CLA	CHC-C1C-C2C	-2.15	120.83	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	602	CLA	CHC-C1C-C2C	-2.15	120.83	126.95
2	F	608	CLA	C2C-C1C-NC	2.15	112.24	109.98
2	G	601	CLA	C2C-C1C-NC	2.15	112.24	109.98
2	E	602	CLA	CHC-C1C-C2C	-2.15	120.84	126.95
2	G	602	CLA	CHC-C1C-C2C	-2.15	120.84	126.95
2	B	602	CLA	CHC-C1C-C2C	-2.15	120.84	126.95
2	D	604	CLA	CHC-C1C-C2C	-2.15	120.84	126.95
2	H	602	CLA	CHC-C1C-C2C	-2.15	120.84	126.95
2	F	604	CLA	CHC-C1C-C2C	-2.15	120.84	126.95
2	C	604	CLA	CHC-C1C-C2C	-2.15	120.84	126.95
2	H	604	CLA	CHC-C1C-C2C	-2.15	120.84	126.95
2	A	602	CLA	CHC-C1C-C2C	-2.15	120.85	126.95
2	F	602	CLA	CHC-C1C-C2C	-2.15	120.85	126.95
2	K	604	CLA	CHC-C1C-C2C	-2.15	120.85	126.95
2	D	608	CLA	C2C-C1C-NC	2.15	112.23	109.98
2	I	604	CLA	CHC-C1C-C2C	-2.14	120.85	126.95
2	K	602	CLA	CHC-C1C-C2C	-2.14	120.85	126.95
2	A	604	CLA	CHC-C1C-C2C	-2.14	120.86	126.95
2	E	604	CLA	CHC-C1C-C2C	-2.14	120.86	126.95
2	J	604	CLA	CHC-C1C-C2C	-2.14	120.86	126.95
2	B	604	CLA	CHC-C1C-C2C	-2.14	120.86	126.95
2	I	601	CLA	C2C-C1C-NC	2.14	112.23	109.98
2	D	601	CLA	C2C-C1C-NC	2.14	112.23	109.98
2	J	605	CLA	CHD-C1D-ND	-2.14	121.79	124.80
2	G	604	CLA	CHC-C1C-C2C	-2.14	120.87	126.95
2	I	608	CLA	C2C-C1C-NC	2.14	112.22	109.98
2	C	608	CLA	C2C-C1C-NC	2.13	112.22	109.98
2	J	601	CLA	C2C-C1C-NC	2.13	112.22	109.98
2	D	605	CLA	CHD-C1D-ND	-2.13	121.80	124.80
2	I	605	CLA	CHD-C1D-ND	-2.13	121.81	124.80
2	H	601	CLA	C2C-C1C-NC	2.12	112.21	109.98
2	K	605	CLA	CHD-C1D-ND	-2.12	121.82	124.80
2	B	611	CLA	C3D-C4D-ND	2.12	113.43	109.99
2	A	608	CLA	C2C-C1C-NC	2.11	112.20	109.98
2	B	608	CLA	C2C-C1C-NC	2.11	112.20	109.98
2	J	607	CLA	C1D-ND-C4D	-2.11	104.83	106.31
2	E	611	CLA	C3D-C4D-ND	2.11	113.42	109.99
2	A	605	CLA	CHD-C1D-ND	-2.11	121.83	124.80
2	F	605	CLA	CHD-C1D-ND	-2.11	121.83	124.80
2	G	608	CLA	C2C-C1C-NC	2.11	112.20	109.98
2	E	605	CLA	CHD-C1D-ND	-2.11	121.83	124.80
2	I	607	CLA	C1D-ND-C4D	-2.11	104.83	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	608	CLA	C2C-C1C-NC	2.10	112.19	109.98
2	B	605	CLA	CHD-C1D-ND	-2.10	121.84	124.80
2	K	606	CLA	CHA-C4D-ND	2.10	136.88	132.55
2	C	603	CLA	CHA-C4D-ND	2.10	136.88	132.55
2	C	611	CLA	C3D-C4D-ND	2.10	113.40	109.99
2	I	611	CLA	C3D-C4D-ND	2.10	113.40	109.99
2	H	603	CLA	CHA-C4D-ND	2.10	136.87	132.55
2	G	602	CLA	C3D-C4D-ND	2.09	113.39	109.99
2	H	605	CLA	CHD-C1D-ND	-2.09	121.86	124.80
2	D	606	CLA	CHA-C4D-ND	2.09	136.87	132.55
2	E	603	CLA	CHA-C4D-ND	2.09	136.87	132.55
2	K	608	CLA	C2C-C1C-NC	2.09	112.18	109.98
2	I	607	CLA	CHC-C1C-C2C	-2.09	121.00	126.95
2	A	603	CLA	CHA-C4D-ND	2.09	136.86	132.55
2	D	602	CLA	C3D-C4D-ND	2.09	113.39	109.99
2	D	611	CLA	C3D-C4D-ND	2.09	113.39	109.99
2	K	603	CLA	CHA-C4D-ND	2.09	136.86	132.55
3	D	612	XAT	C24-C23-C22	2.09	114.70	110.79
2	A	611	CLA	C3D-C4D-ND	2.09	113.38	109.99
2	J	607	CLA	CHC-C1C-C2C	-2.09	121.01	126.95
2	B	603	CLA	CHA-C4D-ND	2.09	136.86	132.55
2	H	611	CLA	C3D-C4D-ND	2.09	113.38	109.99
3	J	612	XAT	C24-C23-C22	2.09	114.69	110.79
2	A	602	CLA	C3D-C4D-ND	2.09	113.38	109.99
2	B	602	CLA	C3D-C4D-ND	2.09	113.38	109.99
2	J	611	CLA	C3D-C4D-ND	2.09	113.38	109.99
2	J	602	CLA	C3D-C4D-ND	2.09	113.38	109.99
2	G	607	CLA	CHC-C1C-C2C	-2.09	121.02	126.95
3	C	612	XAT	C24-C23-C22	2.09	114.69	110.79
3	B	612	XAT	C24-C23-C22	2.08	114.69	110.79
2	J	608	CLA	C2C-C1C-NC	2.08	112.17	109.98
2	E	602	CLA	C3D-C4D-ND	2.08	113.37	109.99
2	G	603	CLA	CHA-C4D-ND	2.08	136.85	132.55
2	C	605	CLA	CHD-C1D-ND	-2.08	121.87	124.80
3	H	612	XAT	C24-C23-C22	2.08	114.69	110.79
2	F	602	CLA	C3D-C4D-ND	2.08	113.37	109.99
3	K	612	XAT	C24-C23-C22	2.08	114.69	110.79
3	A	612	XAT	C24-C23-C22	2.08	114.68	110.79
3	I	612	XAT	C24-C23-C22	2.08	114.68	110.79
2	I	602	CLA	C3D-C4D-ND	2.08	113.37	109.99
3	E	612	XAT	C24-C23-C22	2.08	114.68	110.79
2	F	611	CLA	C3D-C4D-ND	2.08	113.37	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	603	CLA	CHA-C4D-ND	2.08	136.84	132.55
3	G	612	XAT	C24-C23-C22	2.08	114.68	110.79
2	D	607	CLA	CHC-C1C-C2C	-2.08	121.04	126.95
2	A	607	CLA	CHC-C1C-C2C	-2.08	121.04	126.95
2	C	607	CLA	CHC-C1C-C2C	-2.08	121.04	126.95
2	K	607	CLA	CHC-C1C-C2C	-2.08	121.04	126.95
2	H	602	CLA	C3D-C4D-ND	2.08	113.36	109.99
2	D	603	CLA	CHA-C4D-ND	2.08	136.84	132.55
3	F	612	XAT	C24-C23-C22	2.08	114.67	110.79
2	C	602	CLA	C3D-C4D-ND	2.08	113.36	109.99
2	H	607	CLA	CHC-C1C-C2C	-2.08	121.05	126.95
2	K	602	CLA	C3D-C4D-ND	2.08	113.36	109.99
2	I	603	CLA	CHA-C4D-ND	2.07	136.83	132.55
2	F	607	CLA	CHC-C1C-C2C	-2.07	121.06	126.95
2	C	606	CLA	CHA-C4D-ND	2.07	136.82	132.55
2	I	606	CLA	CHA-C4D-ND	2.07	136.82	132.55
2	K	611	CLA	C3D-C4D-ND	2.07	113.35	109.99
2	C	607	CLA	C1D-ND-C4D	-2.07	104.86	106.31
2	B	607	CLA	CHC-C1C-C2C	-2.07	121.06	126.95
2	E	607	CLA	CHC-C1C-C2C	-2.07	121.06	126.95
2	E	606	CLA	CHA-C4D-ND	2.07	136.82	132.55
2	F	603	CLA	CHA-C4D-ND	2.07	136.82	132.55
2	A	606	CLA	CHA-C4D-ND	2.07	136.82	132.55
2	C	608	CLA	CHB-C4A-NA	2.07	127.39	124.40
2	J	606	CLA	CHA-C4D-ND	2.07	136.81	132.55
2	D	608	CLA	CHB-C4A-NA	2.07	127.38	124.40
2	G	605	CLA	CHD-C1D-ND	-2.07	121.90	124.80
2	G	606	CLA	CHA-C4D-ND	2.07	136.81	132.55
2	K	607	CLA	C1D-ND-C4D	-2.07	104.86	106.31
2	H	606	CLA	CHA-C4D-ND	2.06	136.81	132.55
2	G	611	CLA	C3D-C4D-ND	2.06	113.34	109.99
2	J	608	CLA	CHB-C4A-NA	2.06	127.37	124.40
2	G	608	CLA	CHB-C4A-NA	2.06	127.37	124.40
2	H	608	CLA	CHB-C4A-NA	2.06	127.37	124.40
2	B	606	CLA	CHA-C4D-ND	2.06	136.80	132.55
2	K	604	CLA	CHA-C4D-ND	2.06	136.79	132.55
2	A	607	CLA	C1D-ND-C4D	-2.06	104.87	106.31
2	F	606	CLA	CHA-C4D-ND	2.05	136.79	132.55
2	A	608	CLA	CHB-C4A-NA	2.05	127.36	124.40
2	F	608	CLA	CHB-C4A-NA	2.05	127.36	124.40
2	B	608	CLA	CHB-C4A-NA	2.05	127.36	124.40
2	G	604	CLA	C3D-C4D-ND	2.05	113.32	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	604	CLA	CHA-C4D-ND	2.05	136.78	132.55
2	K	608	CLA	CHB-C4A-NA	2.05	127.36	124.40
2	E	607	CLA	C1D-ND-C4D	-2.05	104.88	106.31
2	I	608	CLA	CHB-C4A-NA	2.05	127.35	124.40
2	K	609	CLA	C2C-C1C-NC	2.05	112.13	109.98
2	C	604	CLA	CHA-C4D-ND	2.04	136.77	132.55
2	F	604	CLA	CHA-C4D-ND	2.04	136.77	132.55
2	E	604	CLA	C3D-C4D-ND	2.04	113.31	109.99
2	I	604	CLA	CHA-C4D-ND	2.04	136.76	132.55
2	E	608	CLA	CHB-C4A-NA	2.04	127.35	124.40
2	B	604	CLA	C3D-C4D-ND	2.04	113.30	109.99
2	G	604	CLA	CHA-C4D-ND	2.04	136.76	132.55
2	I	604	CLA	C3D-C4D-ND	2.04	113.30	109.99
2	D	604	CLA	C3D-C4D-ND	2.04	113.30	109.99
2	A	604	CLA	CHA-C4D-ND	2.04	136.75	132.55
2	A	604	CLA	C3D-C4D-ND	2.04	113.30	109.99
2	E	604	CLA	CHA-C4D-ND	2.03	136.75	132.55
2	H	604	CLA	CHA-C4D-ND	2.03	136.74	132.55
2	F	609	CLA	C2C-C1C-NC	2.03	112.12	109.98
2	D	607	CLA	C1D-ND-C4D	-2.03	104.89	106.31
2	H	607	CLA	C1D-ND-C4D	-2.03	104.89	106.31
2	C	604	CLA	C3D-C4D-ND	2.03	113.28	109.99
2	D	604	CLA	CHA-C4D-ND	2.03	136.73	132.55
2	K	604	CLA	C3D-C4D-ND	2.03	113.28	109.99
2	B	604	CLA	CHA-C4D-ND	2.02	136.73	132.55
2	H	609	CLA	C2C-C1C-NC	2.02	112.11	109.98
2	F	604	CLA	C3D-C4D-ND	2.02	113.27	109.99
2	F	607	CLA	C1D-ND-C4D	-2.02	104.89	106.31
2	K	611	CLA	CHA-C4D-ND	2.02	136.72	132.55
2	H	604	CLA	C3D-C4D-ND	2.02	113.27	109.99
2	G	607	CLA	C1D-ND-C4D	-2.02	104.90	106.31
2	F	611	CLA	CHA-C4D-ND	2.02	136.71	132.55
2	E	609	CLA	C2C-C1C-NC	2.02	112.10	109.98
2	I	609	CLA	C2C-C1C-NC	2.02	112.10	109.98
2	G	611	CLA	CHA-C4D-ND	2.02	136.71	132.55
2	J	604	CLA	C3D-C4D-ND	2.02	113.26	109.99
2	D	611	CLA	CHA-C4D-ND	2.02	136.71	132.55
2	G	609	CLA	C2C-C1C-NC	2.02	112.10	109.98
2	A	611	CLA	CHA-C4D-ND	2.02	136.71	132.55
2	C	611	CLA	CHA-C4D-ND	2.01	136.71	132.55
2	B	611	CLA	CHA-C4D-ND	2.01	136.70	132.55
2	E	611	CLA	CHA-C4D-ND	2.01	136.70	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	611	CLA	CHA-C4D-ND	2.01	136.70	132.55
2	H	611	CLA	CHA-C4D-ND	2.01	136.70	132.55
2	J	611	CLA	CHA-C4D-ND	2.01	136.69	132.55
2	C	609	CLA	C2C-C1C-NC	2.01	112.09	109.98
2	J	601	CLA	C3D-C4D-ND	2.01	113.25	109.99
2	B	607	CLA	C1D-ND-C4D	-2.00	104.91	106.31

All (121) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601	CLA	ND
2	A	602	CLA	ND
2	A	603	CLA	ND
2	A	604	CLA	ND
2	A	605	CLA	ND
2	A	606	CLA	ND
2	A	607	CLA	ND
2	A	608	CLA	ND
2	A	609	CLA	ND
2	A	610	CLA	ND
2	A	611	CLA	ND
2	B	601	CLA	ND
2	B	602	CLA	ND
2	B	603	CLA	ND
2	B	604	CLA	ND
2	B	605	CLA	ND
2	B	606	CLA	ND
2	B	607	CLA	ND
2	B	608	CLA	ND
2	B	609	CLA	ND
2	B	610	CLA	ND
2	B	611	CLA	ND
2	C	601	CLA	ND
2	C	602	CLA	ND
2	C	603	CLA	ND
2	C	604	CLA	ND
2	C	605	CLA	ND
2	C	606	CLA	ND
2	C	607	CLA	ND
2	C	608	CLA	ND
2	C	609	CLA	ND
2	C	610	CLA	ND

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Mol	Chain	Res	Type	Atom
2	C	611	CLA	ND
2	D	601	CLA	ND
2	D	602	CLA	ND
2	D	603	CLA	ND
2	D	604	CLA	ND
2	D	605	CLA	ND
2	D	606	CLA	ND
2	D	607	CLA	ND
2	D	608	CLA	ND
2	D	609	CLA	ND
2	D	610	CLA	ND
2	D	611	CLA	ND
2	E	601	CLA	ND
2	E	602	CLA	ND
2	E	603	CLA	ND
2	E	604	CLA	ND
2	E	605	CLA	ND
2	E	606	CLA	ND
2	E	607	CLA	ND
2	E	608	CLA	ND
2	E	609	CLA	ND
2	E	610	CLA	ND
2	E	611	CLA	ND
2	F	601	CLA	ND
2	F	602	CLA	ND
2	F	603	CLA	ND
2	F	604	CLA	ND
2	F	605	CLA	ND
2	F	606	CLA	ND
2	F	607	CLA	ND
2	F	608	CLA	ND
2	F	609	CLA	ND
2	F	610	CLA	ND
2	F	611	CLA	ND
2	G	601	CLA	ND
2	G	602	CLA	ND
2	G	603	CLA	ND
2	G	604	CLA	ND
2	G	605	CLA	ND
2	G	606	CLA	ND
2	G	607	CLA	ND
2	G	608	CLA	ND

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Mol	Chain	Res	Type	Atom
2	G	609	CLA	ND
2	G	610	CLA	ND
2	G	611	CLA	ND
2	H	601	CLA	ND
2	H	602	CLA	ND
2	H	603	CLA	ND
2	H	604	CLA	ND
2	H	605	CLA	ND
2	H	606	CLA	ND
2	H	607	CLA	ND
2	H	608	CLA	ND
2	H	609	CLA	ND
2	H	610	CLA	ND
2	H	611	CLA	ND
2	I	601	CLA	ND
2	I	602	CLA	ND
2	I	603	CLA	ND
2	I	604	CLA	ND
2	I	605	CLA	ND
2	I	606	CLA	ND
2	I	607	CLA	ND
2	I	608	CLA	ND
2	I	609	CLA	ND
2	I	610	CLA	ND
2	I	611	CLA	ND
2	J	601	CLA	ND
2	J	602	CLA	ND
2	J	603	CLA	ND
2	J	604	CLA	ND
2	J	605	CLA	ND
2	J	606	CLA	ND
2	J	607	CLA	ND
2	J	608	CLA	ND
2	J	609	CLA	ND
2	J	610	CLA	ND
2	J	611	CLA	ND
2	K	601	CLA	ND
2	K	602	CLA	ND
2	K	603	CLA	ND
2	K	604	CLA	ND
2	K	605	CLA	ND
2	K	606	CLA	ND

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Mol	Chain	Res	Type	Atom
2	K	607	CLA	ND
2	K	608	CLA	ND
2	K	609	CLA	ND
2	K	610	CLA	ND
2	K	611	CLA	ND

All (1198) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	CLA	C1A-C2A-CAA-CBA
2	A	602	CLA	C3A-C2A-CAA-CBA
2	A	602	CLA	CHA-CBD-CGD-O1D
2	A	602	CLA	CHA-CBD-CGD-O2D
2	A	603	CLA	CHA-CBD-CGD-O2D
2	A	605	CLA	C1A-C2A-CAA-CBA
2	A	606	CLA	C1A-C2A-CAA-CBA
2	A	610	CLA	C11-C12-C13-C15
2	B	602	CLA	C1A-C2A-CAA-CBA
2	B	602	CLA	C3A-C2A-CAA-CBA
2	B	602	CLA	CHA-CBD-CGD-O1D
2	B	602	CLA	CHA-CBD-CGD-O2D
2	B	603	CLA	CHA-CBD-CGD-O2D
2	B	605	CLA	C1A-C2A-CAA-CBA
2	B	606	CLA	C1A-C2A-CAA-CBA
2	B	610	CLA	C11-C12-C13-C15
2	C	602	CLA	C1A-C2A-CAA-CBA
2	C	602	CLA	C3A-C2A-CAA-CBA
2	C	602	CLA	CHA-CBD-CGD-O1D
2	C	602	CLA	CHA-CBD-CGD-O2D
2	C	603	CLA	CHA-CBD-CGD-O2D
2	C	605	CLA	C1A-C2A-CAA-CBA
2	C	606	CLA	C1A-C2A-CAA-CBA
2	C	610	CLA	C11-C12-C13-C15
2	D	602	CLA	C1A-C2A-CAA-CBA
2	D	602	CLA	C3A-C2A-CAA-CBA
2	D	602	CLA	CHA-CBD-CGD-O1D
2	D	602	CLA	CHA-CBD-CGD-O2D
2	D	603	CLA	CHA-CBD-CGD-O2D
2	D	605	CLA	C1A-C2A-CAA-CBA
2	D	606	CLA	C1A-C2A-CAA-CBA
2	D	610	CLA	C11-C12-C13-C15
2	E	602	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
2	E	602	CLA	C3A-C2A-CAA-CBA
2	E	602	CLA	CHA-CBD-CGD-O1D
2	E	602	CLA	CHA-CBD-CGD-O2D
2	E	603	CLA	CHA-CBD-CGD-O2D
2	E	605	CLA	C1A-C2A-CAA-CBA
2	E	606	CLA	C1A-C2A-CAA-CBA
2	E	610	CLA	C11-C12-C13-C15
2	F	602	CLA	C1A-C2A-CAA-CBA
2	F	602	CLA	C3A-C2A-CAA-CBA
2	F	602	CLA	CHA-CBD-CGD-O1D
2	F	602	CLA	CHA-CBD-CGD-O2D
2	F	603	CLA	CHA-CBD-CGD-O2D
2	F	605	CLA	C1A-C2A-CAA-CBA
2	F	606	CLA	C1A-C2A-CAA-CBA
2	F	610	CLA	C11-C12-C13-C15
2	G	602	CLA	C1A-C2A-CAA-CBA
2	G	602	CLA	C3A-C2A-CAA-CBA
2	G	602	CLA	CHA-CBD-CGD-O1D
2	G	602	CLA	CHA-CBD-CGD-O2D
2	G	603	CLA	CHA-CBD-CGD-O2D
2	G	605	CLA	C1A-C2A-CAA-CBA
2	G	606	CLA	C1A-C2A-CAA-CBA
2	G	610	CLA	C11-C12-C13-C15
2	H	602	CLA	C1A-C2A-CAA-CBA
2	H	602	CLA	C3A-C2A-CAA-CBA
2	H	602	CLA	CHA-CBD-CGD-O1D
2	H	602	CLA	CHA-CBD-CGD-O2D
2	H	603	CLA	CHA-CBD-CGD-O2D
2	H	605	CLA	C1A-C2A-CAA-CBA
2	H	606	CLA	C1A-C2A-CAA-CBA
2	H	610	CLA	C11-C12-C13-C15
2	I	602	CLA	C1A-C2A-CAA-CBA
2	I	602	CLA	C3A-C2A-CAA-CBA
2	I	602	CLA	CHA-CBD-CGD-O1D
2	I	602	CLA	CHA-CBD-CGD-O2D
2	I	603	CLA	CHA-CBD-CGD-O2D
2	I	605	CLA	C1A-C2A-CAA-CBA
2	I	606	CLA	C1A-C2A-CAA-CBA
2	I	610	CLA	C11-C12-C13-C15
2	J	602	CLA	C1A-C2A-CAA-CBA
2	J	602	CLA	C3A-C2A-CAA-CBA
2	J	602	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
2	J	602	CLA	CHA-CBD-CGD-O2D
2	J	603	CLA	CHA-CBD-CGD-O2D
2	J	605	CLA	C1A-C2A-CAA-CBA
2	J	606	CLA	C1A-C2A-CAA-CBA
2	J	610	CLA	C11-C12-C13-C15
2	K	602	CLA	C1A-C2A-CAA-CBA
2	K	602	CLA	C3A-C2A-CAA-CBA
2	K	602	CLA	CHA-CBD-CGD-O1D
2	K	602	CLA	CHA-CBD-CGD-O2D
2	K	603	CLA	CHA-CBD-CGD-O2D
2	K	605	CLA	C1A-C2A-CAA-CBA
2	K	606	CLA	C1A-C2A-CAA-CBA
2	K	610	CLA	C11-C12-C13-C15
4	A	613	32N	C27-C28-C29-C34
4	B	613	32N	C27-C28-C29-C34
4	C	613	32N	C27-C28-C29-C34
4	D	613	32N	C27-C28-C29-C34
4	E	613	32N	C27-C28-C29-C34
4	F	613	32N	C27-C28-C29-C34
4	G	613	32N	C27-C28-C29-C34
4	H	613	32N	C27-C28-C29-C34
4	I	613	32N	C27-C28-C29-C34
4	J	613	32N	C27-C28-C29-C34
4	K	613	32N	C27-C28-C29-C34
2	A	603	CLA	C2C-C3C-CAC-CBC
2	B	603	CLA	C2C-C3C-CAC-CBC
2	C	603	CLA	C2C-C3C-CAC-CBC
2	D	603	CLA	C2C-C3C-CAC-CBC
2	E	603	CLA	C2C-C3C-CAC-CBC
2	F	603	CLA	C2C-C3C-CAC-CBC
2	G	603	CLA	C2C-C3C-CAC-CBC
2	H	603	CLA	C2C-C3C-CAC-CBC
2	I	603	CLA	C2C-C3C-CAC-CBC
2	J	603	CLA	C2C-C3C-CAC-CBC
2	K	603	CLA	C2C-C3C-CAC-CBC
2	A	601	CLA	C3-C5-C6-C7
2	B	601	CLA	C3-C5-C6-C7
2	C	601	CLA	C3-C5-C6-C7
2	D	601	CLA	C3-C5-C6-C7
2	E	601	CLA	C3-C5-C6-C7
2	F	601	CLA	C3-C5-C6-C7
2	G	601	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
2	H	601	CLA	C3-C5-C6-C7
2	I	601	CLA	C3-C5-C6-C7
2	J	601	CLA	C3-C5-C6-C7
2	K	601	CLA	C3-C5-C6-C7
2	A	605	CLA	C4-C3-C5-C6
2	A	606	CLA	C4-C3-C5-C6
2	B	605	CLA	C4-C3-C5-C6
2	B	606	CLA	C4-C3-C5-C6
2	C	605	CLA	C4-C3-C5-C6
2	C	606	CLA	C4-C3-C5-C6
2	D	605	CLA	C4-C3-C5-C6
2	D	606	CLA	C4-C3-C5-C6
2	E	605	CLA	C4-C3-C5-C6
2	E	606	CLA	C4-C3-C5-C6
2	F	605	CLA	C4-C3-C5-C6
2	F	606	CLA	C4-C3-C5-C6
2	G	605	CLA	C4-C3-C5-C6
2	G	606	CLA	C4-C3-C5-C6
2	H	605	CLA	C4-C3-C5-C6
2	H	606	CLA	C4-C3-C5-C6
2	I	605	CLA	C4-C3-C5-C6
2	I	606	CLA	C4-C3-C5-C6
2	J	605	CLA	C4-C3-C5-C6
2	J	606	CLA	C4-C3-C5-C6
2	K	605	CLA	C4-C3-C5-C6
2	K	606	CLA	C4-C3-C5-C6
2	A	605	CLA	C2-C3-C5-C6
2	A	606	CLA	C2-C3-C5-C6
2	B	605	CLA	C2-C3-C5-C6
2	B	606	CLA	C2-C3-C5-C6
2	C	605	CLA	C2-C3-C5-C6
2	C	606	CLA	C2-C3-C5-C6
2	D	605	CLA	C2-C3-C5-C6
2	D	606	CLA	C2-C3-C5-C6
2	E	605	CLA	C2-C3-C5-C6
2	E	606	CLA	C2-C3-C5-C6
2	F	605	CLA	C2-C3-C5-C6
2	F	606	CLA	C2-C3-C5-C6
2	G	605	CLA	C2-C3-C5-C6
2	G	606	CLA	C2-C3-C5-C6
2	H	605	CLA	C2-C3-C5-C6
2	H	606	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
2	I	605	CLA	C2-C3-C5-C6
2	I	606	CLA	C2-C3-C5-C6
2	J	605	CLA	C2-C3-C5-C6
2	J	606	CLA	C2-C3-C5-C6
2	K	605	CLA	C2-C3-C5-C6
2	K	606	CLA	C2-C3-C5-C6
2	A	605	CLA	C3-C5-C6-C7
2	B	605	CLA	C3-C5-C6-C7
2	C	605	CLA	C3-C5-C6-C7
2	D	605	CLA	C3-C5-C6-C7
2	E	605	CLA	C3-C5-C6-C7
2	F	605	CLA	C3-C5-C6-C7
2	G	605	CLA	C3-C5-C6-C7
2	H	605	CLA	C3-C5-C6-C7
2	I	605	CLA	C3-C5-C6-C7
2	J	605	CLA	C3-C5-C6-C7
2	K	605	CLA	C3-C5-C6-C7
2	A	603	CLA	C4C-C3C-CAC-CBC
2	B	603	CLA	C4C-C3C-CAC-CBC
2	C	603	CLA	C4C-C3C-CAC-CBC
2	D	603	CLA	C4C-C3C-CAC-CBC
2	E	603	CLA	C4C-C3C-CAC-CBC
2	F	603	CLA	C4C-C3C-CAC-CBC
2	H	603	CLA	C4C-C3C-CAC-CBC
2	I	603	CLA	C4C-C3C-CAC-CBC
2	J	603	CLA	C4C-C3C-CAC-CBC
2	K	603	CLA	C4C-C3C-CAC-CBC
2	G	603	CLA	C4C-C3C-CAC-CBC
2	A	606	CLA	C3-C5-C6-C7
2	B	606	CLA	C3-C5-C6-C7
2	C	606	CLA	C3-C5-C6-C7
2	D	606	CLA	C3-C5-C6-C7
2	E	606	CLA	C3-C5-C6-C7
2	F	606	CLA	C3-C5-C6-C7
2	G	606	CLA	C3-C5-C6-C7
2	H	606	CLA	C3-C5-C6-C7
2	I	606	CLA	C3-C5-C6-C7
2	J	606	CLA	C3-C5-C6-C7
2	K	606	CLA	C3-C5-C6-C7
2	A	603	CLA	CBA-CGA-O2A-C1
2	B	603	CLA	CBA-CGA-O2A-C1
2	C	603	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
2	D	603	CLA	CBA-CGA-O2A-C1
2	E	603	CLA	CBA-CGA-O2A-C1
2	F	603	CLA	CBA-CGA-O2A-C1
2	G	603	CLA	CBA-CGA-O2A-C1
2	H	603	CLA	CBA-CGA-O2A-C1
2	I	603	CLA	CBA-CGA-O2A-C1
2	J	603	CLA	CBA-CGA-O2A-C1
2	K	603	CLA	CBA-CGA-O2A-C1
2	A	601	CLA	C11-C12-C13-C14
2	A	603	CLA	C6-C7-C8-C9
2	A	607	CLA	C6-C7-C8-C9
2	B	601	CLA	C11-C12-C13-C14
2	B	603	CLA	C6-C7-C8-C9
2	B	607	CLA	C6-C7-C8-C9
2	C	601	CLA	C11-C12-C13-C14
2	C	603	CLA	C6-C7-C8-C9
2	C	607	CLA	C6-C7-C8-C9
2	D	601	CLA	C11-C12-C13-C14
2	D	603	CLA	C6-C7-C8-C9
2	D	607	CLA	C6-C7-C8-C9
2	E	601	CLA	C11-C12-C13-C14
2	E	603	CLA	C6-C7-C8-C9
2	E	607	CLA	C6-C7-C8-C9
2	F	601	CLA	C11-C12-C13-C14
2	F	603	CLA	C6-C7-C8-C9
2	F	607	CLA	C6-C7-C8-C9
2	G	601	CLA	C11-C12-C13-C14
2	G	603	CLA	C6-C7-C8-C9
2	G	607	CLA	C6-C7-C8-C9
2	H	601	CLA	C11-C12-C13-C14
2	H	603	CLA	C6-C7-C8-C9
2	H	607	CLA	C6-C7-C8-C9
2	I	601	CLA	C11-C12-C13-C14
2	I	603	CLA	C6-C7-C8-C9
2	I	607	CLA	C6-C7-C8-C9
2	J	601	CLA	C11-C12-C13-C14
2	J	603	CLA	C6-C7-C8-C9
2	J	607	CLA	C6-C7-C8-C9
2	K	601	CLA	C11-C12-C13-C14
2	K	603	CLA	C6-C7-C8-C9
2	K	607	CLA	C6-C7-C8-C9
2	A	606	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
2	B	606	CLA	C2A-CAA-CBA-CGA
2	C	606	CLA	C2A-CAA-CBA-CGA
2	D	606	CLA	C2A-CAA-CBA-CGA
2	E	606	CLA	C2A-CAA-CBA-CGA
2	F	606	CLA	C2A-CAA-CBA-CGA
2	G	606	CLA	C2A-CAA-CBA-CGA
2	H	606	CLA	C2A-CAA-CBA-CGA
2	I	606	CLA	C2A-CAA-CBA-CGA
2	J	606	CLA	C2A-CAA-CBA-CGA
2	K	606	CLA	C2A-CAA-CBA-CGA
2	A	601	CLA	C11-C10-C8-C7
2	B	601	CLA	C11-C10-C8-C7
2	C	601	CLA	C11-C10-C8-C7
2	D	601	CLA	C11-C10-C8-C7
2	E	601	CLA	C11-C10-C8-C7
2	F	601	CLA	C11-C10-C8-C7
2	G	601	CLA	C11-C10-C8-C7
2	H	601	CLA	C11-C10-C8-C7
2	I	601	CLA	C11-C10-C8-C7
2	J	601	CLA	C11-C10-C8-C7
2	K	601	CLA	C11-C10-C8-C7
2	B	607	CLA	C15-C16-C17-C18
2	H	607	CLA	C15-C16-C17-C18
2	J	607	CLA	C15-C16-C17-C18
2	B	603	CLA	O1A-CGA-O2A-C1
2	E	603	CLA	O1A-CGA-O2A-C1
2	A	607	CLA	C10-C11-C12-C13
2	A	607	CLA	C15-C16-C17-C18
2	B	607	CLA	C10-C11-C12-C13
2	C	607	CLA	C10-C11-C12-C13
2	C	607	CLA	C15-C16-C17-C18
2	D	607	CLA	C10-C11-C12-C13
2	D	607	CLA	C15-C16-C17-C18
2	E	607	CLA	C10-C11-C12-C13
2	E	607	CLA	C15-C16-C17-C18
2	F	607	CLA	C10-C11-C12-C13
2	F	607	CLA	C15-C16-C17-C18
2	G	607	CLA	C10-C11-C12-C13
2	G	607	CLA	C15-C16-C17-C18
2	H	607	CLA	C10-C11-C12-C13
2	I	607	CLA	C10-C11-C12-C13
2	I	607	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
2	J	607	CLA	C10-C11-C12-C13
2	K	607	CLA	C10-C11-C12-C13
2	K	607	CLA	C15-C16-C17-C18
2	A	603	CLA	O1A-CGA-O2A-C1
2	C	603	CLA	O1A-CGA-O2A-C1
2	D	603	CLA	O1A-CGA-O2A-C1
2	F	603	CLA	O1A-CGA-O2A-C1
2	G	603	CLA	O1A-CGA-O2A-C1
2	H	603	CLA	O1A-CGA-O2A-C1
2	I	603	CLA	O1A-CGA-O2A-C1
2	J	603	CLA	O1A-CGA-O2A-C1
2	K	603	CLA	O1A-CGA-O2A-C1
2	A	601	CLA	C5-C6-C7-C8
2	A	605	CLA	C15-C16-C17-C18
2	B	601	CLA	C5-C6-C7-C8
2	B	605	CLA	C15-C16-C17-C18
2	C	601	CLA	C5-C6-C7-C8
2	C	605	CLA	C15-C16-C17-C18
2	D	601	CLA	C5-C6-C7-C8
2	D	605	CLA	C15-C16-C17-C18
2	E	601	CLA	C5-C6-C7-C8
2	E	605	CLA	C15-C16-C17-C18
2	F	601	CLA	C5-C6-C7-C8
2	F	605	CLA	C15-C16-C17-C18
2	G	601	CLA	C5-C6-C7-C8
2	G	605	CLA	C15-C16-C17-C18
2	H	601	CLA	C5-C6-C7-C8
2	H	605	CLA	C15-C16-C17-C18
2	I	601	CLA	C5-C6-C7-C8
2	I	605	CLA	C15-C16-C17-C18
2	J	601	CLA	C5-C6-C7-C8
2	J	605	CLA	C15-C16-C17-C18
2	K	601	CLA	C5-C6-C7-C8
2	K	605	CLA	C15-C16-C17-C18
2	C	607	CLA	CBD-CGD-O2D-CED
2	A	607	CLA	CBD-CGD-O2D-CED
2	B	607	CLA	CBD-CGD-O2D-CED
2	D	607	CLA	CBD-CGD-O2D-CED
2	E	607	CLA	CBD-CGD-O2D-CED
2	K	607	CLA	CBD-CGD-O2D-CED
2	F	607	CLA	CBD-CGD-O2D-CED
2	G	607	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
2	H	607	CLA	CBD-CGD-O2D-CED
2	I	607	CLA	CBD-CGD-O2D-CED
2	J	607	CLA	CBD-CGD-O2D-CED
2	A	610	CLA	C4B-C3B-CAB-CBB
2	B	610	CLA	C4B-C3B-CAB-CBB
2	C	610	CLA	C4B-C3B-CAB-CBB
2	D	610	CLA	C4B-C3B-CAB-CBB
2	E	610	CLA	C4B-C3B-CAB-CBB
2	F	610	CLA	C4B-C3B-CAB-CBB
2	G	610	CLA	C4B-C3B-CAB-CBB
2	H	610	CLA	C4B-C3B-CAB-CBB
2	I	610	CLA	C4B-C3B-CAB-CBB
2	J	610	CLA	C4B-C3B-CAB-CBB
2	K	610	CLA	C4B-C3B-CAB-CBB
2	A	605	CLA	C3A-C2A-CAA-CBA
2	B	605	CLA	C3A-C2A-CAA-CBA
2	C	605	CLA	C3A-C2A-CAA-CBA
2	D	605	CLA	C3A-C2A-CAA-CBA
2	E	605	CLA	C3A-C2A-CAA-CBA
2	F	605	CLA	C3A-C2A-CAA-CBA
2	G	605	CLA	C3A-C2A-CAA-CBA
2	H	605	CLA	C3A-C2A-CAA-CBA
2	I	605	CLA	C3A-C2A-CAA-CBA
2	J	605	CLA	C3A-C2A-CAA-CBA
2	K	605	CLA	C3A-C2A-CAA-CBA
2	A	601	CLA	C10-C11-C12-C13
2	G	601	CLA	C10-C11-C12-C13
2	J	601	CLA	C10-C11-C12-C13
2	A	610	CLA	C2B-C3B-CAB-CBB
2	B	610	CLA	C2B-C3B-CAB-CBB
2	C	610	CLA	C2B-C3B-CAB-CBB
2	D	610	CLA	C2B-C3B-CAB-CBB
2	E	610	CLA	C2B-C3B-CAB-CBB
2	F	610	CLA	C2B-C3B-CAB-CBB
2	G	610	CLA	C2B-C3B-CAB-CBB
2	H	610	CLA	C2B-C3B-CAB-CBB
2	I	610	CLA	C2B-C3B-CAB-CBB
2	J	610	CLA	C2B-C3B-CAB-CBB
2	K	610	CLA	C2B-C3B-CAB-CBB
4	A	613	32N	C1-C2-C9-C10
4	A	613	32N	C3-C2-C9-C10
4	B	613	32N	C1-C2-C9-C10

