



## wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 01:16 PM UTC

PDB ID : 7Y8A / pdb\_00007y8a  
EMDB ID : EMD-33683  
Title : Cryo-EM structure of cryptophyte photosystem I  
Authors : Zhao, L.S.; Zhang, Y.Z.; Liu, L.N.; Li, K.  
Deposited on : 2022-06-23  
Resolution : 2.71 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

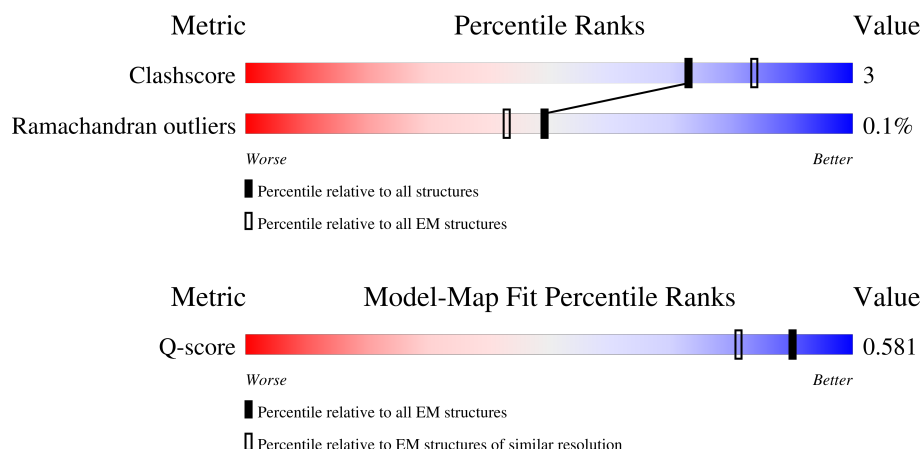
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 2.71 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Q-score               | -                           | 25397                       | 10297 ( 2.21 - 3.21 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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   | 1     | 222    |  71% 10% 19% |
| 2   | 2     | 216    |  69% 8% 22%  |
| 3   | 3     | 236    |  74% 24%     |
| 4   | 4     | 217    |  77% 19%     |
| 5   | 5     | 229    |  67% 15% 18% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 6   | 6     | 215    |                  |
| 7   | 7     | 230    |                  |
| 8   | 8     | 227    |                  |
| 9   | 9     | 220    |                  |
| 10  | A     | 752    |                  |
| 11  | B     | 734    |                  |
| 12  | C     | 81     |                  |
| 13  | D     | 141    |                  |
| 14  | E     | 64     |                  |
| 15  | F     | 183    |                  |
| 16  | I     | 36     |                  |
| 17  | J     | 42     |                  |
| 18  | K     | 87     |                  |
| 19  | L     | 153    |                  |
| 20  | M     | 30     |                  |
| 21  | O     | 154    |                  |
| 22  | R     | 133    |                  |
| 23  | X     | 164    |                  |
| 24  | Z     | 242    |                  |
| 25  | a     | 215    |                  |
| 26  | b     | 218    |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 27  | CLA  | 1     | 601 | X         | -        | -       | -                |
| 27  | CLA  | 1     | 602 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 27  | CLA  | 1     | 603 | X         | -        | -       | -                |
| 27  | CLA  | 1     | 604 | X         | -        | -       | -                |
| 27  | CLA  | 1     | 605 | X         | -        | -       | -                |
| 27  | CLA  | 1     | 606 | X         | -        | -       | -                |
| 27  | CLA  | 1     | 607 | X         | -        | -       | -                |
| 27  | CLA  | 1     | 608 | X         