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Mol	Chain	Res	Type	Atoms
4	B	613	32N	C3-C2-C9-C10
4	C	613	32N	C1-C2-C9-C10
4	C	613	32N	C3-C2-C9-C10
4	D	613	32N	C1-C2-C9-C10
4	D	613	32N	C3-C2-C9-C10
4	E	613	32N	C1-C2-C9-C10
4	E	613	32N	C3-C2-C9-C10
4	F	613	32N	C1-C2-C9-C10
4	F	613	32N	C3-C2-C9-C10
4	G	613	32N	C1-C2-C9-C10
4	G	613	32N	C3-C2-C9-C10
4	H	613	32N	C1-C2-C9-C10
4	H	613	32N	C3-C2-C9-C10
4	I	613	32N	C1-C2-C9-C10
4	I	613	32N	C3-C2-C9-C10
4	J	613	32N	C1-C2-C9-C10
4	J	613	32N	C3-C2-C9-C10
4	K	613	32N	C1-C2-C9-C10
4	K	613	32N	C3-C2-C9-C10
2	B	601	CLA	C10-C11-C12-C13
2	C	601	CLA	C10-C11-C12-C13
2	D	601	CLA	C10-C11-C12-C13
2	E	601	CLA	C10-C11-C12-C13
2	F	601	CLA	C10-C11-C12-C13
2	H	601	CLA	C10-C11-C12-C13
2	I	601	CLA	C10-C11-C12-C13
2	K	601	CLA	C10-C11-C12-C13
2	A	603	CLA	C2A-CAA-CBA-CGA
2	B	603	CLA	C2A-CAA-CBA-CGA
2	C	603	CLA	C2A-CAA-CBA-CGA
2	D	603	CLA	C2A-CAA-CBA-CGA
2	E	603	CLA	C2A-CAA-CBA-CGA
2	F	603	CLA	C2A-CAA-CBA-CGA
2	G	603	CLA	C2A-CAA-CBA-CGA
2	H	603	CLA	C2A-CAA-CBA-CGA
2	I	603	CLA	C2A-CAA-CBA-CGA
2	J	603	CLA	C2A-CAA-CBA-CGA
2	K	603	CLA	C2A-CAA-CBA-CGA
2	A	610	CLA	C6-C7-C8-C9
2	B	610	CLA	C6-C7-C8-C9
2	C	610	CLA	C6-C7-C8-C9
2	D	610	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	E	610	CLA	C6-C7-C8-C9
2	F	610	CLA	C6-C7-C8-C9
2	G	610	CLA	C6-C7-C8-C9
2	H	610	CLA	C6-C7-C8-C9
2	I	610	CLA	C6-C7-C8-C9
2	J	610	CLA	C6-C7-C8-C9
2	K	610	CLA	C6-C7-C8-C9
2	A	603	CLA	C3-C5-C6-C7
2	B	603	CLA	C3-C5-C6-C7
2	C	603	CLA	C3-C5-C6-C7
2	D	603	CLA	C3-C5-C6-C7
2	E	603	CLA	C3-C5-C6-C7
2	F	603	CLA	C3-C5-C6-C7
2	G	603	CLA	C3-C5-C6-C7
2	H	603	CLA	C3-C5-C6-C7
2	I	603	CLA	C3-C5-C6-C7
2	J	603	CLA	C3-C5-C6-C7
2	K	603	CLA	C3-C5-C6-C7
2	A	607	CLA	C16-C17-C18-C20
2	B	607	CLA	C16-C17-C18-C20
2	C	607	CLA	C16-C17-C18-C20
2	D	607	CLA	C16-C17-C18-C20
2	G	607	CLA	C16-C17-C18-C20
2	H	607	CLA	C16-C17-C18-C20
2	I	607	CLA	C16-C17-C18-C20
2	E	607	CLA	C16-C17-C18-C20
2	F	607	CLA	C16-C17-C18-C20
2	J	607	CLA	C16-C17-C18-C20
2	K	607	CLA	C16-C17-C18-C20
2	A	607	CLA	C11-C12-C13-C15
2	A	607	CLA	C12-C13-C15-C16
2	B	607	CLA	C11-C12-C13-C15
2	B	607	CLA	C12-C13-C15-C16
2	C	607	CLA	C11-C12-C13-C15
2	C	607	CLA	C12-C13-C15-C16
2	D	607	CLA	C11-C12-C13-C15
2	D	607	CLA	C12-C13-C15-C16
2	E	607	CLA	C11-C12-C13-C15
2	E	607	CLA	C12-C13-C15-C16
2	F	607	CLA	C11-C12-C13-C15
2	F	607	CLA	C12-C13-C15-C16
2	G	607	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
2	G	607	CLA	C12-C13-C15-C16
2	H	607	CLA	C11-C12-C13-C15
2	H	607	CLA	C12-C13-C15-C16
2	I	607	CLA	C11-C12-C13-C15
2	I	607	CLA	C12-C13-C15-C16
2	J	607	CLA	C11-C12-C13-C15
2	J	607	CLA	C12-C13-C15-C16
2	K	607	CLA	C11-C12-C13-C15
2	K	607	CLA	C12-C13-C15-C16
2	J	610	CLA	C8-C10-C11-C12
2	A	610	CLA	C8-C10-C11-C12
2	B	610	CLA	C8-C10-C11-C12
2	C	610	CLA	C8-C10-C11-C12
2	D	610	CLA	C8-C10-C11-C12
2	E	610	CLA	C8-C10-C11-C12
2	F	610	CLA	C8-C10-C11-C12
2	G	610	CLA	C8-C10-C11-C12
2	H	610	CLA	C8-C10-C11-C12
2	I	610	CLA	C8-C10-C11-C12
2	K	610	CLA	C8-C10-C11-C12
2	A	602	CLA	C11-C10-C8-C9
2	A	605	CLA	C11-C10-C8-C9
2	A	607	CLA	C14-C13-C15-C16
2	B	602	CLA	C11-C10-C8-C9
2	B	605	CLA	C11-C10-C8-C9
2	B	607	CLA	C14-C13-C15-C16
2	C	602	CLA	C11-C10-C8-C9
2	C	605	CLA	C11-C10-C8-C9
2	C	607	CLA	C14-C13-C15-C16
2	D	602	CLA	C11-C10-C8-C9
2	D	605	CLA	C11-C10-C8-C9
2	D	607	CLA	C14-C13-C15-C16
2	E	602	CLA	C11-C10-C8-C9
2	E	605	CLA	C11-C10-C8-C9
2	E	607	CLA	C14-C13-C15-C16
2	F	602	CLA	C11-C10-C8-C9
2	F	605	CLA	C11-C10-C8-C9
2	F	607	CLA	C14-C13-C15-C16
2	G	602	CLA	C11-C10-C8-C9
2	G	605	CLA	C11-C10-C8-C9
2	G	607	CLA	C14-C13-C15-C16
2	H	602	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
2	H	605	CLA	C11-C10-C8-C9
2	H	607	CLA	C14-C13-C15-C16
2	I	602	CLA	C11-C10-C8-C9
2	I	605	CLA	C11-C10-C8-C9
2	I	607	CLA	C14-C13-C15-C16
2	J	602	CLA	C11-C10-C8-C9
2	J	605	CLA	C11-C10-C8-C9
2	J	607	CLA	C14-C13-C15-C16
2	K	602	CLA	C11-C10-C8-C9
2	K	605	CLA	C11-C10-C8-C9
2	K	607	CLA	C14-C13-C15-C16
2	A	605	CLA	CBA-CGA-O2A-C1
2	B	605	CLA	CBA-CGA-O2A-C1
2	C	605	CLA	CBA-CGA-O2A-C1
2	D	605	CLA	CBA-CGA-O2A-C1
2	E	605	CLA	CBA-CGA-O2A-C1
2	F	605	CLA	CBA-CGA-O2A-C1
2	G	605	CLA	CBA-CGA-O2A-C1
2	H	605	CLA	CBA-CGA-O2A-C1
2	I	605	CLA	CBA-CGA-O2A-C1
2	J	605	CLA	CBA-CGA-O2A-C1
2	K	605	CLA	CBA-CGA-O2A-C1
2	A	610	CLA	C10-C11-C12-C13
2	B	610	CLA	C10-C11-C12-C13
2	C	610	CLA	C10-C11-C12-C13
2	D	610	CLA	C10-C11-C12-C13
2	E	610	CLA	C10-C11-C12-C13
2	F	610	CLA	C10-C11-C12-C13
2	G	610	CLA	C10-C11-C12-C13
2	H	610	CLA	C10-C11-C12-C13
2	I	610	CLA	C10-C11-C12-C13
2	J	610	CLA	C10-C11-C12-C13
2	K	610	CLA	C10-C11-C12-C13
2	C	605	CLA	O1A-CGA-O2A-C1
2	E	605	CLA	O1A-CGA-O2A-C1
2	A	605	CLA	O1A-CGA-O2A-C1
2	G	605	CLA	O1A-CGA-O2A-C1
2	H	605	CLA	O1A-CGA-O2A-C1
2	I	605	CLA	O1A-CGA-O2A-C1
2	B	605	CLA	O1A-CGA-O2A-C1
2	D	605	CLA	O1A-CGA-O2A-C1
2	J	605	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
2	K	605	CLA	O1A-CGA-O2A-C1
2	F	605	CLA	O1A-CGA-O2A-C1
2	A	607	CLA	C11-C12-C13-C14
2	B	607	CLA	C11-C12-C13-C14
2	C	607	CLA	C11-C12-C13-C14
2	D	607	CLA	C11-C12-C13-C14
2	E	607	CLA	C11-C12-C13-C14
2	F	607	CLA	C11-C12-C13-C14
2	G	607	CLA	C11-C12-C13-C14
2	H	607	CLA	C11-C12-C13-C14
2	I	607	CLA	C11-C12-C13-C14
2	J	607	CLA	C11-C12-C13-C14
2	K	607	CLA	C11-C12-C13-C14
2	A	604	CLA	C4B-C3B-CAB-CBB
2	A	611	CLA	C4B-C3B-CAB-CBB
2	B	604	CLA	C4B-C3B-CAB-CBB
2	B	611	CLA	C4B-C3B-CAB-CBB
2	C	604	CLA	C4B-C3B-CAB-CBB
2	C	611	CLA	C4B-C3B-CAB-CBB
2	D	604	CLA	C4B-C3B-CAB-CBB
2	D	611	CLA	C4B-C3B-CAB-CBB
2	E	604	CLA	C4B-C3B-CAB-CBB
2	E	611	CLA	C4B-C3B-CAB-CBB
2	F	604	CLA	C4B-C3B-CAB-CBB
2	F	611	CLA	C4B-C3B-CAB-CBB
2	G	604	CLA	C4B-C3B-CAB-CBB
2	G	611	CLA	C4B-C3B-CAB-CBB
2	H	604	CLA	C4B-C3B-CAB-CBB
2	H	611	CLA	C4B-C3B-CAB-CBB
2	I	604	CLA	C4B-C3B-CAB-CBB
2	I	611	CLA	C4B-C3B-CAB-CBB
2	J	604	CLA	C4B-C3B-CAB-CBB
2	J	611	CLA	C4B-C3B-CAB-CBB
2	K	604	CLA	C4B-C3B-CAB-CBB
2	K	611	CLA	C4B-C3B-CAB-CBB
2	A	602	CLA	C11-C10-C8-C7
2	A	605	CLA	C11-C10-C8-C7
2	B	602	CLA	C11-C10-C8-C7
2	B	605	CLA	C11-C10-C8-C7
2	C	602	CLA	C11-C10-C8-C7
2	C	605	CLA	C11-C10-C8-C7
2	D	602	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
2	D	605	CLA	C11-C10-C8-C7
2	E	602	CLA	C11-C10-C8-C7
2	E	605	CLA	C11-C10-C8-C7
2	F	602	CLA	C11-C10-C8-C7
2	F	605	CLA	C11-C10-C8-C7
2	G	602	CLA	C11-C10-C8-C7
2	G	605	CLA	C11-C10-C8-C7
2	H	602	CLA	C11-C10-C8-C7
2	H	605	CLA	C11-C10-C8-C7
2	I	602	CLA	C11-C10-C8-C7
2	I	605	CLA	C11-C10-C8-C7
2	J	602	CLA	C11-C10-C8-C7
2	J	605	CLA	C11-C10-C8-C7
2	K	602	CLA	C11-C10-C8-C7
2	K	605	CLA	C11-C10-C8-C7
2	A	606	CLA	C3A-C2A-CAA-CBA
2	B	606	CLA	C3A-C2A-CAA-CBA
2	C	606	CLA	C3A-C2A-CAA-CBA
2	D	606	CLA	C3A-C2A-CAA-CBA
2	E	606	CLA	C3A-C2A-CAA-CBA
2	F	606	CLA	C3A-C2A-CAA-CBA
2	G	606	CLA	C3A-C2A-CAA-CBA
2	H	606	CLA	C3A-C2A-CAA-CBA
2	I	606	CLA	C3A-C2A-CAA-CBA
2	J	606	CLA	C3A-C2A-CAA-CBA
2	K	606	CLA	C3A-C2A-CAA-CBA
2	A	611	CLA	C2A-CAA-CBA-CGA
2	B	611	CLA	C2A-CAA-CBA-CGA
2	C	611	CLA	C2A-CAA-CBA-CGA
2	D	611	CLA	C2A-CAA-CBA-CGA
2	E	611	CLA	C2A-CAA-CBA-CGA
2	F	611	CLA	C2A-CAA-CBA-CGA
2	G	611	CLA	C2A-CAA-CBA-CGA
2	H	611	CLA	C2A-CAA-CBA-CGA
2	I	611	CLA	C2A-CAA-CBA-CGA
2	J	611	CLA	C2A-CAA-CBA-CGA
2	K	611	CLA	C2A-CAA-CBA-CGA
2	E	607	CLA	O1D-CGD-O2D-CED
2	A	611	CLA	C11-C10-C8-C9
2	B	611	CLA	C11-C10-C8-C9
2	C	611	CLA	C11-C10-C8-C9
2	D	611	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
2	E	611	CLA	C11-C10-C8-C9
2	F	611	CLA	C11-C10-C8-C9
2	G	611	CLA	C11-C10-C8-C9
2	H	611	CLA	C11-C10-C8-C9
2	I	611	CLA	C11-C10-C8-C9
2	J	611	CLA	C11-C10-C8-C9
2	K	611	CLA	C11-C10-C8-C9
2	A	607	CLA	O1D-CGD-O2D-CED
2	B	607	CLA	O1D-CGD-O2D-CED
2	C	607	CLA	O1D-CGD-O2D-CED
2	F	607	CLA	O1D-CGD-O2D-CED
2	I	607	CLA	O1D-CGD-O2D-CED
2	J	607	CLA	O1D-CGD-O2D-CED
2	K	607	CLA	O1D-CGD-O2D-CED
2	D	607	CLA	O1D-CGD-O2D-CED
2	H	607	CLA	O1D-CGD-O2D-CED
2	G	607	CLA	O1D-CGD-O2D-CED
2	A	611	CLA	C11-C10-C8-C7
2	B	611	CLA	C11-C10-C8-C7
2	C	611	CLA	C11-C10-C8-C7
2	D	611	CLA	C11-C10-C8-C7
2	F	611	CLA	C11-C10-C8-C7
2	G	611	CLA	C11-C10-C8-C7
2	H	611	CLA	C11-C10-C8-C7
2	J	611	CLA	C11-C10-C8-C7
2	K	611	CLA	C11-C10-C8-C7
2	A	601	CLA	C4-C3-C5-C6
2	B	601	CLA	C4-C3-C5-C6
2	C	601	CLA	C4-C3-C5-C6
2	D	601	CLA	C4-C3-C5-C6
2	E	601	CLA	C4-C3-C5-C6
2	F	601	CLA	C4-C3-C5-C6
2	G	601	CLA	C4-C3-C5-C6
2	H	601	CLA	C4-C3-C5-C6
2	I	601	CLA	C4-C3-C5-C6
2	J	601	CLA	C4-C3-C5-C6
2	K	601	CLA	C4-C3-C5-C6
2	A	601	CLA	C2-C3-C5-C6
2	B	601	CLA	C2-C3-C5-C6
2	C	601	CLA	C2-C3-C5-C6
2	D	601	CLA	C2-C3-C5-C6
2	E	601	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
2	F	601	CLA	C2-C3-C5-C6
2	G	601	CLA	C2-C3-C5-C6
2	H	601	CLA	C2-C3-C5-C6
2	I	601	CLA	C2-C3-C5-C6
2	J	601	CLA	C2-C3-C5-C6
2	K	601	CLA	C2-C3-C5-C6
2	A	601	CLA	C6-C7-C8-C9
2	B	601	CLA	C6-C7-C8-C9
2	C	601	CLA	C6-C7-C8-C9
2	D	601	CLA	C6-C7-C8-C9
2	E	601	CLA	C6-C7-C8-C9
2	F	601	CLA	C6-C7-C8-C9
2	G	601	CLA	C6-C7-C8-C9
2	H	601	CLA	C6-C7-C8-C9
2	I	601	CLA	C6-C7-C8-C9
2	J	601	CLA	C6-C7-C8-C9
2	K	601	CLA	C6-C7-C8-C9
2	A	609	CLA	C3-C5-C6-C7
2	B	609	CLA	C3-C5-C6-C7
2	C	609	CLA	C3-C5-C6-C7
2	D	609	CLA	C3-C5-C6-C7
2	E	609	CLA	C3-C5-C6-C7
2	F	609	CLA	C3-C5-C6-C7
2	G	609	CLA	C3-C5-C6-C7
2	H	609	CLA	C3-C5-C6-C7
2	I	609	CLA	C3-C5-C6-C7
2	J	609	CLA	C3-C5-C6-C7
2	K	609	CLA	C3-C5-C6-C7
2	A	605	CLA	C16-C17-C18-C19
2	B	605	CLA	C16-C17-C18-C19
2	C	605	CLA	C16-C17-C18-C19
2	D	605	CLA	C16-C17-C18-C19
2	E	605	CLA	C16-C17-C18-C19
2	F	605	CLA	C16-C17-C18-C19
2	G	605	CLA	C16-C17-C18-C19
2	H	605	CLA	C16-C17-C18-C19
2	I	605	CLA	C16-C17-C18-C19
2	J	605	CLA	C16-C17-C18-C19
2	K	605	CLA	C16-C17-C18-C19
2	A	607	CLA	C16-C17-C18-C19
2	B	607	CLA	C16-C17-C18-C19
2	C	607	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
2	D	607	CLA	C16-C17-C18-C19
2	E	607	CLA	C16-C17-C18-C19
2	F	607	CLA	C16-C17-C18-C19
2	G	607	CLA	C16-C17-C18-C19
2	H	607	CLA	C16-C17-C18-C19
2	I	607	CLA	C16-C17-C18-C19
2	J	607	CLA	C16-C17-C18-C19
2	K	607	CLA	C16-C17-C18-C19
2	A	601	CLA	C6-C7-C8-C10
2	A	601	CLA	C11-C12-C13-C15
2	A	610	CLA	C11-C10-C8-C7
2	B	601	CLA	C6-C7-C8-C10
2	B	601	CLA	C11-C12-C13-C15
2	B	610	CLA	C11-C10-C8-C7
2	C	601	CLA	C6-C7-C8-C10
2	C	601	CLA	C11-C12-C13-C15
2	C	610	CLA	C11-C10-C8-C7
2	D	601	CLA	C6-C7-C8-C10
2	D	601	CLA	C11-C12-C13-C15
2	D	610	CLA	C11-C10-C8-C7
2	E	601	CLA	C6-C7-C8-C10
2	E	601	CLA	C11-C12-C13-C15
2	E	610	CLA	C11-C10-C8-C7
2	F	601	CLA	C6-C7-C8-C10
2	F	601	CLA	C11-C12-C13-C15
2	F	610	CLA	C11-C10-C8-C7
2	G	601	CLA	C6-C7-C8-C10
2	G	601	CLA	C11-C12-C13-C15
2	G	610	CLA	C11-C10-C8-C7
2	H	601	CLA	C6-C7-C8-C10
2	H	601	CLA	C11-C12-C13-C15
2	H	610	CLA	C11-C10-C8-C7
2	I	601	CLA	C6-C7-C8-C10
2	I	601	CLA	C11-C12-C13-C15
2	I	610	CLA	C11-C10-C8-C7
2	J	601	CLA	C6-C7-C8-C10
2	J	601	CLA	C11-C12-C13-C15
2	J	610	CLA	C11-C10-C8-C7
2	K	601	CLA	C6-C7-C8-C10
2	K	601	CLA	C11-C12-C13-C15
2	K	610	CLA	C11-C10-C8-C7
2	A	610	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
2	B	610	CLA	C2A-CAA-CBA-CGA
2	C	610	CLA	C2A-CAA-CBA-CGA
2	D	610	CLA	C2A-CAA-CBA-CGA
2	E	610	CLA	C2A-CAA-CBA-CGA
2	F	610	CLA	C2A-CAA-CBA-CGA
2	G	610	CLA	C2A-CAA-CBA-CGA
2	H	610	CLA	C2A-CAA-CBA-CGA
2	I	610	CLA	C2A-CAA-CBA-CGA
2	J	610	CLA	C2A-CAA-CBA-CGA
2	K	610	CLA	C2A-CAA-CBA-CGA
2	A	604	CLA	C4-C3-C5-C6
2	B	604	CLA	C4-C3-C5-C6
2	C	604	CLA	C4-C3-C5-C6
2	D	604	CLA	C4-C3-C5-C6
2	E	604	CLA	C4-C3-C5-C6
2	F	604	CLA	C4-C3-C5-C6
2	G	604	CLA	C4-C3-C5-C6
2	H	604	CLA	C4-C3-C5-C6
2	J	604	CLA	C4-C3-C5-C6
2	K	604	CLA	C4-C3-C5-C6
2	I	604	CLA	C4-C3-C5-C6
2	A	603	CLA	C5-C6-C7-C8
2	B	603	CLA	C5-C6-C7-C8
2	C	603	CLA	C5-C6-C7-C8
2	D	603	CLA	C5-C6-C7-C8
2	E	603	CLA	C5-C6-C7-C8
2	F	603	CLA	C5-C6-C7-C8
2	G	603	CLA	C5-C6-C7-C8
2	H	603	CLA	C5-C6-C7-C8
2	I	603	CLA	C5-C6-C7-C8
2	J	603	CLA	C5-C6-C7-C8
2	K	603	CLA	C5-C6-C7-C8
2	A	608	CLA	C4B-C3B-CAB-CBB
2	B	608	CLA	C4B-C3B-CAB-CBB
2	C	608	CLA	C4B-C3B-CAB-CBB
2	D	608	CLA	C4B-C3B-CAB-CBB
2	E	608	CLA	C4B-C3B-CAB-CBB
2	F	608	CLA	C4B-C3B-CAB-CBB
2	G	608	CLA	C4B-C3B-CAB-CBB
2	H	608	CLA	C4B-C3B-CAB-CBB
2	I	608	CLA	C4B-C3B-CAB-CBB
2	J	608	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
2	K	608	CLA	C4B-C3B-CAB-CBB
2	A	610	CLA	C11-C10-C8-C9
2	B	610	CLA	C11-C10-C8-C9
2	C	610	CLA	C11-C10-C8-C9
2	D	610	CLA	C11-C10-C8-C9
2	E	610	CLA	C11-C10-C8-C9
2	F	610	CLA	C11-C10-C8-C9
2	G	610	CLA	C11-C10-C8-C9
2	H	610	CLA	C11-C10-C8-C9
2	I	610	CLA	C11-C10-C8-C9
2	J	610	CLA	C11-C10-C8-C9
2	K	610	CLA	C11-C10-C8-C9
2	A	603	CLA	CHA-CBD-CGD-O1D
2	B	603	CLA	CHA-CBD-CGD-O1D
2	C	603	CLA	CHA-CBD-CGD-O1D
2	D	603	CLA	CHA-CBD-CGD-O1D
2	E	603	CLA	CHA-CBD-CGD-O1D
2	F	603	CLA	CHA-CBD-CGD-O1D
2	G	603	CLA	CHA-CBD-CGD-O1D
2	H	603	CLA	CHA-CBD-CGD-O1D
2	I	603	CLA	CHA-CBD-CGD-O1D
2	J	603	CLA	CHA-CBD-CGD-O1D
2	K	603	CLA	CHA-CBD-CGD-O1D
2	A	611	CLA	C4-C3-C5-C6
2	B	611	CLA	C4-C3-C5-C6
2	C	611	CLA	C4-C3-C5-C6
2	D	611	CLA	C4-C3-C5-C6
2	E	611	CLA	C4-C3-C5-C6
2	F	611	CLA	C4-C3-C5-C6
2	G	611	CLA	C4-C3-C5-C6
2	H	611	CLA	C4-C3-C5-C6
2	I	611	CLA	C4-C3-C5-C6
2	J	611	CLA	C4-C3-C5-C6
2	K	611	CLA	C4-C3-C5-C6
2	A	604	CLA	C2B-C3B-CAB-CBB
2	B	604	CLA	C2B-C3B-CAB-CBB
2	C	604	CLA	C2B-C3B-CAB-CBB
2	D	604	CLA	C2B-C3B-CAB-CBB
2	E	604	CLA	C2B-C3B-CAB-CBB
2	F	604	CLA	C2B-C3B-CAB-CBB
2	G	604	CLA	C2B-C3B-CAB-CBB
2	H	604	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
2	I	604	CLA	C2B-C3B-CAB-CBB
2	J	604	CLA	C2B-C3B-CAB-CBB
2	K	604	CLA	C2B-C3B-CAB-CBB
2	E	611	CLA	C11-C10-C8-C7
2	I	611	CLA	C11-C10-C8-C7
2	A	604	CLA	C2-C3-C5-C6
2	B	604	CLA	C2-C3-C5-C6
2	C	604	CLA	C2-C3-C5-C6
2	D	604	CLA	C2-C3-C5-C6
2	E	604	CLA	C2-C3-C5-C6
2	F	604	CLA	C2-C3-C5-C6
2	G	604	CLA	C2-C3-C5-C6
2	H	604	CLA	C2-C3-C5-C6
2	I	604	CLA	C2-C3-C5-C6
2	J	604	CLA	C2-C3-C5-C6
2	K	604	CLA	C2-C3-C5-C6
2	A	605	CLA	C16-C17-C18-C20
2	B	605	CLA	C16-C17-C18-C20
2	C	605	CLA	C16-C17-C18-C20
2	D	605	CLA	C16-C17-C18-C20
2	E	605	CLA	C16-C17-C18-C20
2	F	605	CLA	C16-C17-C18-C20
2	G	605	CLA	C16-C17-C18-C20
2	H	605	CLA	C16-C17-C18-C20
2	I	605	CLA	C16-C17-C18-C20
2	J	605	CLA	C16-C17-C18-C20
2	K	605	CLA	C16-C17-C18-C20
2	A	601	CLA	C11-C10-C8-C9
2	A	602	CLA	C14-C13-C15-C16
2	B	601	CLA	C11-C10-C8-C9
2	B	602	CLA	C14-C13-C15-C16
2	C	601	CLA	C11-C10-C8-C9
2	C	602	CLA	C14-C13-C15-C16
2	D	601	CLA	C11-C10-C8-C9
2	D	602	CLA	C14-C13-C15-C16
2	E	601	CLA	C11-C10-C8-C9
2	E	602	CLA	C14-C13-C15-C16
2	F	601	CLA	C11-C10-C8-C9
2	F	602	CLA	C14-C13-C15-C16
2	G	601	CLA	C11-C10-C8-C9
2	G	602	CLA	C14-C13-C15-C16
2	H	601	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
2	H	602	CLA	C14-C13-C15-C16
2	I	601	CLA	C11-C10-C8-C9
2	I	602	CLA	C14-C13-C15-C16
2	J	601	CLA	C11-C10-C8-C9
2	J	602	CLA	C14-C13-C15-C16
2	K	601	CLA	C11-C10-C8-C9
2	K	602	CLA	C14-C13-C15-C16
2	A	602	CLA	C2A-CAA-CBA-CGA
2	A	609	CLA	C2A-CAA-CBA-CGA
2	B	602	CLA	C2A-CAA-CBA-CGA
2	B	609	CLA	C2A-CAA-CBA-CGA
2	C	602	CLA	C2A-CAA-CBA-CGA
2	C	609	CLA	C2A-CAA-CBA-CGA
2	D	602	CLA	C2A-CAA-CBA-CGA
2	D	609	CLA	C2A-CAA-CBA-CGA
2	E	602	CLA	C2A-CAA-CBA-CGA
2	E	609	CLA	C2A-CAA-CBA-CGA
2	F	602	CLA	C2A-CAA-CBA-CGA
2	F	609	CLA	C2A-CAA-CBA-CGA
2	G	602	CLA	C2A-CAA-CBA-CGA
2	G	609	CLA	C2A-CAA-CBA-CGA
2	H	602	CLA	C2A-CAA-CBA-CGA
2	H	609	CLA	C2A-CAA-CBA-CGA
2	I	602	CLA	C2A-CAA-CBA-CGA
2	I	609	CLA	C2A-CAA-CBA-CGA
2	J	602	CLA	C2A-CAA-CBA-CGA
2	J	609	CLA	C2A-CAA-CBA-CGA
2	K	602	CLA	C2A-CAA-CBA-CGA
2	K	609	CLA	C2A-CAA-CBA-CGA
2	A	605	CLA	C4B-C3B-CAB-CBB
2	B	605	CLA	C4B-C3B-CAB-CBB
2	C	605	CLA	C4B-C3B-CAB-CBB
2	D	605	CLA	C4B-C3B-CAB-CBB
2	E	605	CLA	C4B-C3B-CAB-CBB
2	F	605	CLA	C4B-C3B-CAB-CBB
2	G	605	CLA	C4B-C3B-CAB-CBB
2	H	605	CLA	C4B-C3B-CAB-CBB
2	I	605	CLA	C4B-C3B-CAB-CBB
2	J	605	CLA	C4B-C3B-CAB-CBB
2	K	605	CLA	C4B-C3B-CAB-CBB
2	A	601	CLA	C3A-C2A-CAA-CBA
2	B	601	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
2	C	601	CLA	C3A-C2A-CAA-CBA
2	D	601	CLA	C3A-C2A-CAA-CBA
2	E	601	CLA	C3A-C2A-CAA-CBA
2	F	601	CLA	C3A-C2A-CAA-CBA
2	G	601	CLA	C3A-C2A-CAA-CBA
2	H	601	CLA	C3A-C2A-CAA-CBA
2	I	601	CLA	C3A-C2A-CAA-CBA
2	J	601	CLA	C3A-C2A-CAA-CBA
2	K	601	CLA	C3A-C2A-CAA-CBA
2	B	601	CLA	C15-C16-C17-C18
2	C	601	CLA	C15-C16-C17-C18
2	D	601	CLA	C15-C16-C17-C18
2	F	601	CLA	C15-C16-C17-C18
2	J	601	CLA	C15-C16-C17-C18
2	K	601	CLA	C15-C16-C17-C18
2	A	611	CLA	C2-C3-C5-C6
2	B	611	CLA	C2-C3-C5-C6
2	C	611	CLA	C2-C3-C5-C6
2	D	611	CLA	C2-C3-C5-C6
2	E	611	CLA	C2-C3-C5-C6
2	F	611	CLA	C2-C3-C5-C6
2	G	611	CLA	C2-C3-C5-C6
2	H	611	CLA	C2-C3-C5-C6
2	I	611	CLA	C2-C3-C5-C6
2	J	611	CLA	C2-C3-C5-C6
2	K	611	CLA	C2-C3-C5-C6
2	A	601	CLA	C15-C16-C17-C18
2	E	601	CLA	C15-C16-C17-C18
2	G	601	CLA	C15-C16-C17-C18
2	H	601	CLA	C15-C16-C17-C18
2	I	601	CLA	C15-C16-C17-C18
2	B	609	CLA	C5-C6-C7-C8
2	F	609	CLA	C5-C6-C7-C8
2	J	609	CLA	C5-C6-C7-C8
2	A	609	CLA	C5-C6-C7-C8
2	C	609	CLA	C5-C6-C7-C8
2	D	609	CLA	C5-C6-C7-C8
2	E	609	CLA	C5-C6-C7-C8
2	G	609	CLA	C5-C6-C7-C8
2	H	609	CLA	C5-C6-C7-C8
2	I	609	CLA	C5-C6-C7-C8
2	K	609	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	A	605	CLA	C11-C12-C13-C14
2	B	605	CLA	C11-C12-C13-C14
2	C	605	CLA	C11-C12-C13-C14
2	D	605	CLA	C11-C12-C13-C14
2	E	605	CLA	C11-C12-C13-C14
2	F	605	CLA	C11-C12-C13-C14
2	G	605	CLA	C11-C12-C13-C14
2	H	605	CLA	C11-C12-C13-C14
2	I	605	CLA	C11-C12-C13-C14
2	J	605	CLA	C11-C12-C13-C14
2	K	605	CLA	C11-C12-C13-C14
2	A	605	CLA	C2B-C3B-CAB-CBB
2	A	608	CLA	C2B-C3B-CAB-CBB
2	B	605	CLA	C2B-C3B-CAB-CBB
2	B	608	CLA	C2B-C3B-CAB-CBB
2	C	605	CLA	C2B-C3B-CAB-CBB
2	C	608	CLA	C2B-C3B-CAB-CBB
2	D	605	CLA	C2B-C3B-CAB-CBB
2	D	608	CLA	C2B-C3B-CAB-CBB
2	E	605	CLA	C2B-C3B-CAB-CBB
2	E	608	CLA	C2B-C3B-CAB-CBB
2	F	605	CLA	C2B-C3B-CAB-CBB
2	F	608	CLA	C2B-C3B-CAB-CBB
2	G	605	CLA	C2B-C3B-CAB-CBB
2	G	608	CLA	C2B-C3B-CAB-CBB
2	H	605	CLA	C2B-C3B-CAB-CBB
2	H	608	CLA	C2B-C3B-CAB-CBB
2	I	605	CLA	C2B-C3B-CAB-CBB
2	I	608	CLA	C2B-C3B-CAB-CBB
2	J	605	CLA	C2B-C3B-CAB-CBB
2	J	608	CLA	C2B-C3B-CAB-CBB
2	K	605	CLA	C2B-C3B-CAB-CBB
2	K	608	CLA	C2B-C3B-CAB-CBB
2	A	606	CLA	C12-C13-C15-C16
2	A	608	CLA	C6-C7-C8-C10
2	B	606	CLA	C12-C13-C15-C16
2	B	608	CLA	C6-C7-C8-C10
2	C	606	CLA	C12-C13-C15-C16
2	C	608	CLA	C6-C7-C8-C10
2	D	606	CLA	C12-C13-C15-C16
2	D	608	CLA	C6-C7-C8-C10
2	E	606	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
2	E	608	CLA	C6-C7-C8-C10
2	F	606	CLA	C12-C13-C15-C16
2	F	608	CLA	C6-C7-C8-C10
2	G	606	CLA	C12-C13-C15-C16
2	G	608	CLA	C6-C7-C8-C10
2	H	606	CLA	C12-C13-C15-C16
2	H	608	CLA	C6-C7-C8-C10
2	I	606	CLA	C12-C13-C15-C16
2	I	608	CLA	C6-C7-C8-C10
2	J	606	CLA	C12-C13-C15-C16
2	J	608	CLA	C6-C7-C8-C10
2	K	606	CLA	C12-C13-C15-C16
2	K	608	CLA	C6-C7-C8-C10
2	A	605	CLA	C5-C6-C7-C8
2	B	605	CLA	C5-C6-C7-C8
2	C	605	CLA	C5-C6-C7-C8
2	D	605	CLA	C5-C6-C7-C8
2	E	605	CLA	C5-C6-C7-C8
2	F	605	CLA	C5-C6-C7-C8
2	G	605	CLA	C5-C6-C7-C8
2	H	605	CLA	C5-C6-C7-C8
2	I	605	CLA	C5-C6-C7-C8
2	J	605	CLA	C5-C6-C7-C8
2	K	605	CLA	C5-C6-C7-C8
2	A	603	CLA	C11-C10-C8-C9
2	B	603	CLA	C11-C10-C8-C9
2	C	603	CLA	C11-C10-C8-C9
2	D	603	CLA	C11-C10-C8-C9
2	E	603	CLA	C11-C10-C8-C9
2	F	603	CLA	C11-C10-C8-C9
2	G	603	CLA	C11-C10-C8-C9
2	H	603	CLA	C11-C10-C8-C9
2	I	603	CLA	C11-C10-C8-C9
2	J	603	CLA	C11-C10-C8-C9
2	K	603	CLA	C11-C10-C8-C9
2	A	604	CLA	C11-C12-C13-C14
2	A	610	CLA	C11-C12-C13-C14
2	B	604	CLA	C11-C12-C13-C14
2	B	610	CLA	C11-C12-C13-C14
2	C	604	CLA	C11-C12-C13-C14
2	C	610	CLA	C11-C12-C13-C14
2	D	604	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
2	D	610	CLA	C11-C12-C13-C14
2	E	604	CLA	C11-C12-C13-C14
2	E	610	CLA	C11-C12-C13-C14
2	F	604	CLA	C11-C12-C13-C14
2	F	610	CLA	C11-C12-C13-C14
2	G	604	CLA	C11-C12-C13-C14
2	G	610	CLA	C11-C12-C13-C14
2	H	604	CLA	C11-C12-C13-C14
2	H	610	CLA	C11-C12-C13-C14
2	I	604	CLA	C11-C12-C13-C14
2	I	610	CLA	C11-C12-C13-C14
2	J	604	CLA	C11-C12-C13-C14
2	J	610	CLA	C11-C12-C13-C14
2	K	604	CLA	C11-C12-C13-C14
2	K	610	CLA	C11-C12-C13-C14
2	A	608	CLA	C3A-C2A-CAA-CBA
2	B	608	CLA	C3A-C2A-CAA-CBA
2	C	608	CLA	C3A-C2A-CAA-CBA
2	D	608	CLA	C3A-C2A-CAA-CBA
2	E	608	CLA	C3A-C2A-CAA-CBA
2	F	608	CLA	C3A-C2A-CAA-CBA
2	G	608	CLA	C3A-C2A-CAA-CBA
2	H	608	CLA	C3A-C2A-CAA-CBA
2	I	608	CLA	C3A-C2A-CAA-CBA
2	J	608	CLA	C3A-C2A-CAA-CBA
2	K	608	CLA	C3A-C2A-CAA-CBA
2	A	607	CLA	CAA-CBA-CGA-O2A
2	G	607	CLA	CAA-CBA-CGA-O2A
2	I	607	CLA	CAA-CBA-CGA-O2A
2	K	607	CLA	CAA-CBA-CGA-O2A
2	C	607	CLA	CAA-CBA-CGA-O2A
2	B	607	CLA	CAA-CBA-CGA-O2A
2	D	607	CLA	CAA-CBA-CGA-O2A
2	E	607	CLA	CAA-CBA-CGA-O2A
2	F	607	CLA	CAA-CBA-CGA-O2A
2	H	607	CLA	CAA-CBA-CGA-O2A
2	J	607	CLA	CAA-CBA-CGA-O2A
2	C	603	CLA	C6-C7-C8-C10
2	D	603	CLA	C6-C7-C8-C10
2	E	603	CLA	C6-C7-C8-C10
2	F	603	CLA	C6-C7-C8-C10
2	G	603	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
2	I	603	CLA	C6-C7-C8-C10
2	J	603	CLA	C6-C7-C8-C10
2	A	611	CLA	C2B-C3B-CAB-CBB
2	B	611	CLA	C2B-C3B-CAB-CBB
2	C	611	CLA	C2B-C3B-CAB-CBB
2	D	611	CLA	C2B-C3B-CAB-CBB
2	E	611	CLA	C2B-C3B-CAB-CBB
2	F	611	CLA	C2B-C3B-CAB-CBB
2	G	611	CLA	C2B-C3B-CAB-CBB
2	H	611	CLA	C2B-C3B-CAB-CBB
2	I	611	CLA	C2B-C3B-CAB-CBB
2	J	611	CLA	C2B-C3B-CAB-CBB
2	K	611	CLA	C2B-C3B-CAB-CBB
2	A	604	CLA	C2A-CAA-CBA-CGA
2	B	604	CLA	C2A-CAA-CBA-CGA
2	C	604	CLA	C2A-CAA-CBA-CGA
2	D	604	CLA	C2A-CAA-CBA-CGA
2	E	604	CLA	C2A-CAA-CBA-CGA
2	F	604	CLA	C2A-CAA-CBA-CGA
2	G	604	CLA	C2A-CAA-CBA-CGA
2	H	604	CLA	C2A-CAA-CBA-CGA
2	I	604	CLA	C2A-CAA-CBA-CGA
2	J	604	CLA	C2A-CAA-CBA-CGA
2	K	604	CLA	C2A-CAA-CBA-CGA
2	A	606	CLA	CAA-CBA-CGA-O2A
2	B	606	CLA	CAA-CBA-CGA-O2A
2	C	606	CLA	CAA-CBA-CGA-O2A
2	D	606	CLA	CAA-CBA-CGA-O2A
2	E	606	CLA	CAA-CBA-CGA-O2A
2	F	606	CLA	CAA-CBA-CGA-O2A
2	G	606	CLA	CAA-CBA-CGA-O2A
2	H	606	CLA	CAA-CBA-CGA-O2A
2	I	606	CLA	CAA-CBA-CGA-O2A
2	J	606	CLA	CAA-CBA-CGA-O2A
2	K	606	CLA	CAA-CBA-CGA-O2A
2	A	607	CLA	C3-C5-C6-C7
2	B	607	CLA	C3-C5-C6-C7
2	C	607	CLA	C3-C5-C6-C7
2	D	607	CLA	C3-C5-C6-C7
2	E	607	CLA	C3-C5-C6-C7
2	F	607	CLA	C3-C5-C6-C7
2	G	607	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
2	I	607	CLA	C3-C5-C6-C7
2	J	607	CLA	C3-C5-C6-C7
2	K	607	CLA	C3-C5-C6-C7
2	A	605	CLA	CAA-CBA-CGA-O2A
2	D	605	CLA	CAA-CBA-CGA-O2A
2	E	605	CLA	CAA-CBA-CGA-O2A
2	F	605	CLA	CAA-CBA-CGA-O2A
2	G	605	CLA	CAA-CBA-CGA-O2A
2	I	605	CLA	CAA-CBA-CGA-O2A
2	J	605	CLA	CAA-CBA-CGA-O2A
2	H	607	CLA	C3-C5-C6-C7
2	B	605	CLA	CAA-CBA-CGA-O2A
2	H	605	CLA	CAA-CBA-CGA-O2A
2	K	605	CLA	CAA-CBA-CGA-O2A
2	C	605	CLA	CAA-CBA-CGA-O2A
2	A	603	CLA	C6-C7-C8-C10
2	B	603	CLA	C6-C7-C8-C10
2	B	604	CLA	C11-C10-C8-C7
2	C	604	CLA	C11-C10-C8-C7
2	E	604	CLA	C11-C10-C8-C7
2	H	603	CLA	C6-C7-C8-C10
2	H	604	CLA	C11-C10-C8-C7
2	I	604	CLA	C11-C10-C8-C7
2	J	604	CLA	C11-C10-C8-C7
2	K	603	CLA	C6-C7-C8-C10
2	K	604	CLA	C11-C10-C8-C7
2	A	607	CLA	C3A-C2A-CAA-CBA
2	B	607	CLA	C3A-C2A-CAA-CBA
2	C	607	CLA	C3A-C2A-CAA-CBA
2	D	607	CLA	C3A-C2A-CAA-CBA
2	E	607	CLA	C3A-C2A-CAA-CBA
2	F	607	CLA	C3A-C2A-CAA-CBA
2	G	607	CLA	C3A-C2A-CAA-CBA
2	H	607	CLA	C3A-C2A-CAA-CBA
2	I	607	CLA	C3A-C2A-CAA-CBA
2	J	607	CLA	C3A-C2A-CAA-CBA
2	K	607	CLA	C3A-C2A-CAA-CBA
2	A	606	CLA	C14-C13-C15-C16
2	B	606	CLA	C14-C13-C15-C16
2	C	606	CLA	C14-C13-C15-C16
2	D	606	CLA	C14-C13-C15-C16
2	E	606	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
2	F	606	CLA	C14-C13-C15-C16
2	G	606	CLA	C14-C13-C15-C16
2	H	606	CLA	C14-C13-C15-C16
2	I	606	CLA	C14-C13-C15-C16
2	J	606	CLA	C14-C13-C15-C16
2	K	606	CLA	C14-C13-C15-C16
2	G	606	CLA	CAA-CBA-CGA-O1A
2	A	606	CLA	CAA-CBA-CGA-O1A
2	B	606	CLA	CAA-CBA-CGA-O1A
2	C	606	CLA	CAA-CBA-CGA-O1A
2	D	606	CLA	CAA-CBA-CGA-O1A
2	E	606	CLA	CAA-CBA-CGA-O1A
2	F	606	CLA	CAA-CBA-CGA-O1A
2	H	606	CLA	CAA-CBA-CGA-O1A
2	I	606	CLA	CAA-CBA-CGA-O1A
2	J	606	CLA	CAA-CBA-CGA-O1A
2	K	606	CLA	CAA-CBA-CGA-O1A
2	A	610	CLA	CAA-CBA-CGA-O2A
2	B	610	CLA	CAA-CBA-CGA-O2A
2	C	610	CLA	CAA-CBA-CGA-O2A
2	D	610	CLA	CAA-CBA-CGA-O2A
2	E	610	CLA	CAA-CBA-CGA-O2A
2	F	610	CLA	CAA-CBA-CGA-O2A
2	G	610	CLA	CAA-CBA-CGA-O2A
2	I	610	CLA	CAA-CBA-CGA-O2A
2	J	610	CLA	CAA-CBA-CGA-O2A
2	K	610	CLA	CAA-CBA-CGA-O2A
2	H	610	CLA	CAA-CBA-CGA-O2A
2	A	604	CLA	C11-C10-C8-C7
2	F	604	CLA	C11-C10-C8-C7
2	G	604	CLA	C11-C10-C8-C7

There are no ring outliers.

113 monomers are involved in 438 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	607	CLA	12	0
2	D	608	CLA	2	0
2	E	601	CLA	6	0
2	B	601	CLA	7	0
2	G	605	CLA	3	0
2	D	611	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	603	CLA	3	0
2	A	608	CLA	2	0
2	I	602	CLA	4	0
2	E	608	CLA	2	0
2	B	607	CLA	12	0
2	F	601	CLA	7	0
2	J	611	CLA	1	0
2	A	609	CLA	3	0
3	I	612	XAT	4	0
2	K	608	CLA	2	0
2	K	602	CLA	5	0
2	G	601	CLA	8	0
2	K	611	CLA	1	0
3	K	612	XAT	4	0
2	J	609	CLA	3	0
2	A	606	CLA	6	0
3	A	612	XAT	4	0
2	H	609	CLA	3	0
2	B	605	CLA	2	0
2	E	605	CLA	3	0
2	D	601	CLA	7	0
2	I	605	CLA	3	0
3	D	612	XAT	4	0
2	E	610	CLA	1	0
2	K	609	CLA	3	0
2	G	608	CLA	2	0
3	C	612	XAT	4	0
2	F	606	CLA	7	0
2	E	611	CLA	1	0
2	A	605	CLA	3	0
2	F	602	CLA	4	0
2	C	605	CLA	3	0
3	J	612	XAT	4	0
2	E	606	CLA	7	0
2	I	606	CLA	7	0
2	F	605	CLA	2	0
2	D	607	CLA	12	0
2	B	606	CLA	7	0
2	J	603	CLA	4	0
2	G	602	CLA	4	0
2	G	611	CLA	1	0
2	H	602	CLA	5	0

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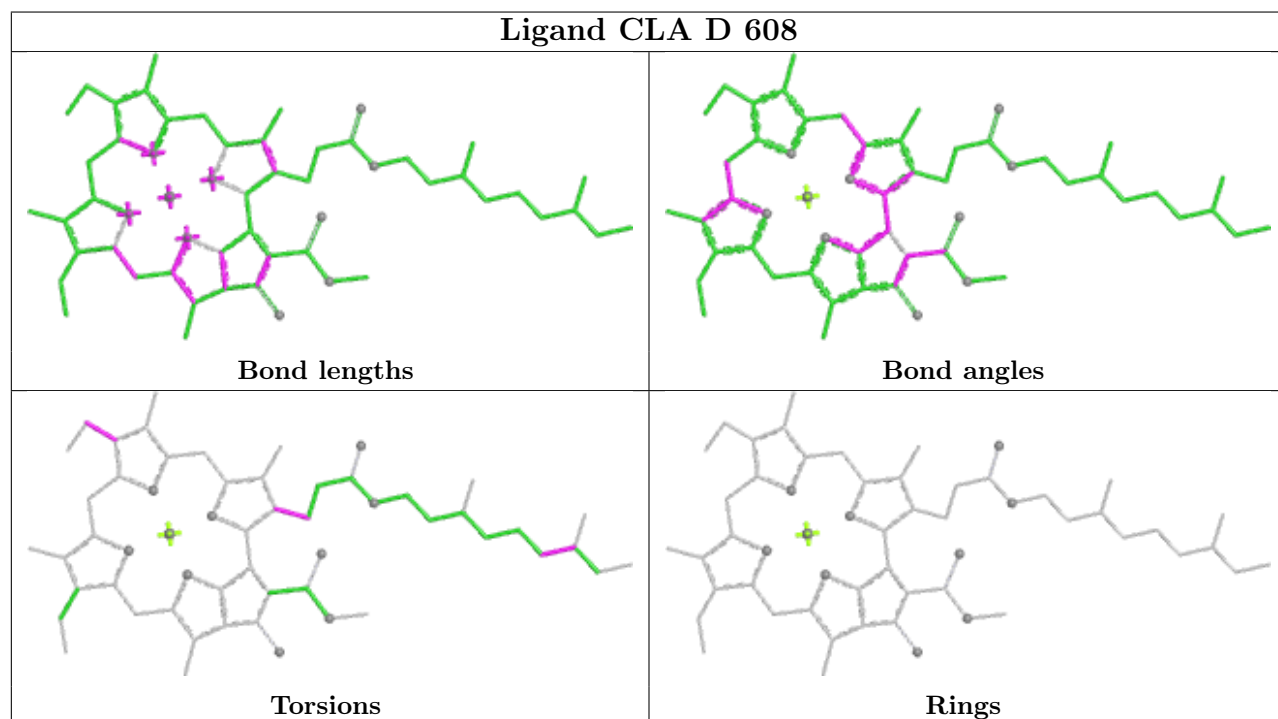
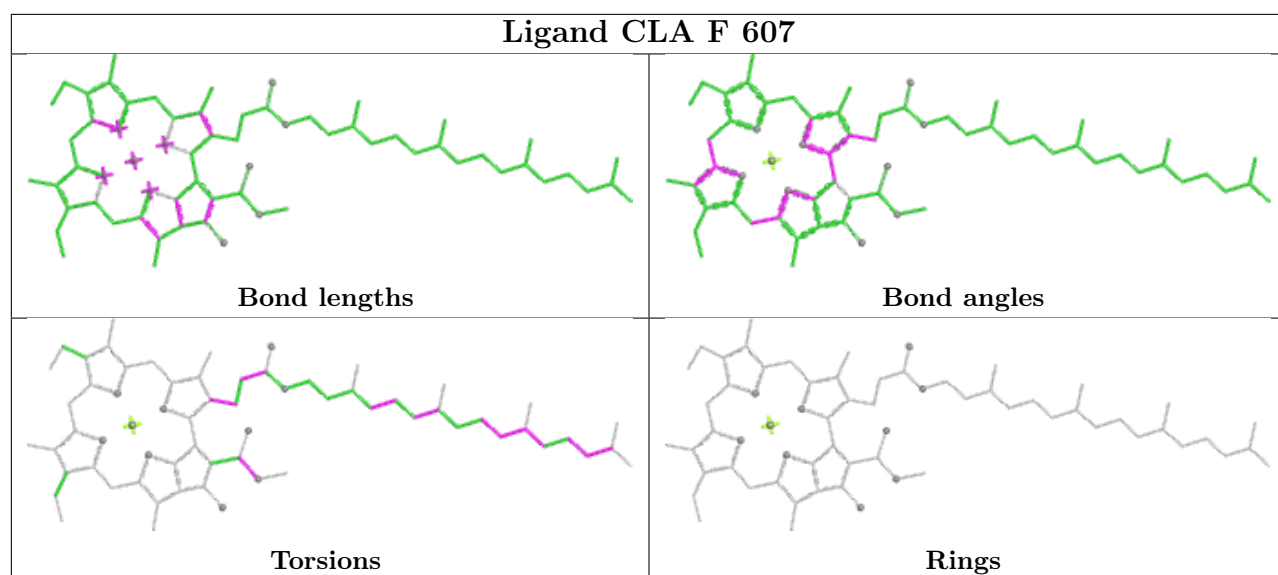
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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2	H	606	CLA	7	0
2	C	606	CLA	7	0
2	I	607	CLA	12	0
2	K	603	CLA	3	0
3	B	612	XAT	4	0
3	E	612	XAT	4	0
2	D	602	CLA	4	0
2	J	607	CLA	11	0
2	D	605	CLA	2	0
2	C	603	CLA	3	0
2	J	605	CLA	3	0
2	B	602	CLA	4	0
2	G	603	CLA	3	0
2	C	601	CLA	6	0
2	G	607	CLA	12	0
2	J	606	CLA	7	0
2	C	602	CLA	5	0
2	C	608	CLA	2	0
2	F	608	CLA	2	0
2	E	609	CLA	3	0
2	H	601	CLA	6	0
2	D	606	CLA	7	0
2	E	603	CLA	4	0
2	I	601	CLA	7	0
2	I	611	CLA	1	0
2	I	608	CLA	2	0
2	B	603	CLA	4	0
2	J	608	CLA	2	0
2	K	601	CLA	6	0
2	A	602	CLA	4	0
2	K	605	CLA	3	0
2	A	611	CLA	1	0
2	F	603	CLA	4	0
2	H	611	CLA	1	0
2	I	603	CLA	5	0
3	H	612	XAT	4	0
2	B	608	CLA	2	0
2	B	609	CLA	3	0
2	A	607	CLA	13	0
2	A	601	CLA	9	0
2	J	602	CLA	4	0

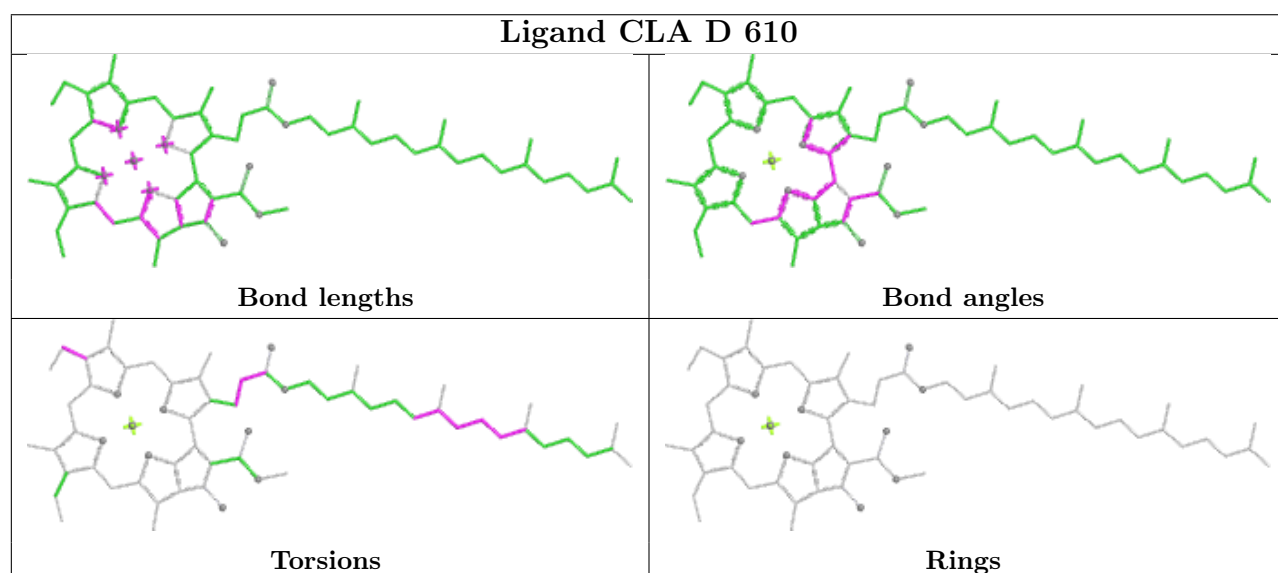
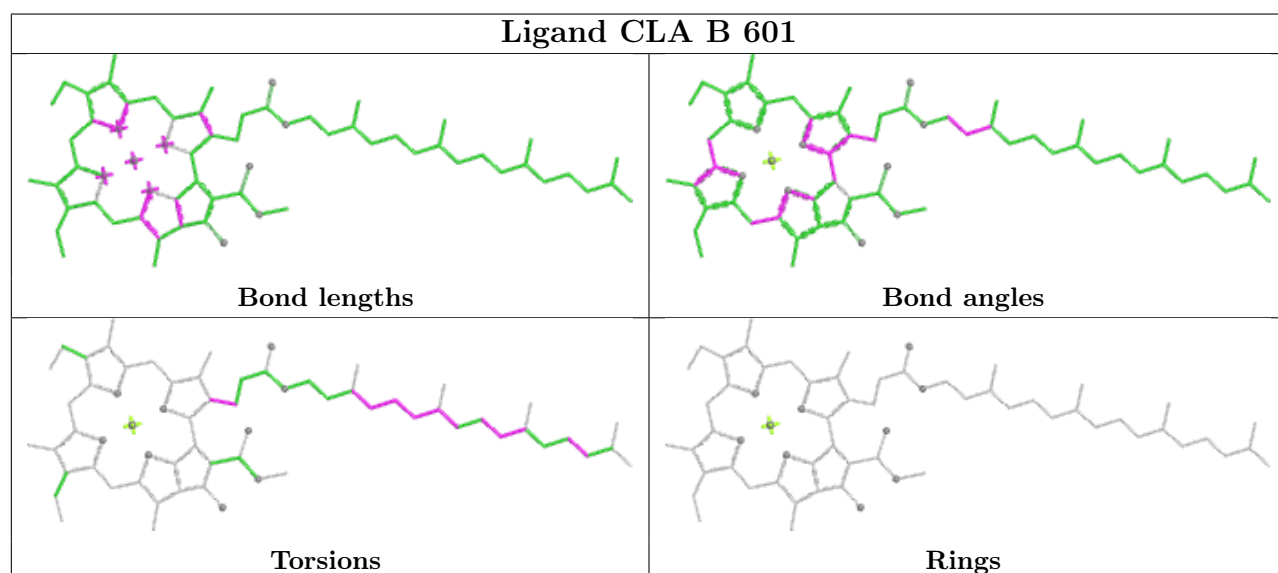
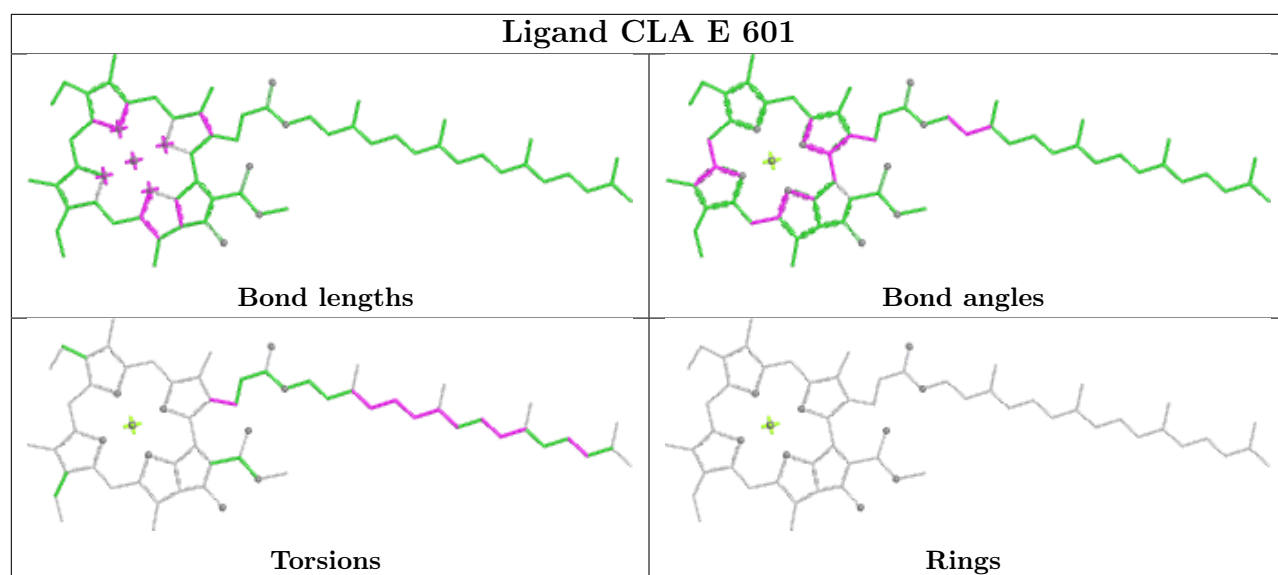
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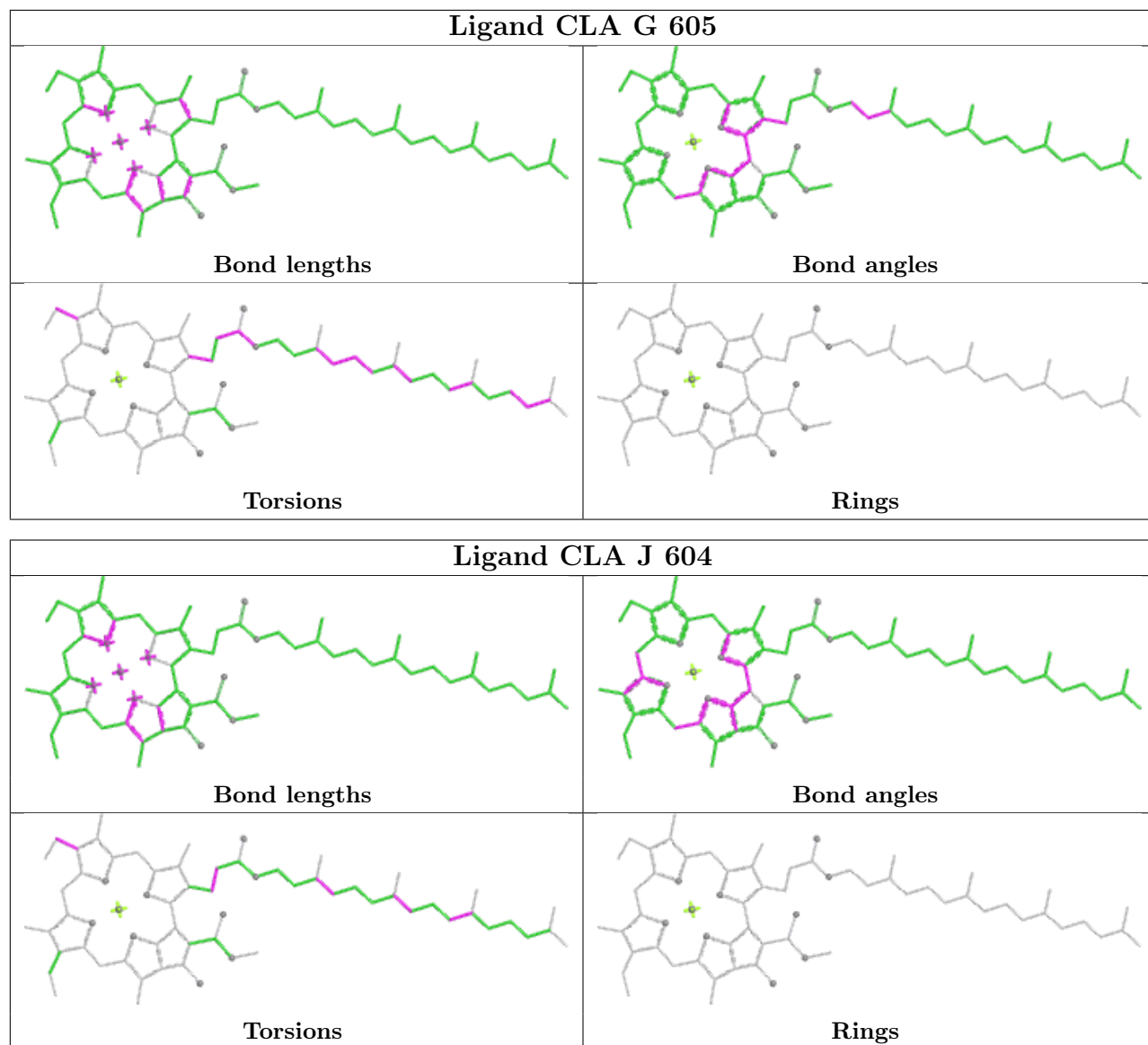
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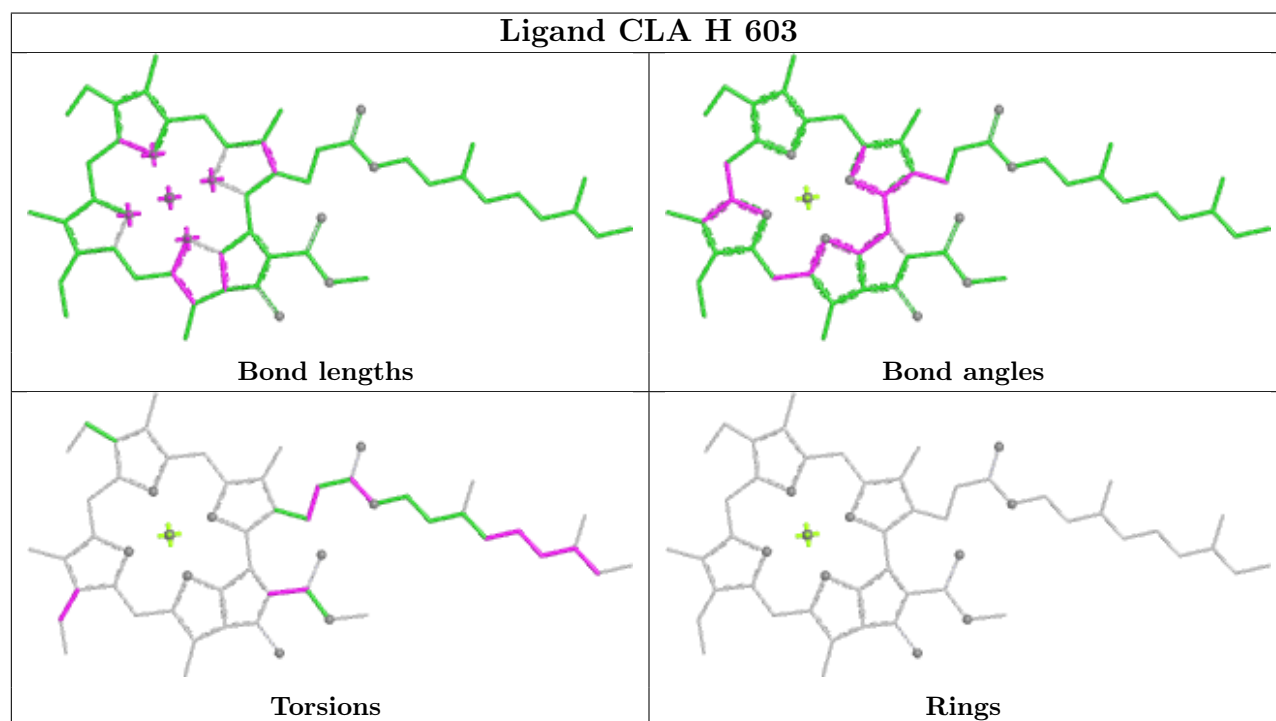
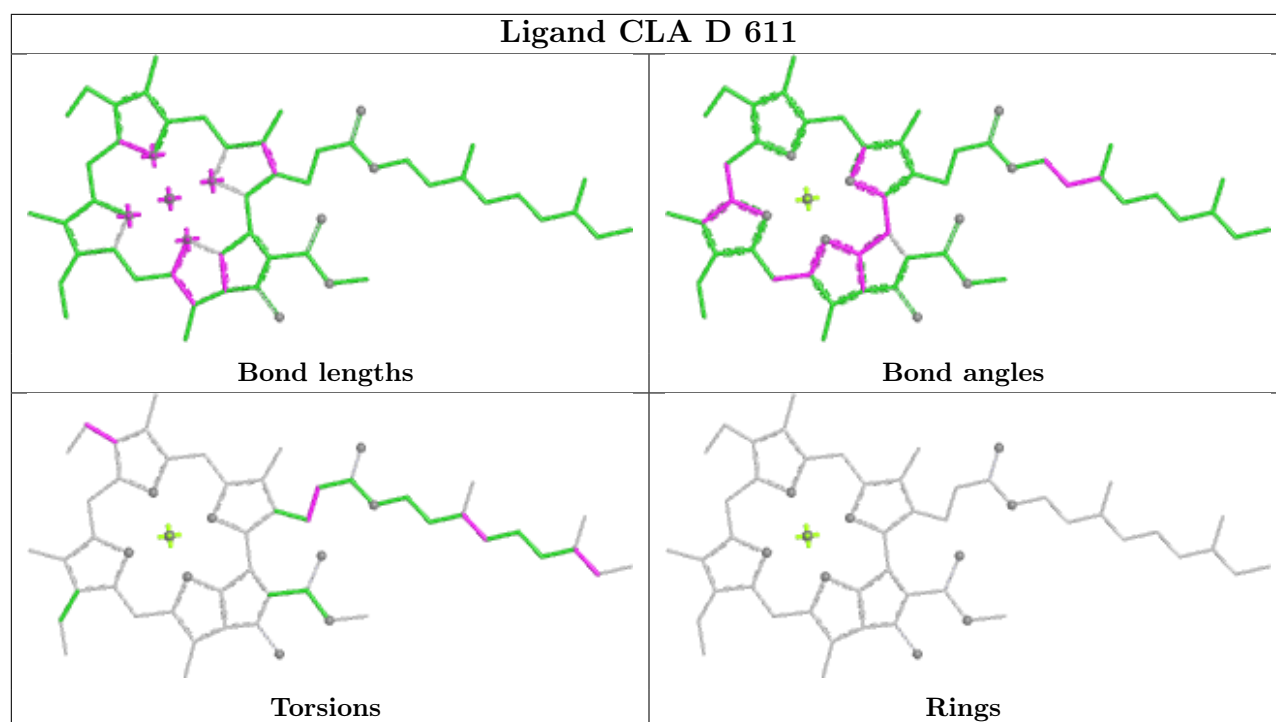
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	611	CLA	1	0
2	G	609	CLA	3	0
2	D	609	CLA	3	0
2	F	611	CLA	1	0
3	F	612	XAT	4	0
2	K	607	CLA	12	0
2	A	603	CLA	4	0
2	H	608	CLA	2	0
2	K	606	CLA	6	0
2	H	607	CLA	12	0
2	C	607	CLA	12	0
2	E	602	CLA	4	0
2	G	606	CLA	7	0
2	J	601	CLA	9	0
3	G	612	XAT	4	0
2	I	610	CLA	1	0
2	D	603	CLA	4	0
2	H	605	CLA	3	0
2	C	609	CLA	3	0
2	B	611	CLA	1	0
2	J	610	CLA	1	0
2	F	609	CLA	3	0
2	I	609	CLA	3	0

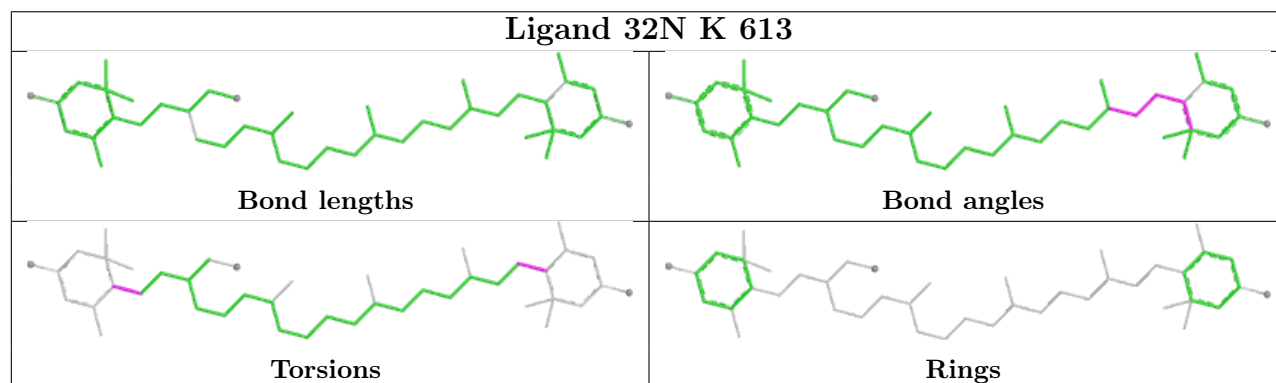
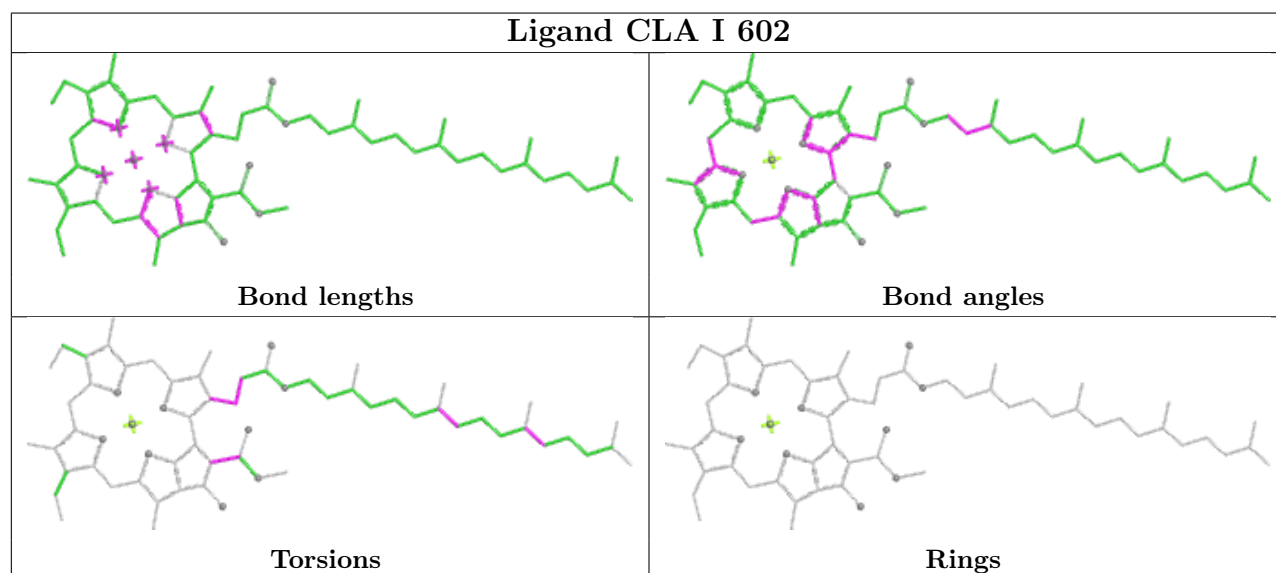
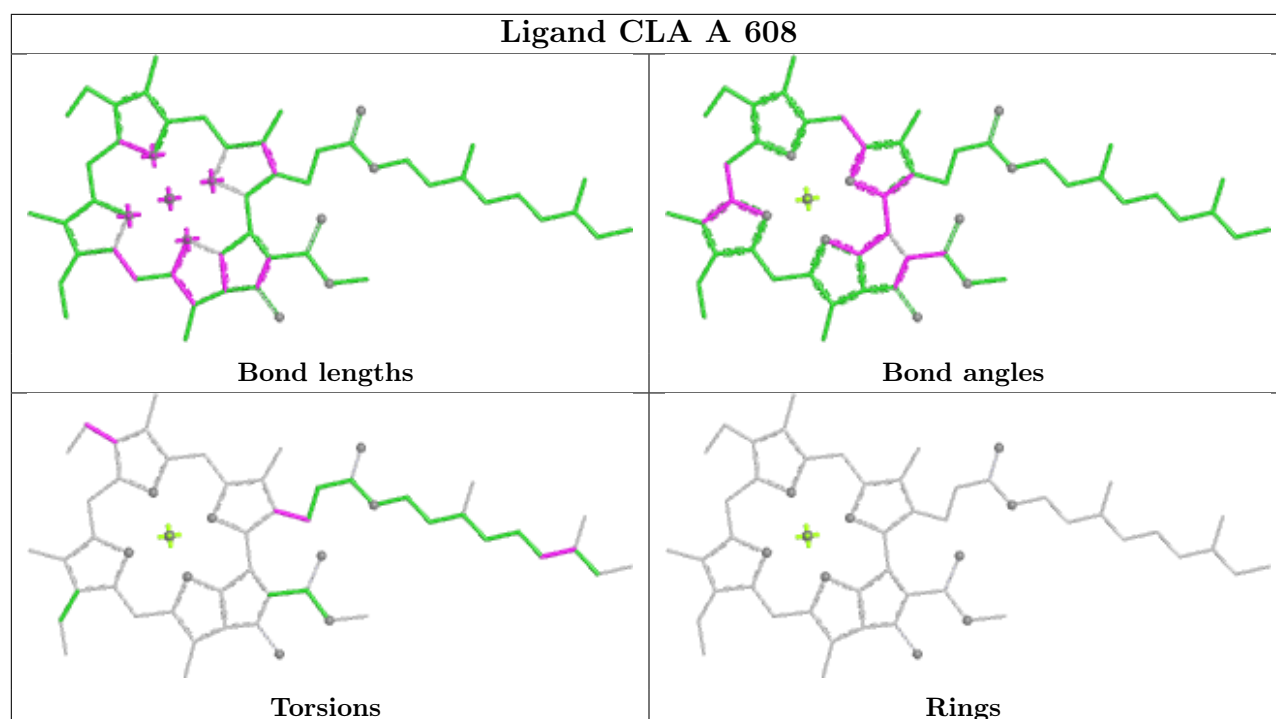
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

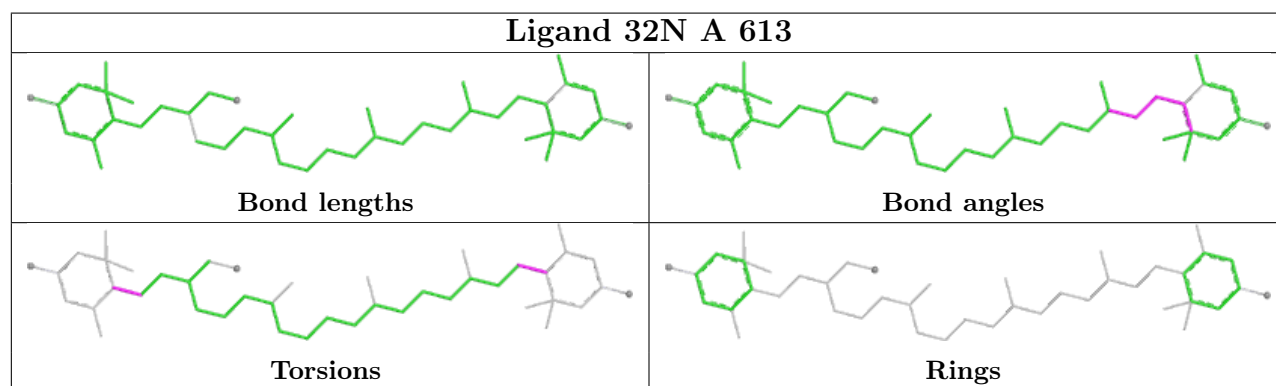
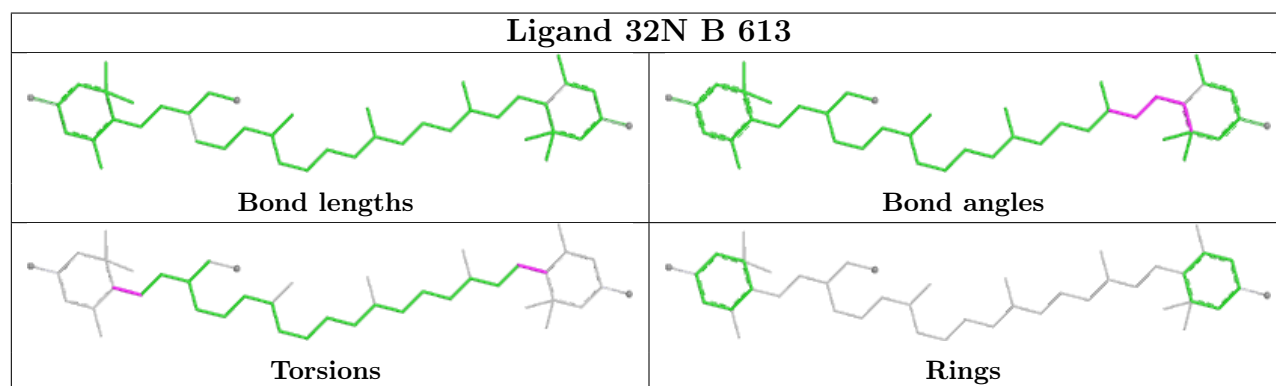
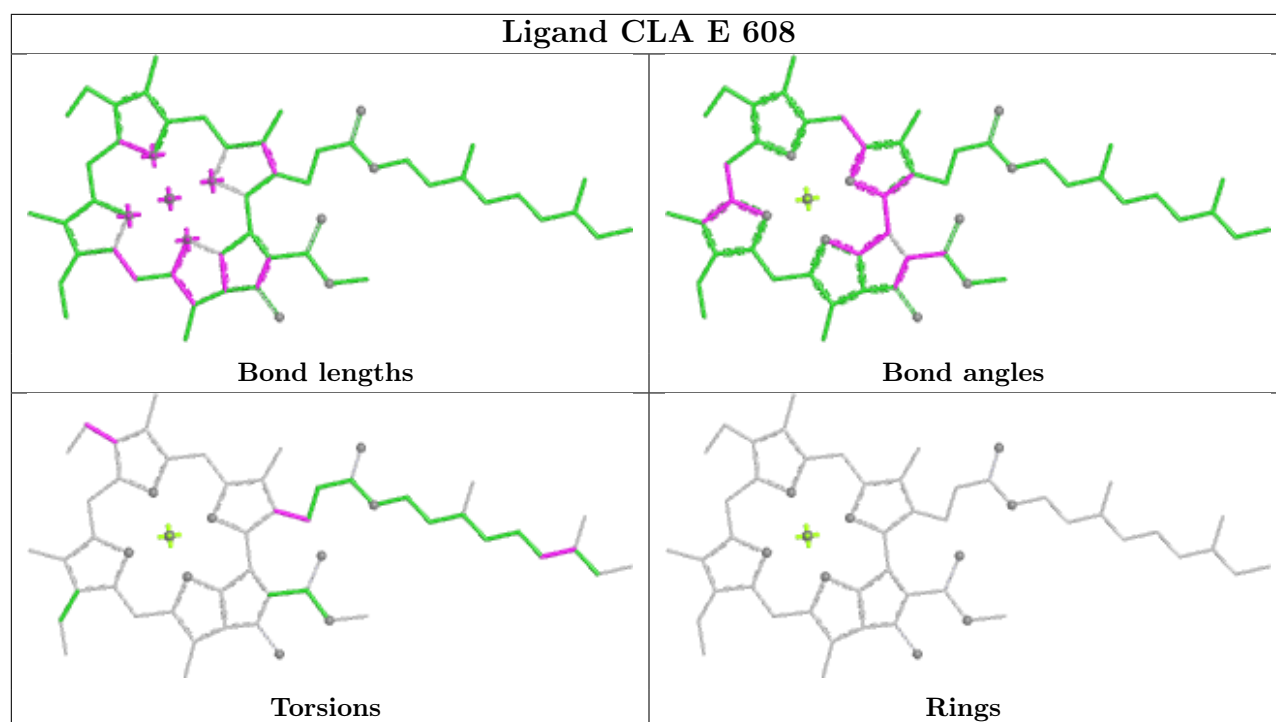


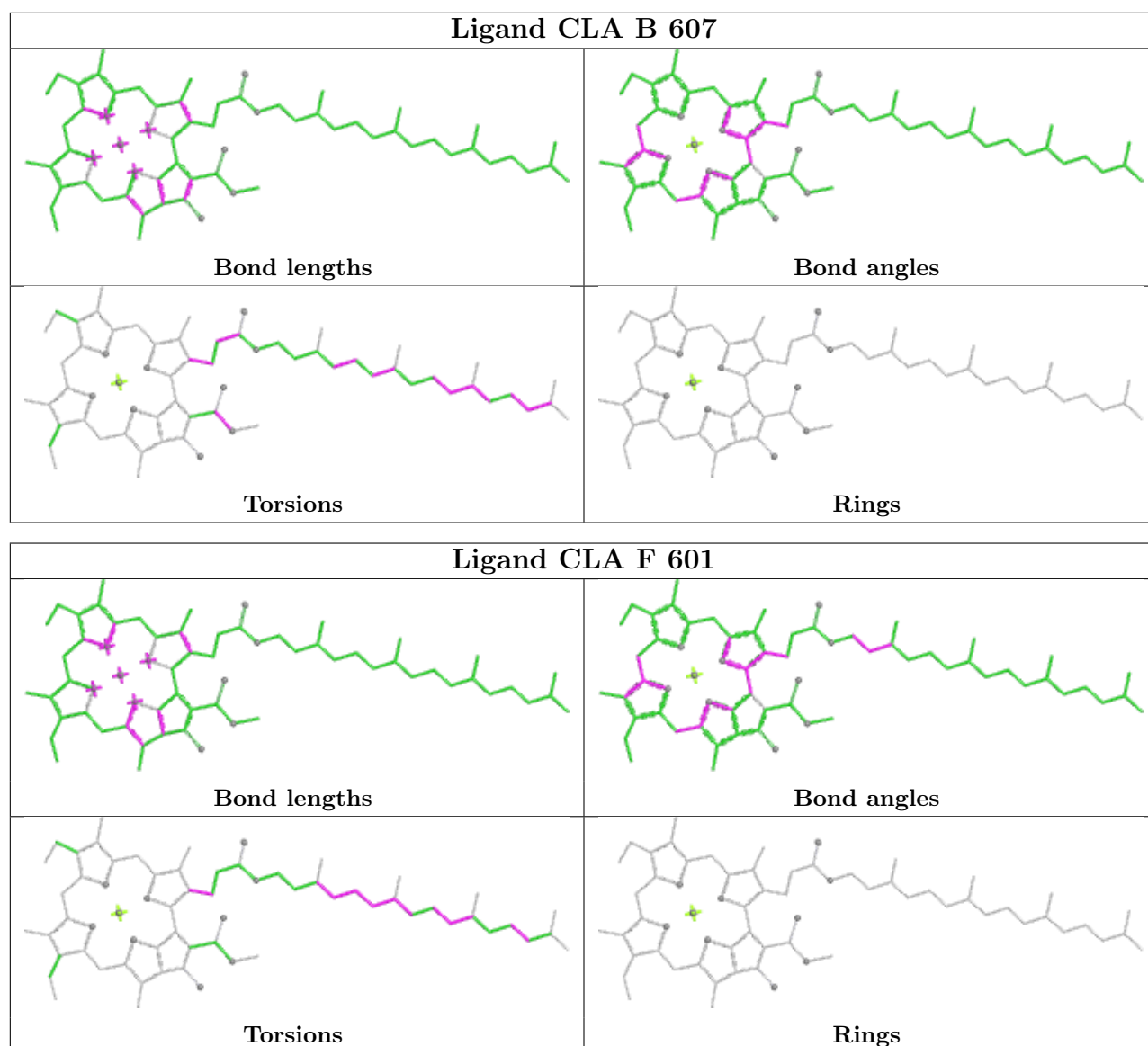


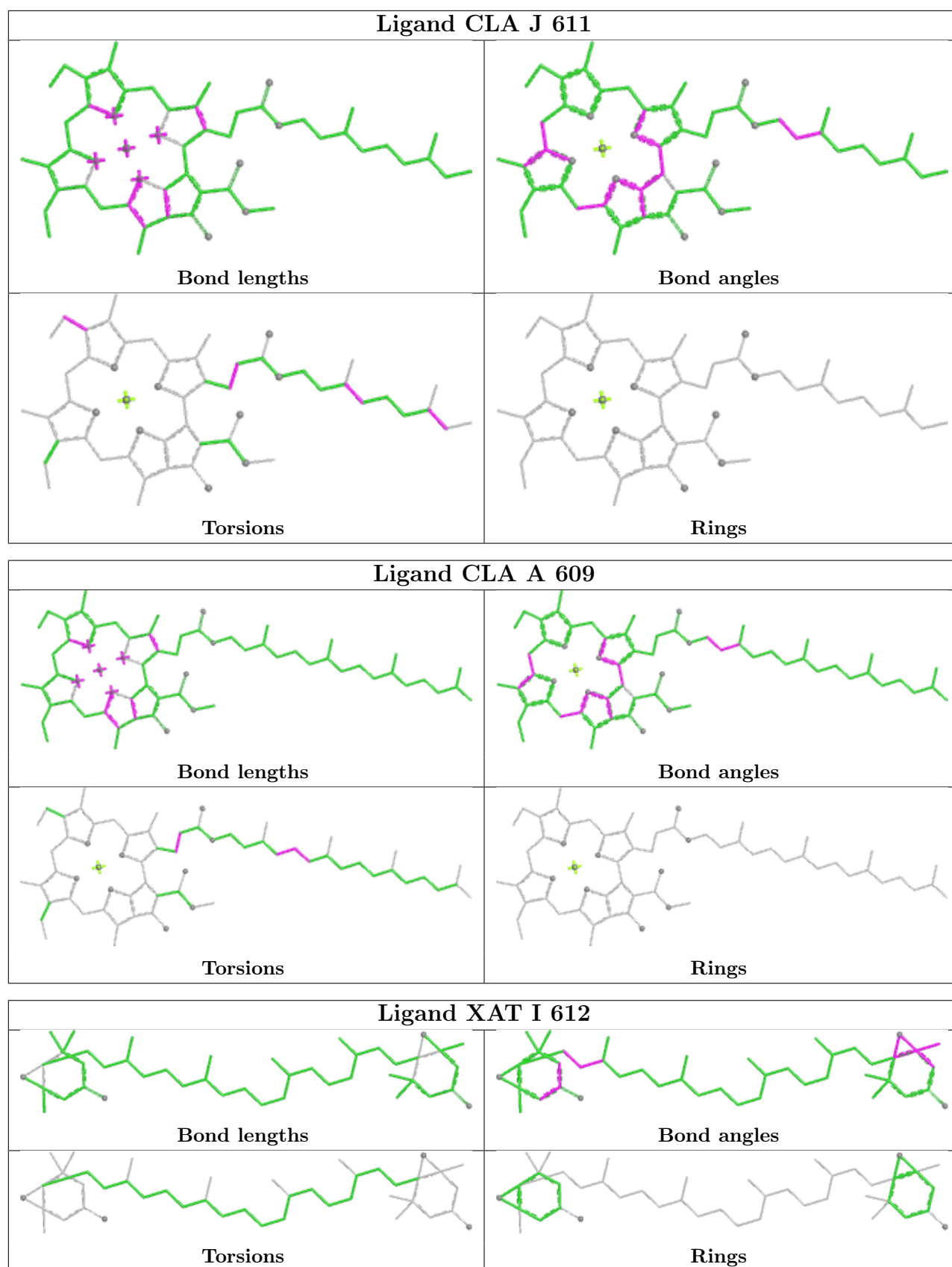


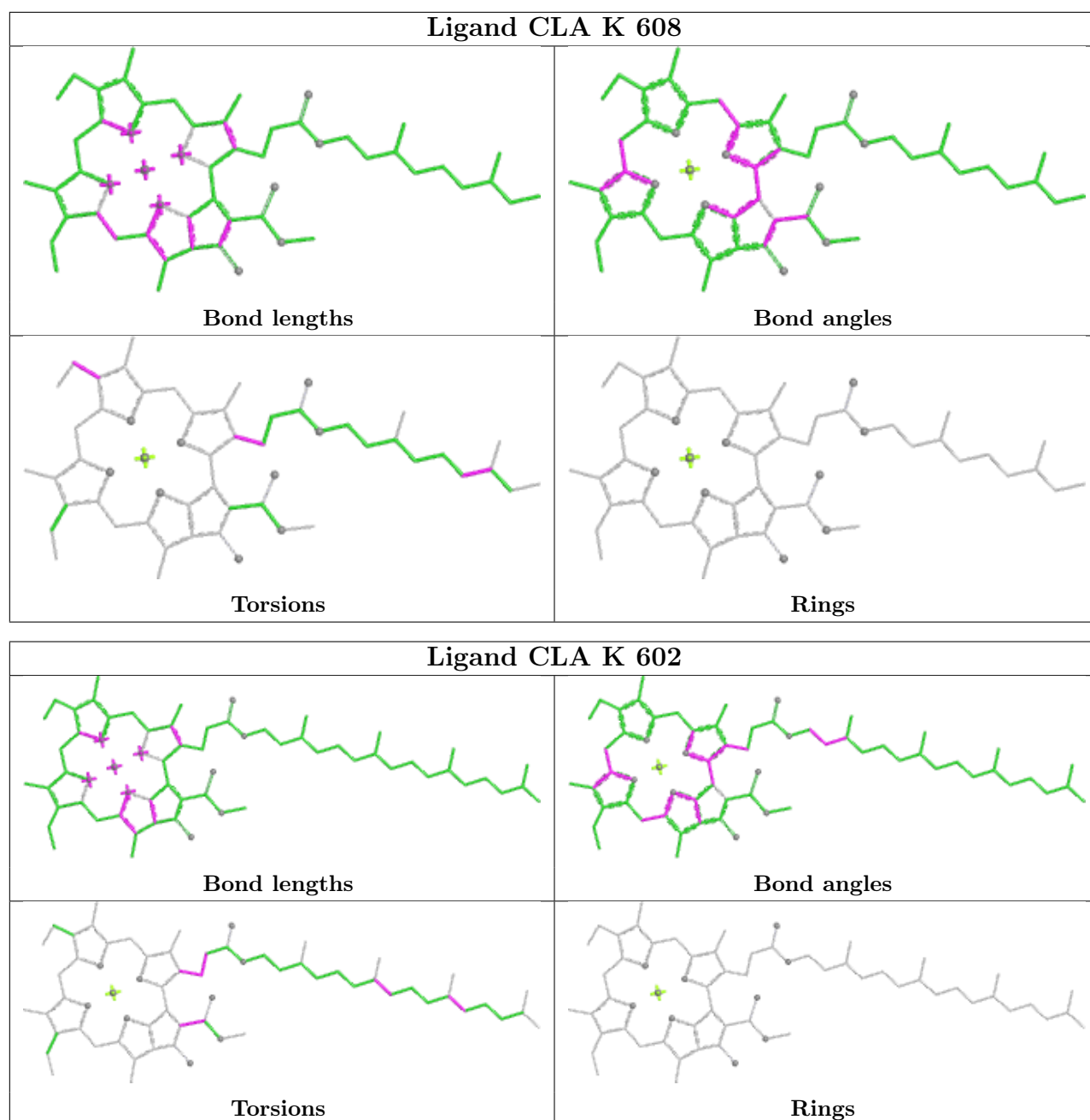


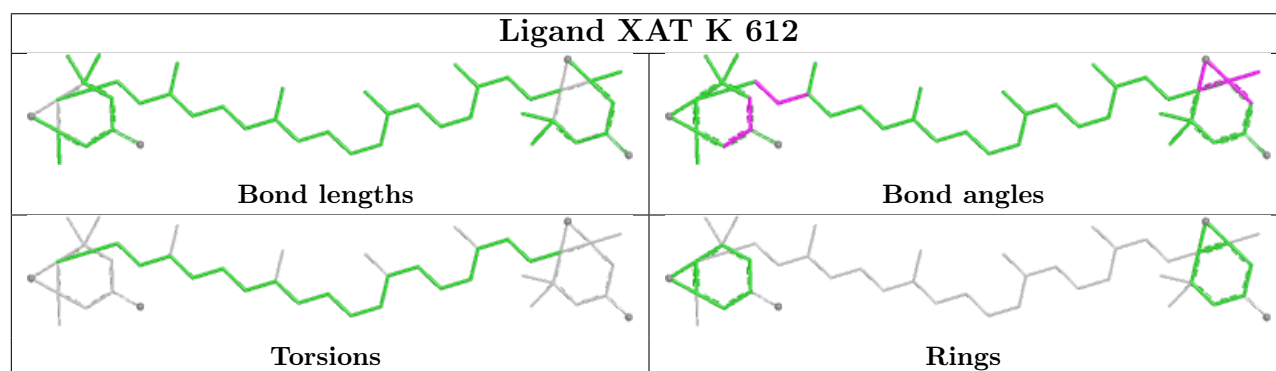
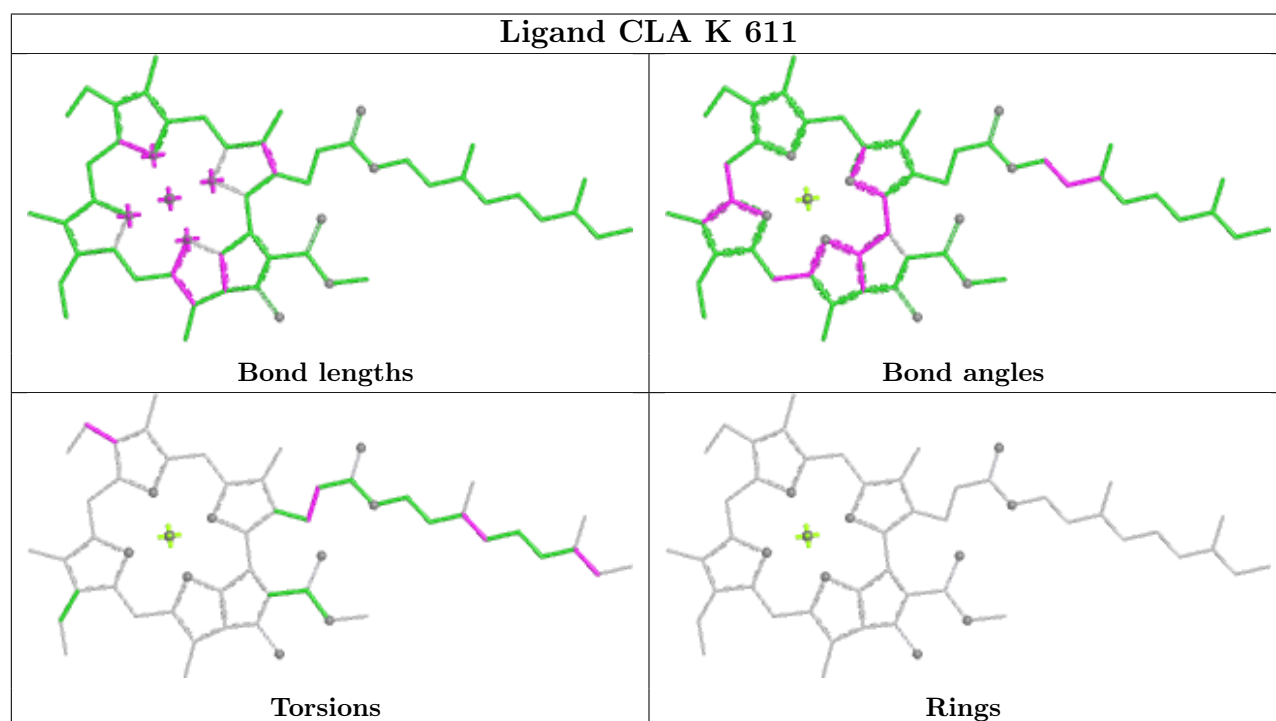
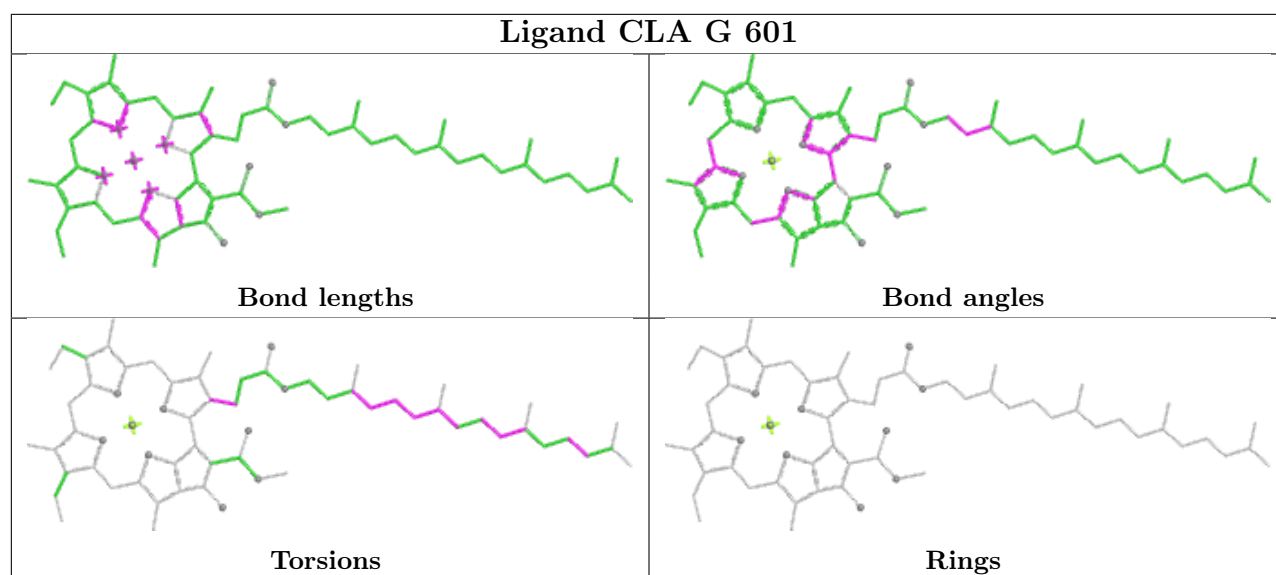


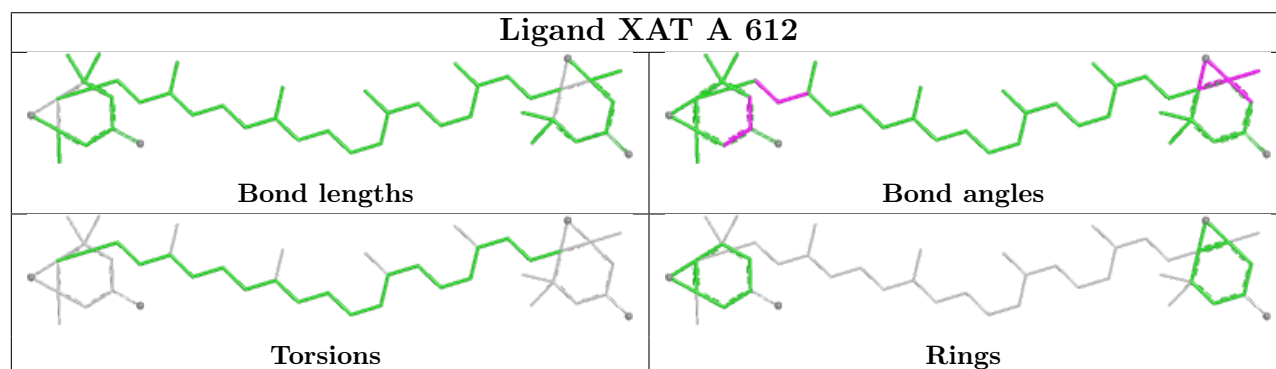
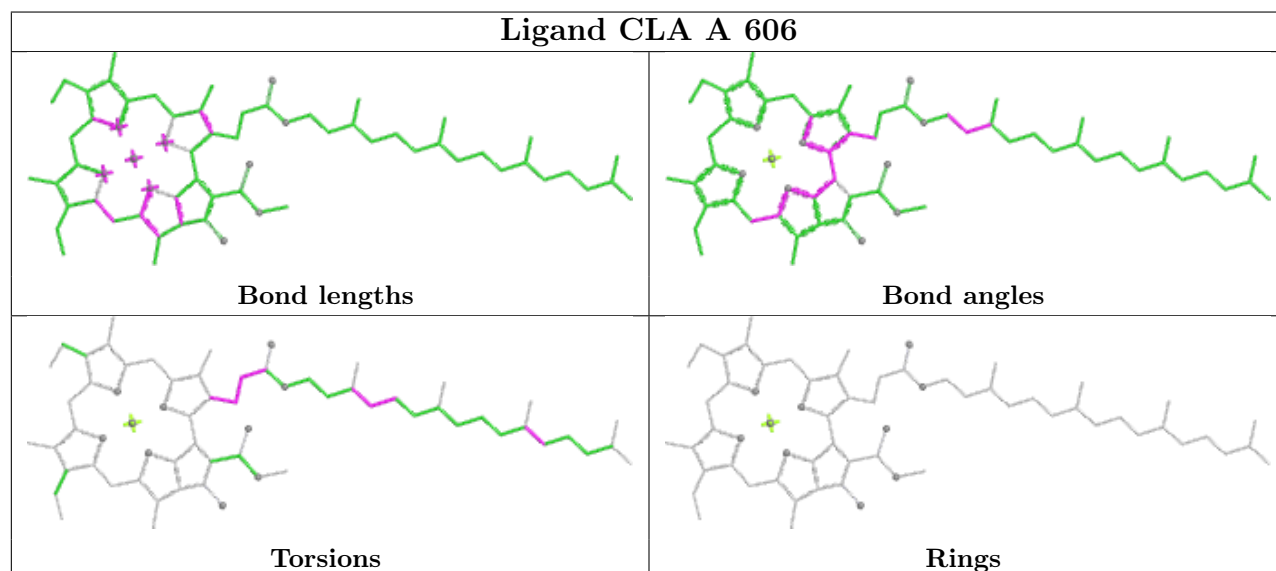
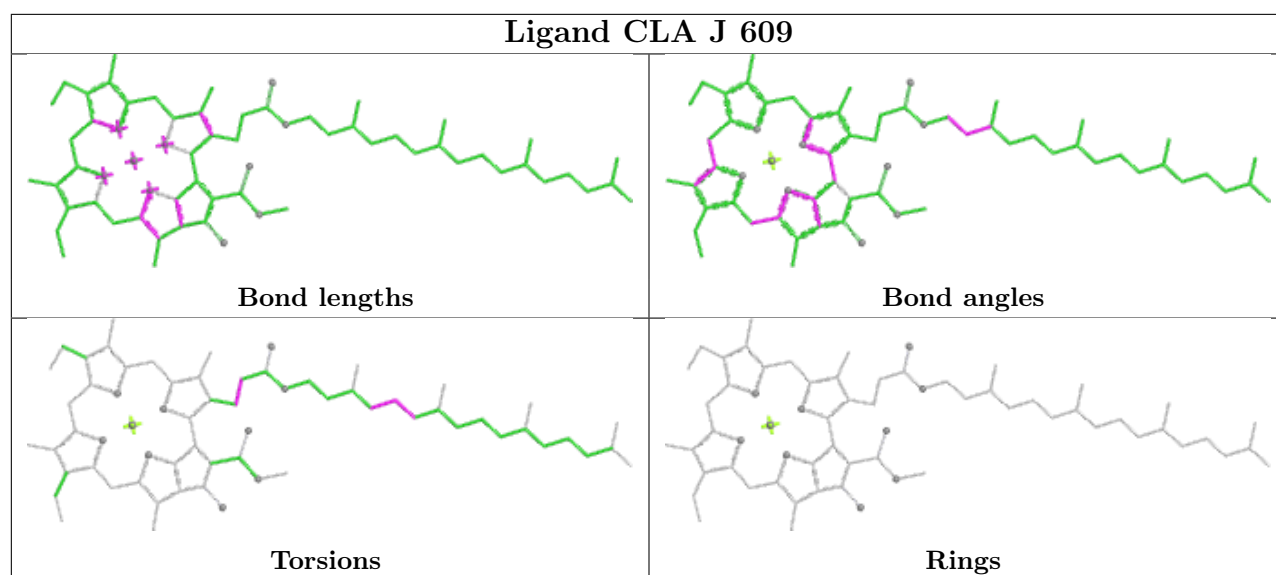


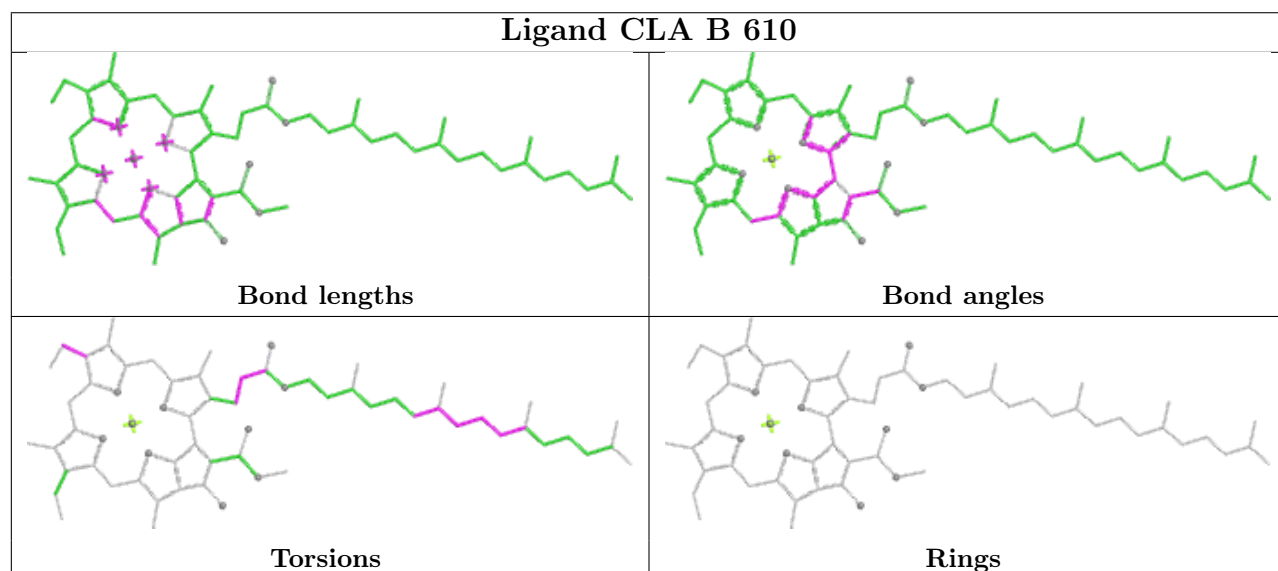
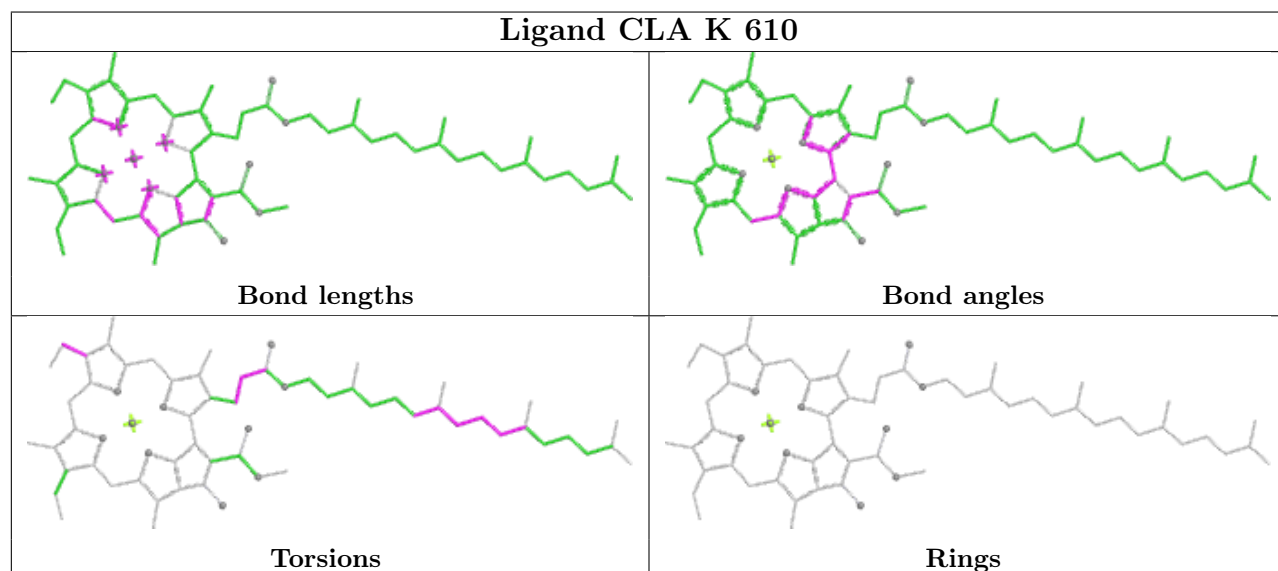
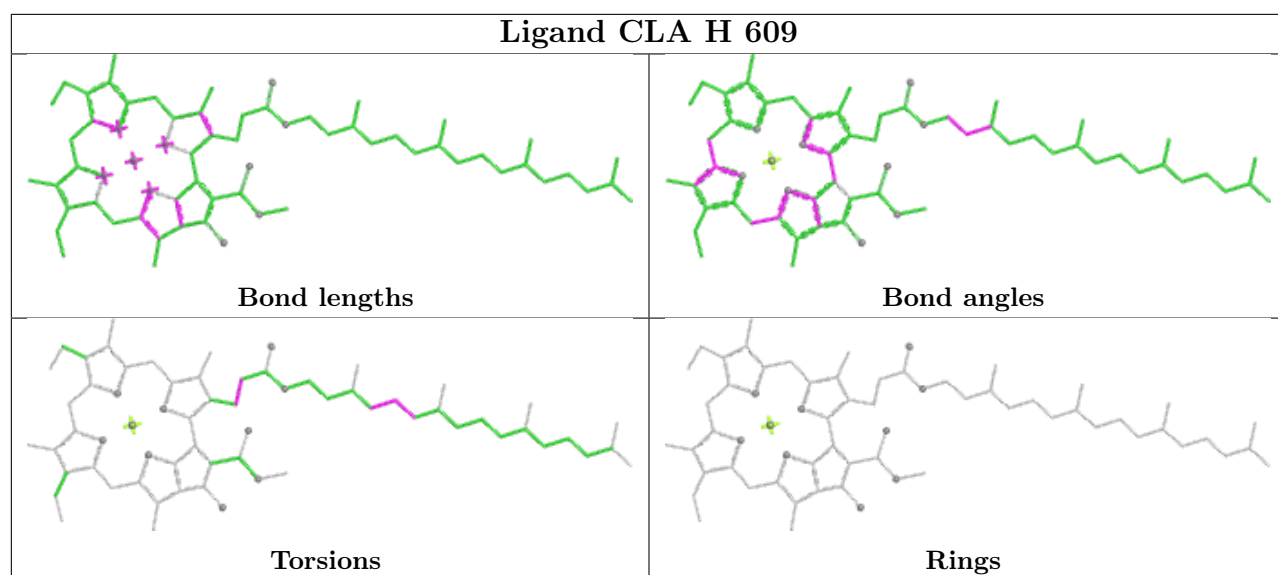


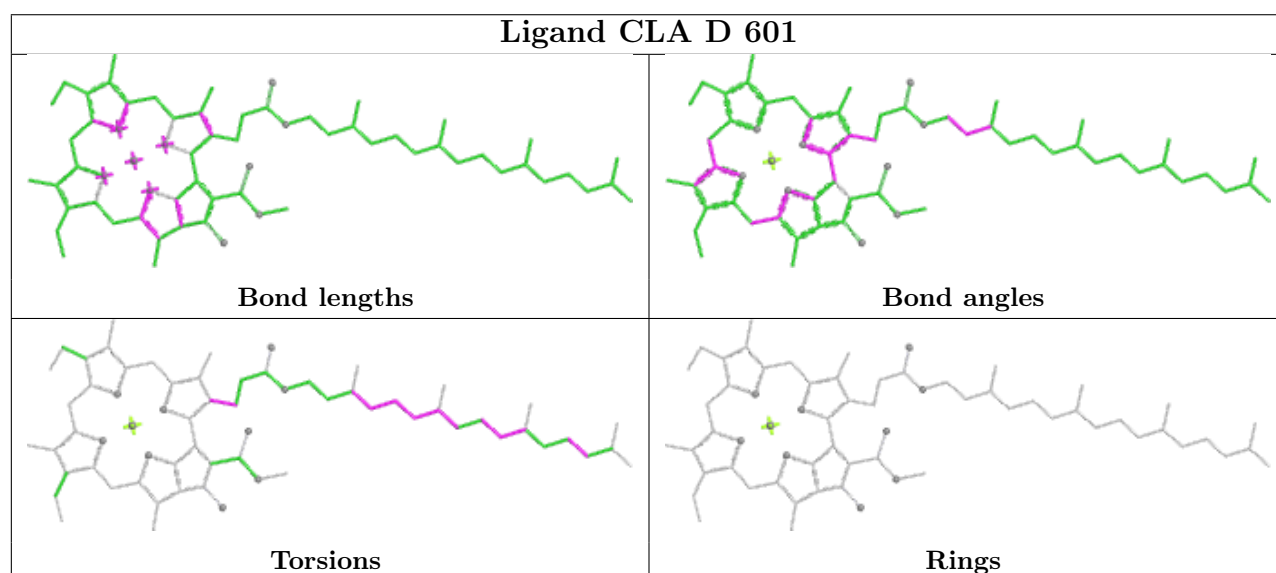
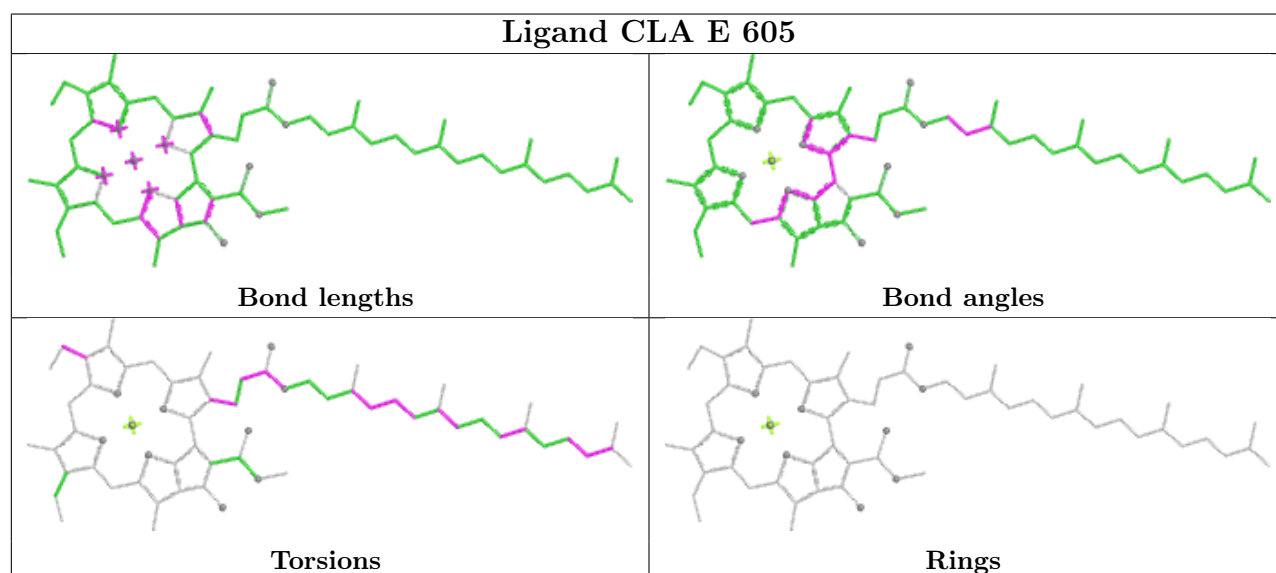
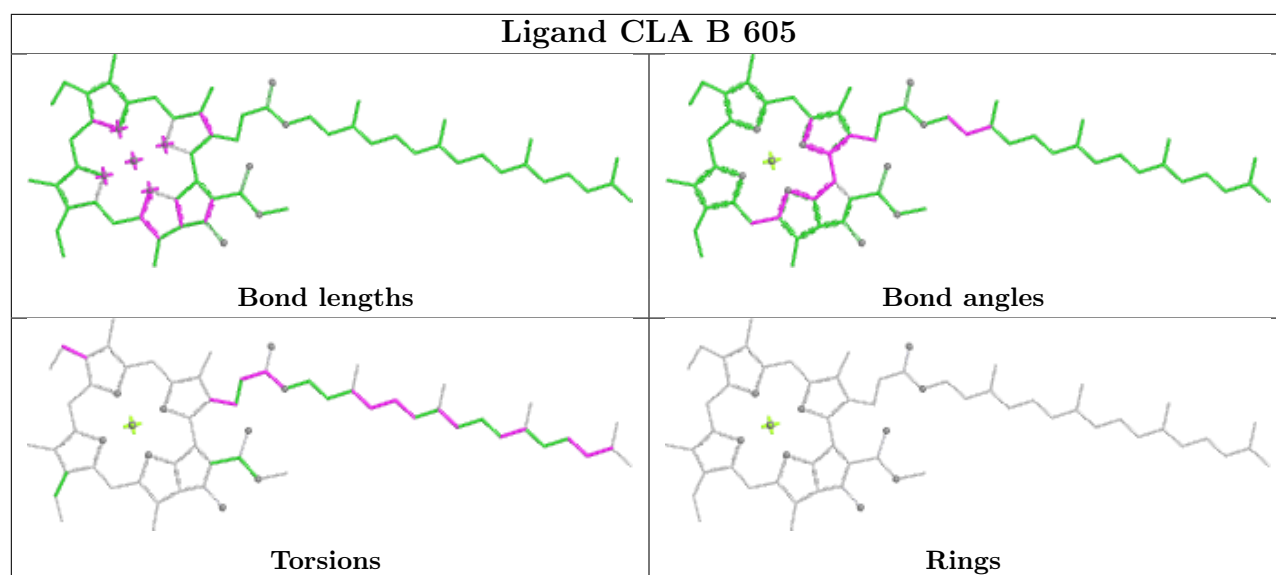


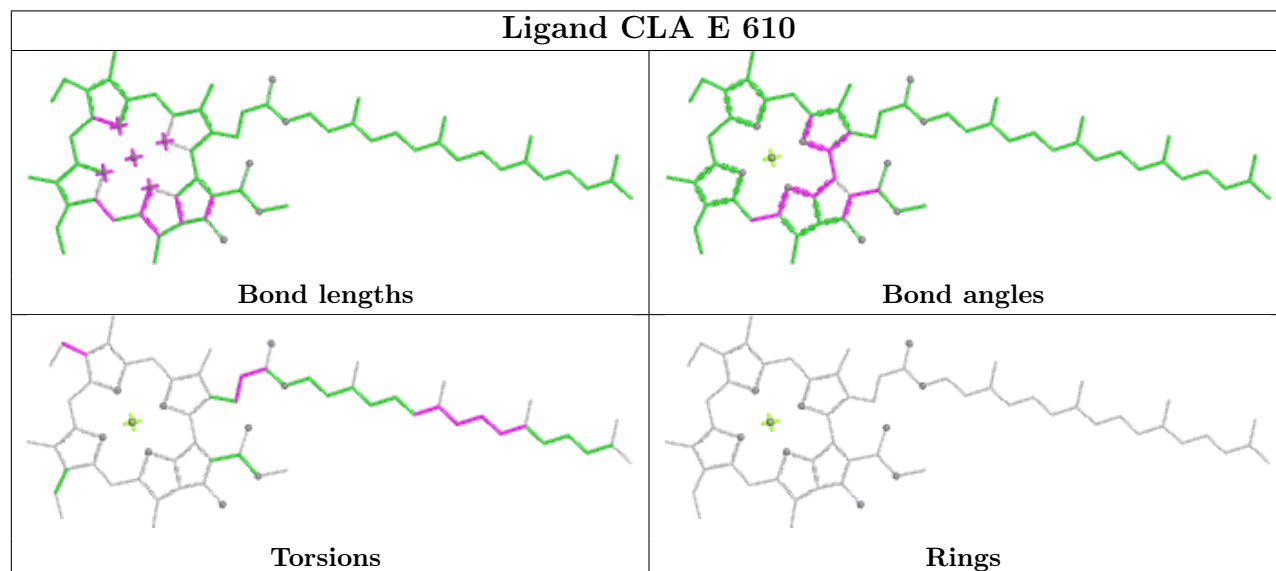
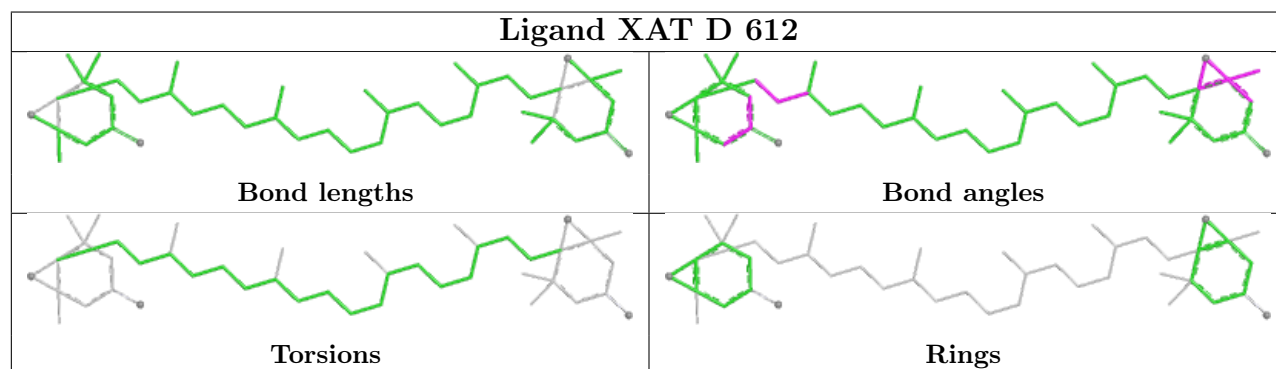
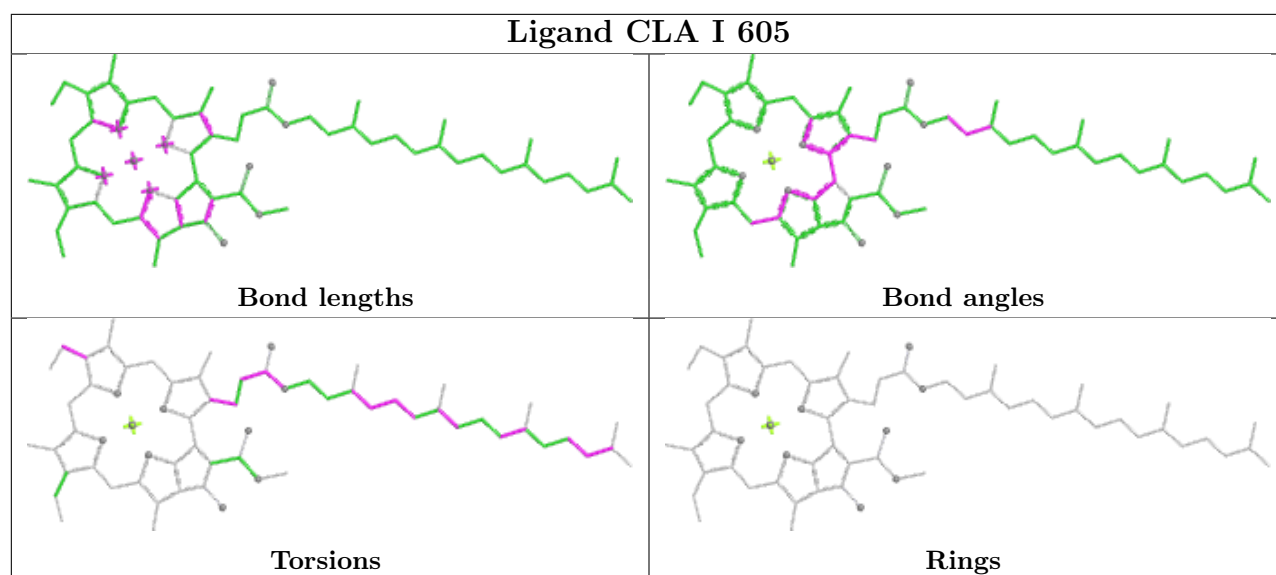


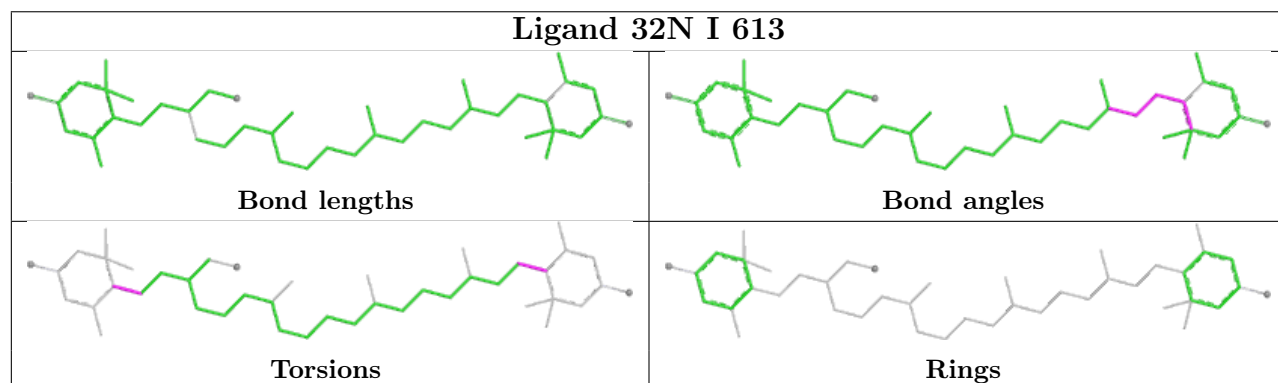
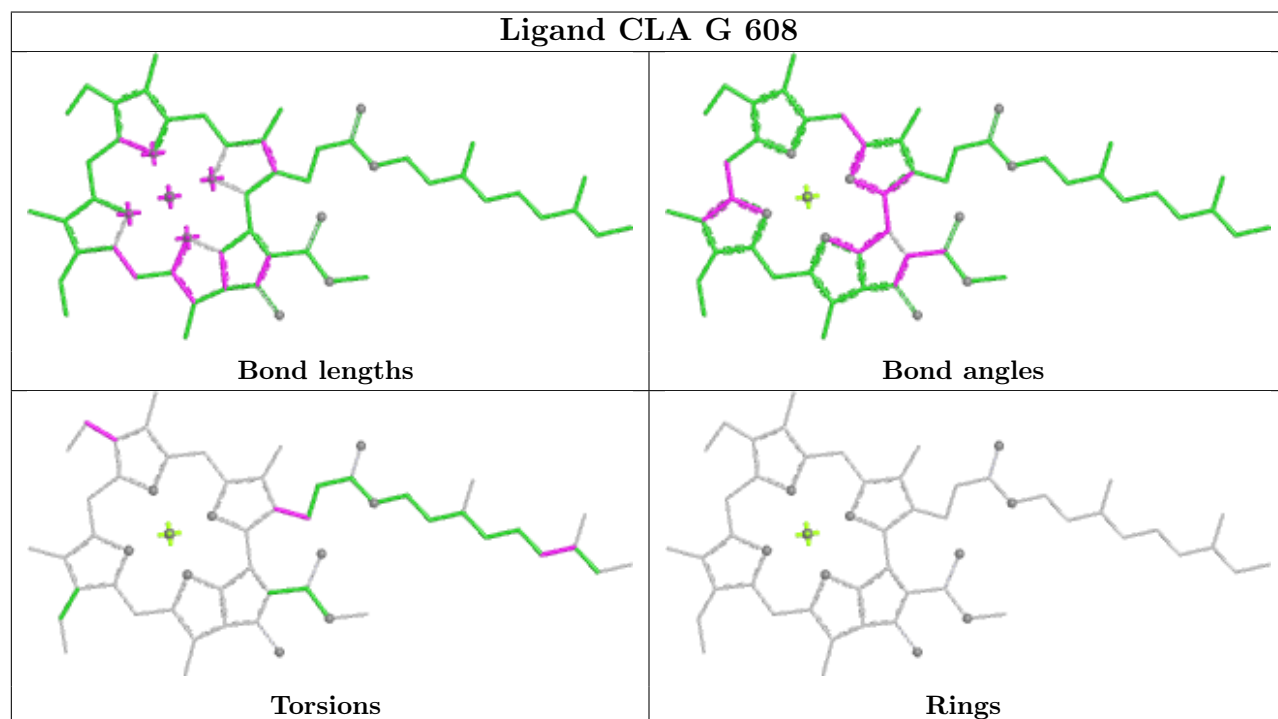
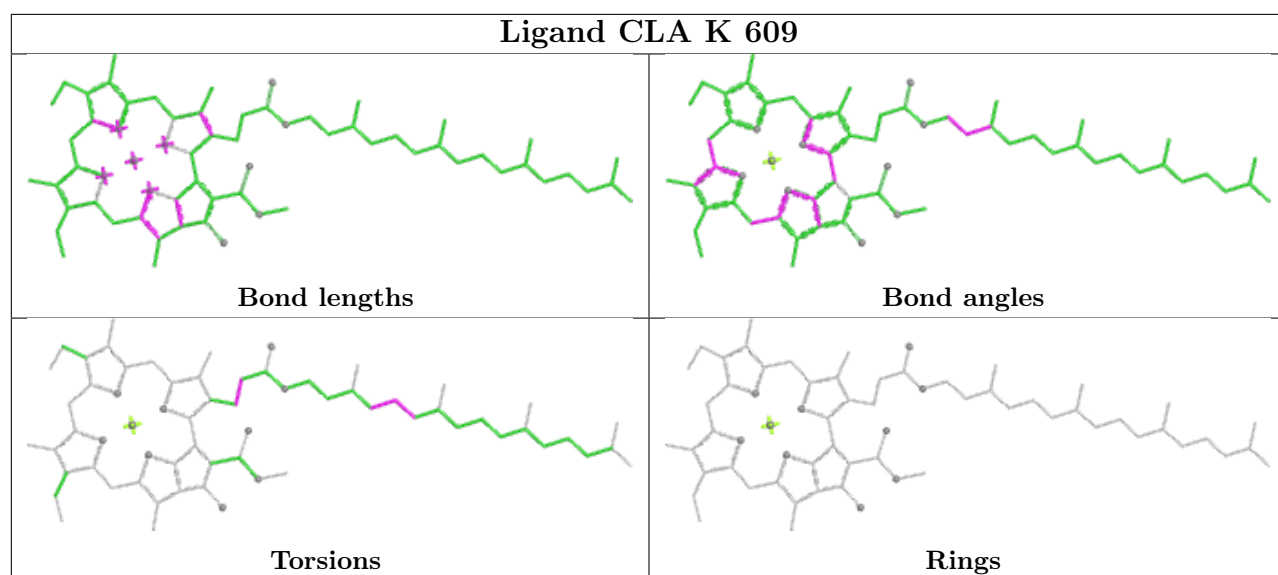


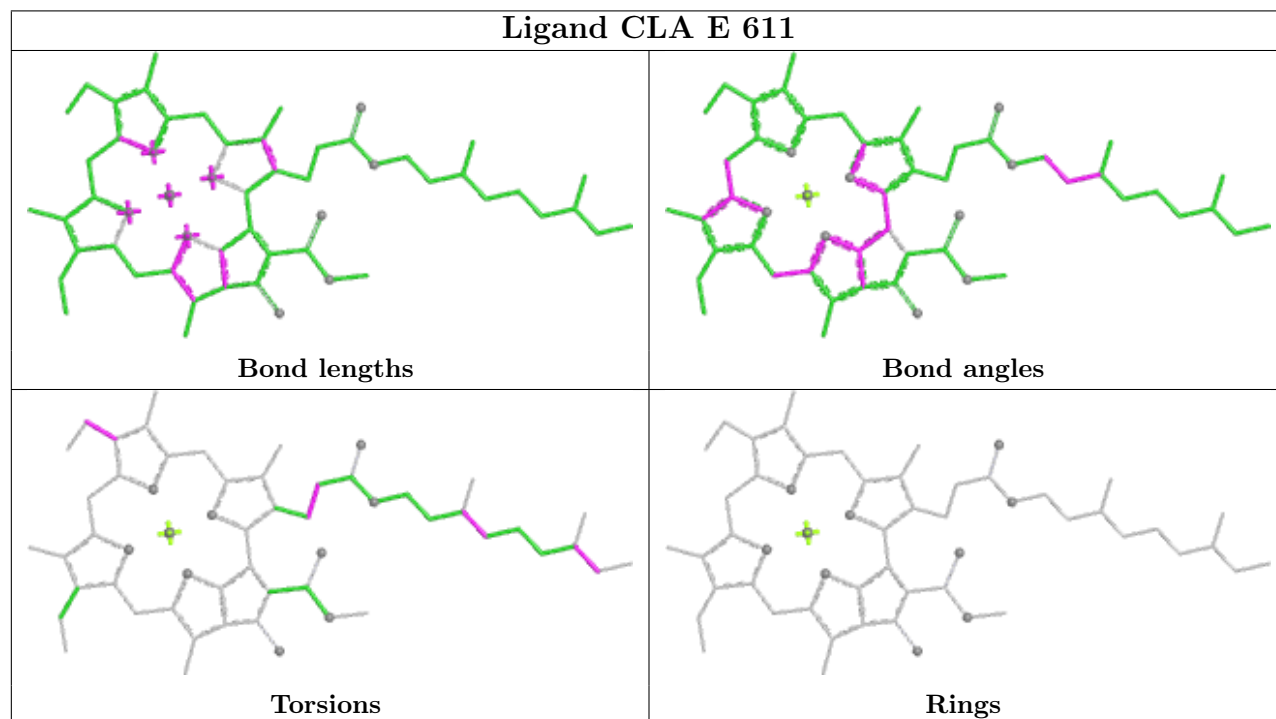
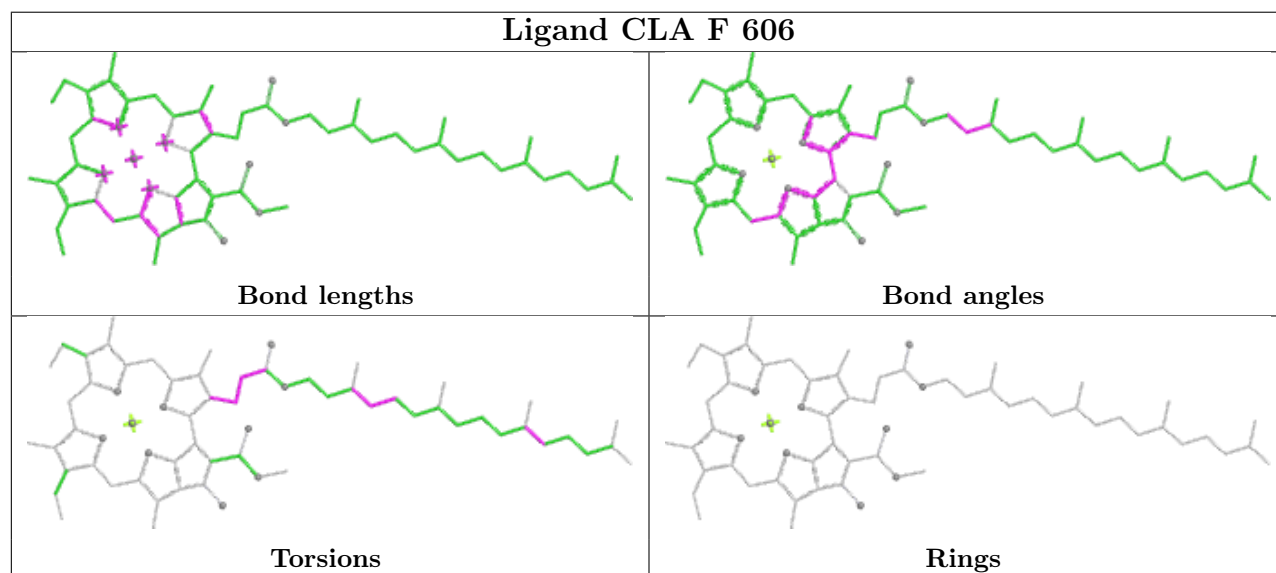
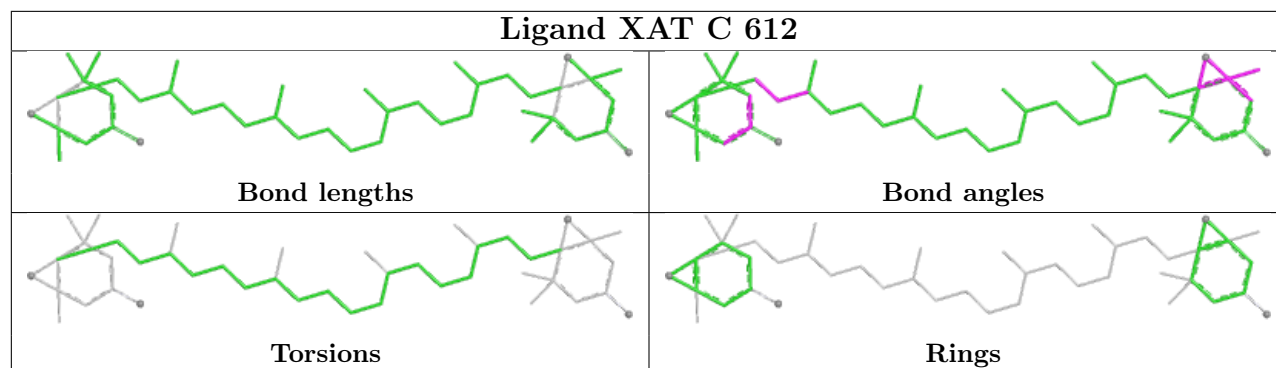


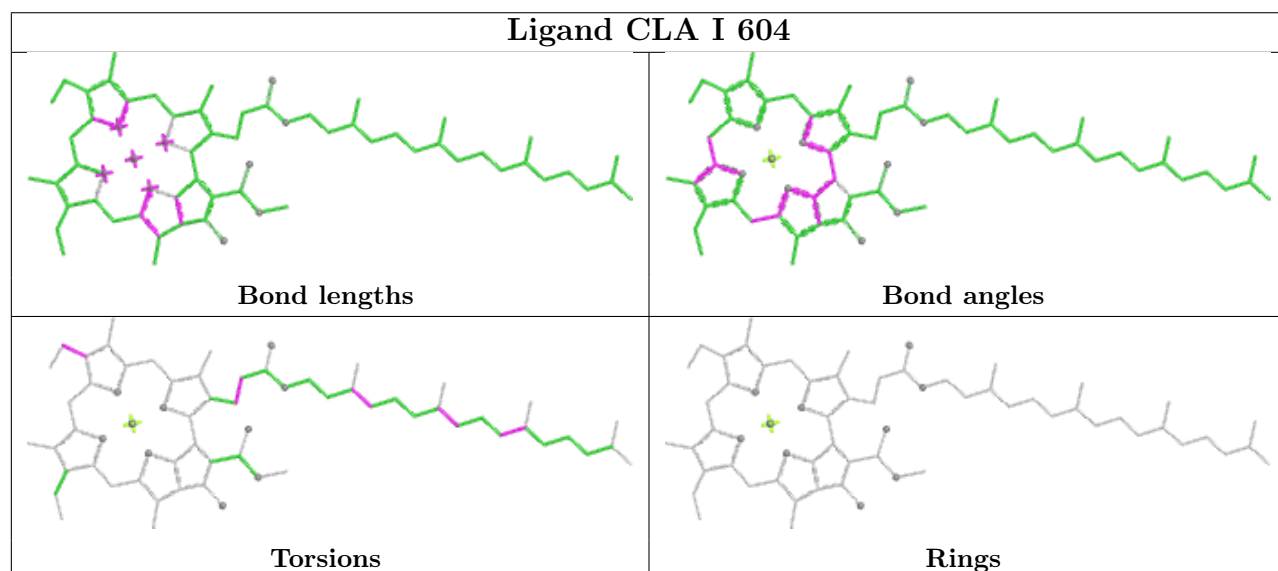
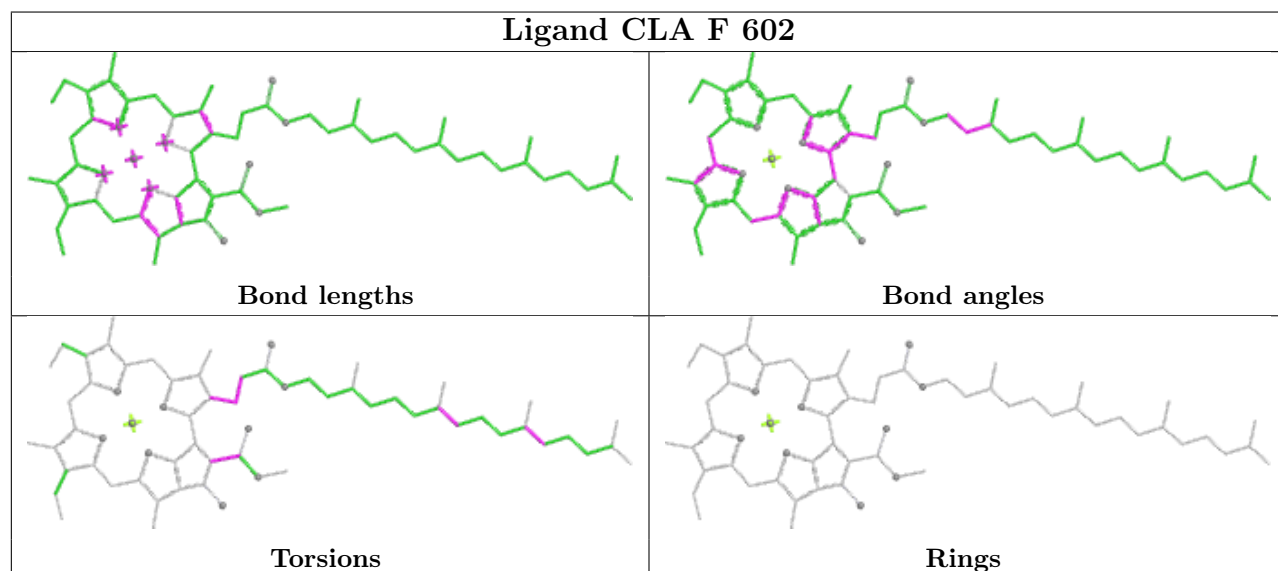
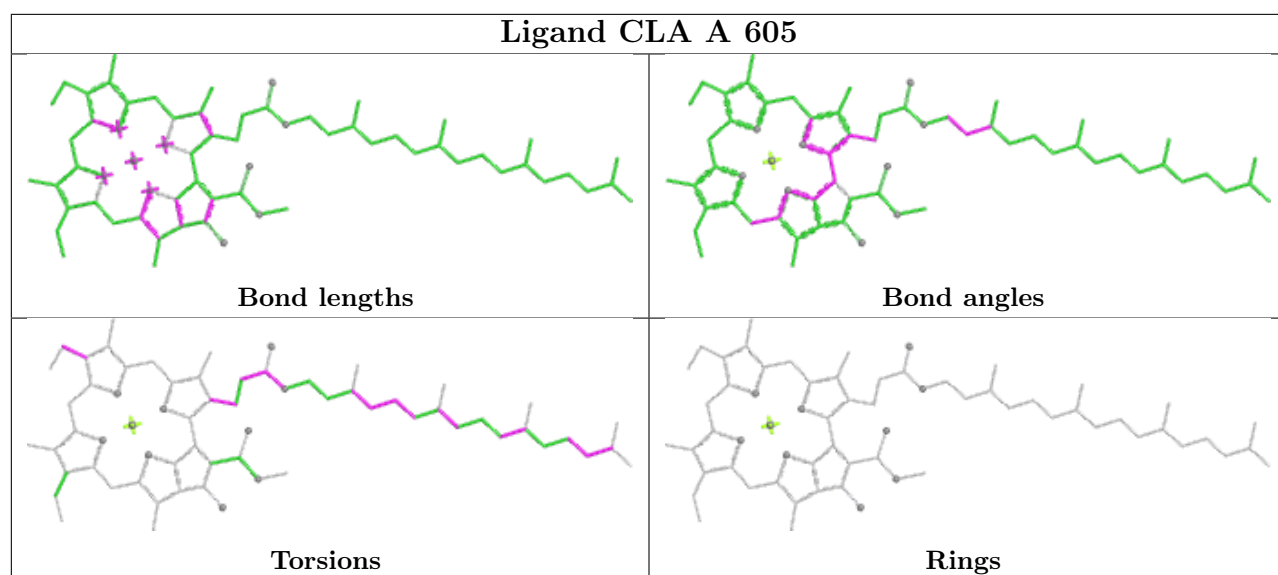


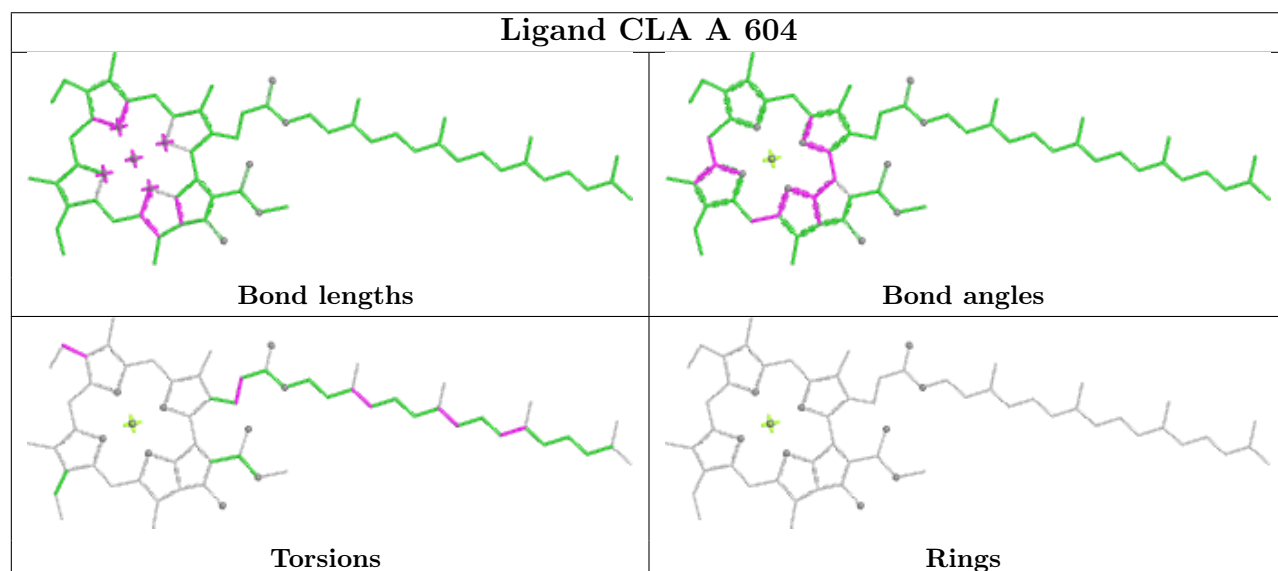
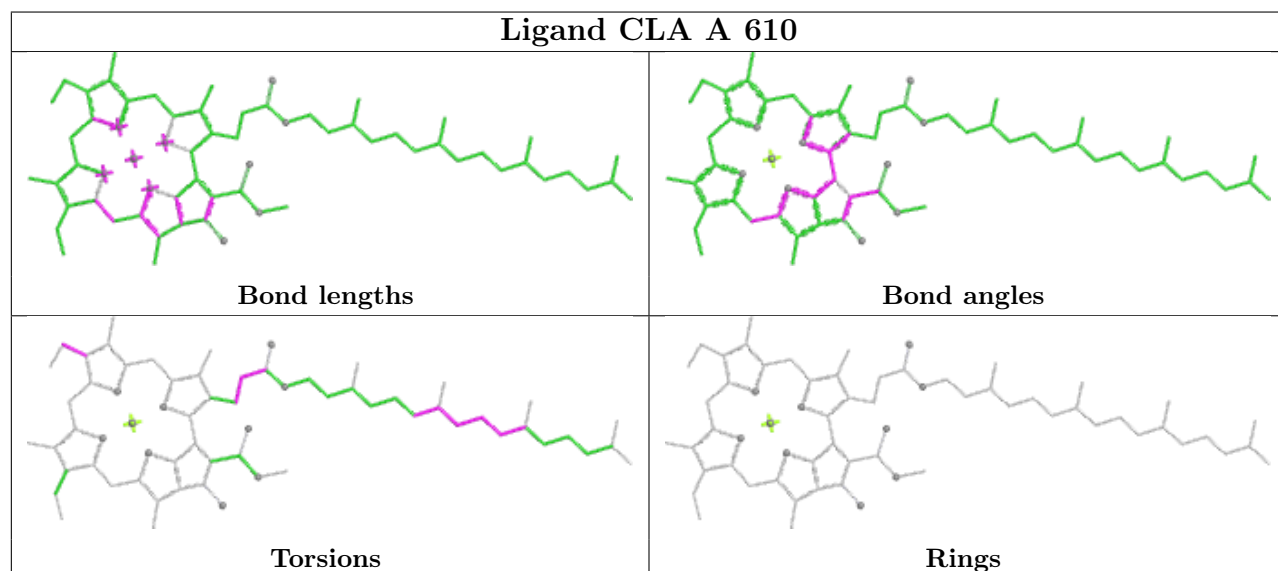
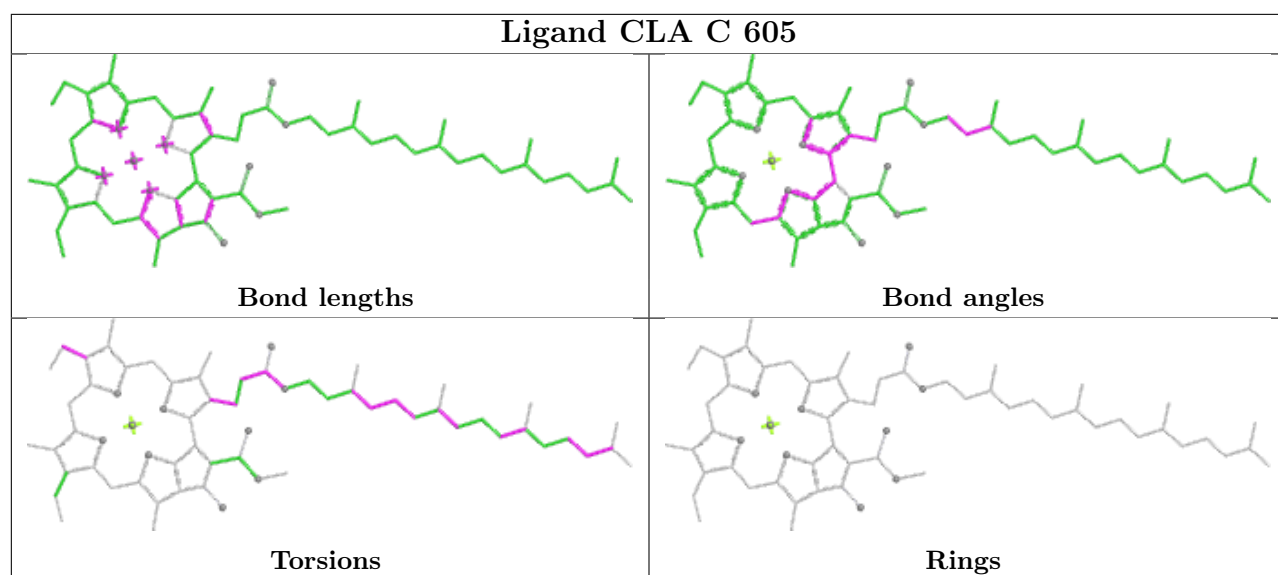


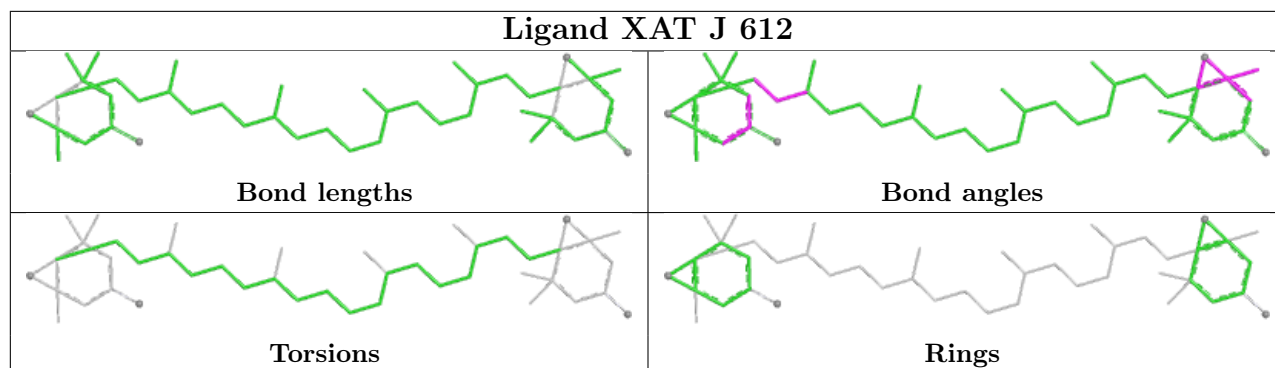
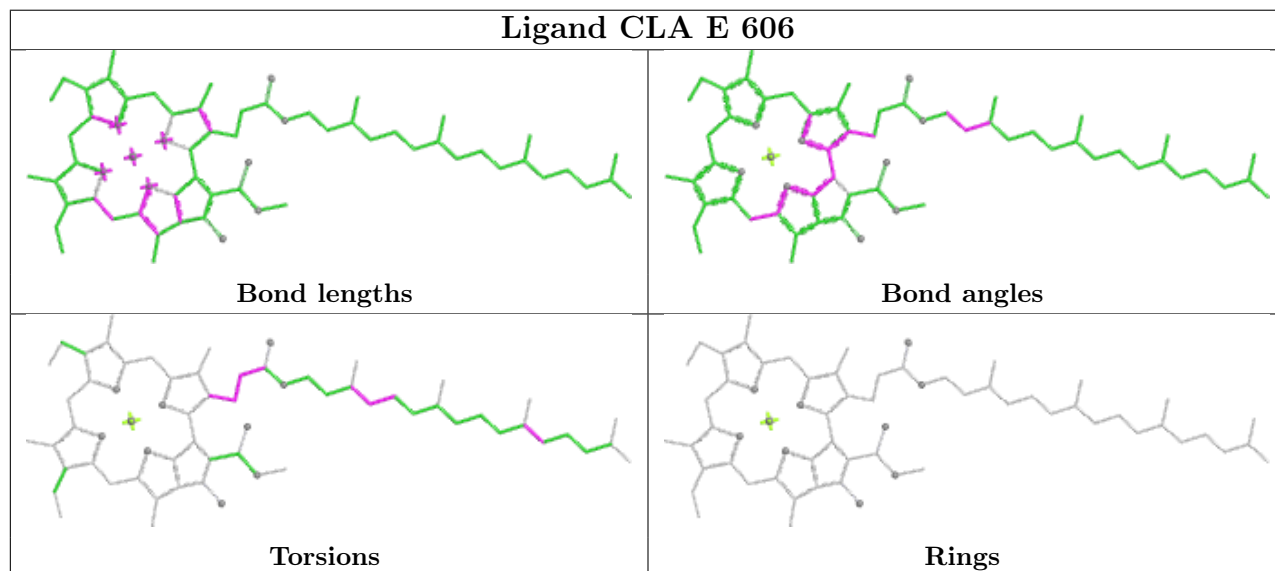
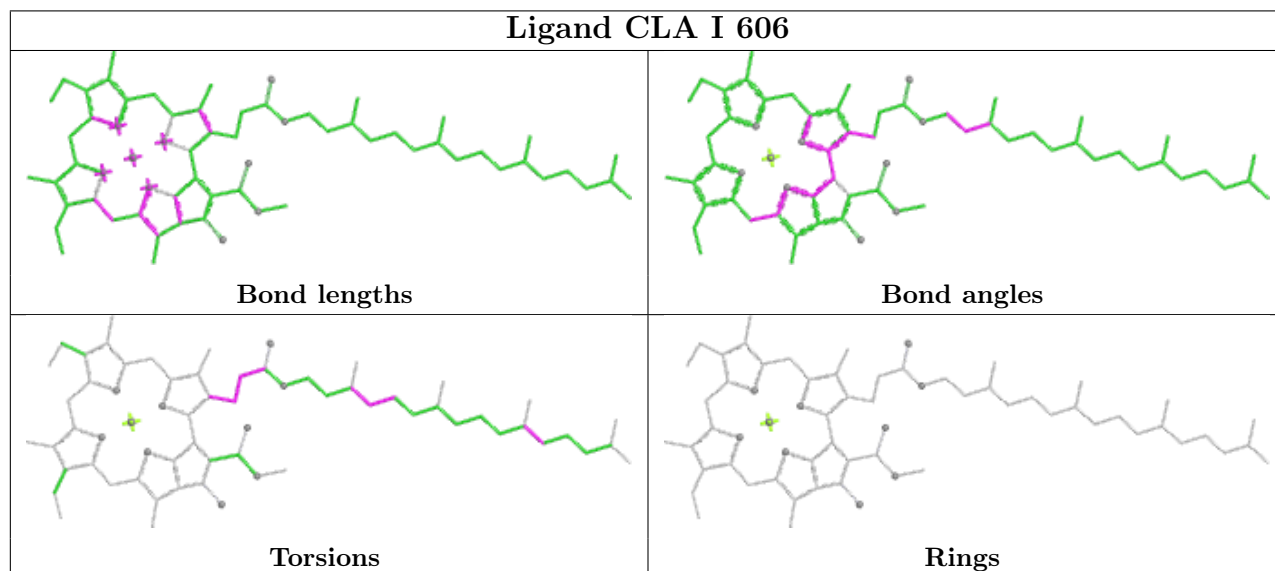


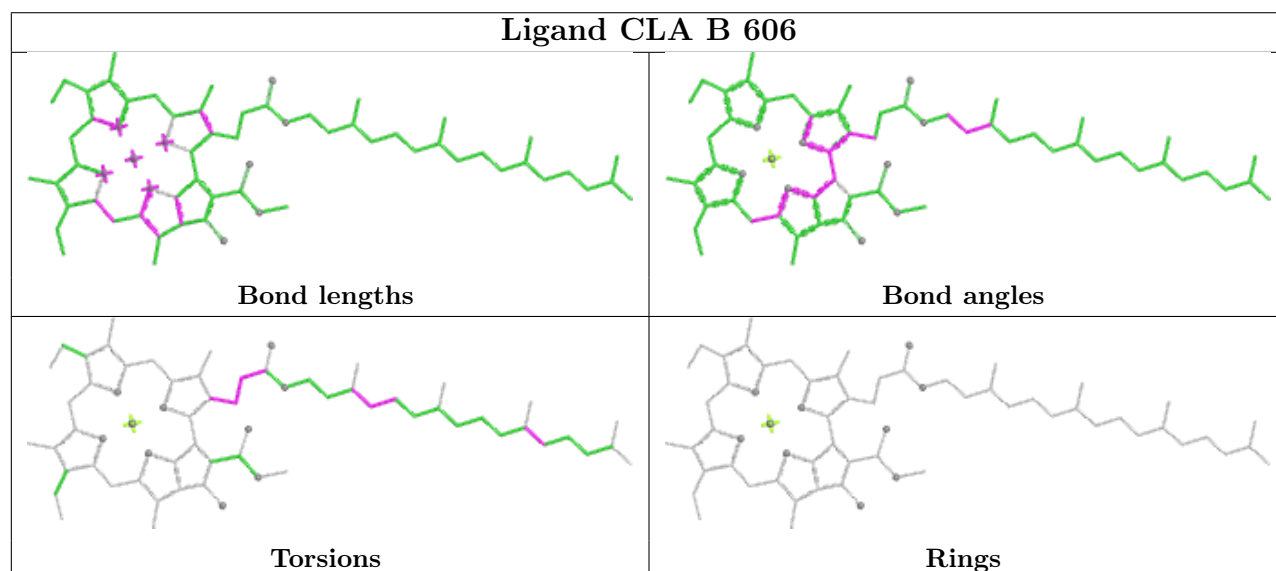
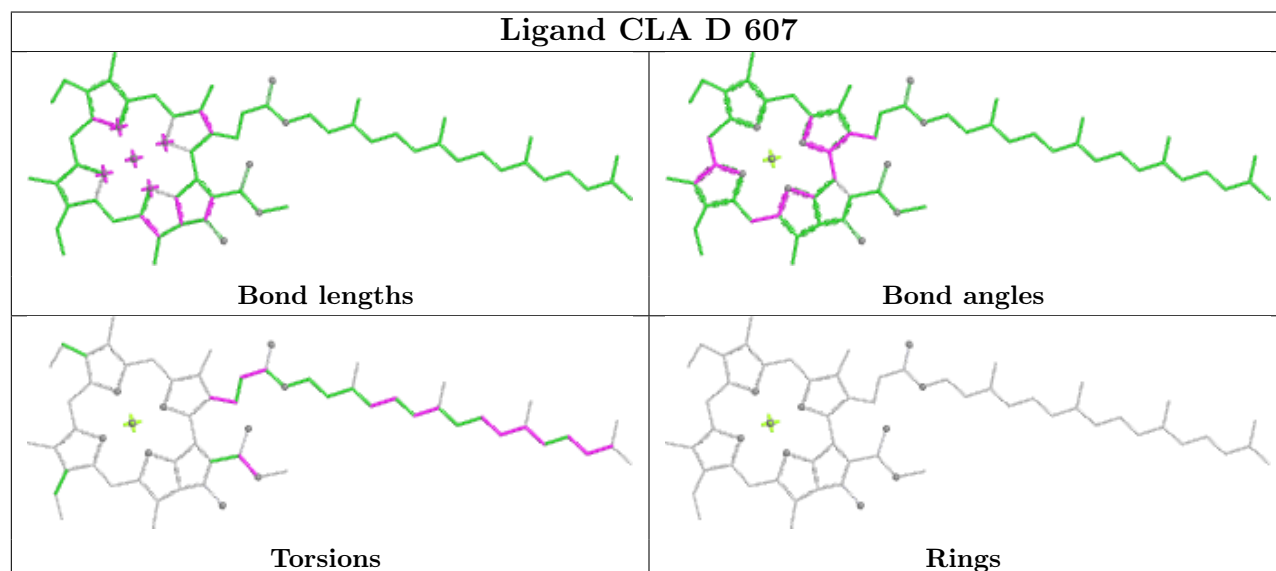
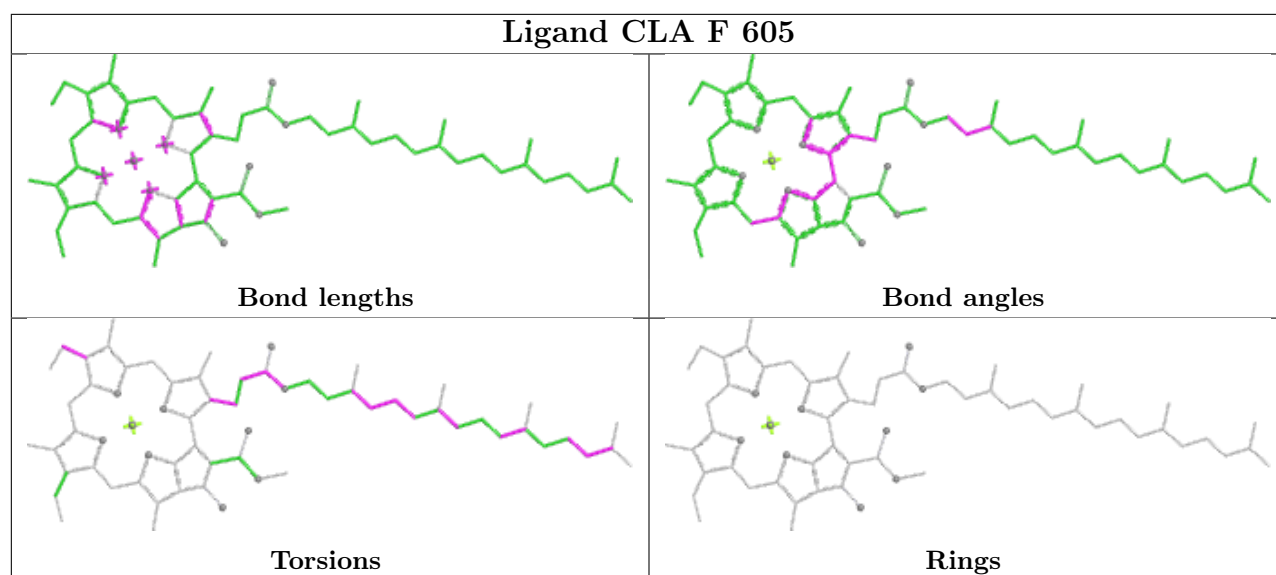


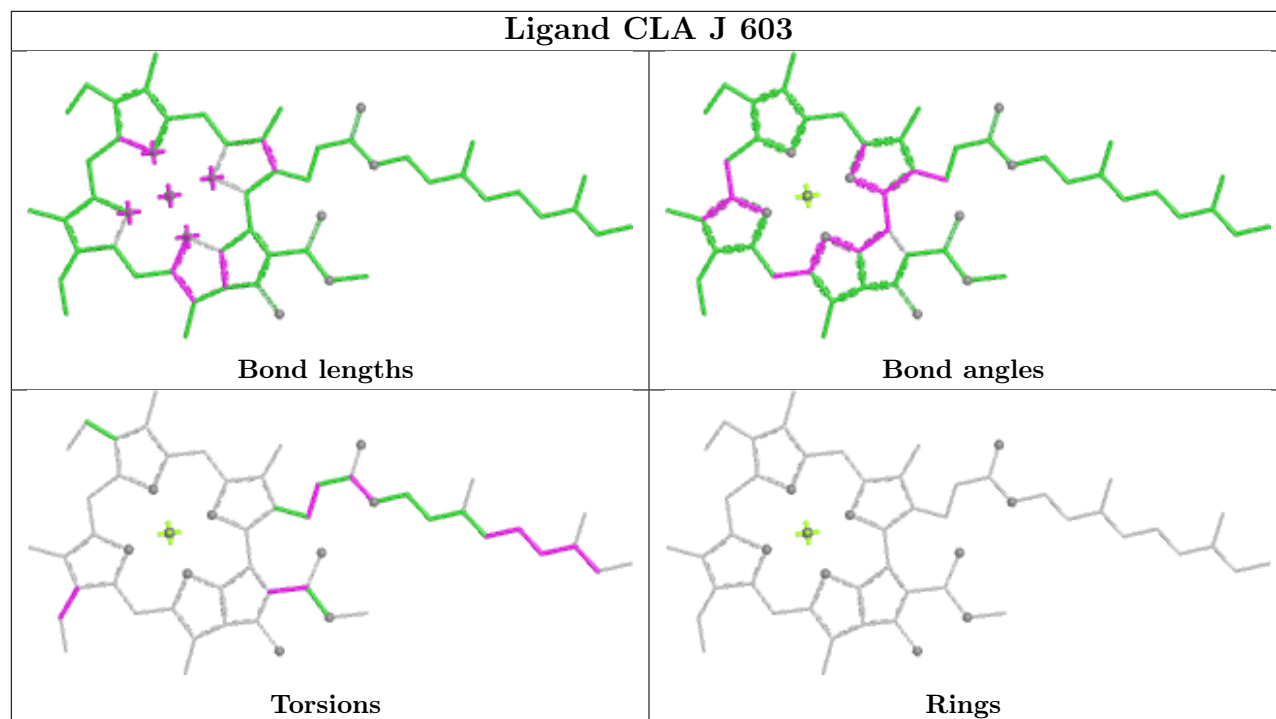
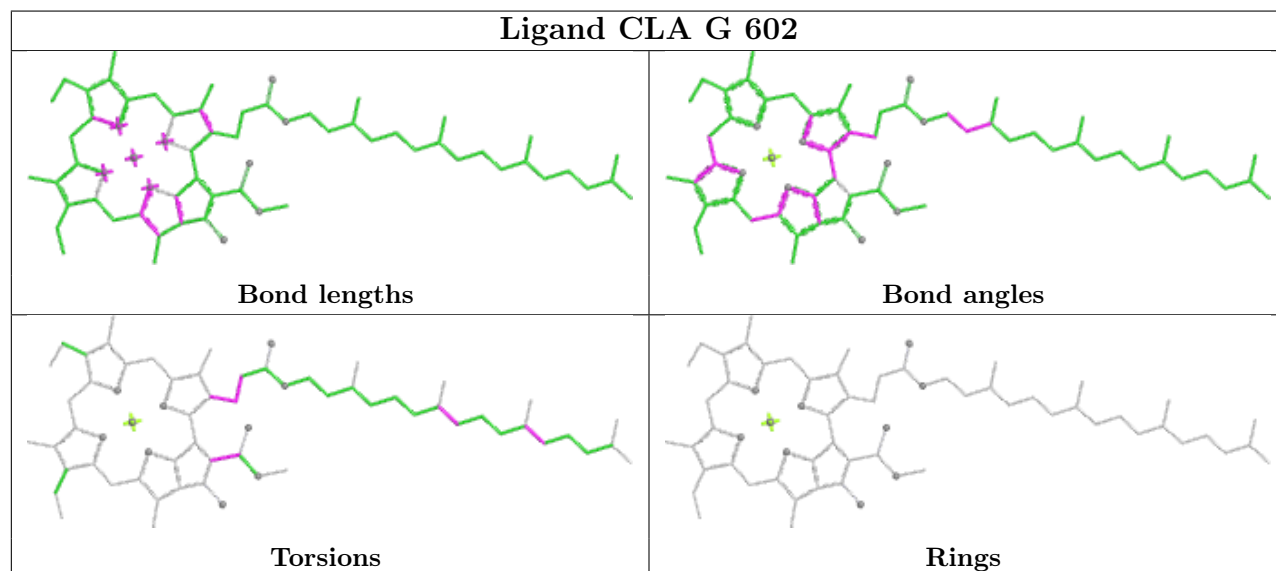
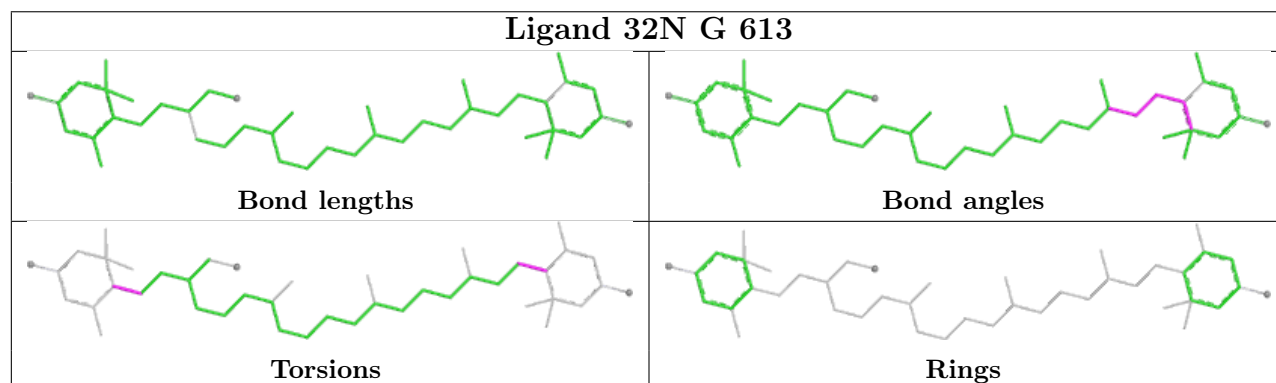


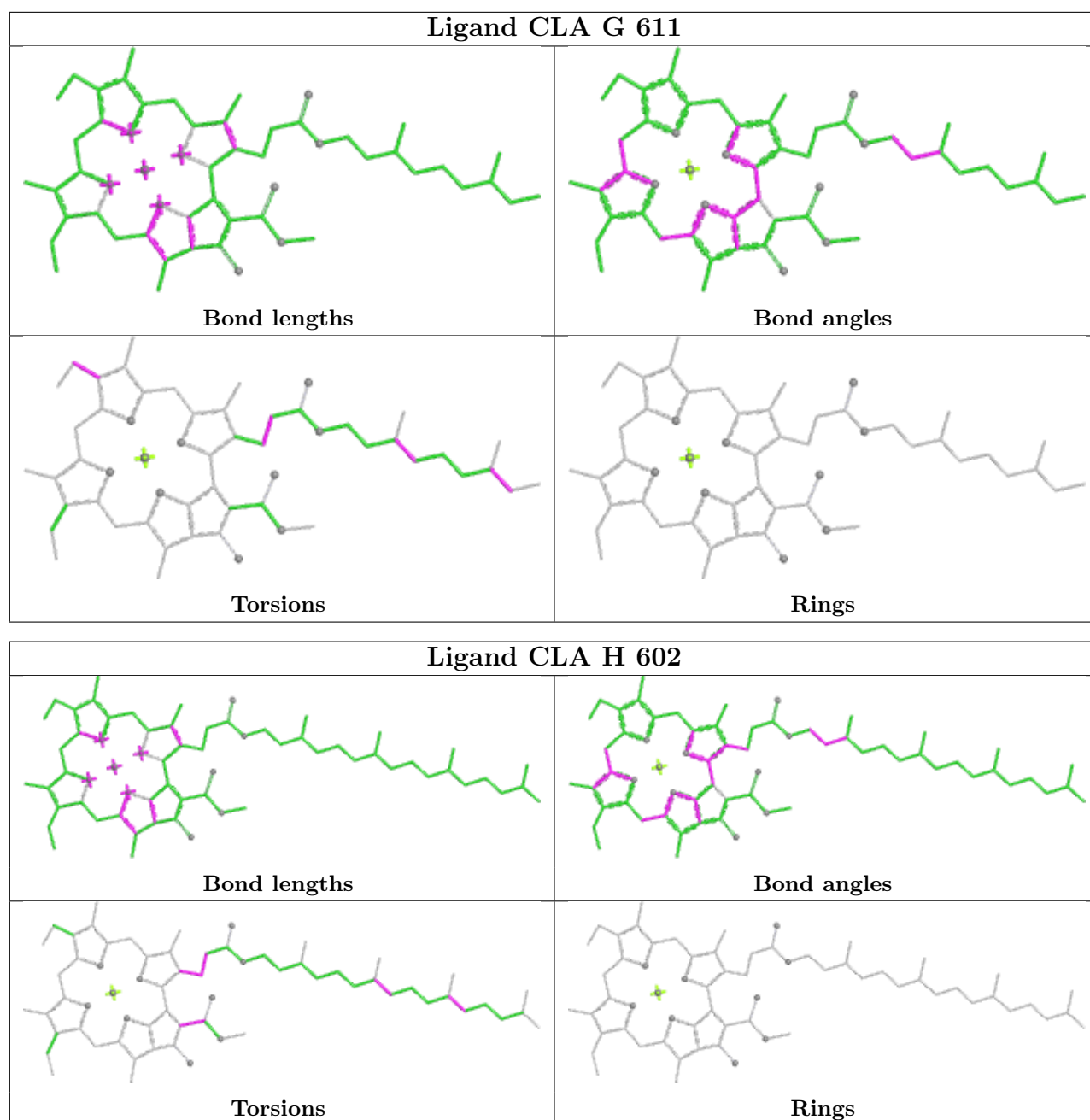


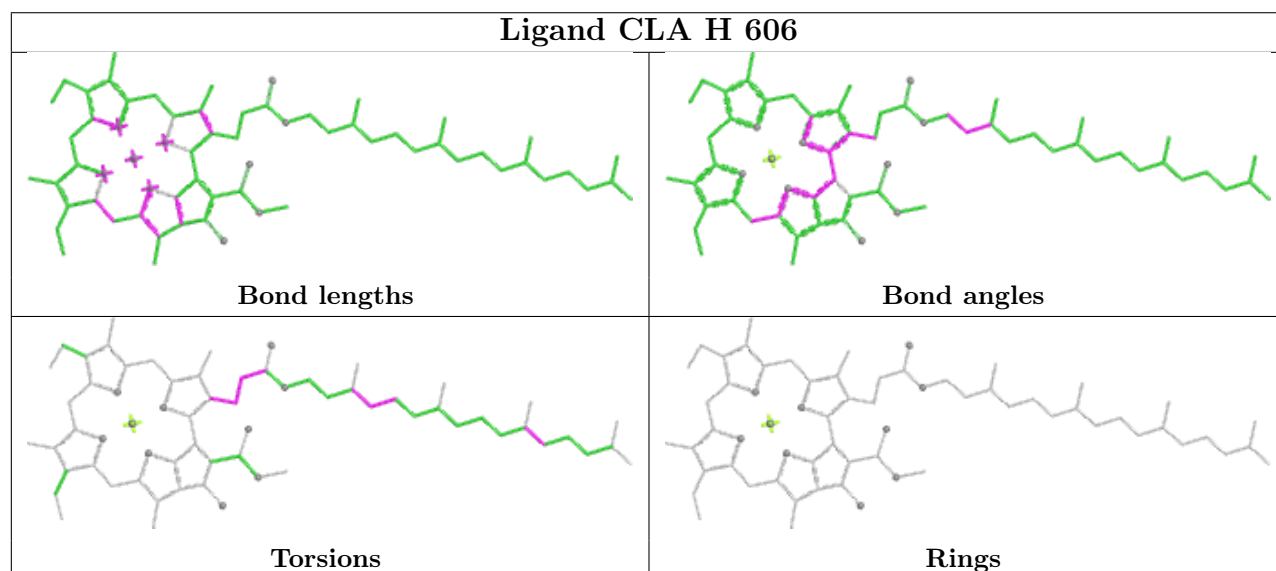
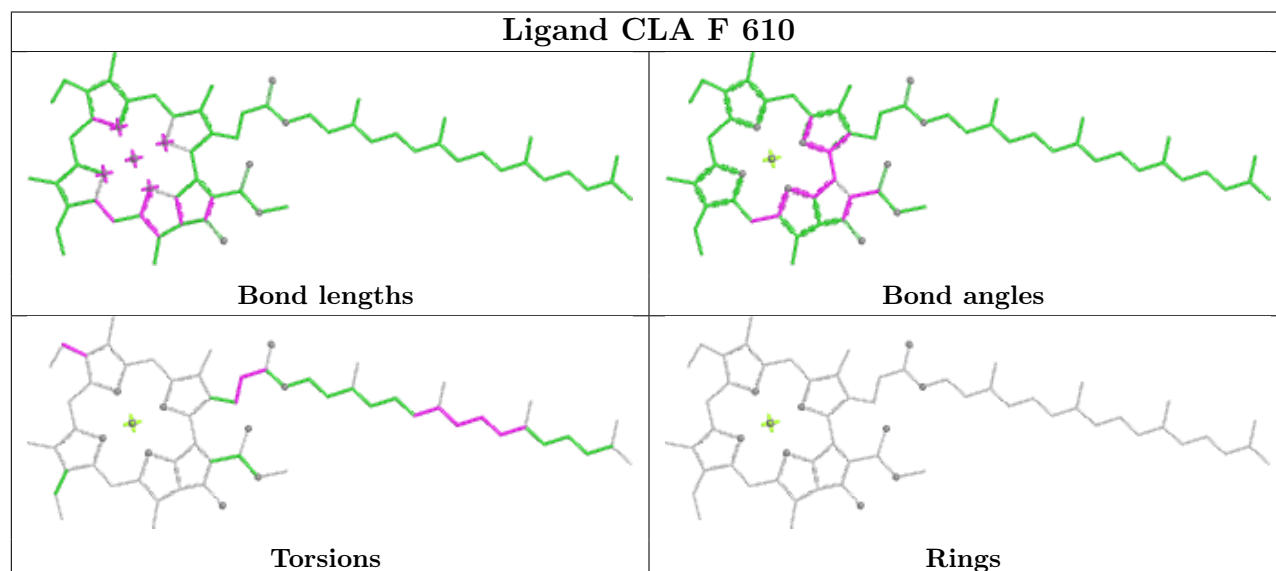
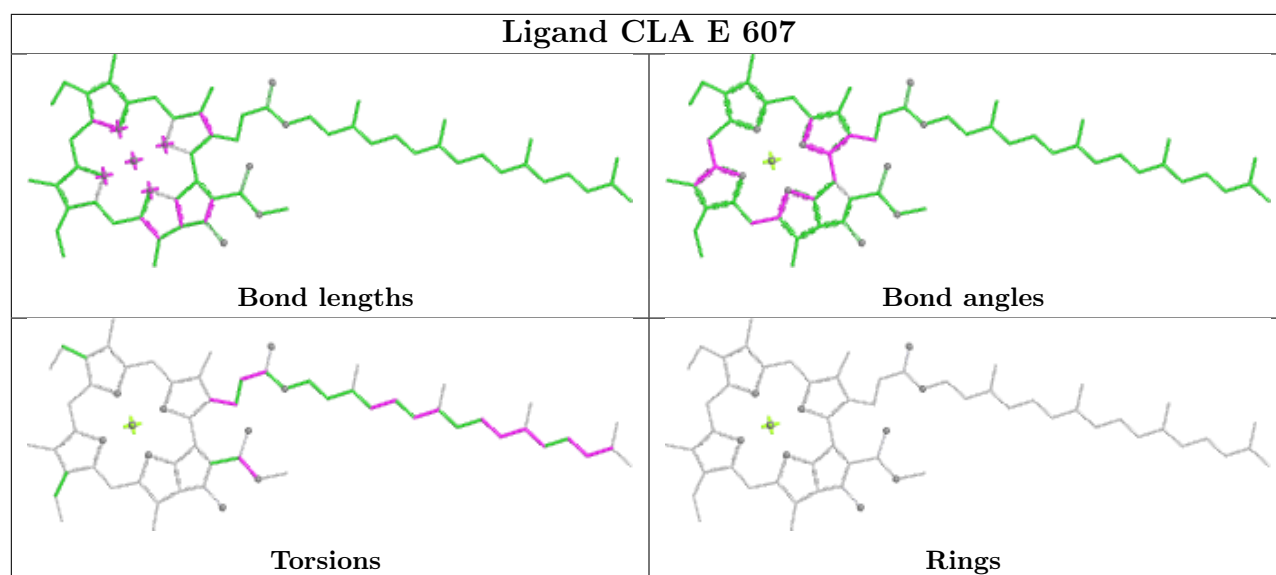


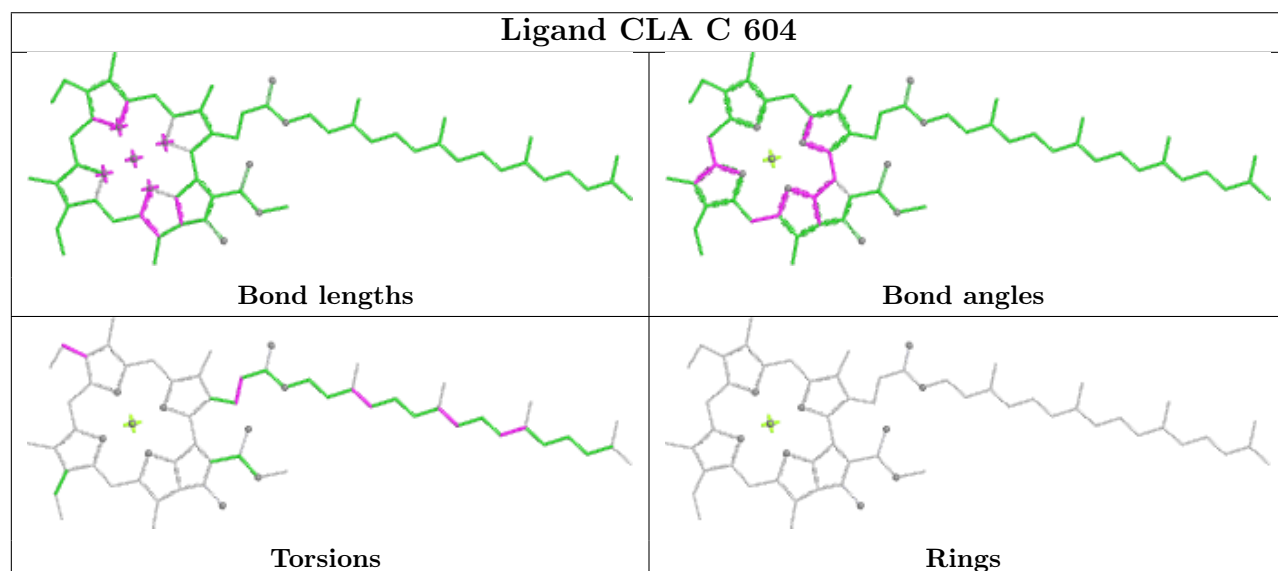
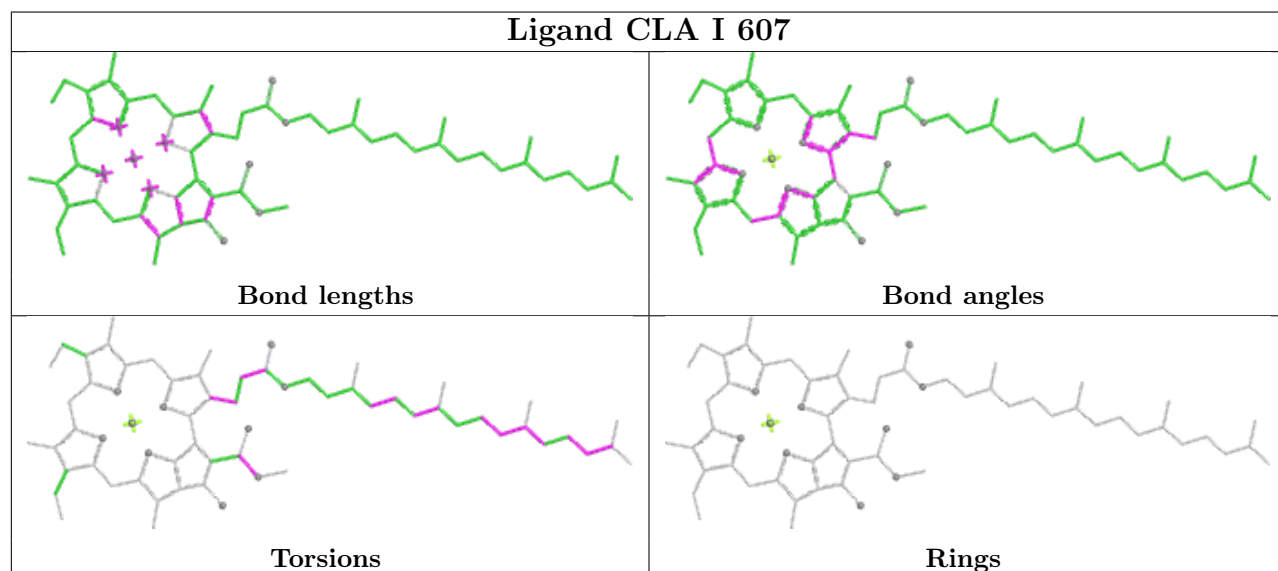
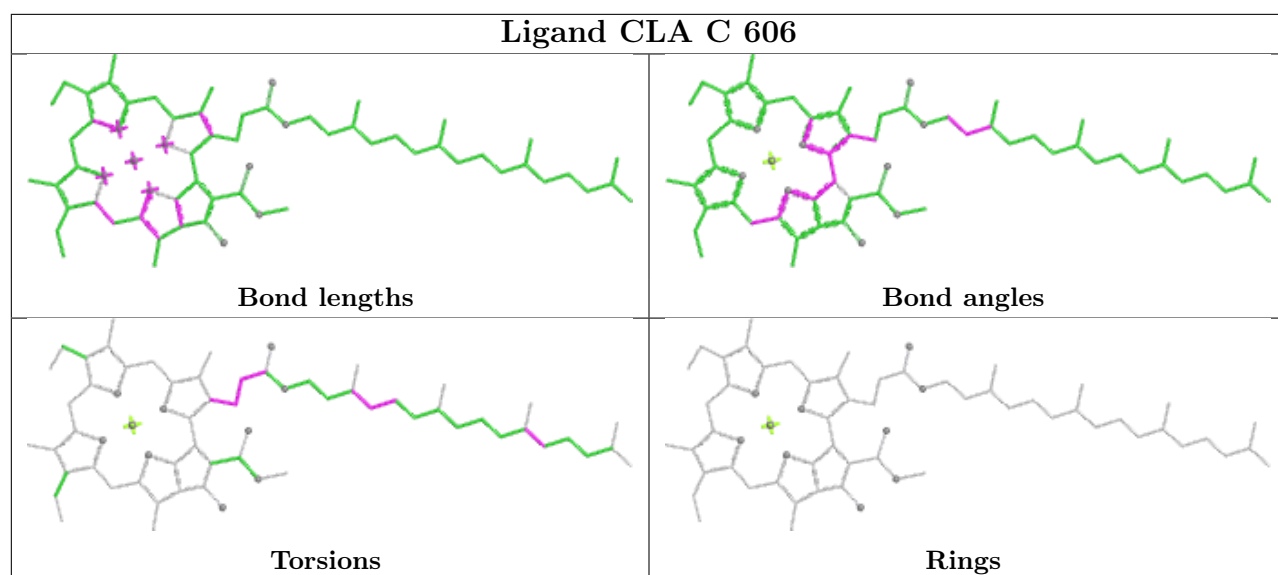
Ligand XAT J 612**Ligand CLA E 606****Ligand CLA I 606**

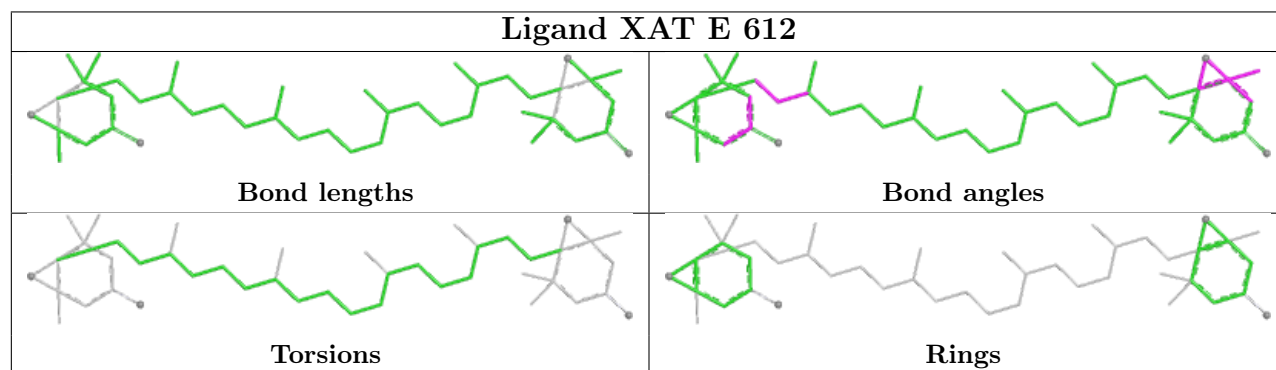
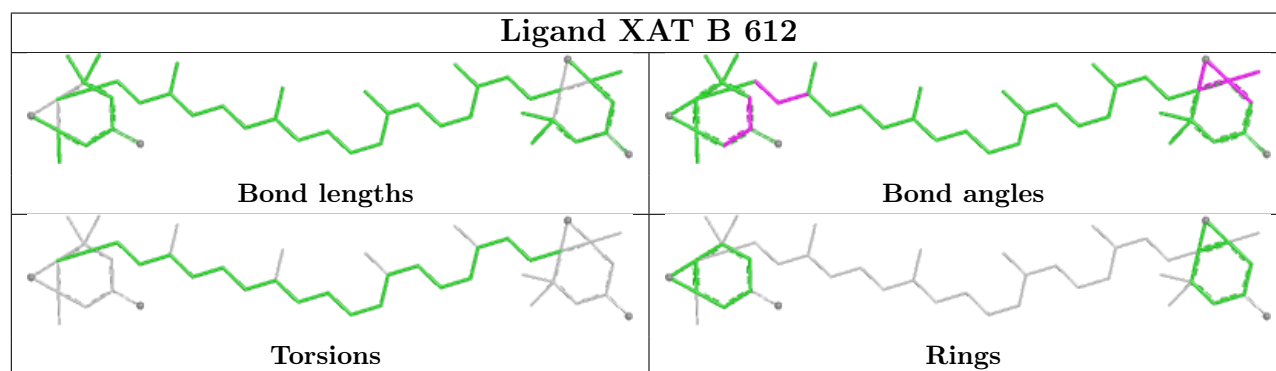
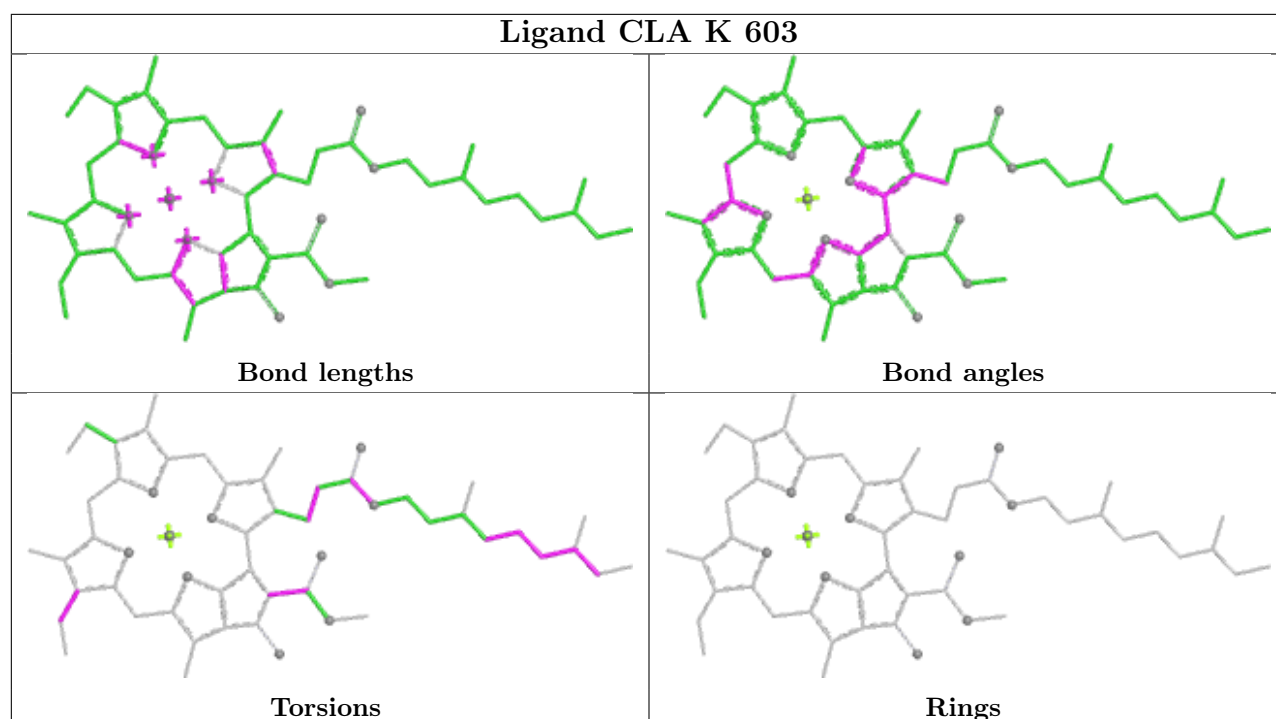


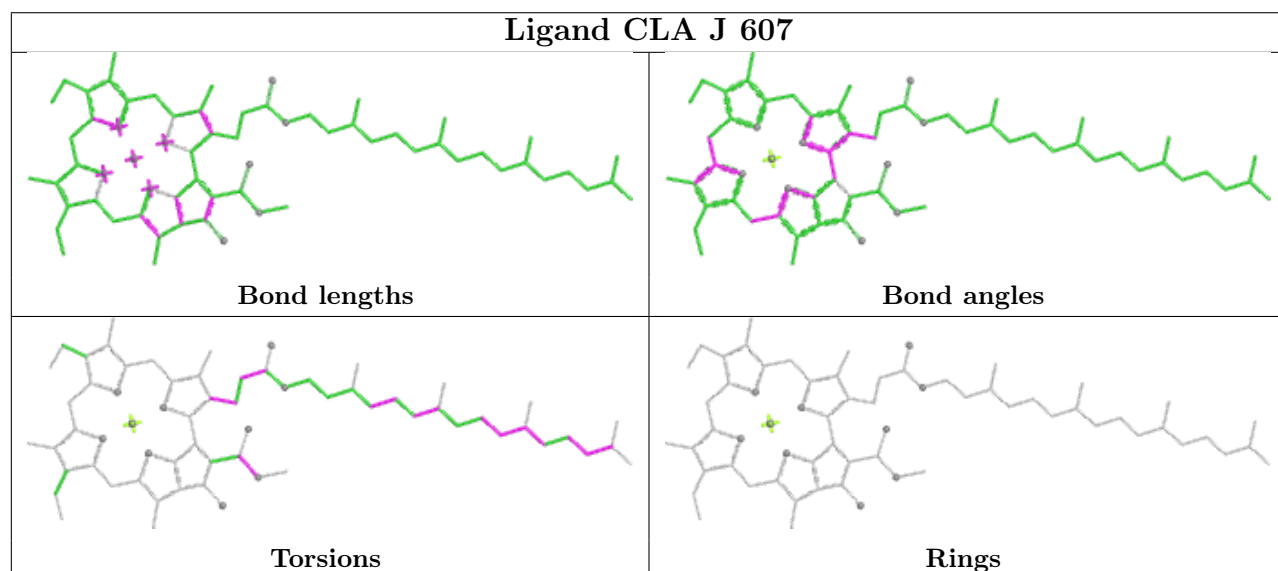
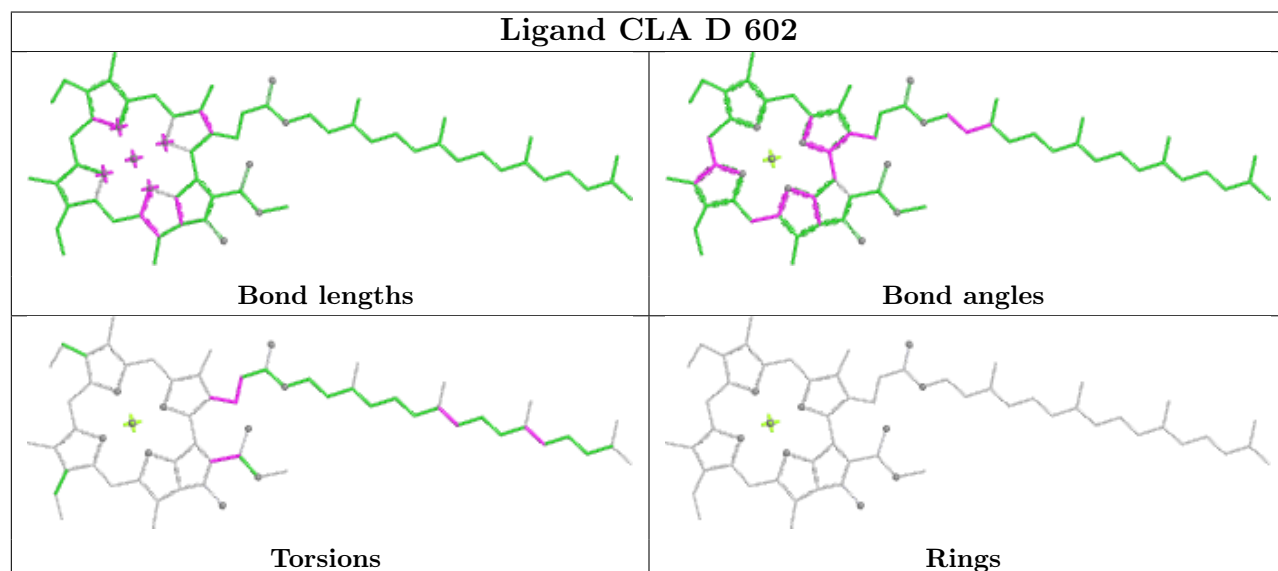
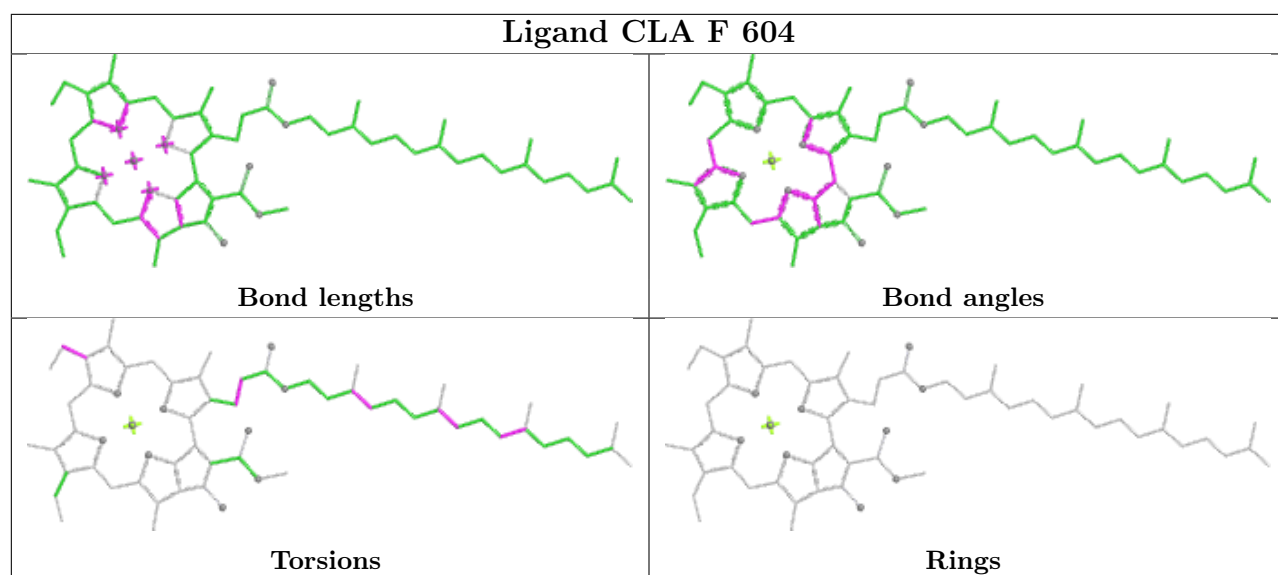
Ligand CLA J 603**Ligand CLA G 602****Ligand 32N G 613**

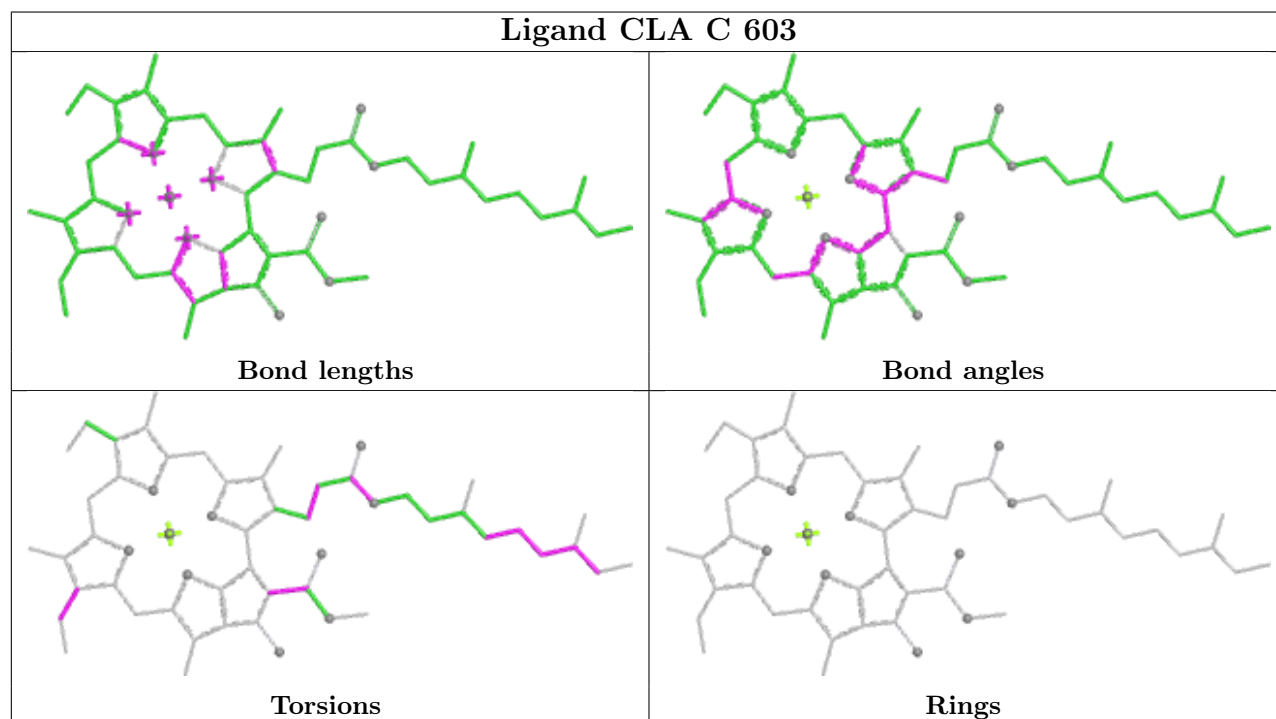
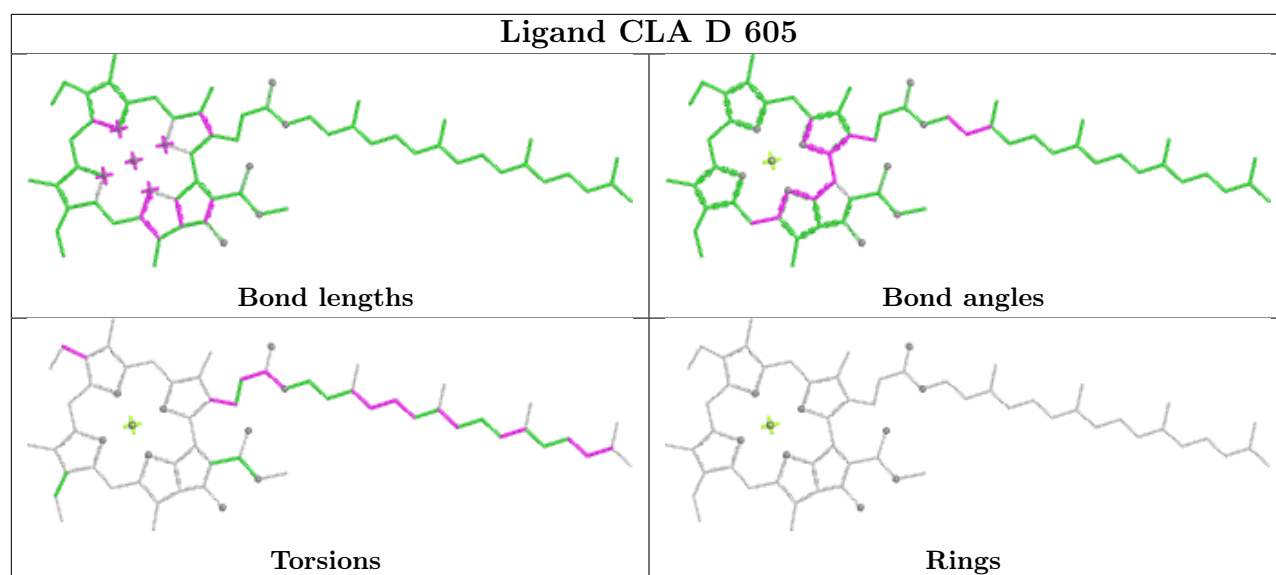


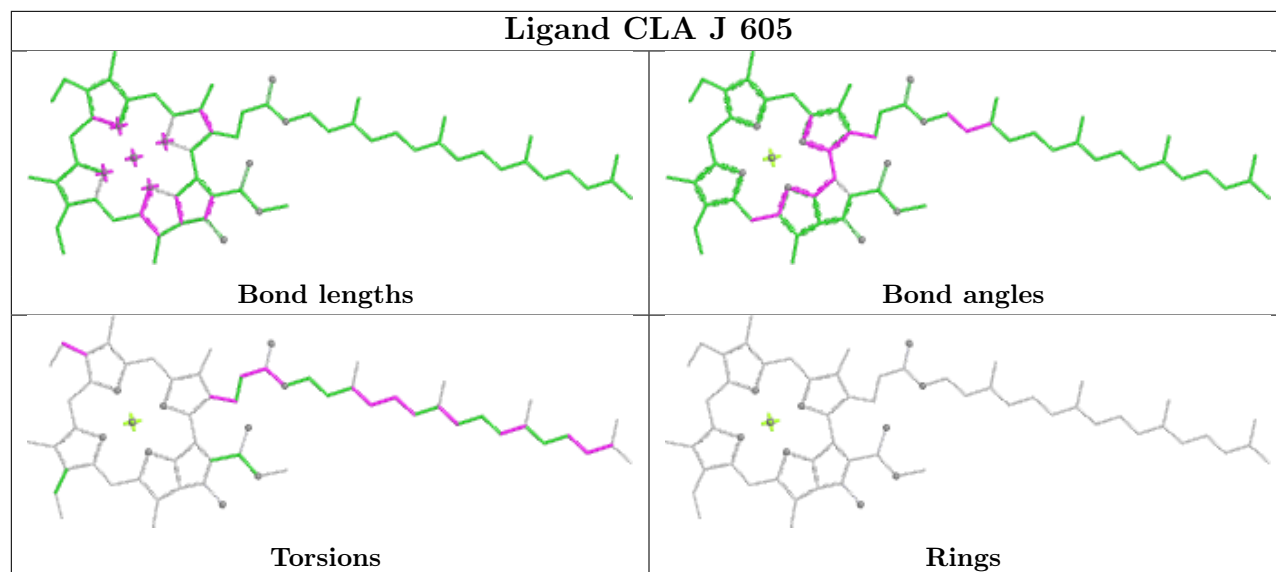
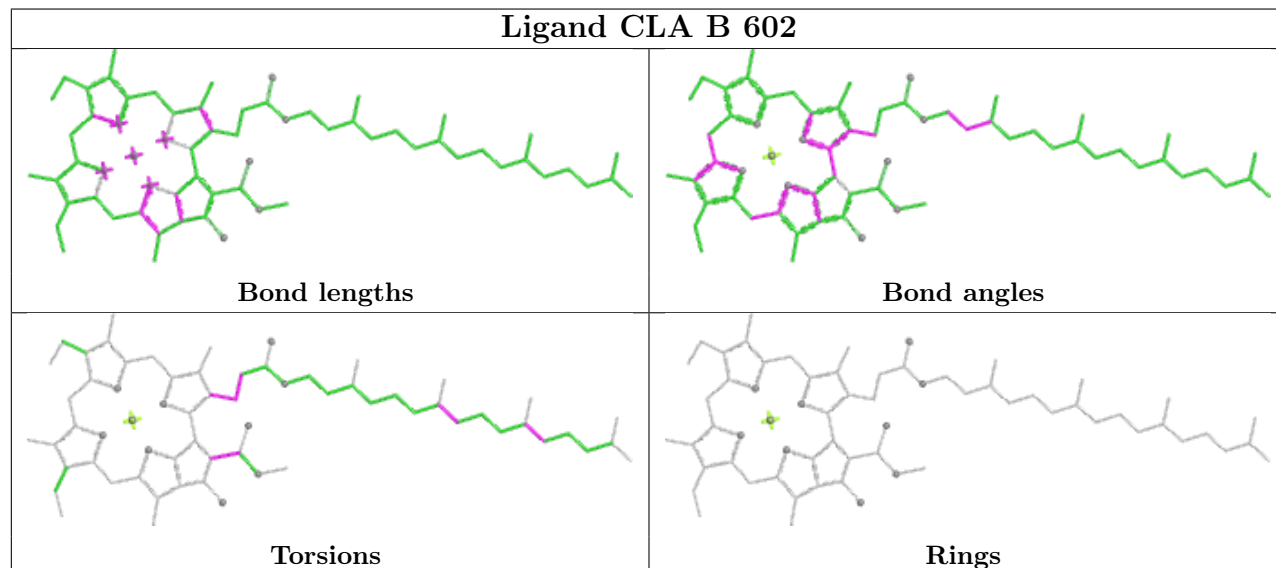


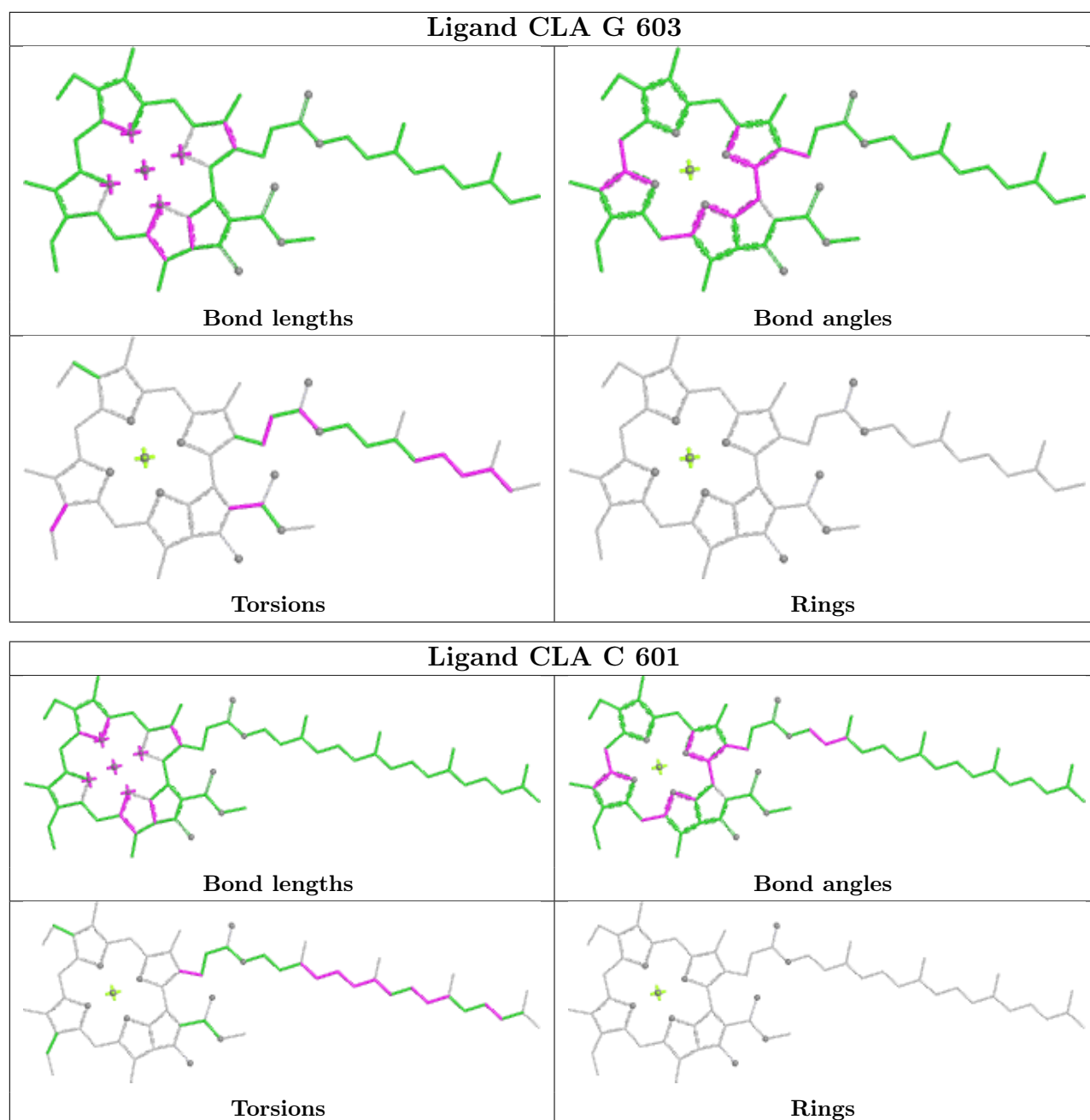


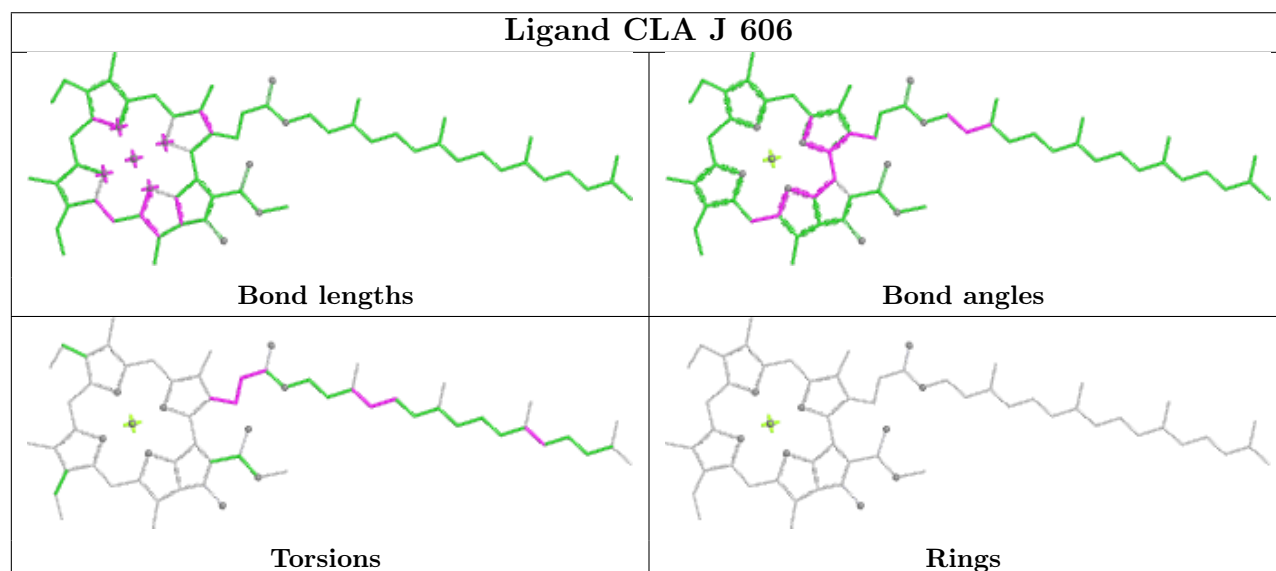
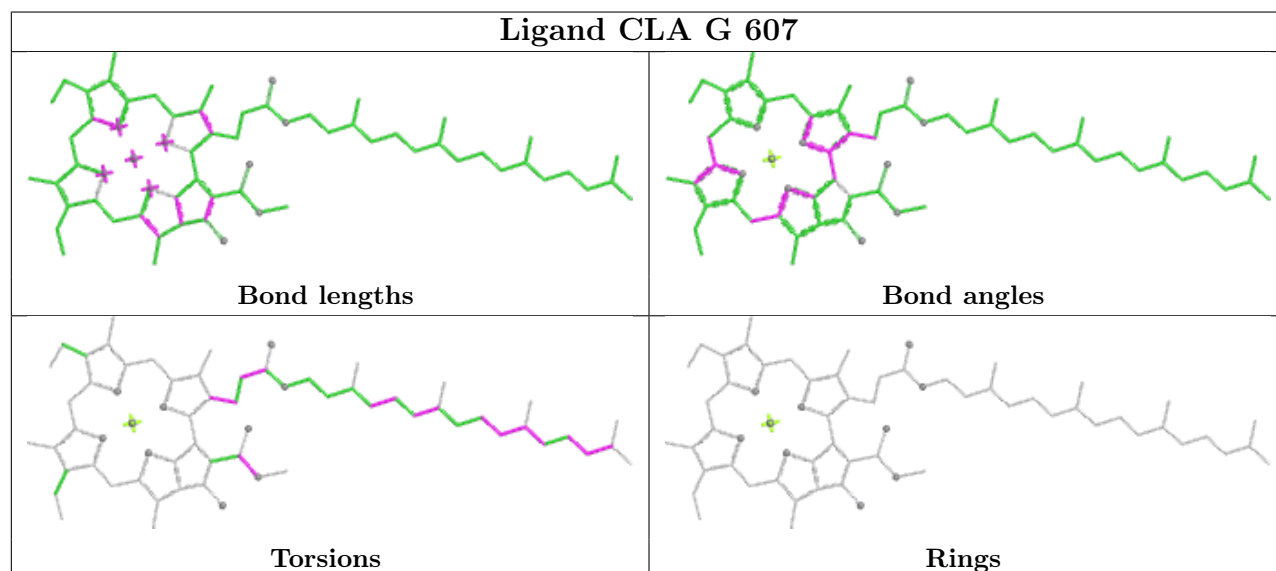
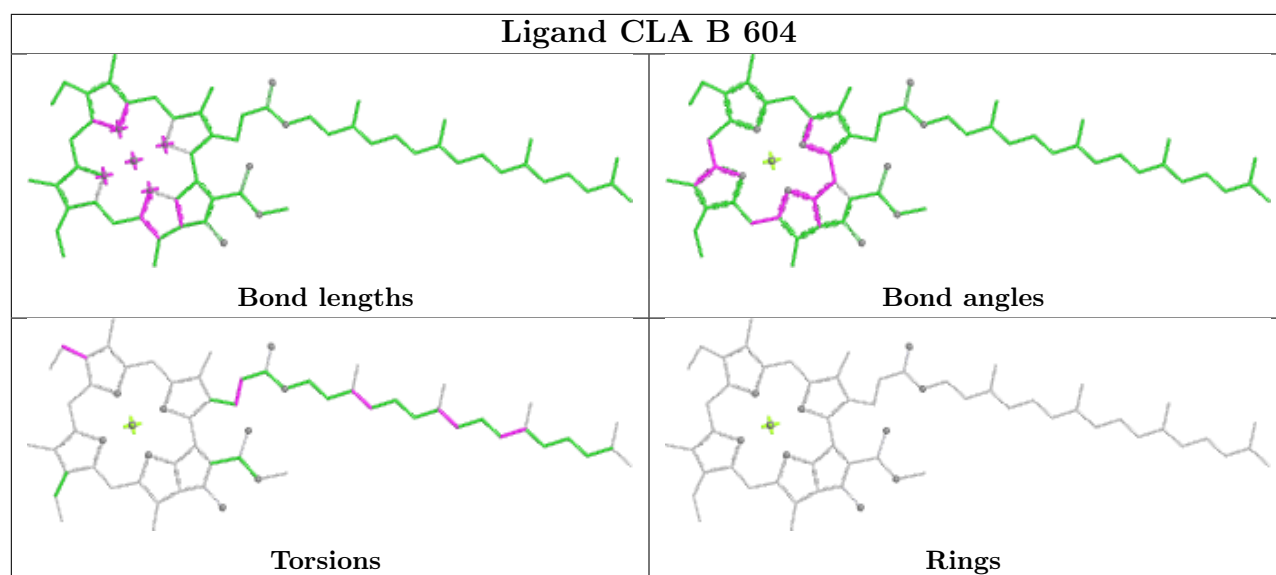


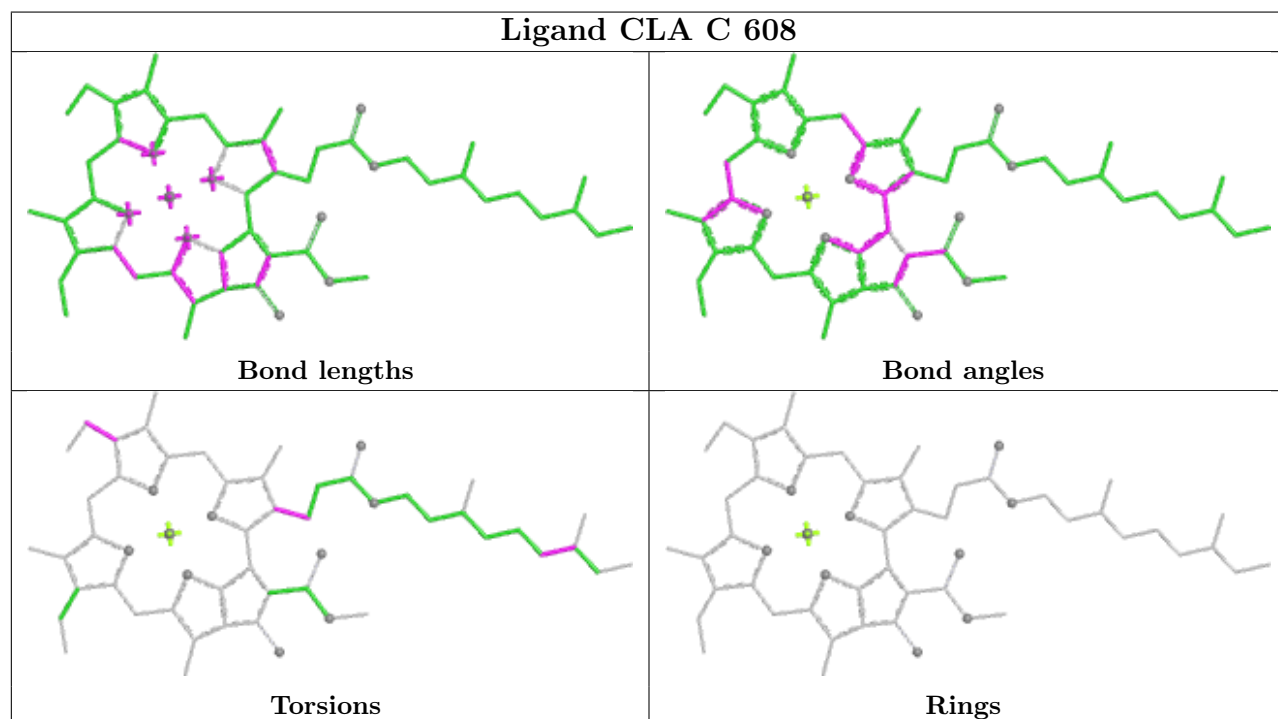
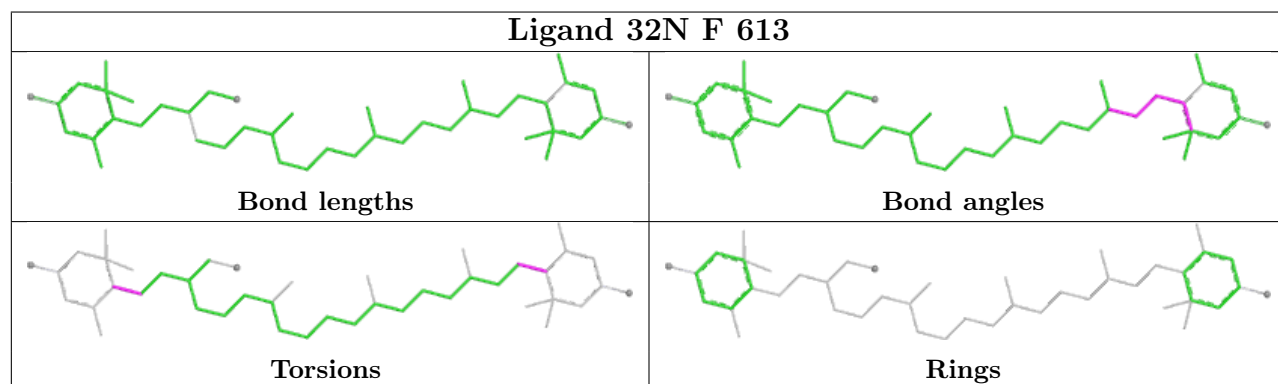
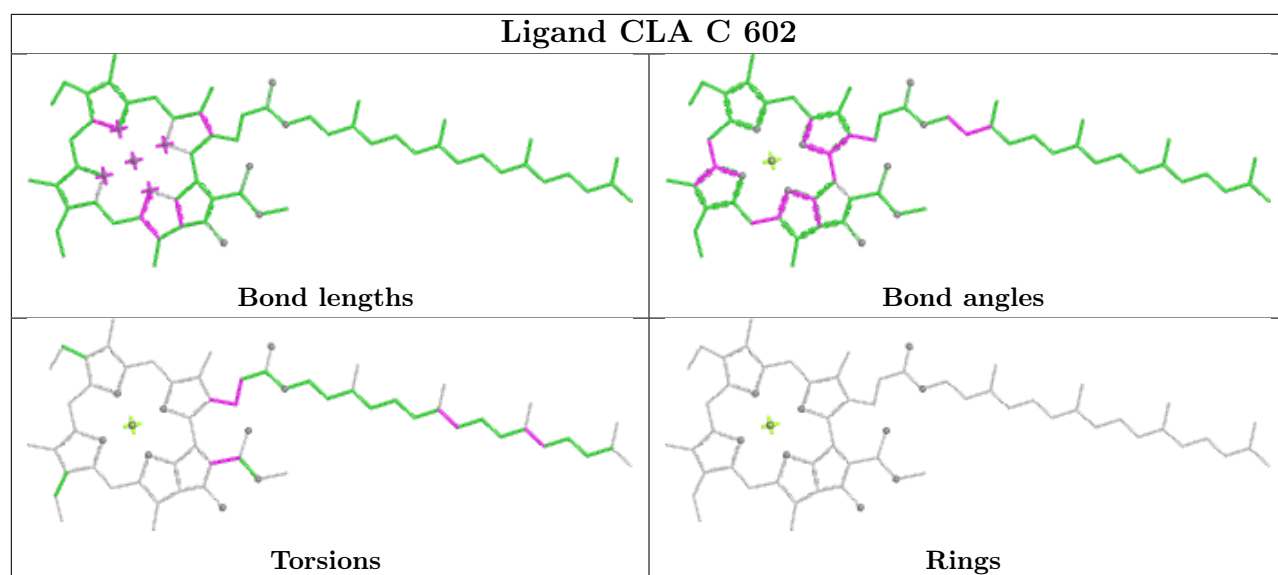




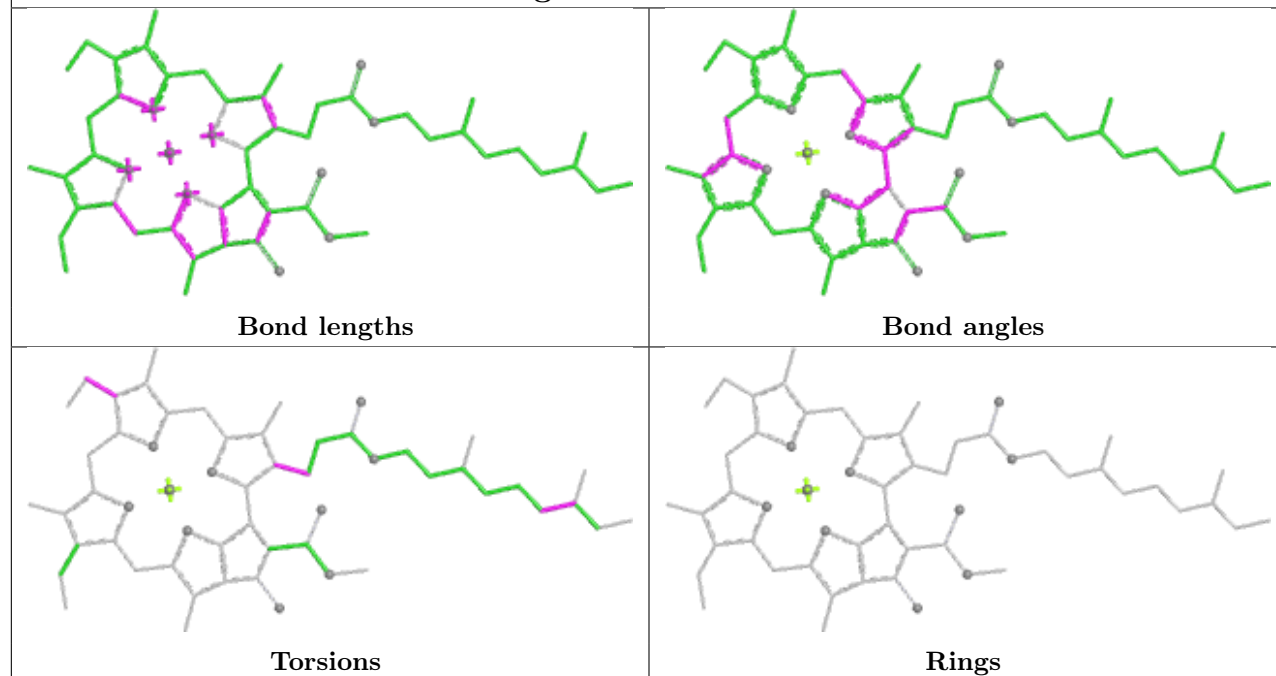
Ligand CLA J 605**Ligand CLA B 602**



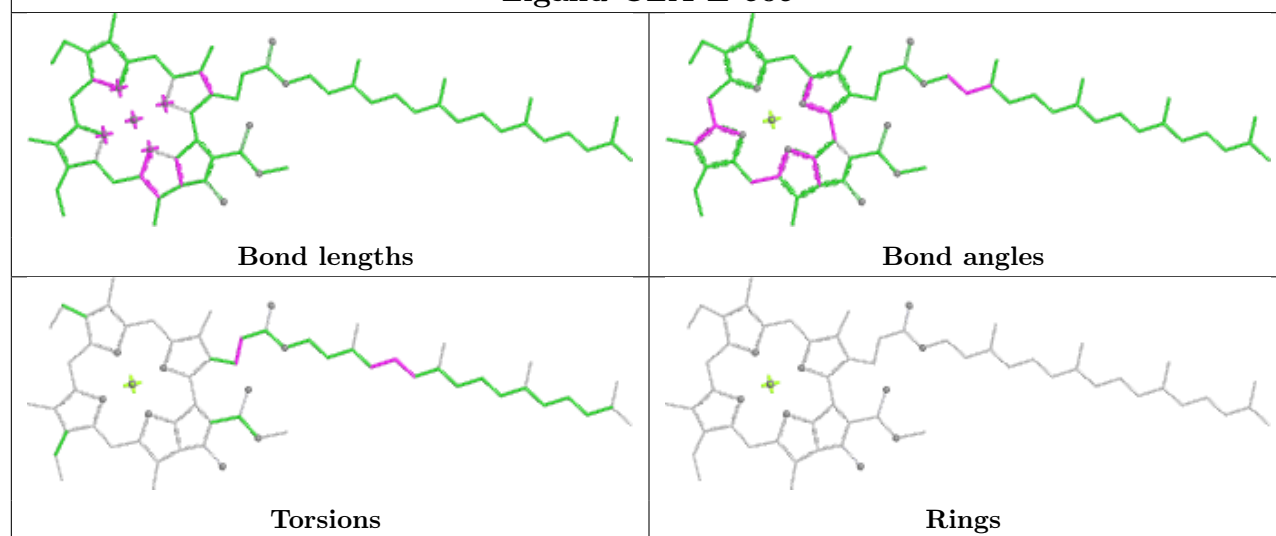


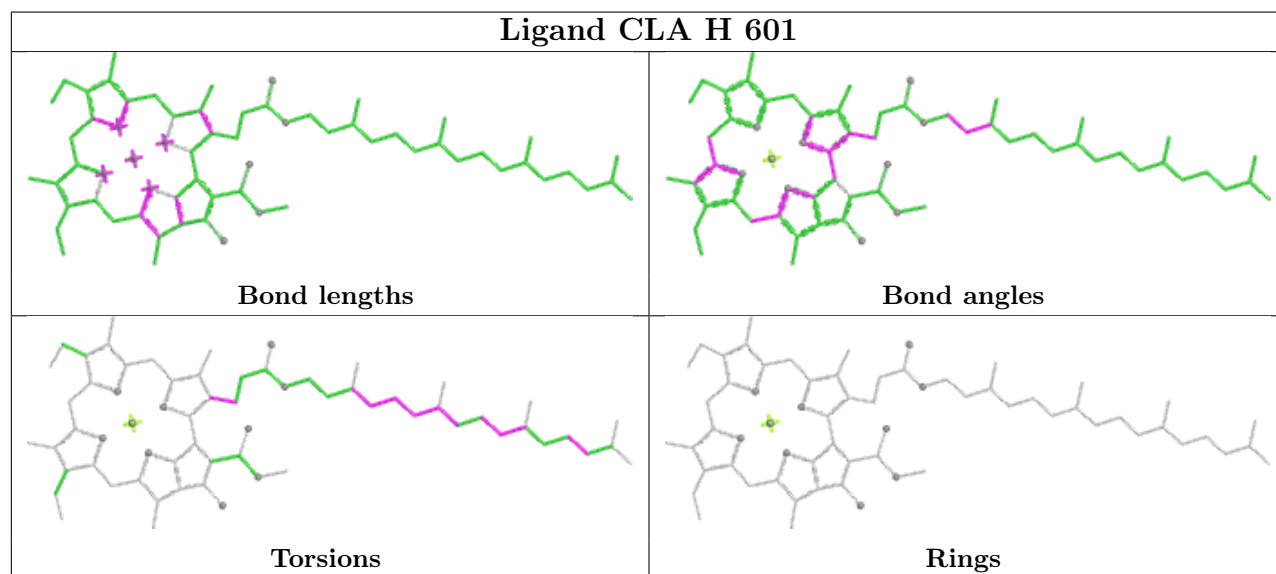
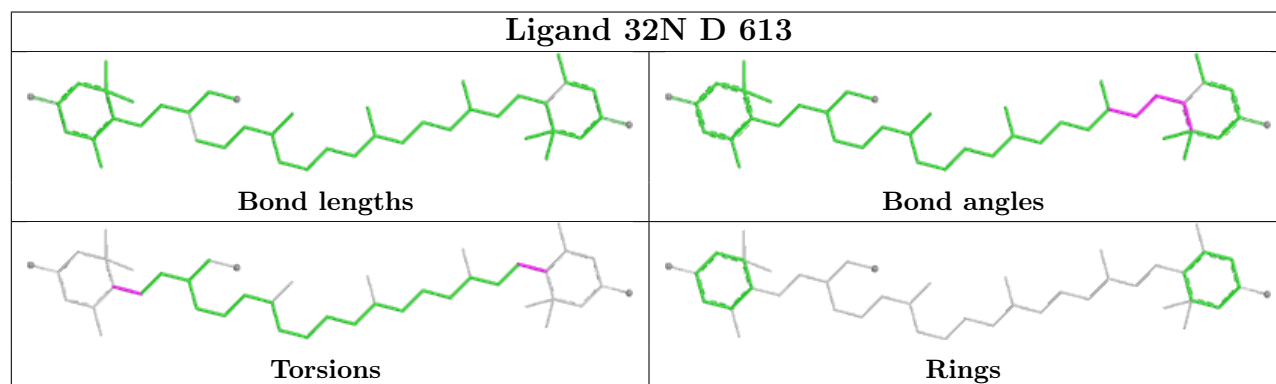
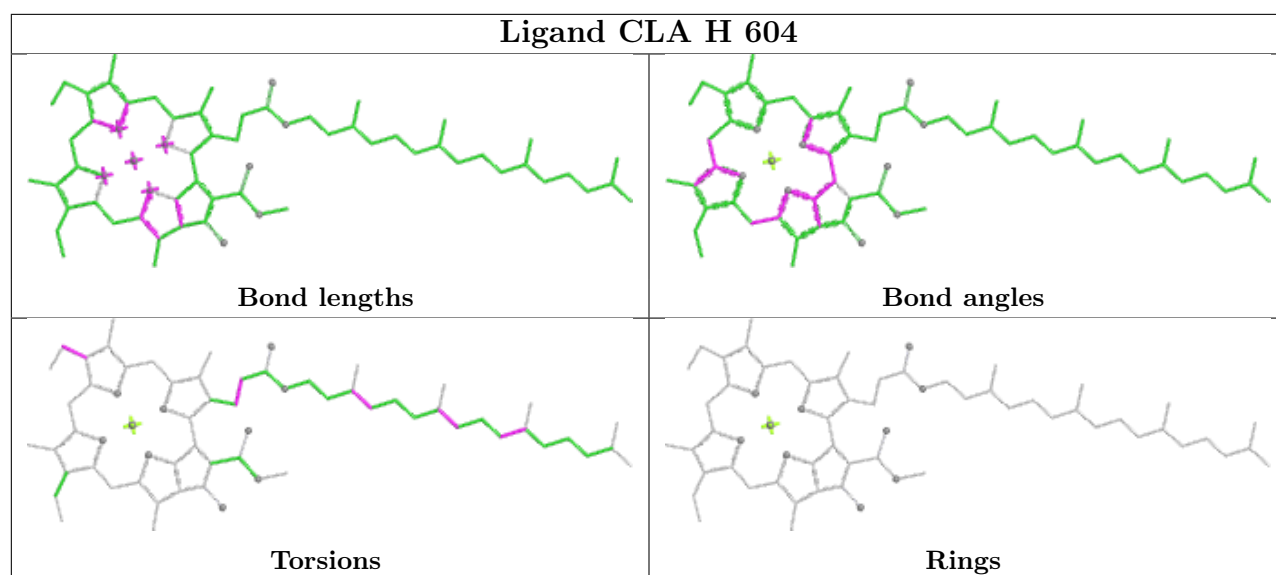


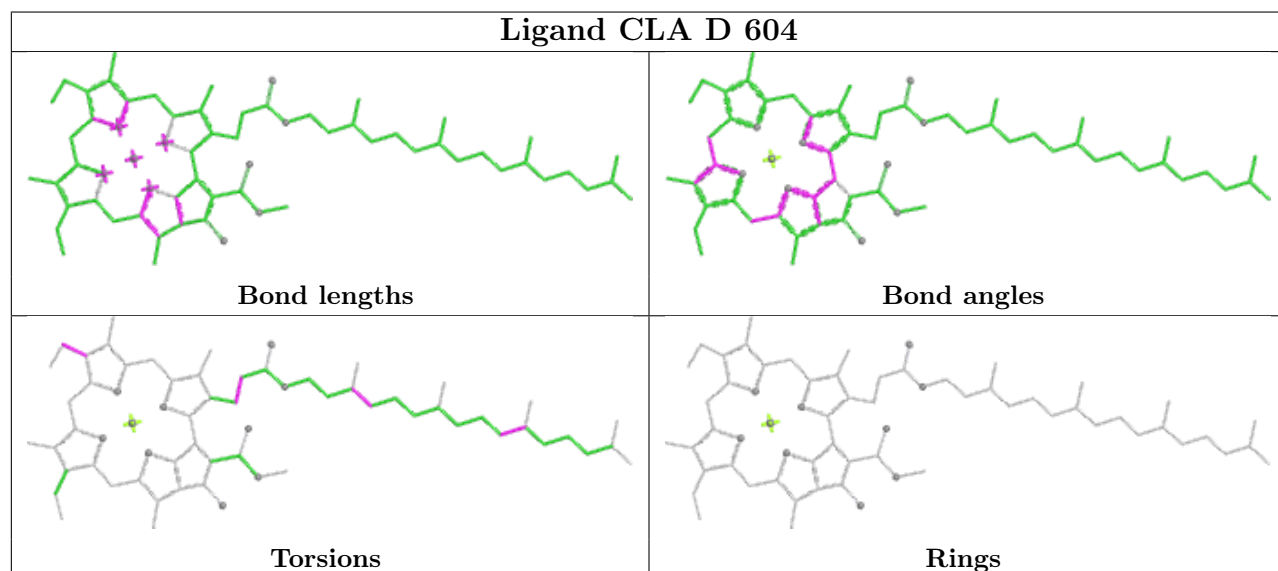
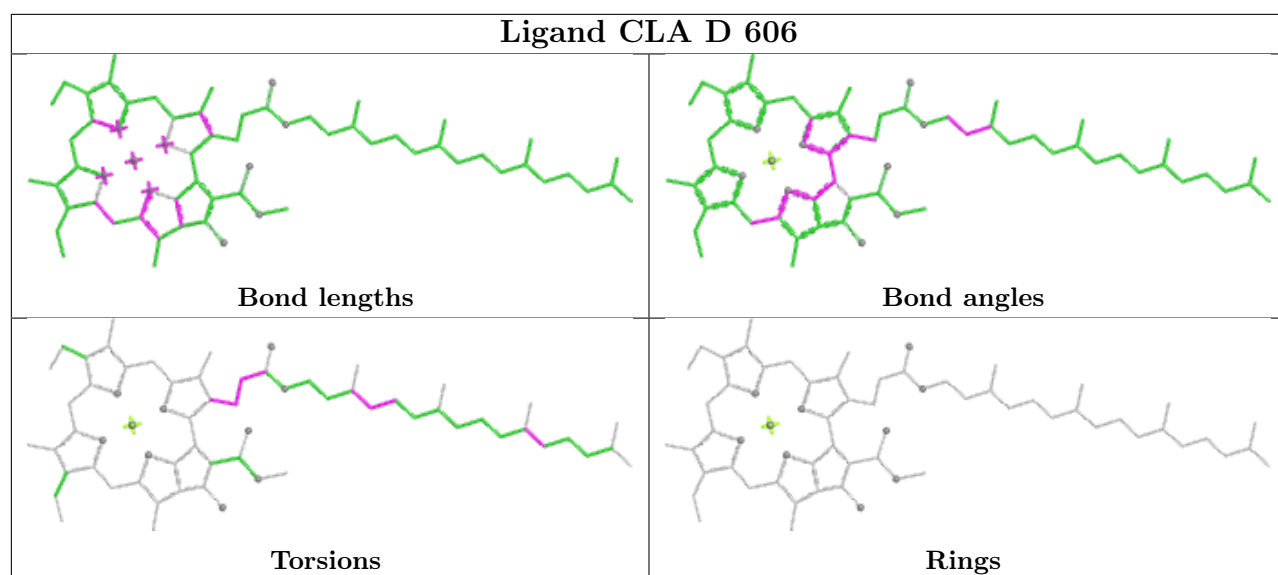
Ligand CLA F 608

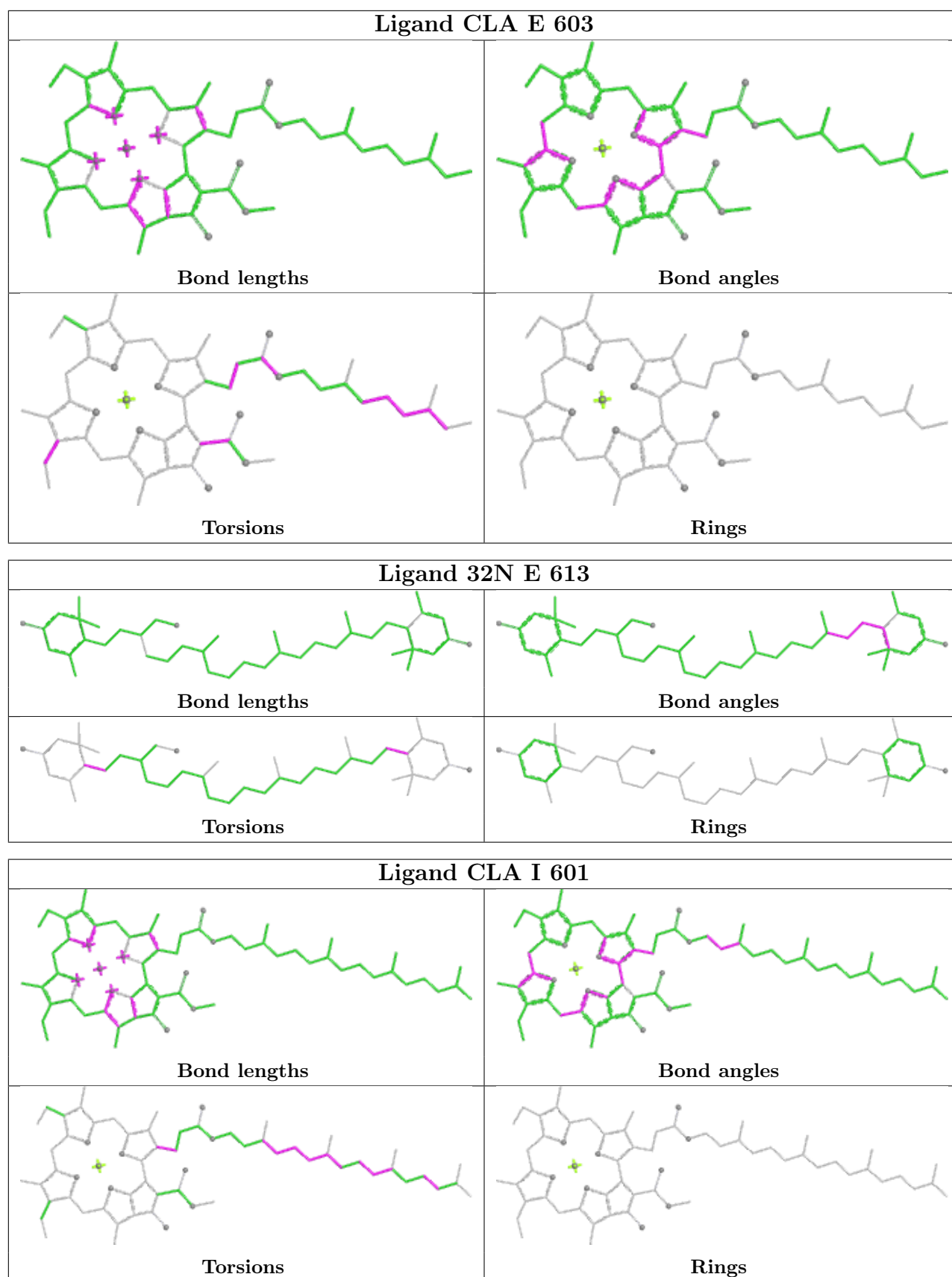


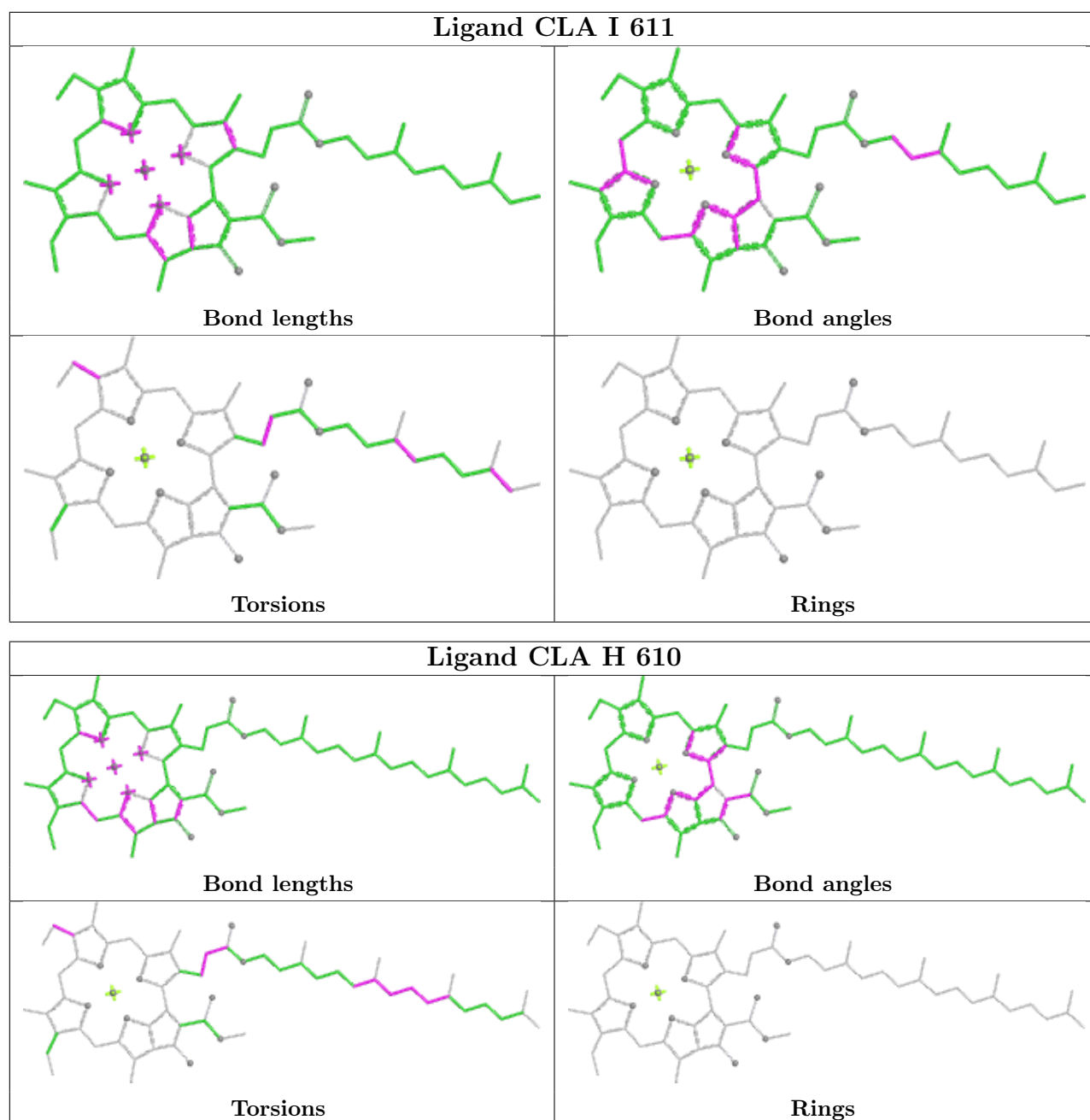
Ligand CLA E 609

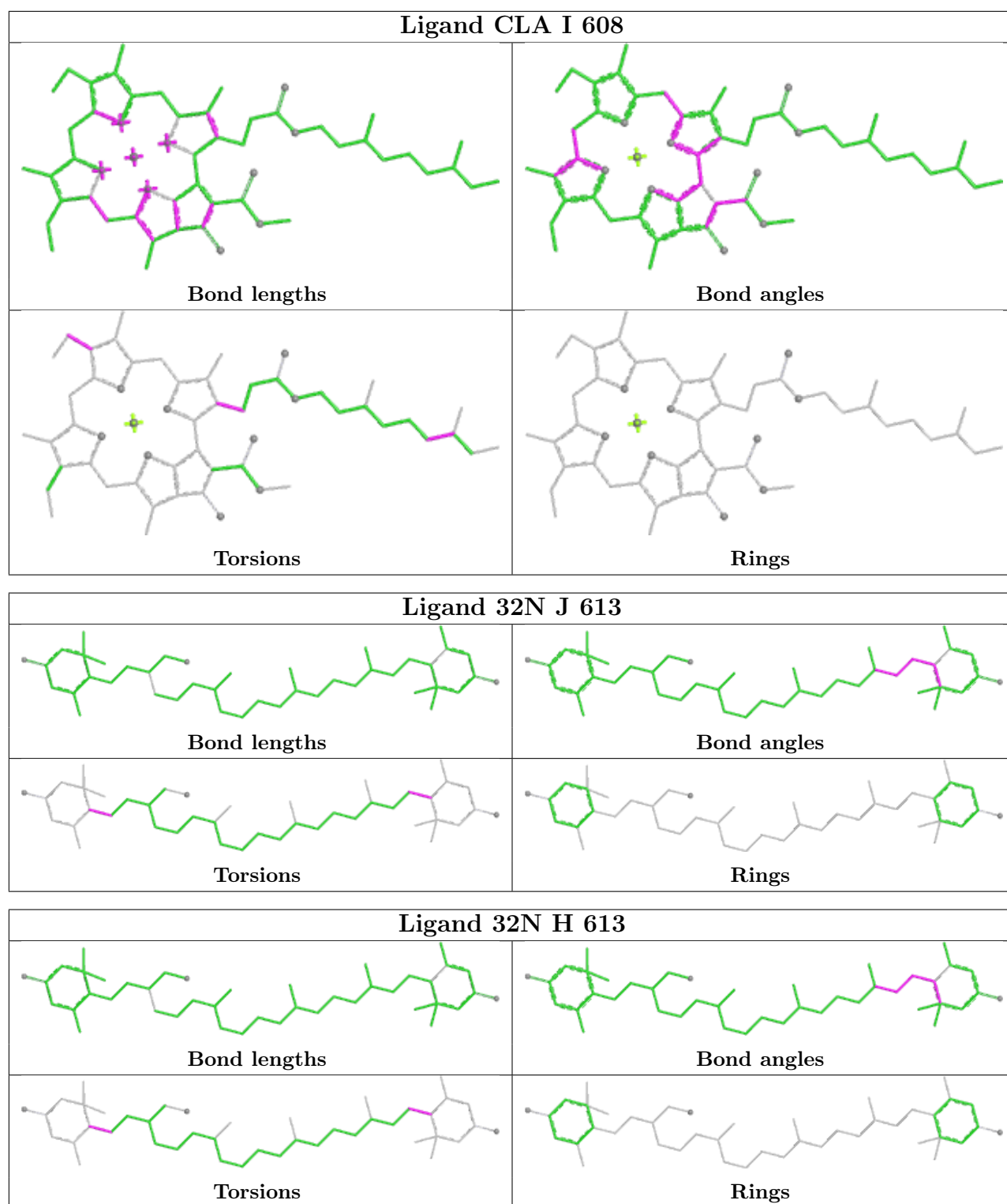


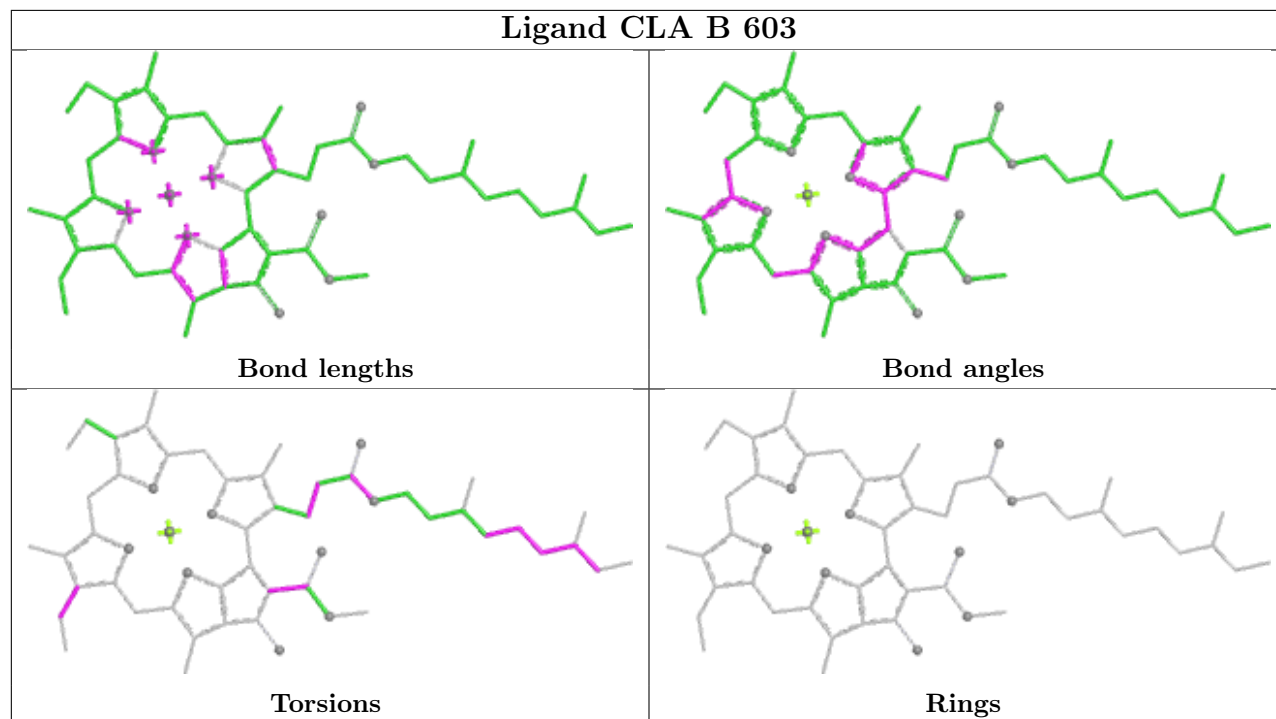
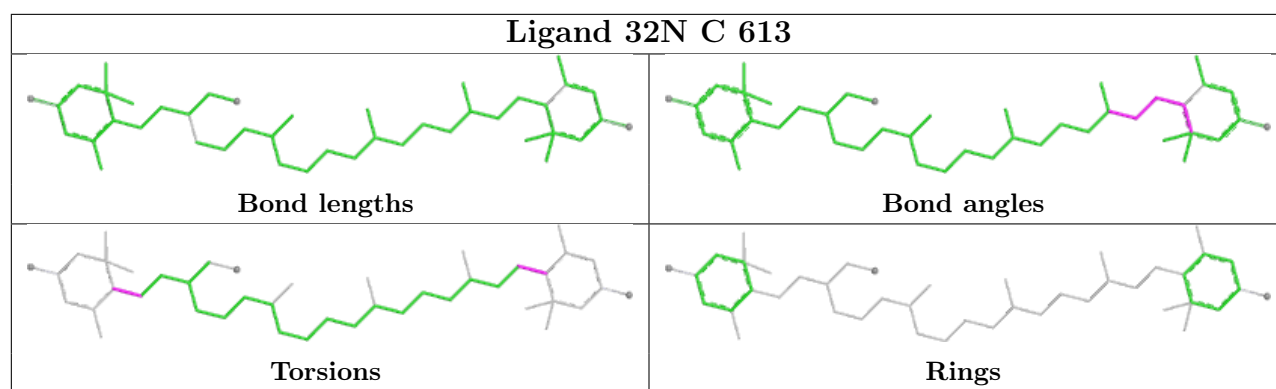


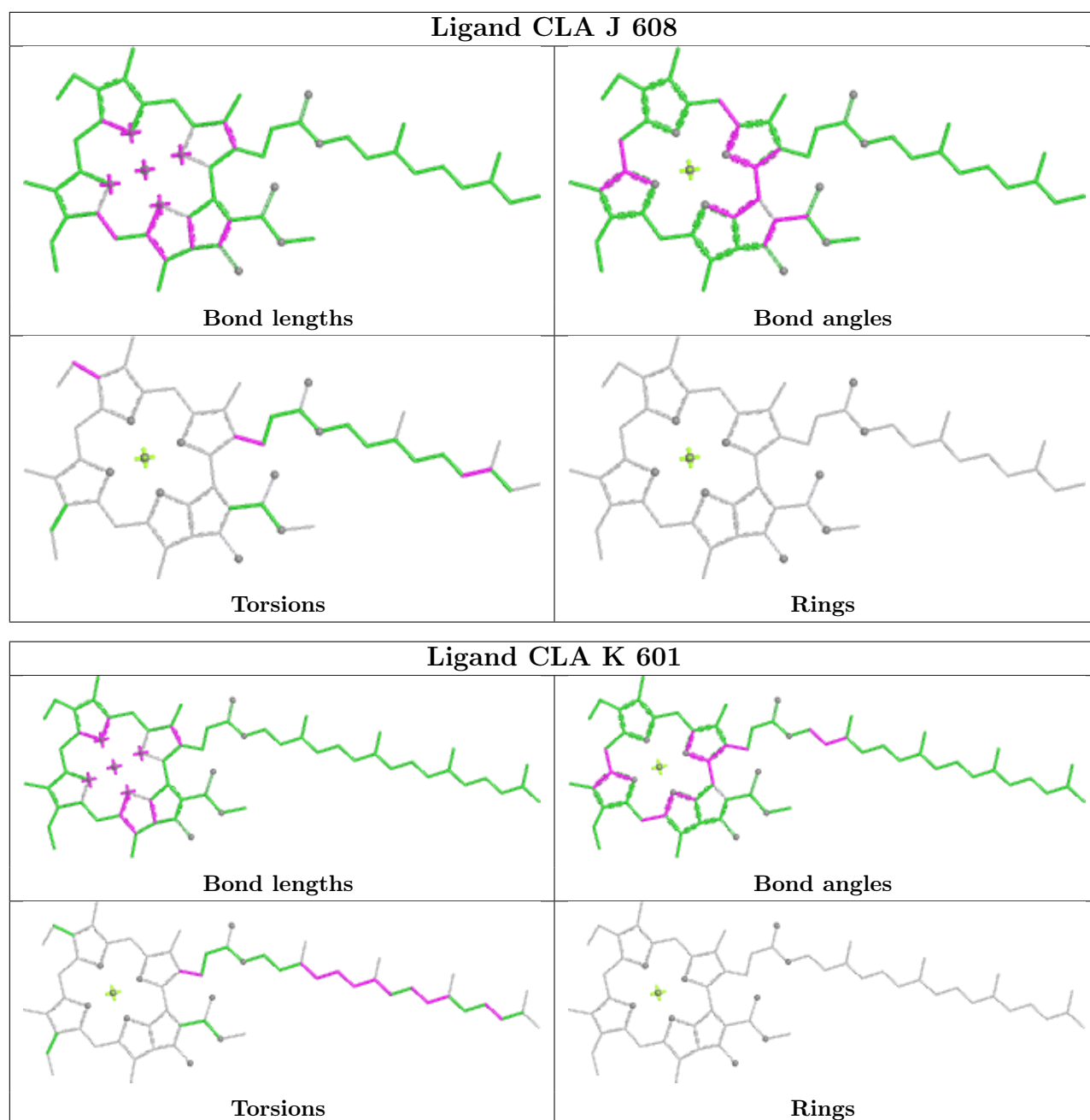


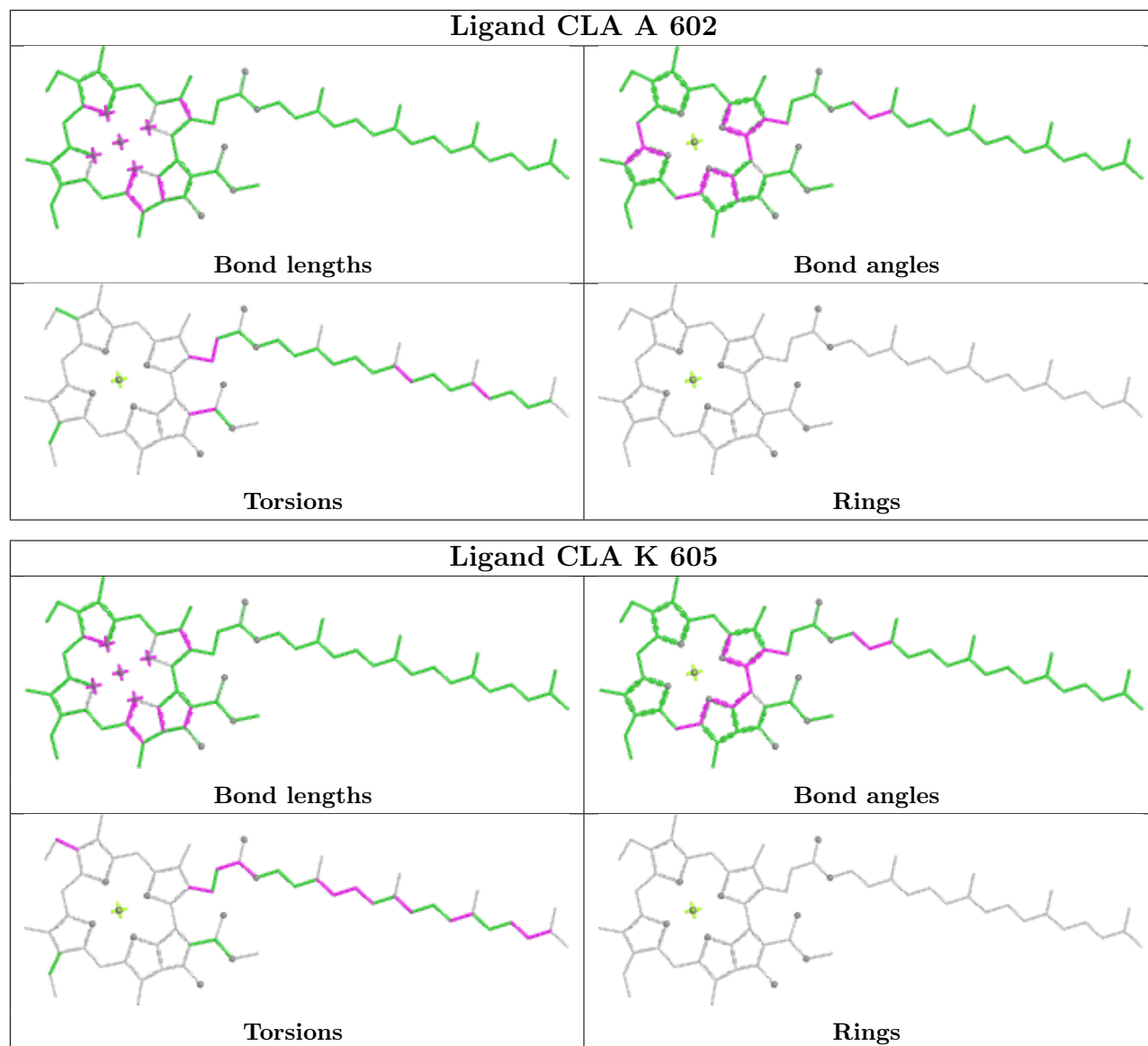




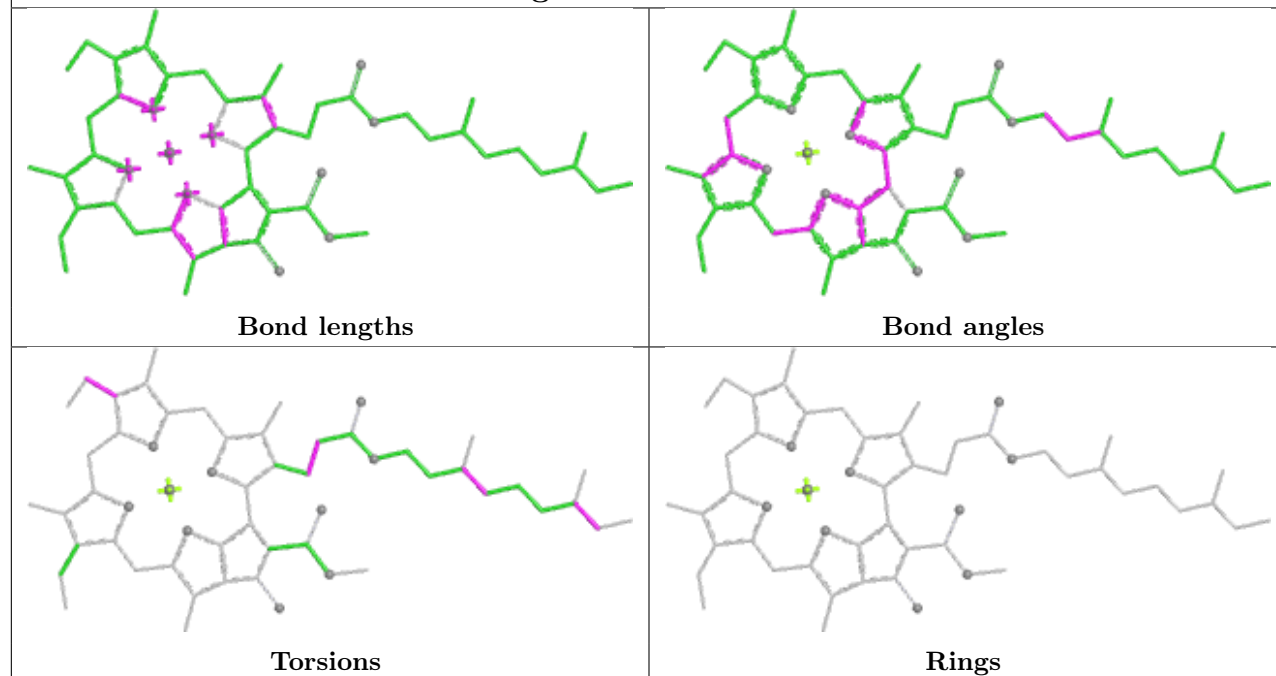




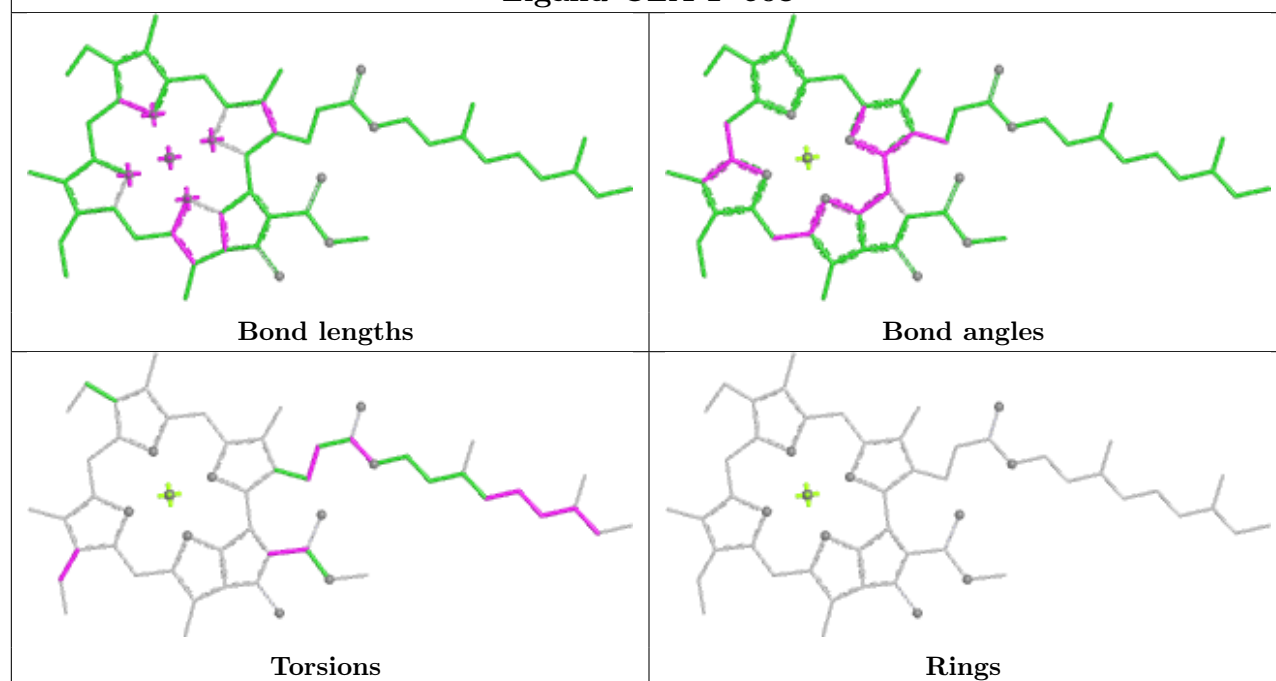




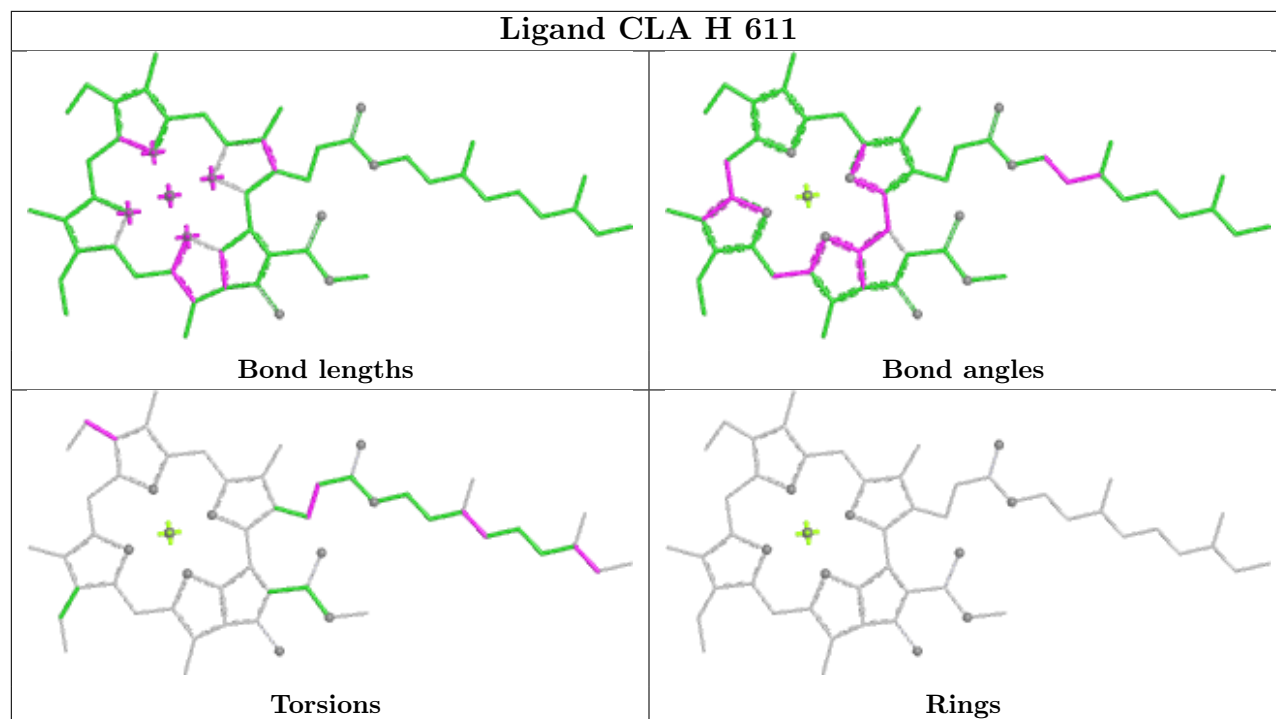
Ligand CLA A 611



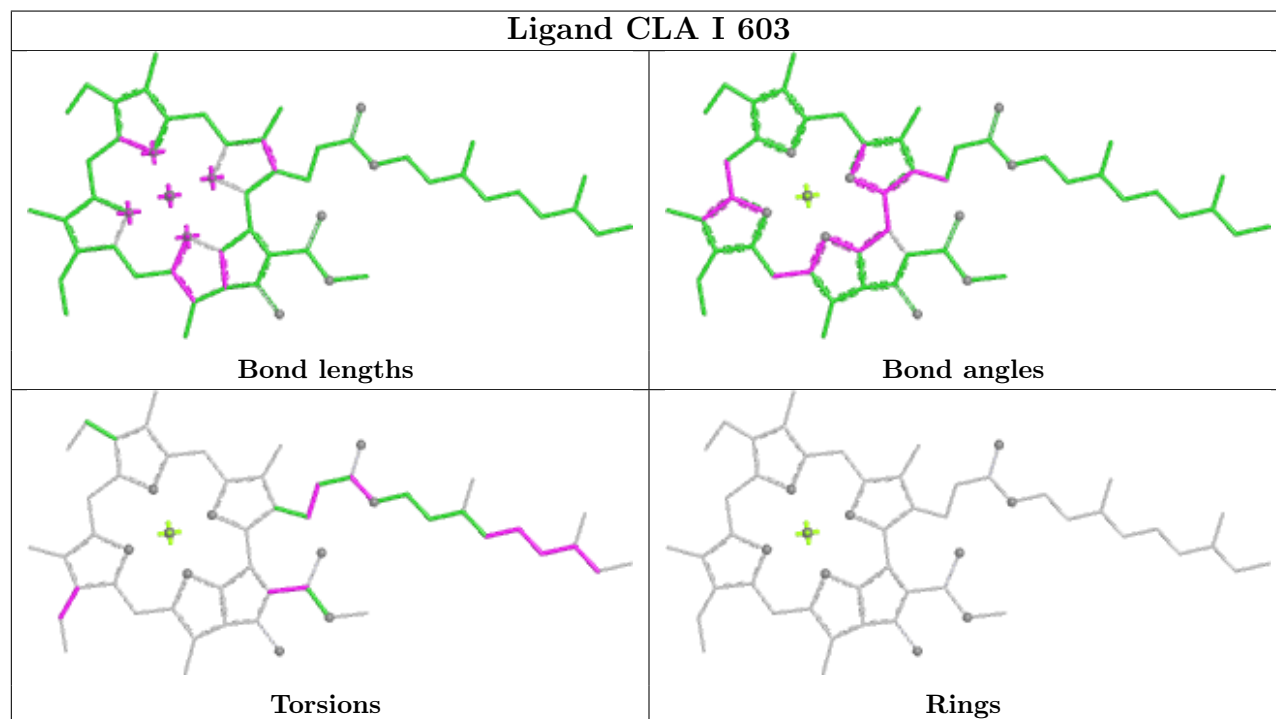
Ligand CLA F 603

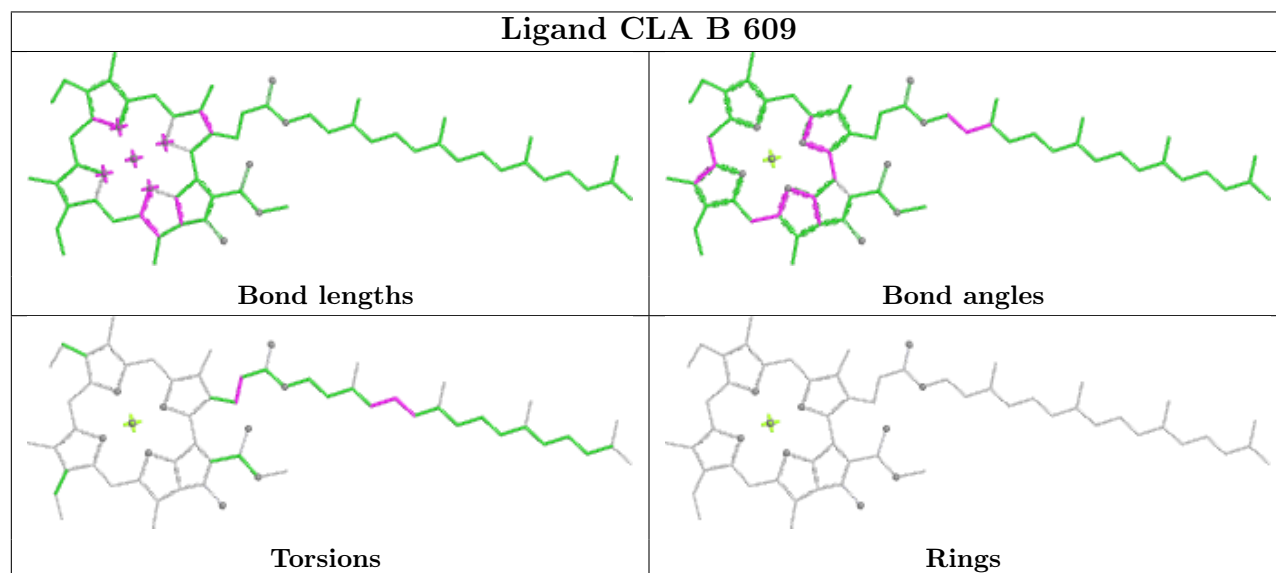
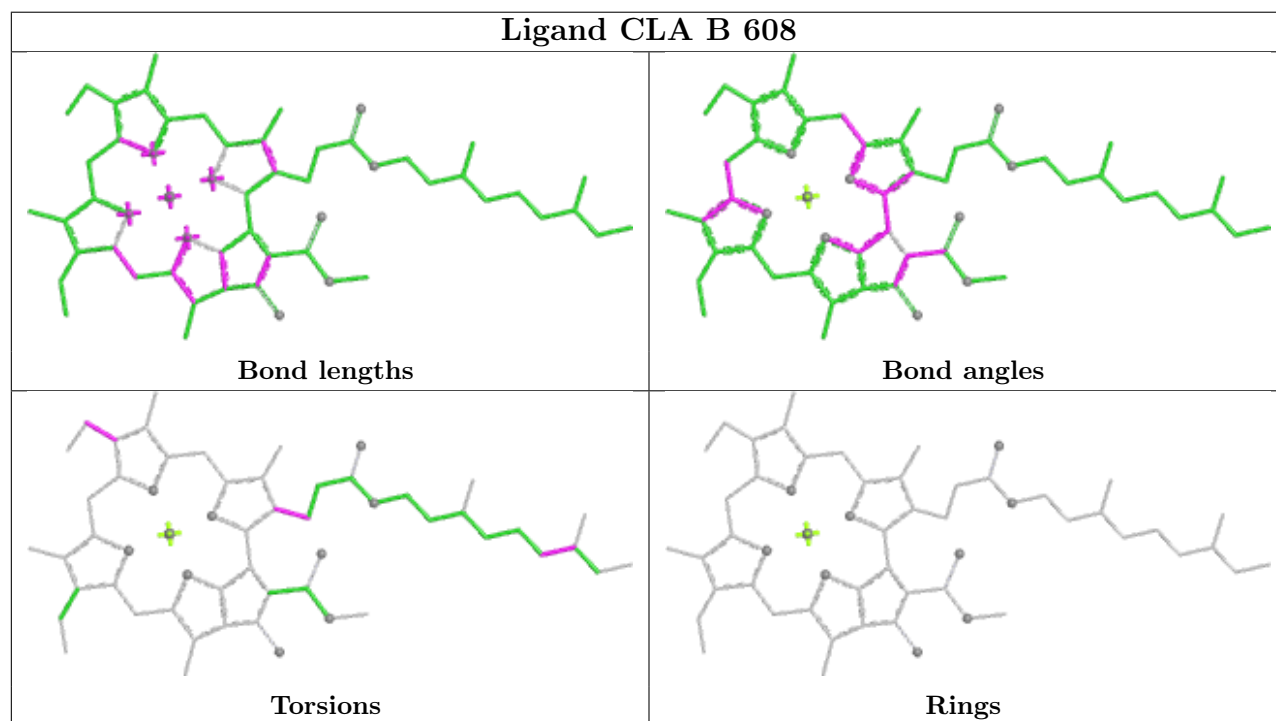
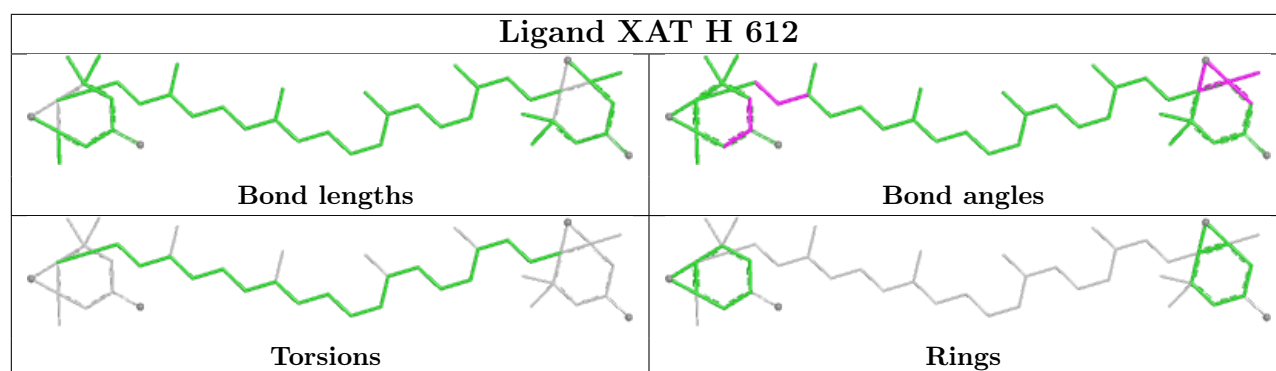


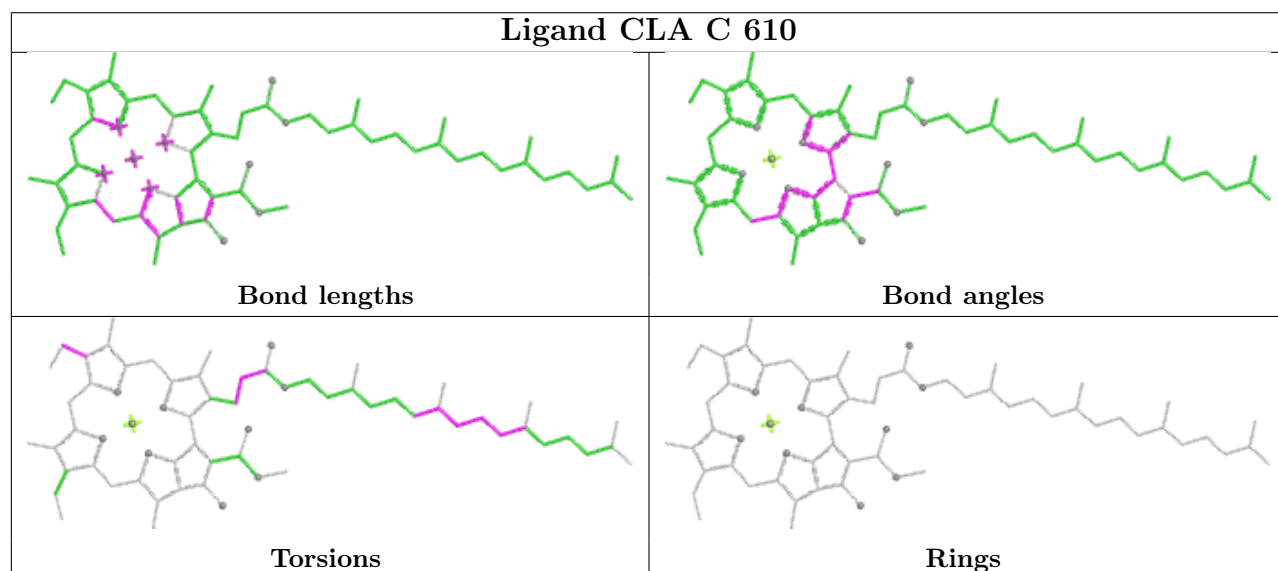
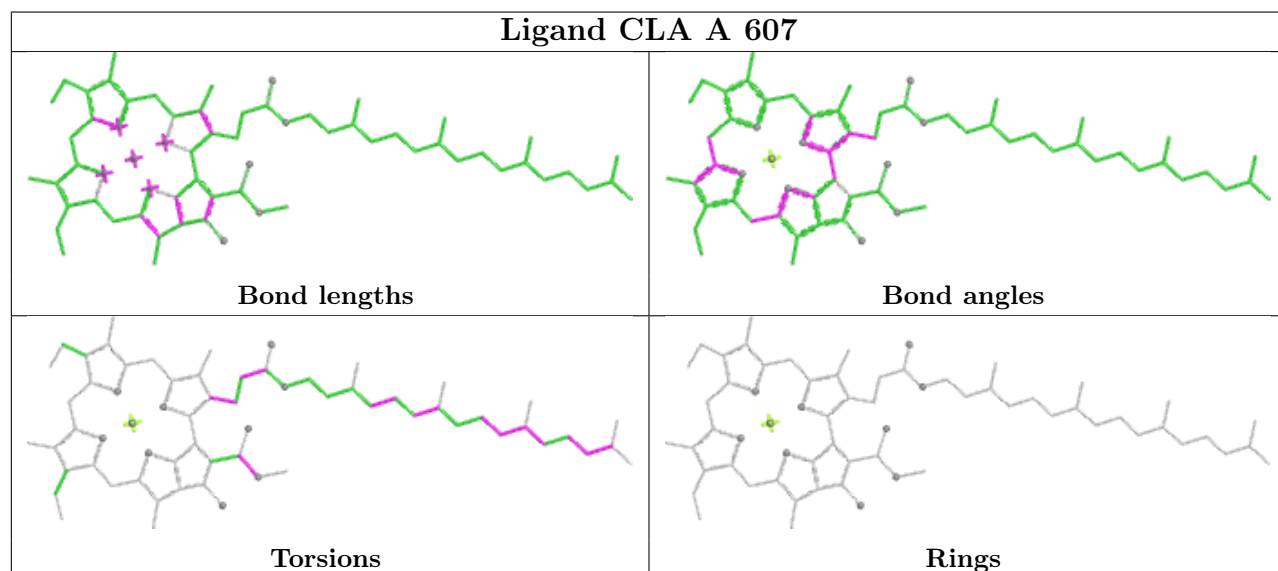
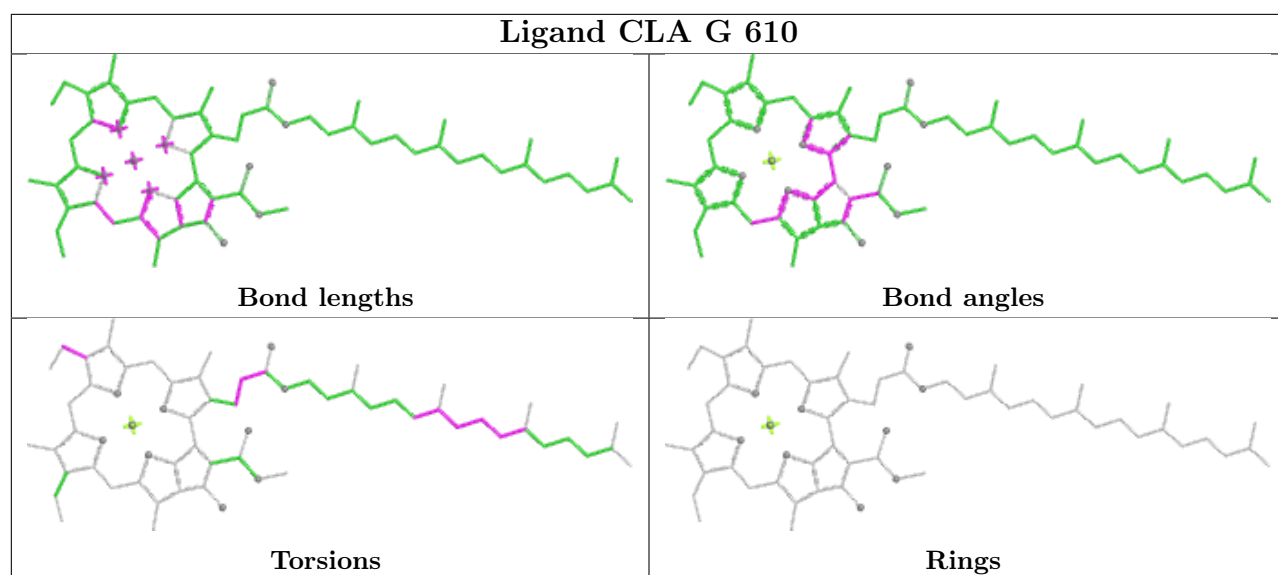
Ligand CLA H 611

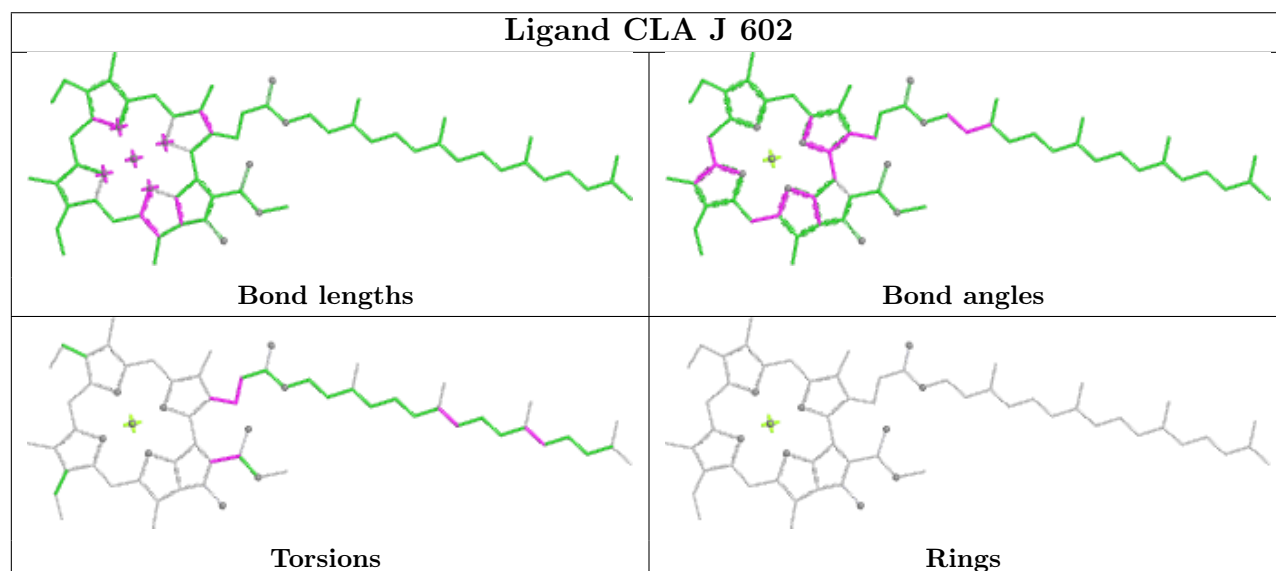
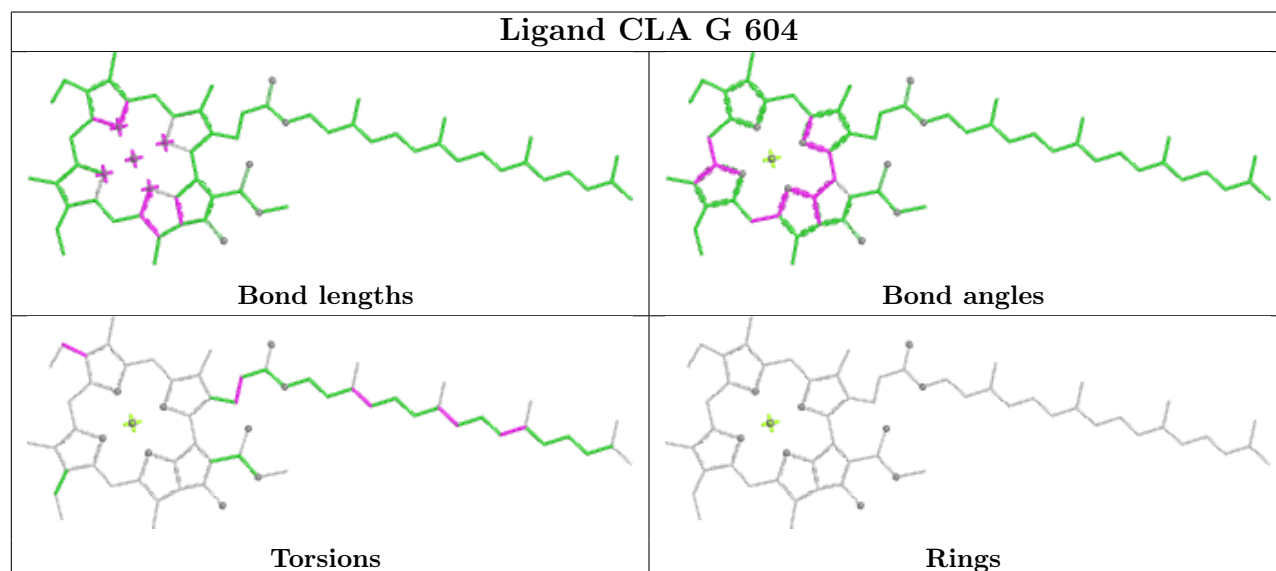
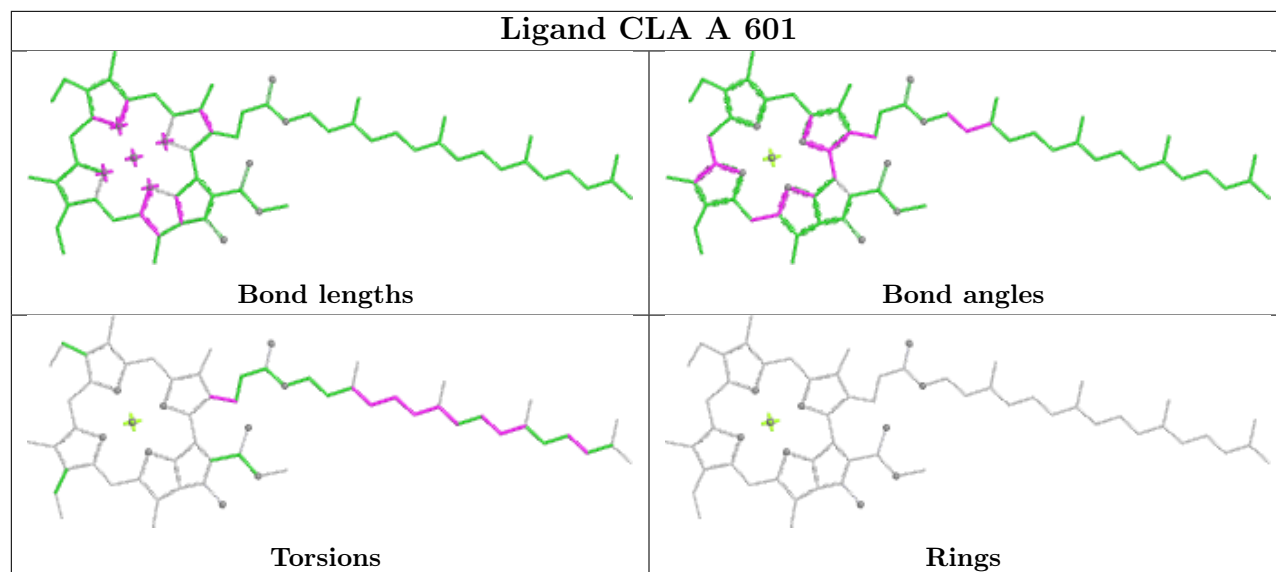


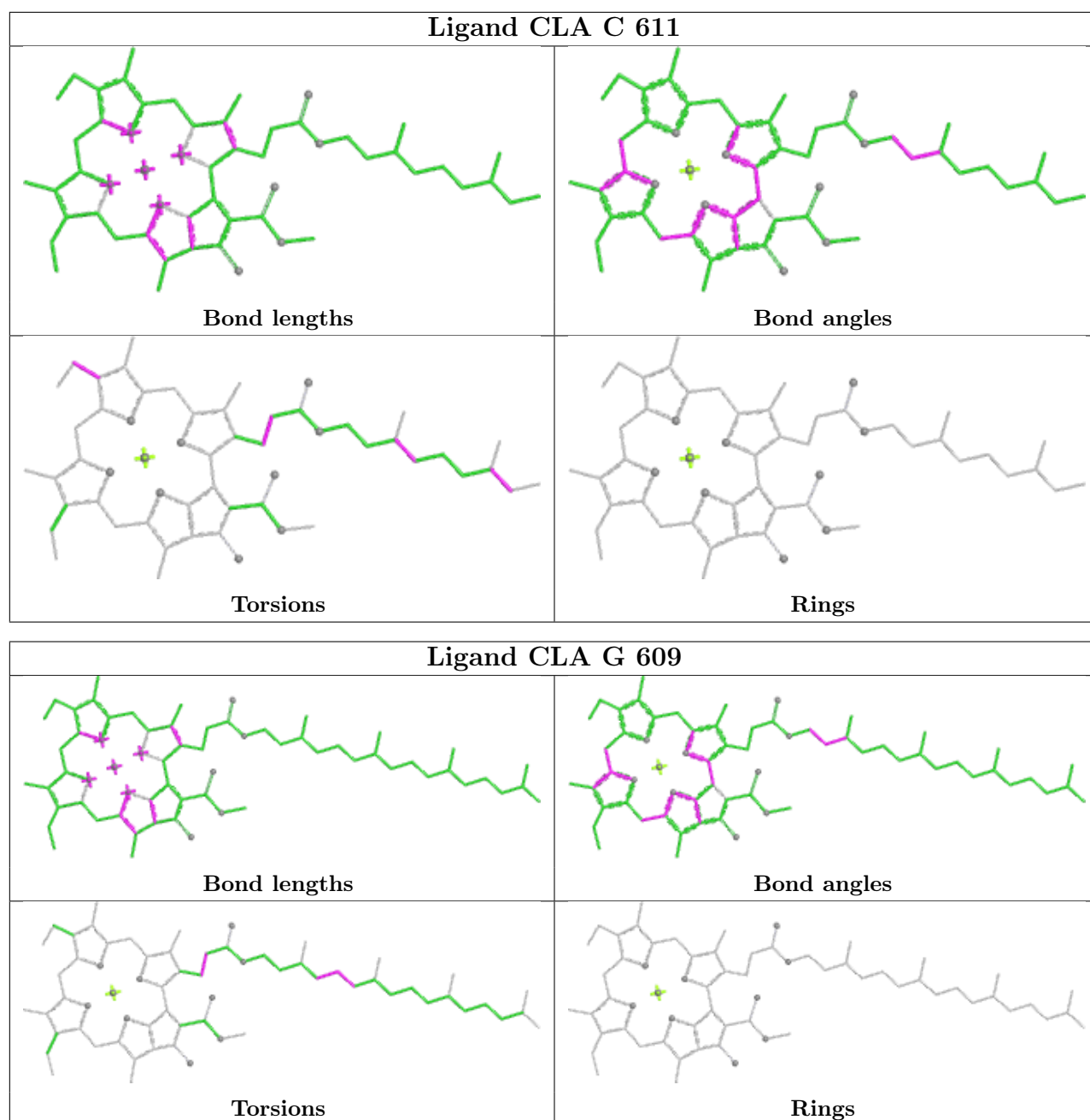
Ligand CLA I 603

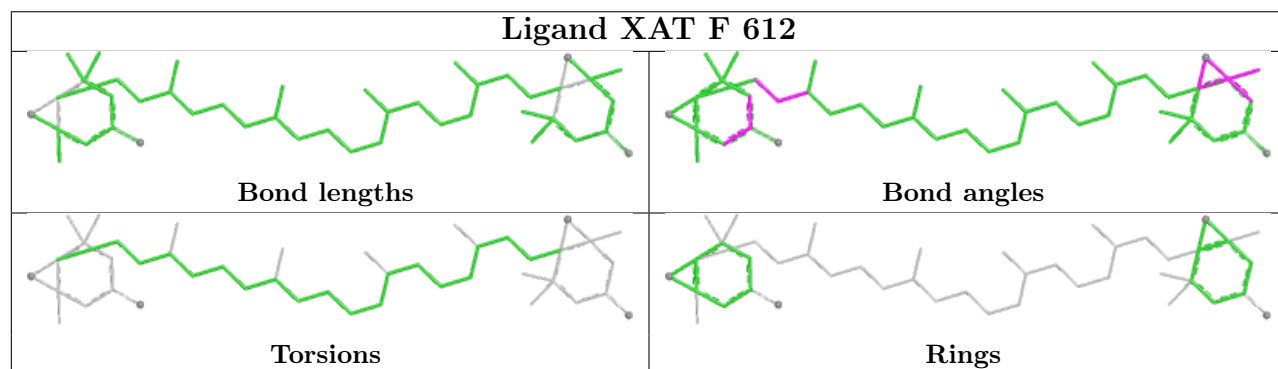
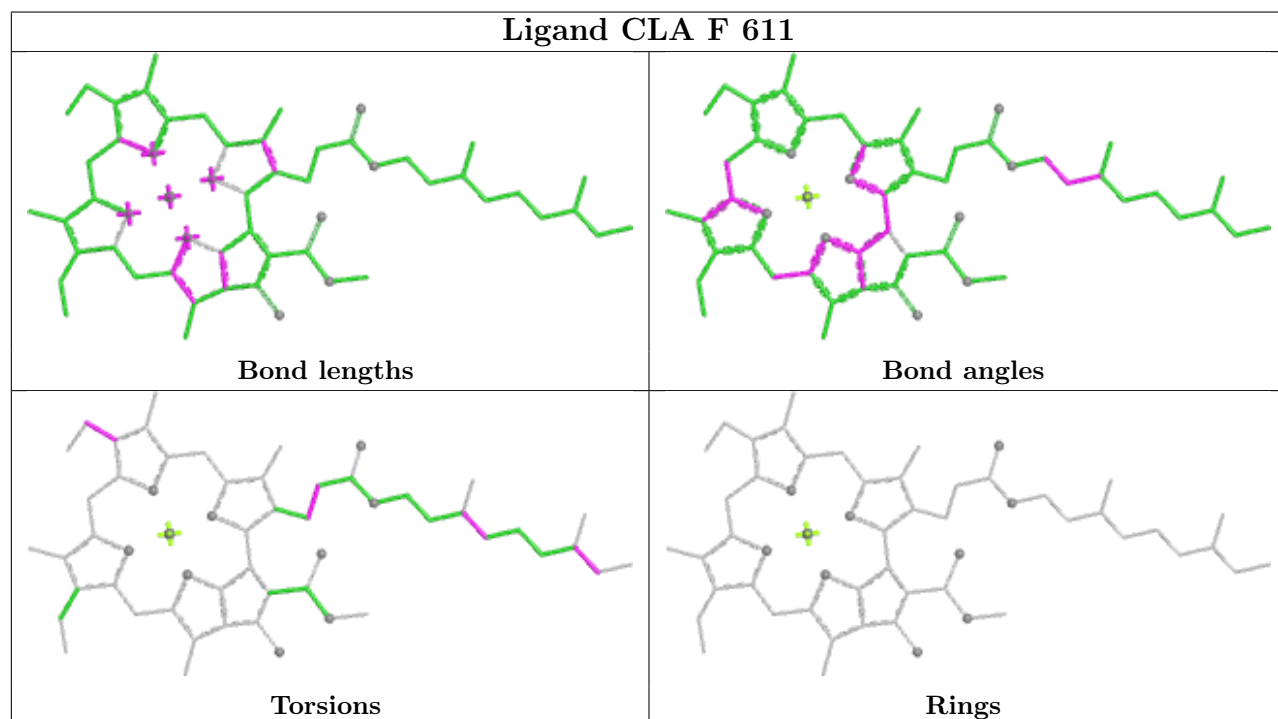
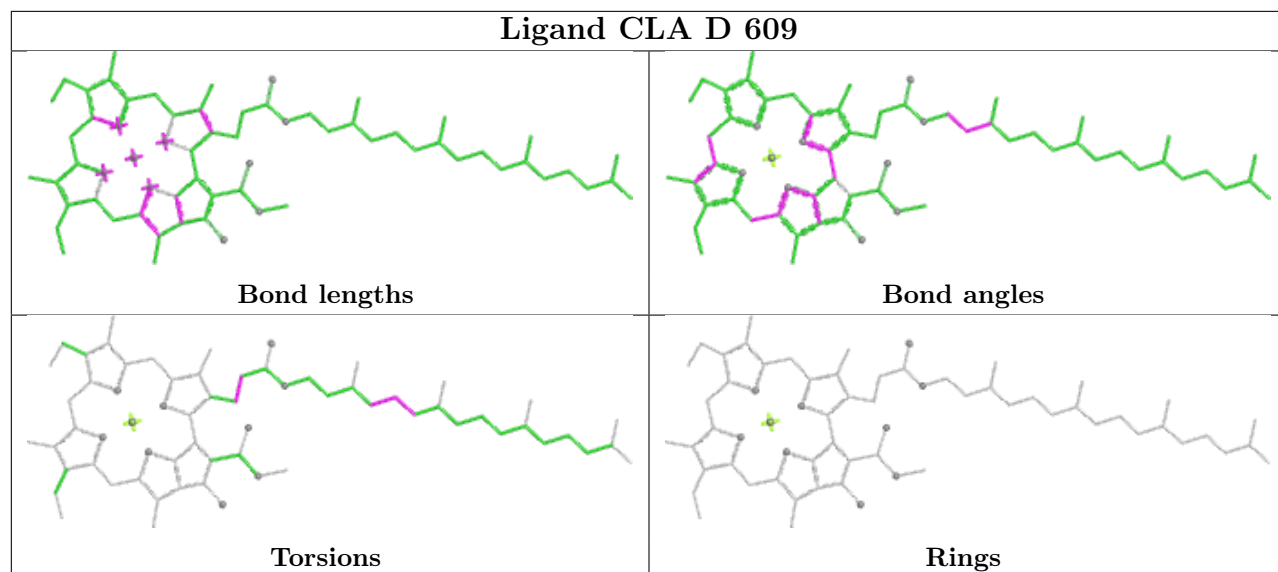


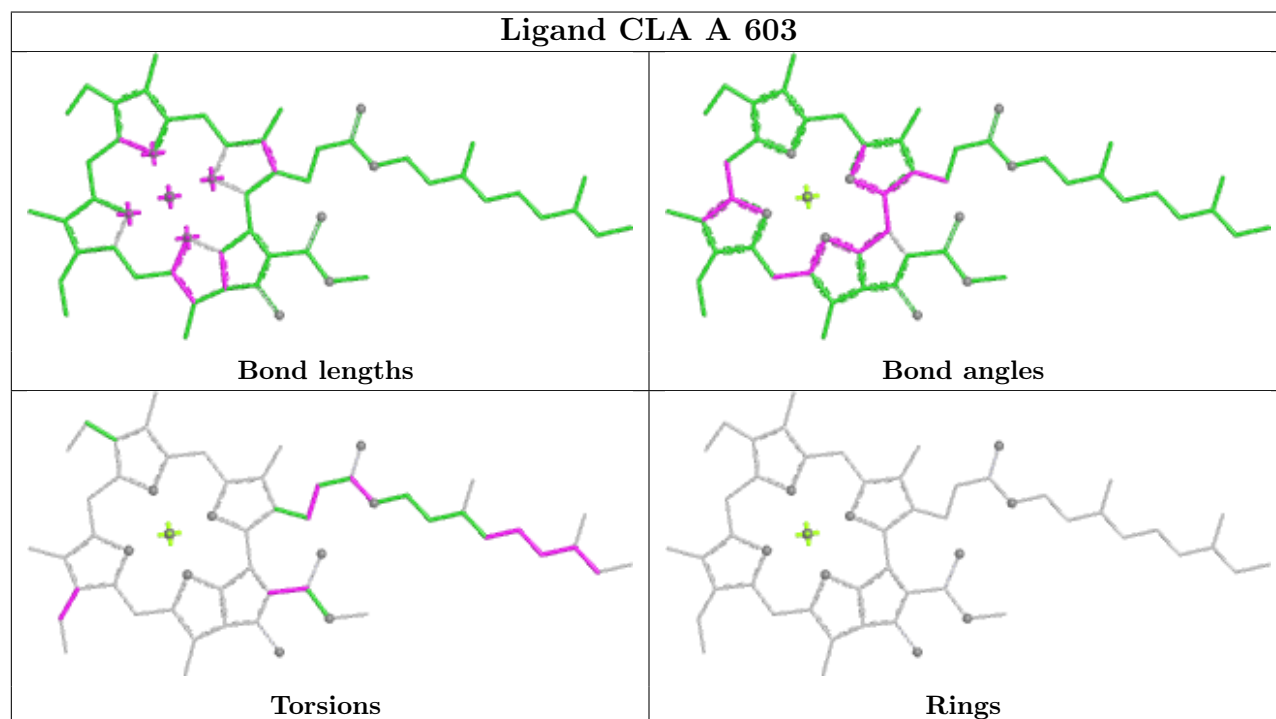
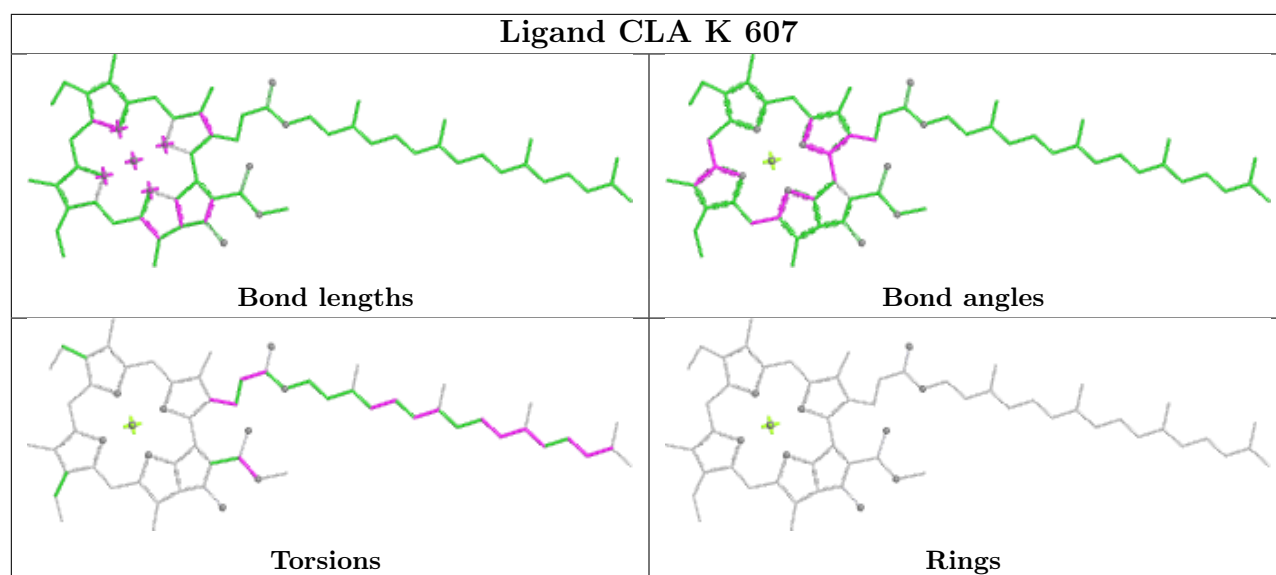


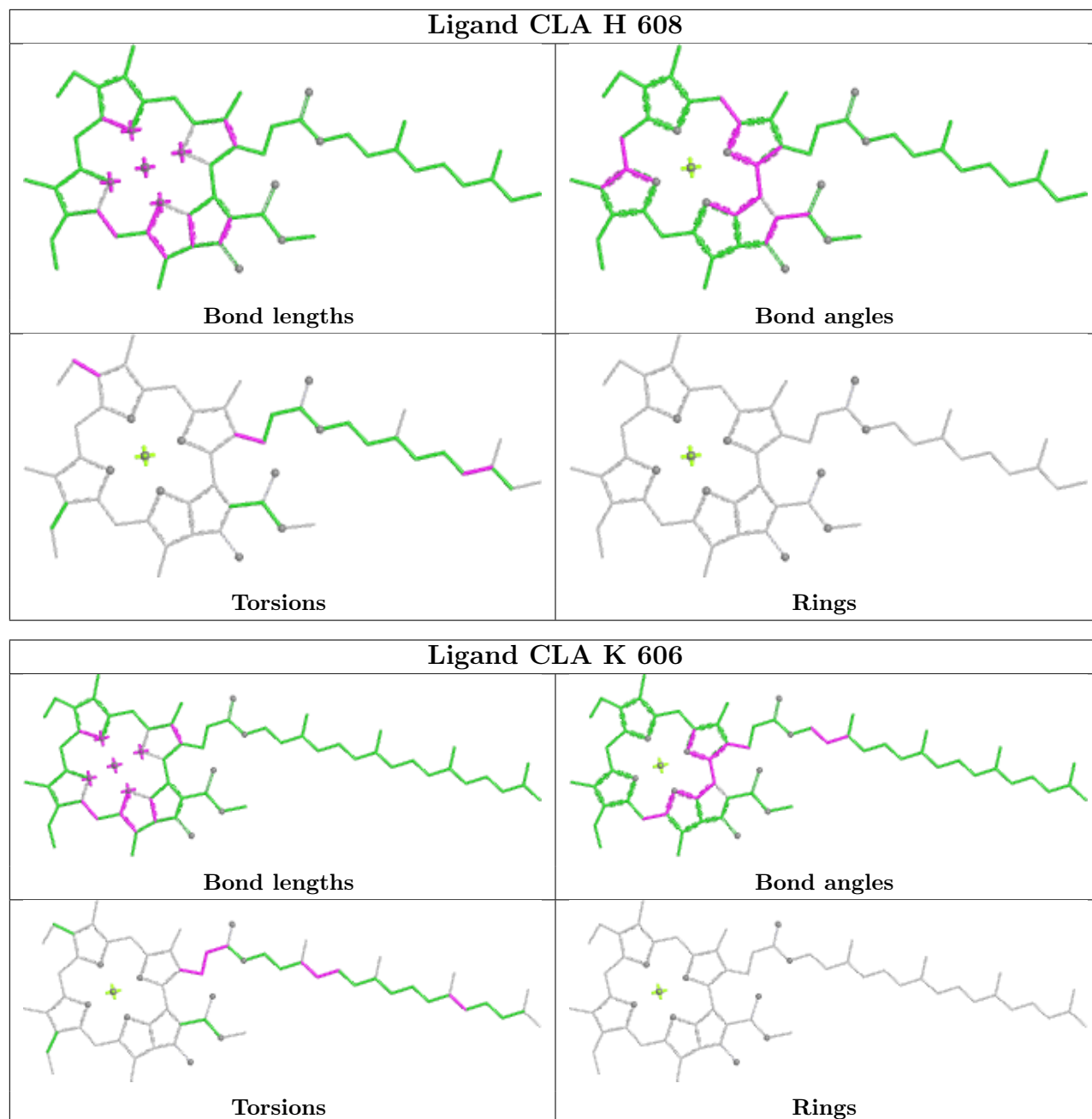


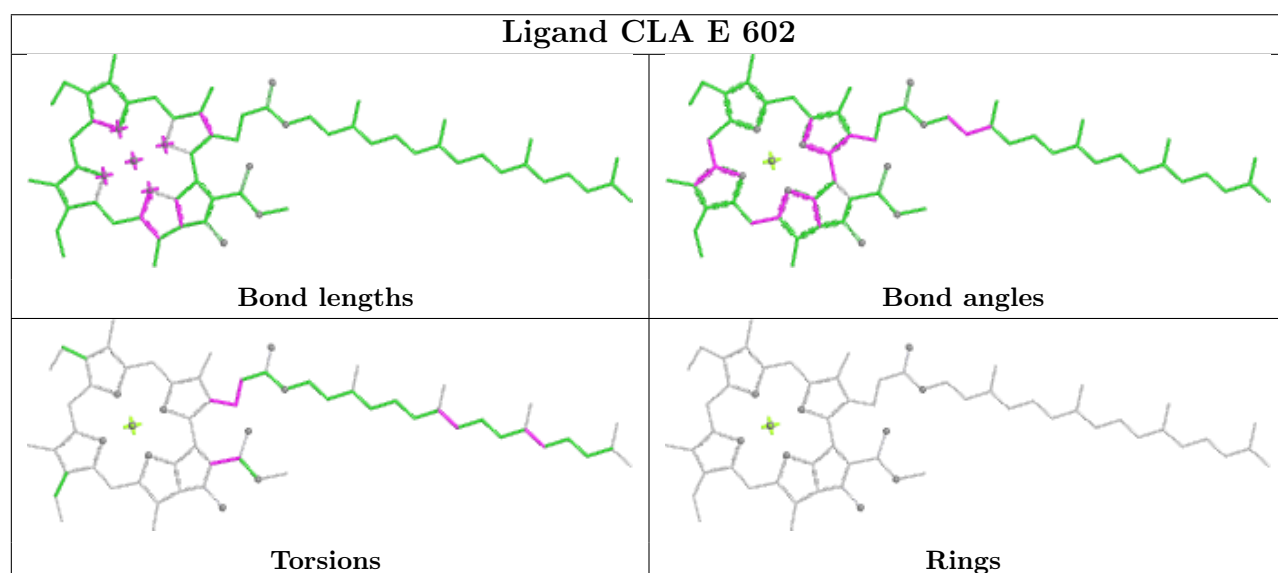
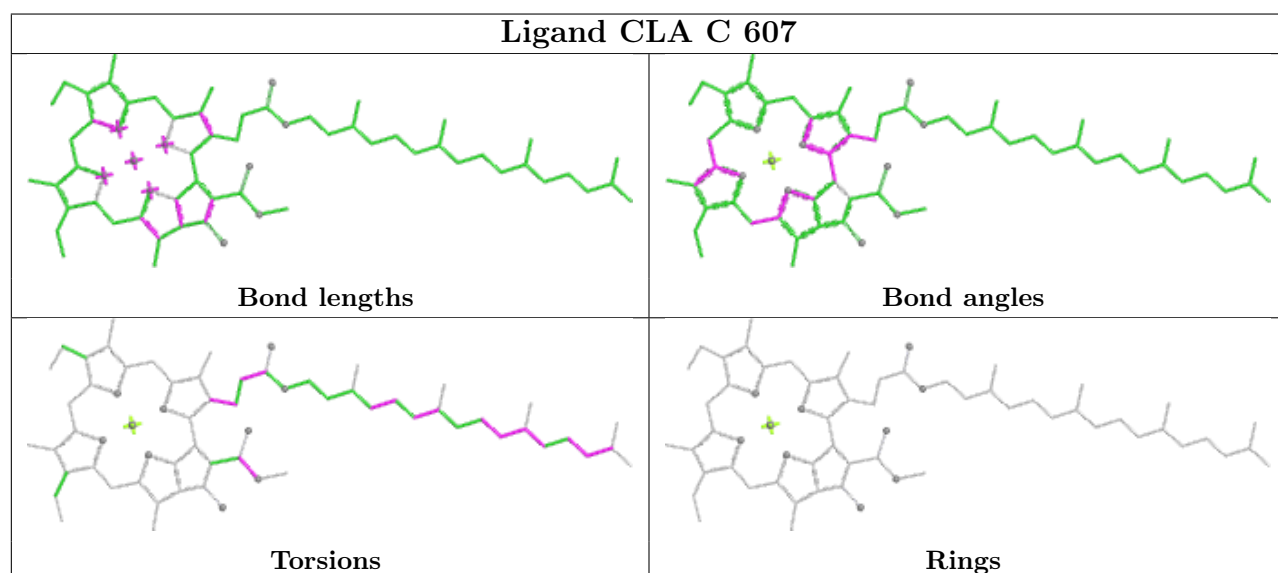
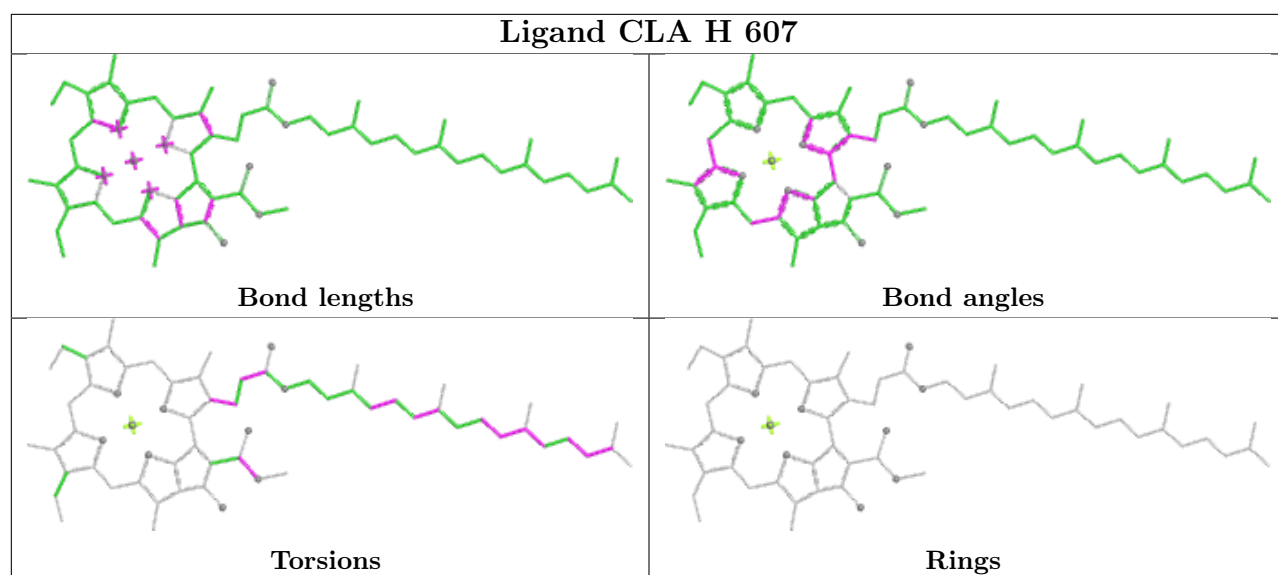


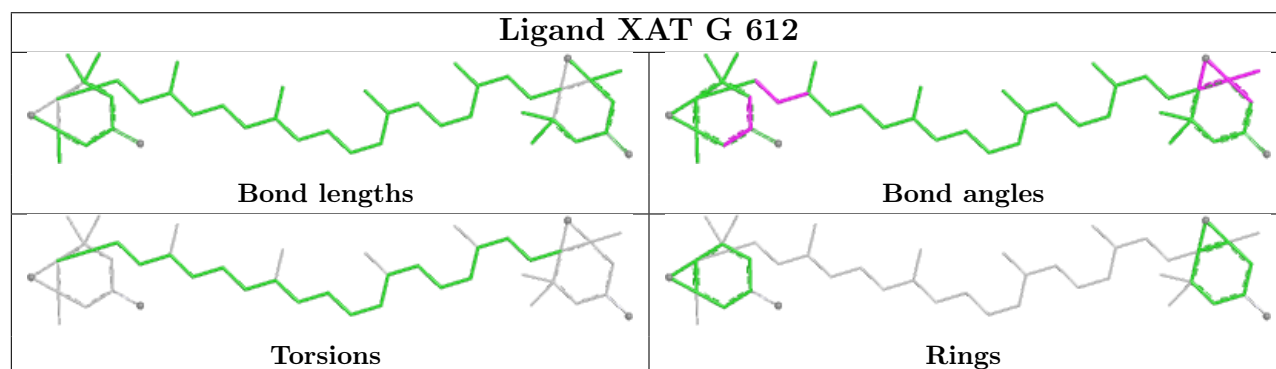
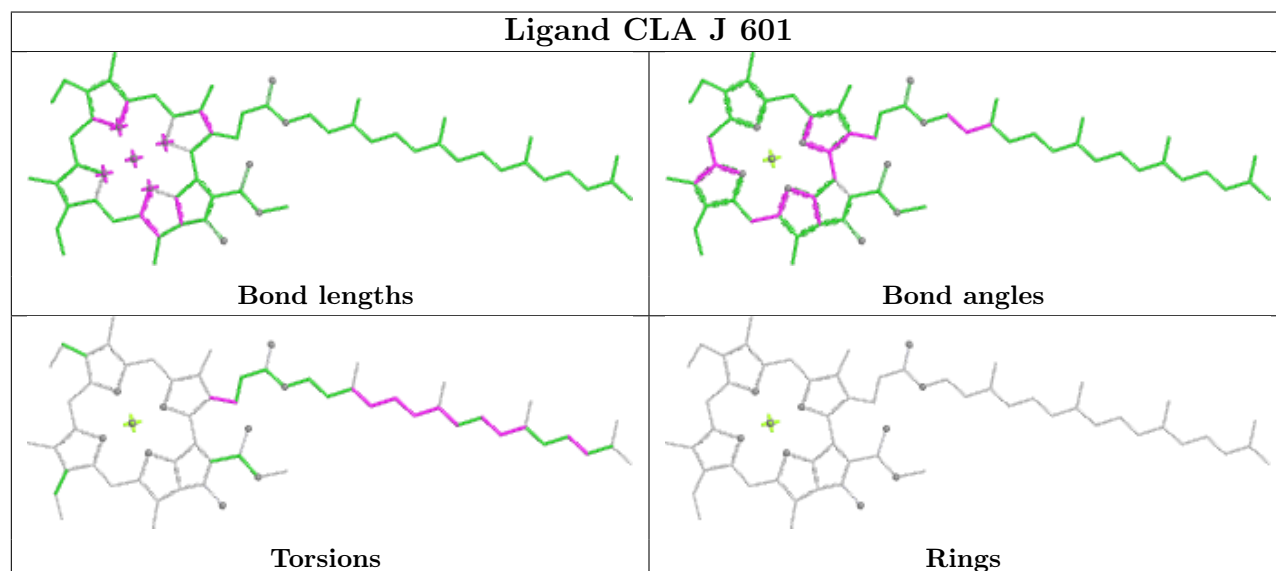
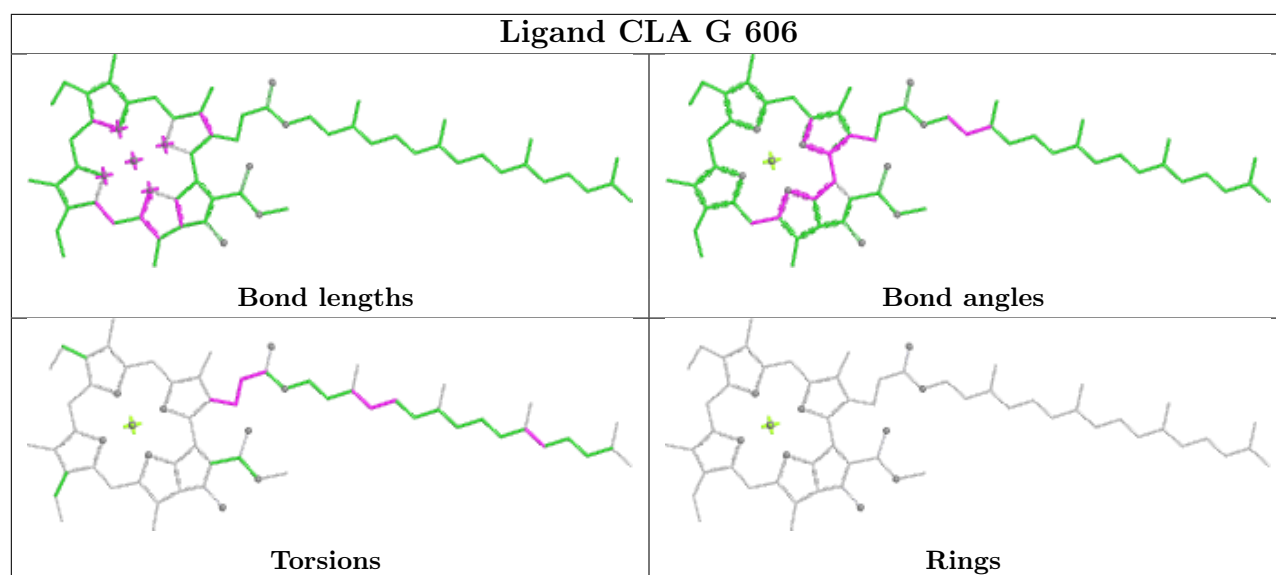


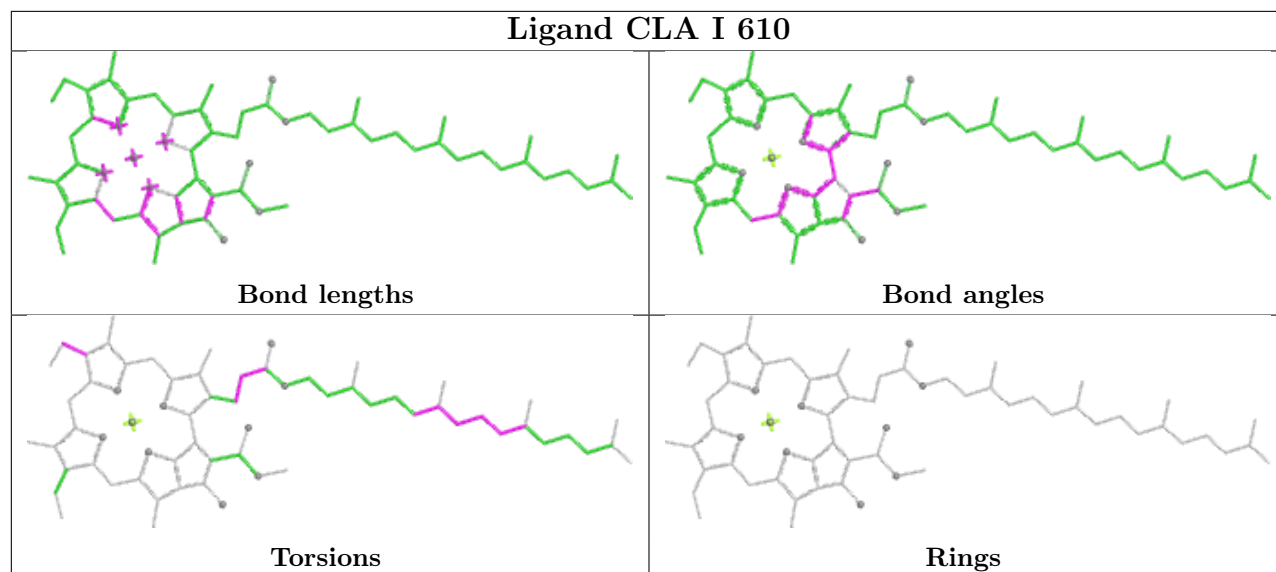
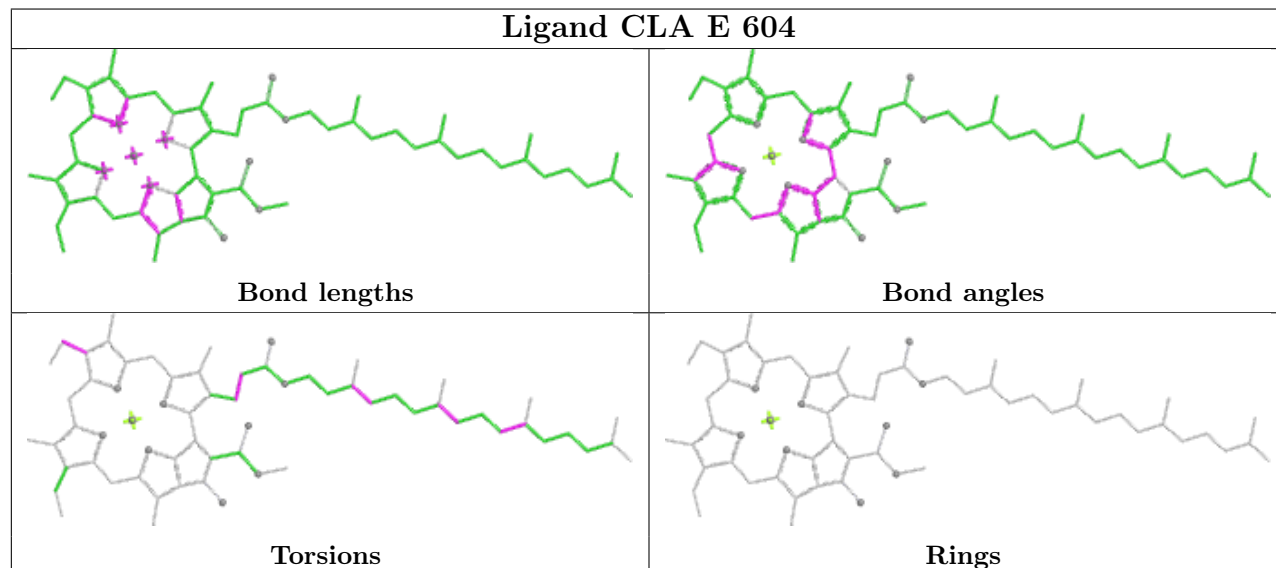


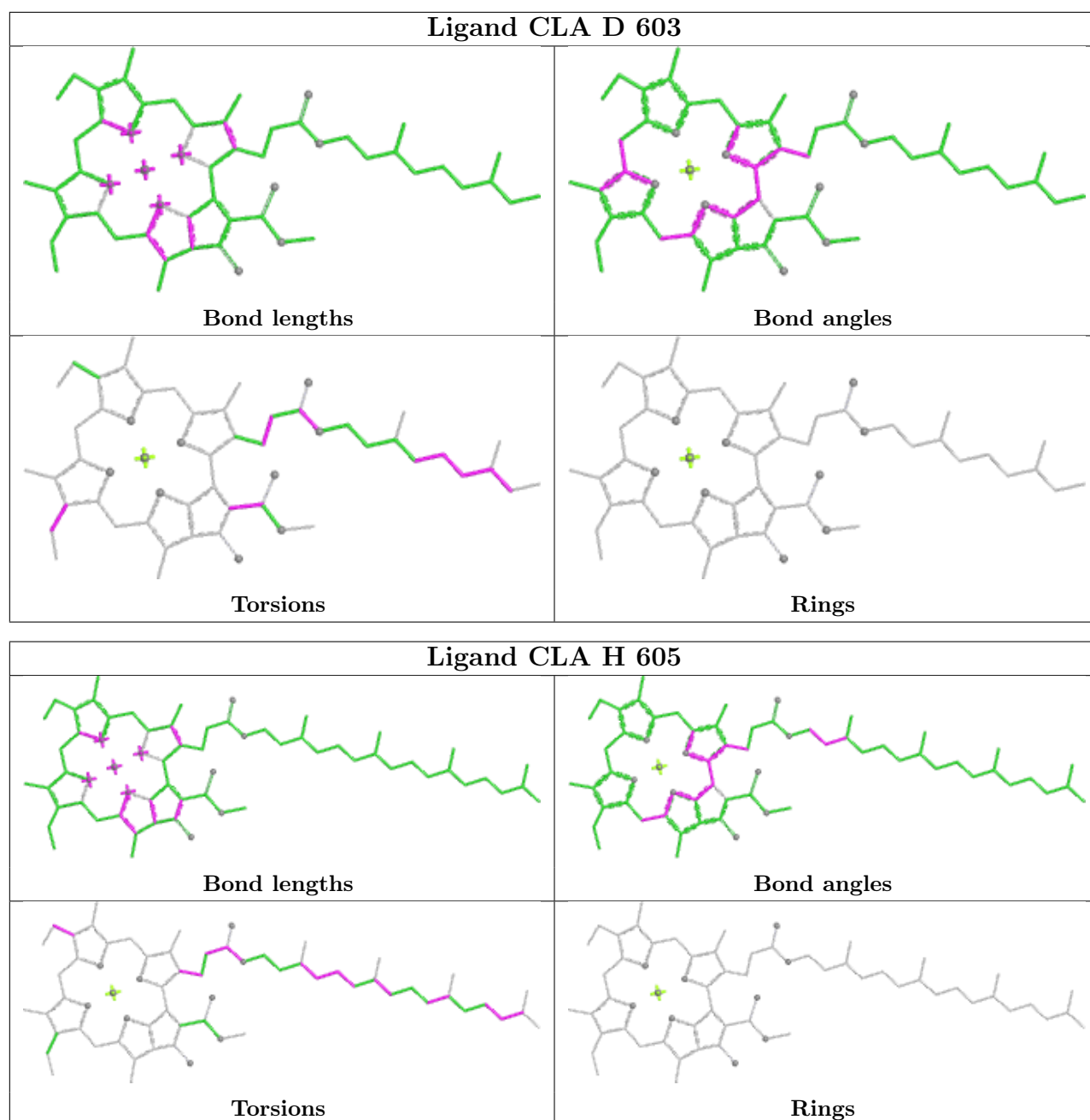


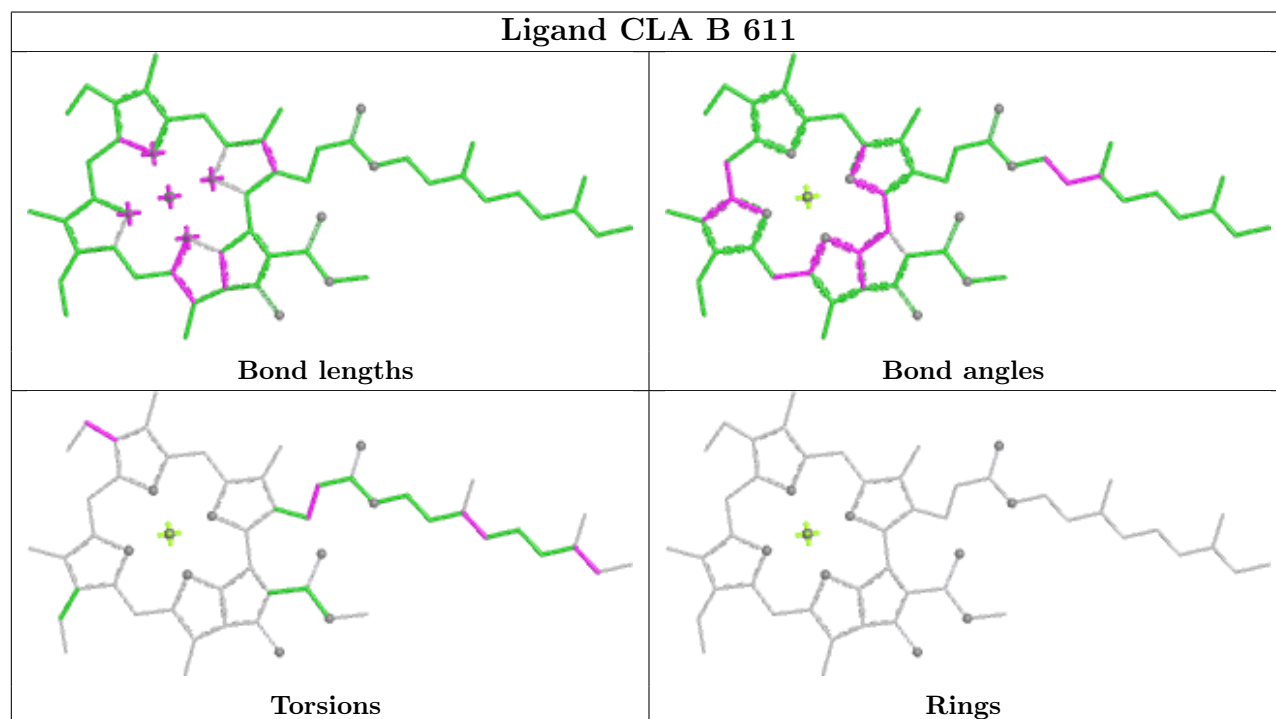
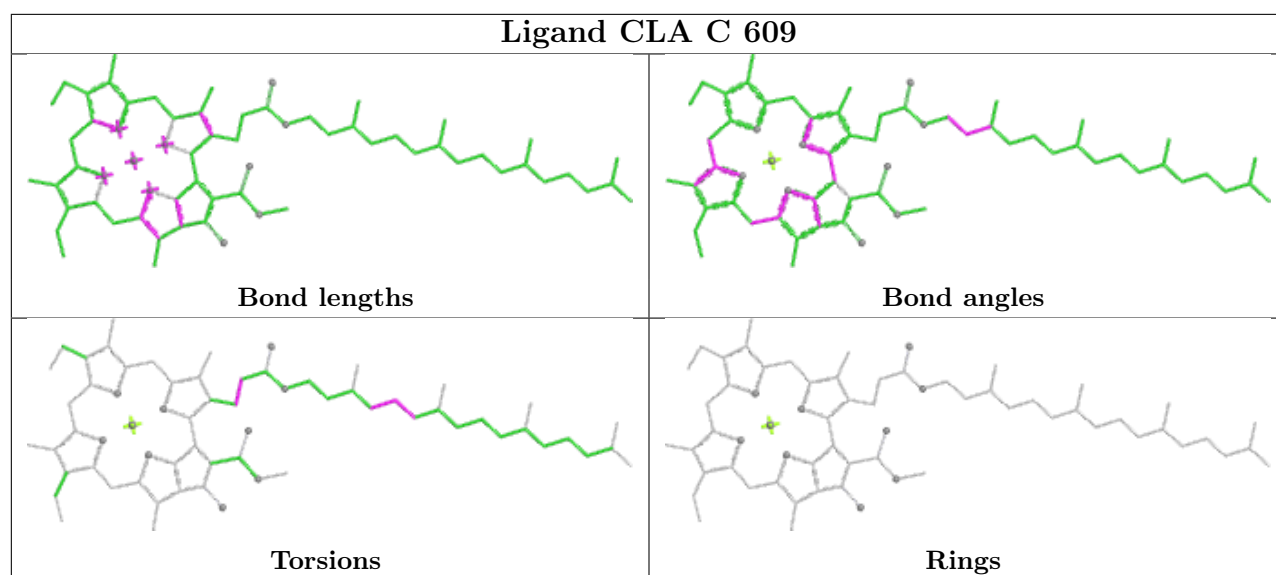


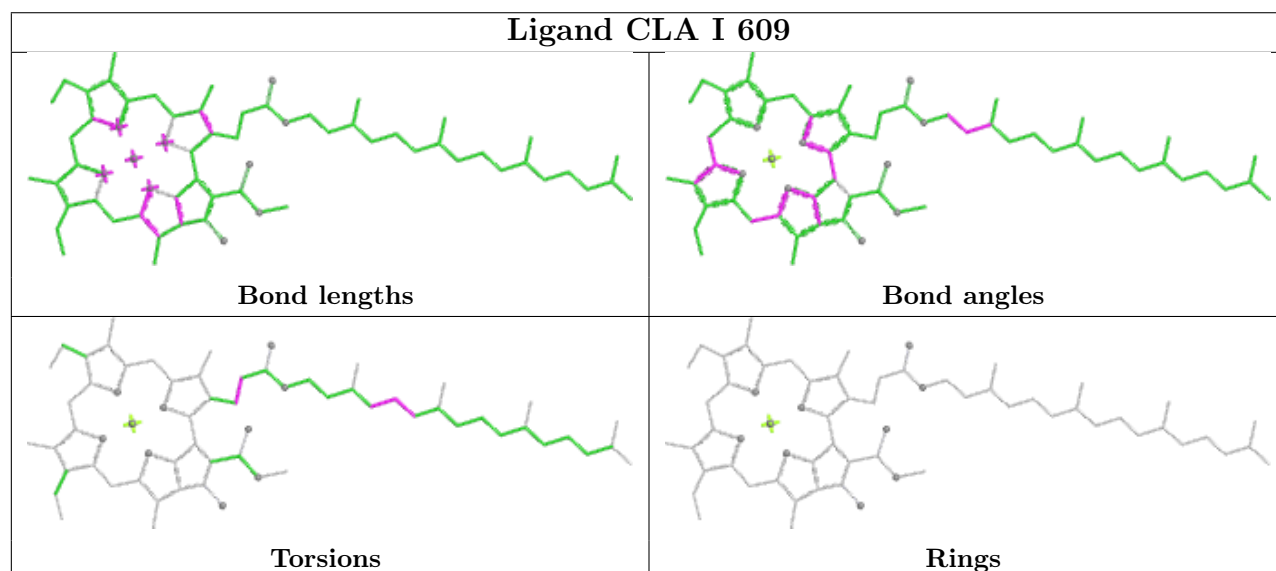
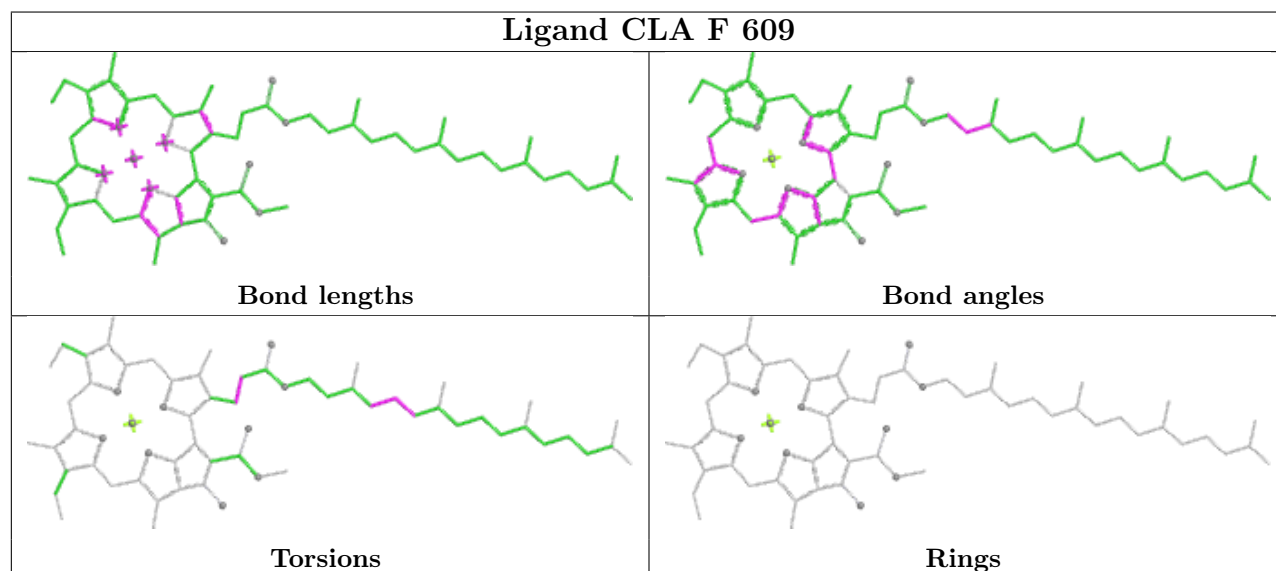
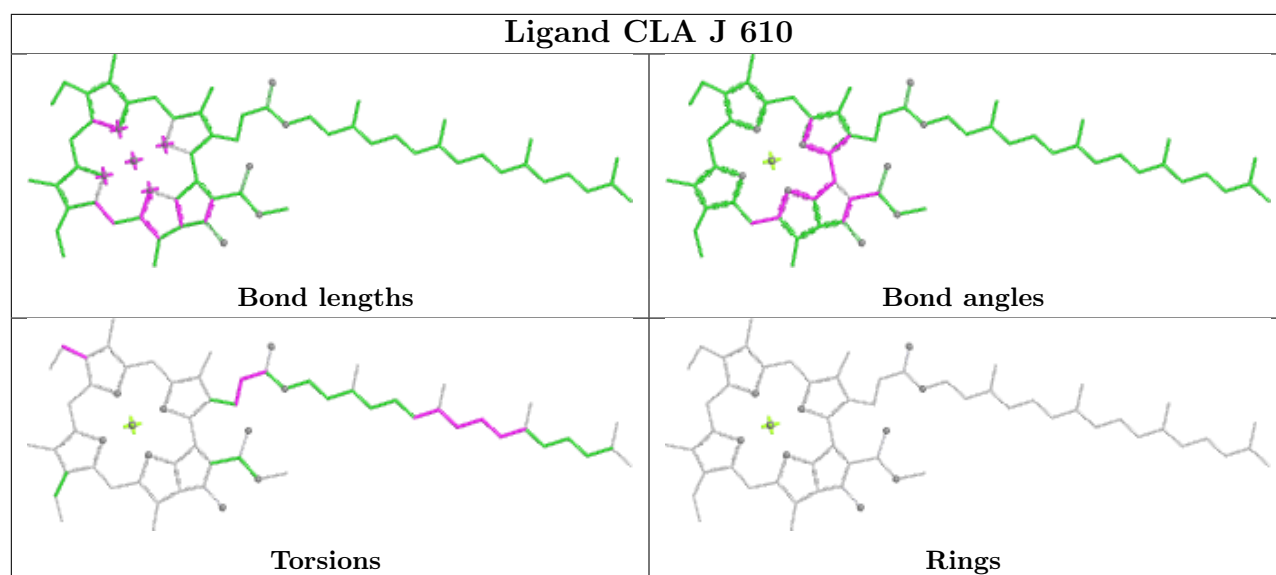


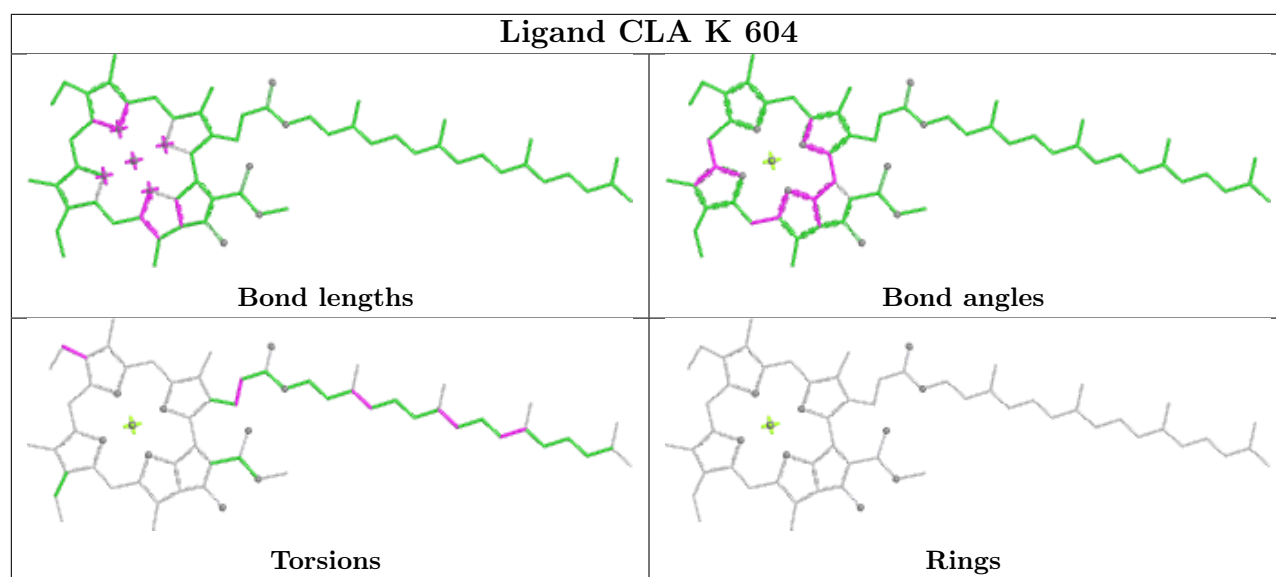


Ligand CLA I 610**Ligand CLA E 604**









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.

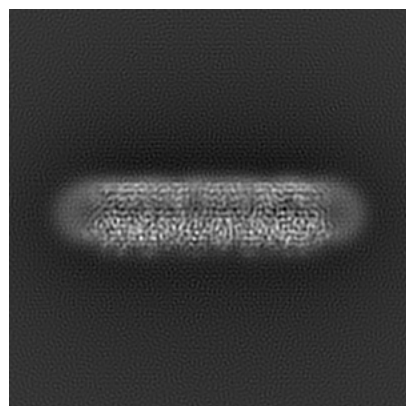
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35080. These allow visual inspection of the internal detail of the map and identification of artifacts.

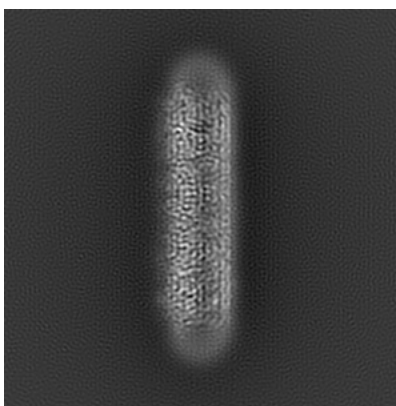
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

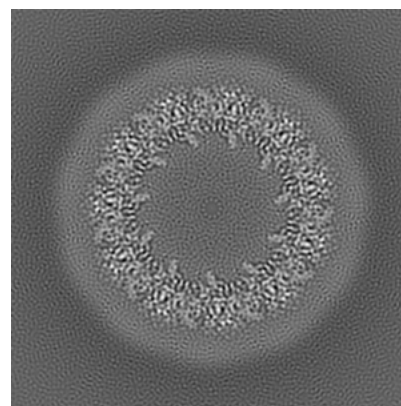
6.1.1 Primary map



X

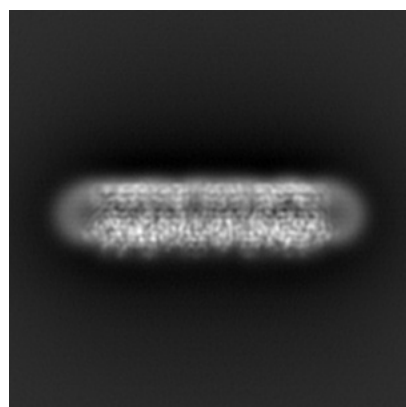


Y

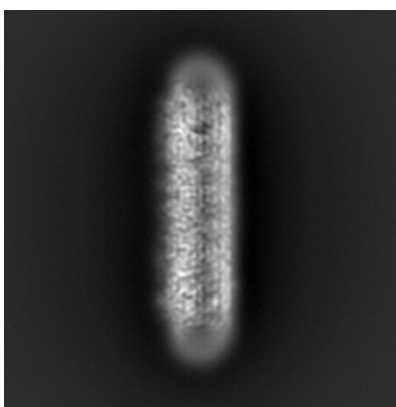


Z

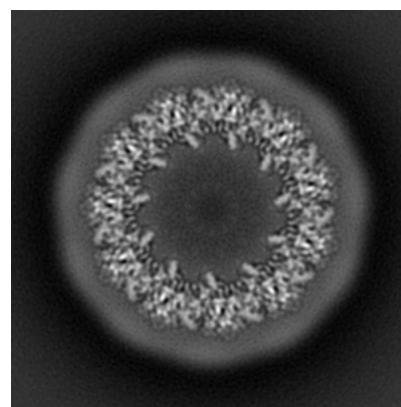
6.1.2 Raw map



X



Y

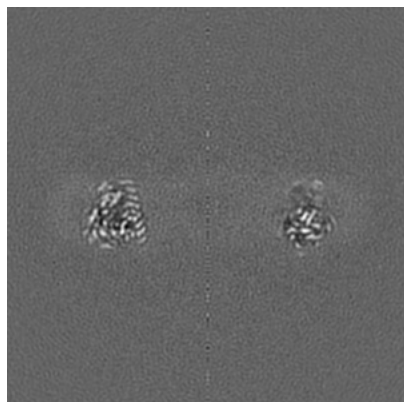


Z

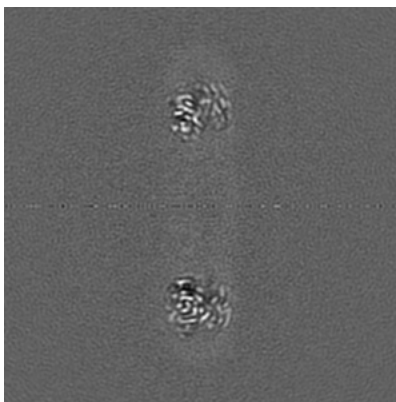
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

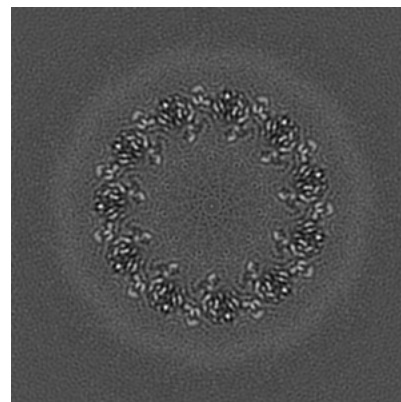
6.2.1 Primary map



X Index: 125

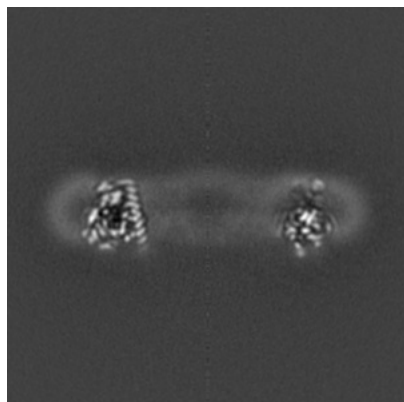


Y Index: 125

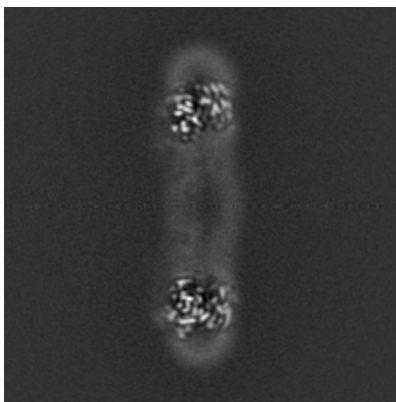


Z Index: 125

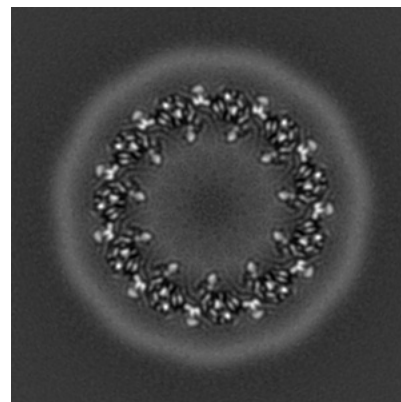
6.2.2 Raw map



X Index: 125



Y Index: 125

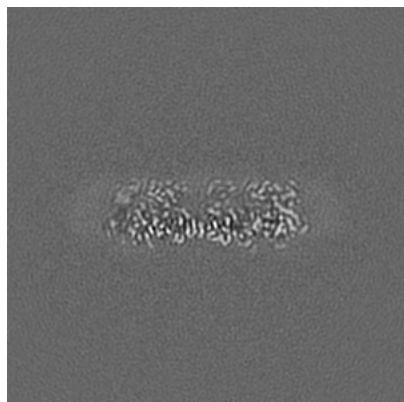


Z Index: 125

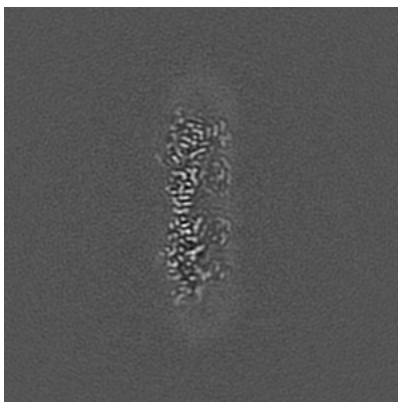
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

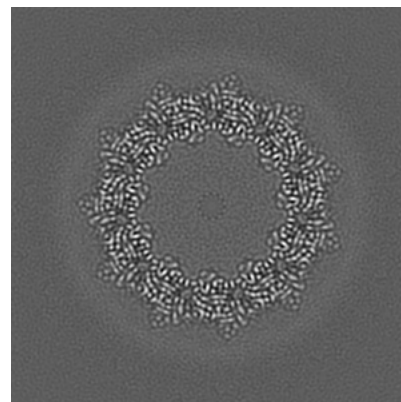
6.3.1 Primary map



X Index: 175

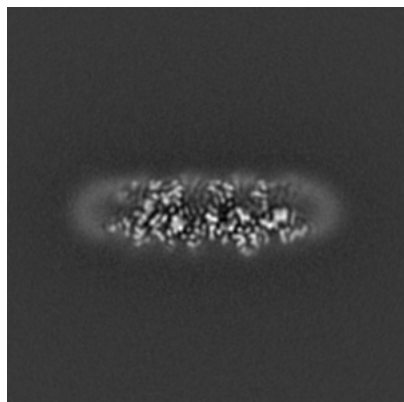


Y Index: 175

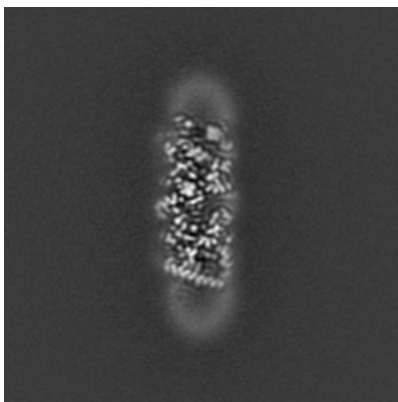


Z Index: 113

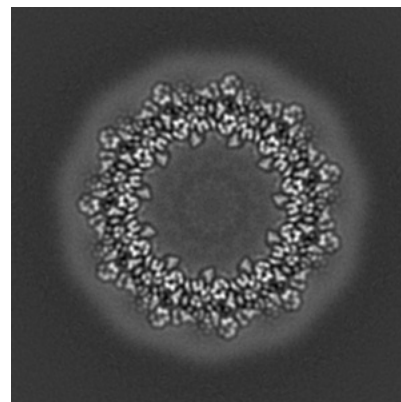
6.3.2 Raw map



X Index: 179



Y Index: 182

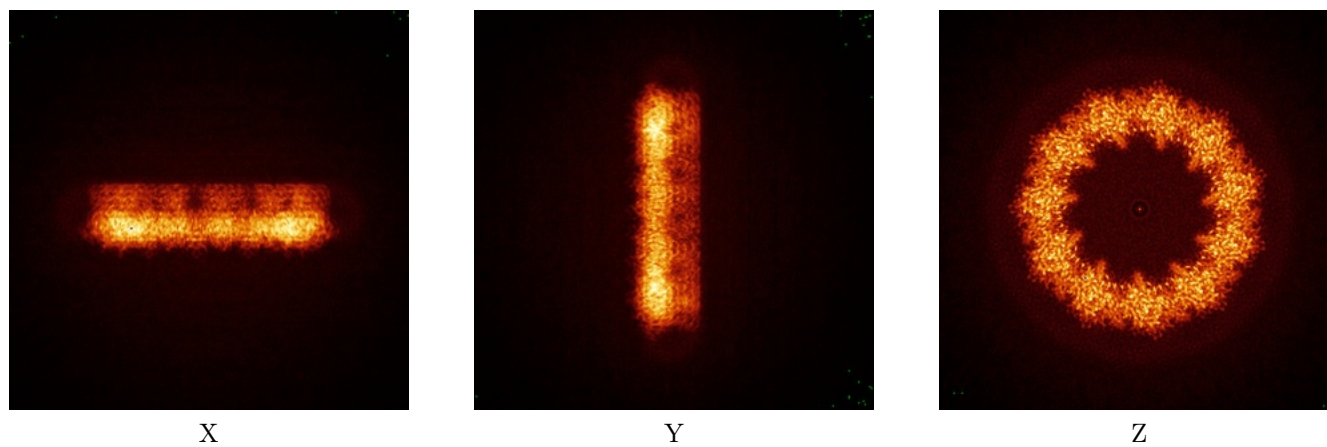


Z Index: 111

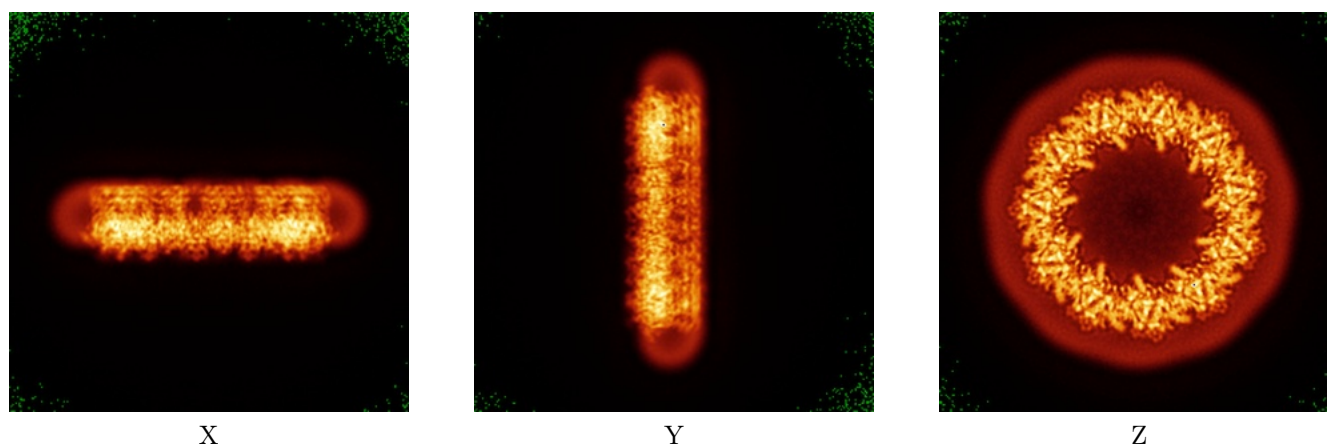
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

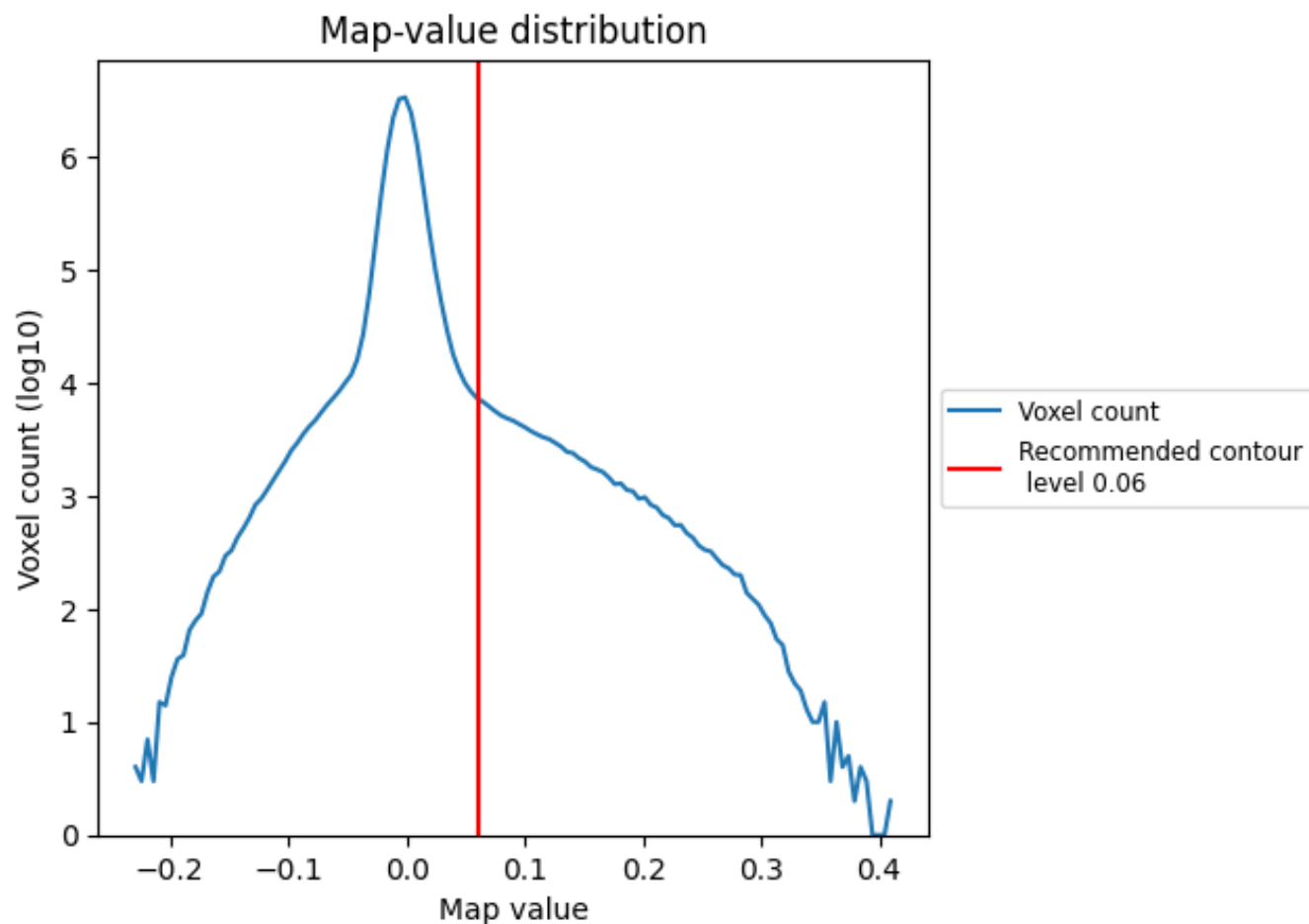
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

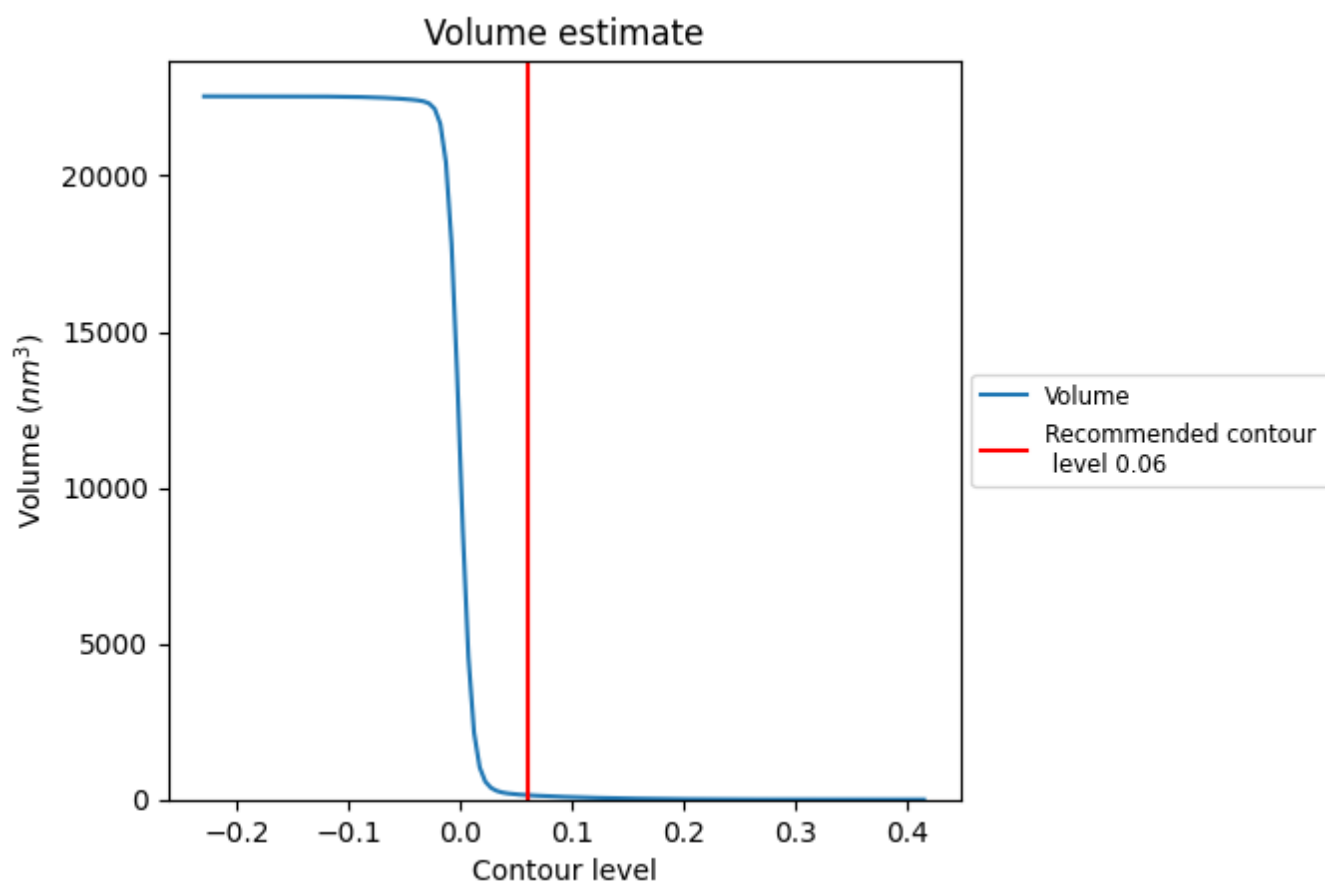
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

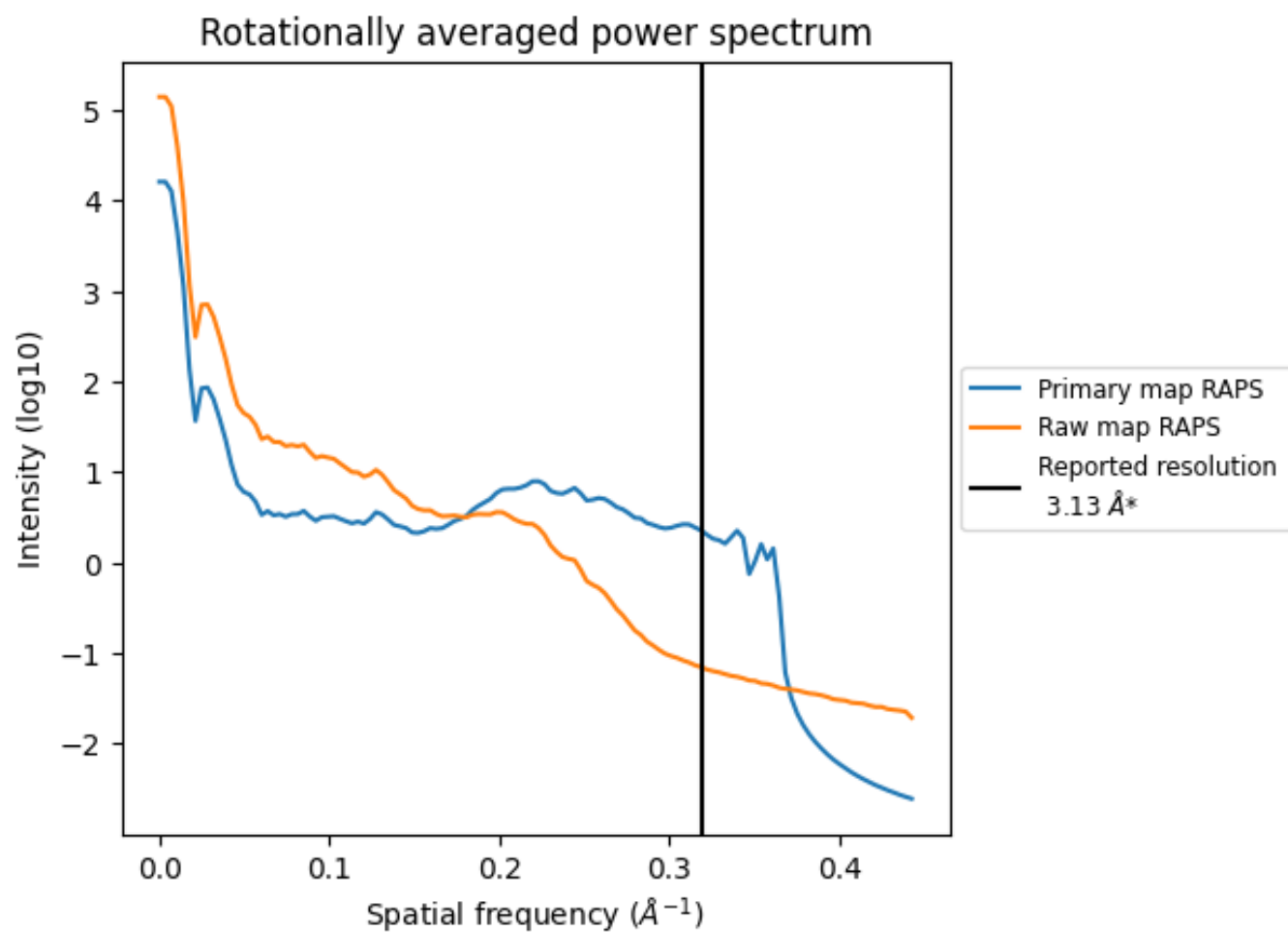
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 142 nm^3 ; this corresponds to an approximate mass of 128 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 ⓘ

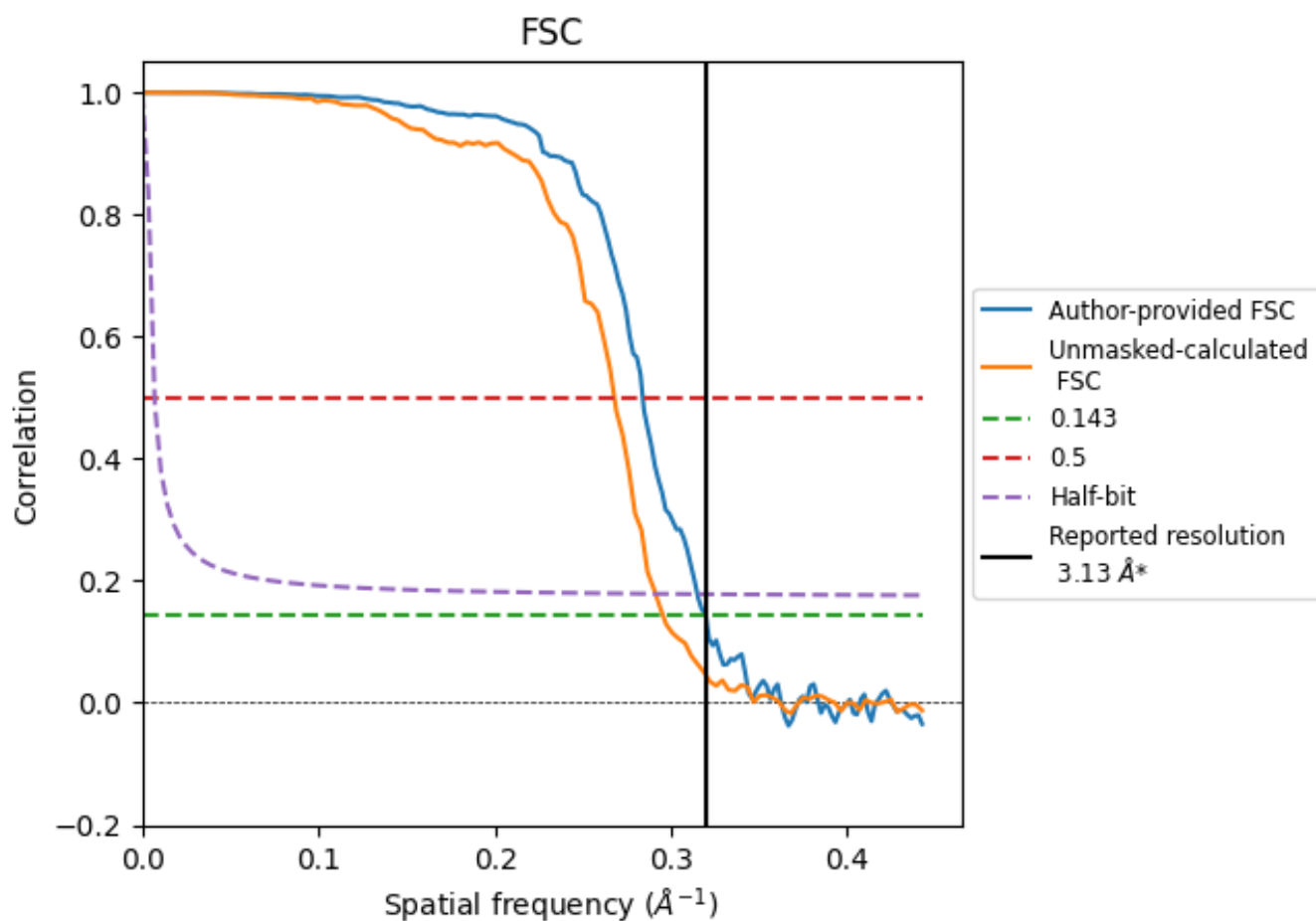


*Reported resolution corresponds to spatial frequency of 0.319 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.319 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

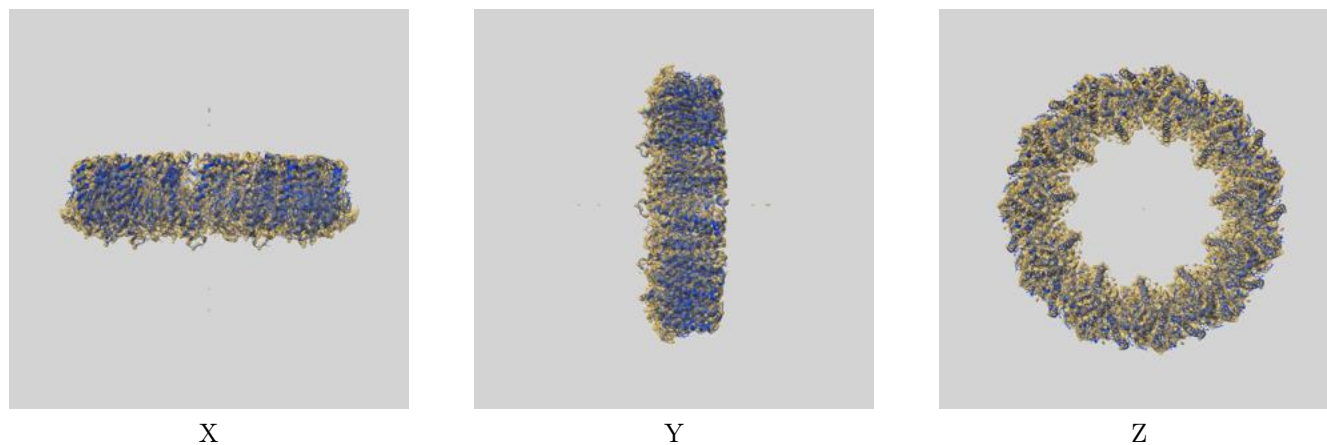
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.13	-	-
Author-provided FSC curve	3.13	3.52	3.17
Unmasked-calculated*	3.38	3.73	3.43

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

9 Map-model fit [i](#)

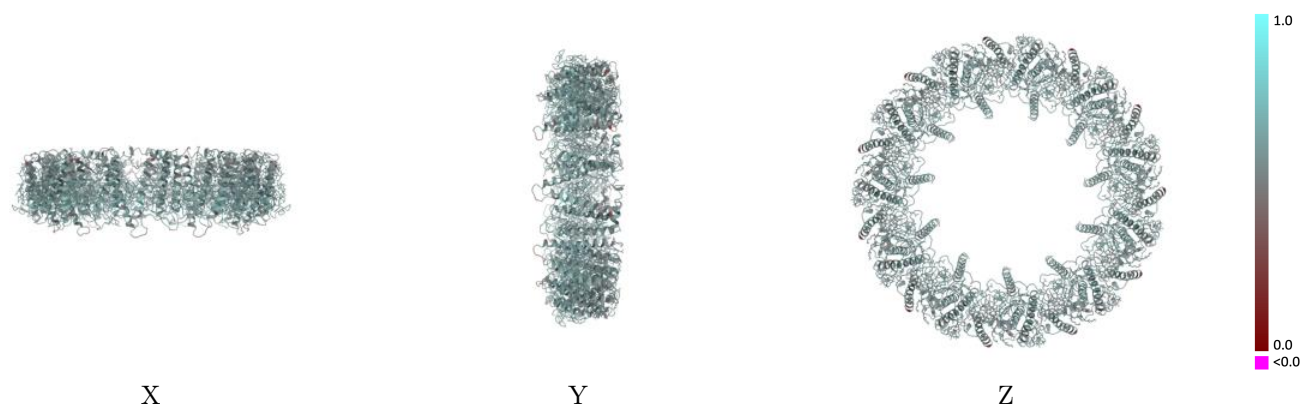
This section contains information regarding the fit between EMDB map EMD-35080 and PDB model 8HW1. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



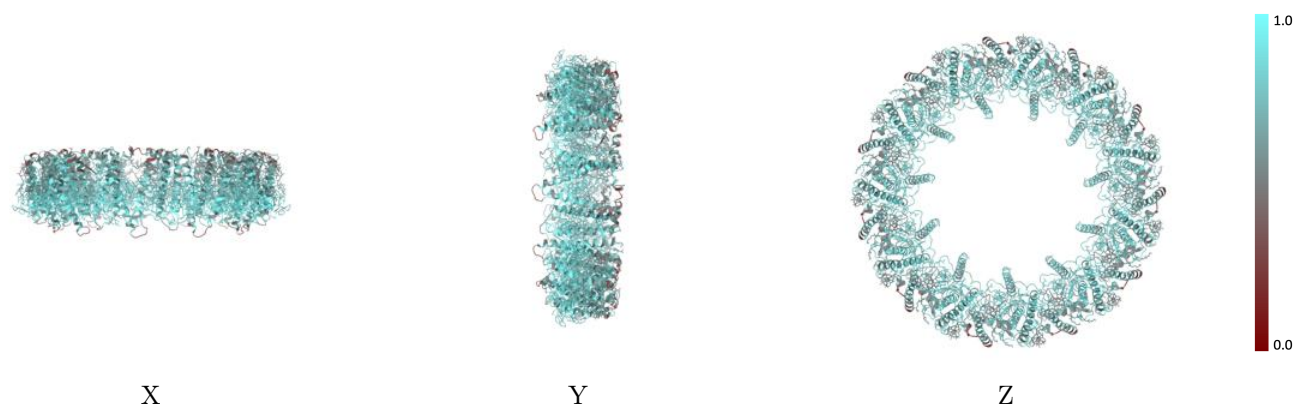
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



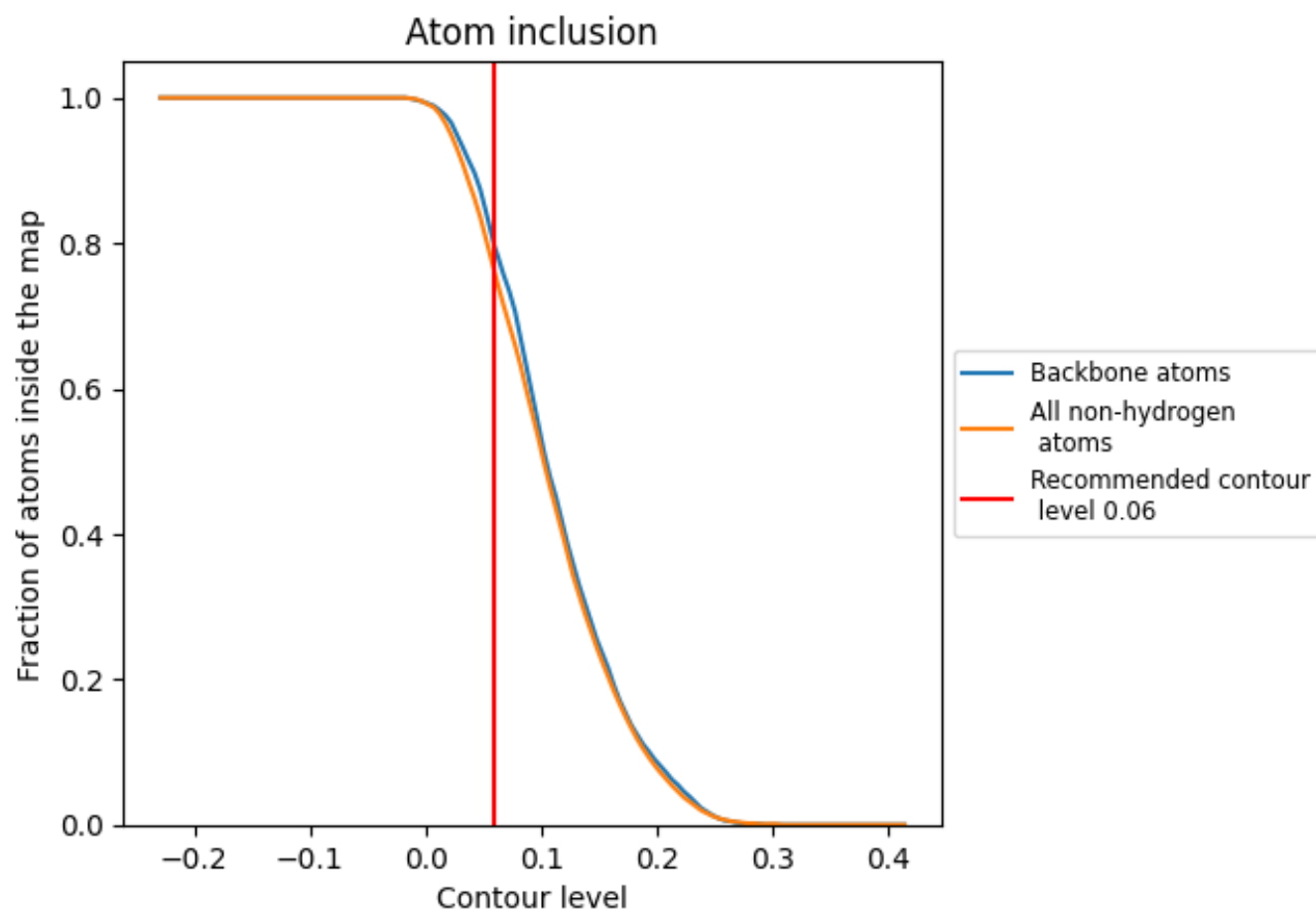
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion ⓘ



At the recommended contour level, 79% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7590	0.5800
A	0.7580	0.5810
B	0.7550	0.5810
C	0.7560	0.5790
D	0.7600	0.5810
E	0.7560	0.5800
F	0.7570	0.5780
G	0.7620	0.5780
H	0.7610	0.5800
I	0.7590	0.5790
J	0.7610	0.5800
K	0.7610	0.5810

1.0

0.0

<0.0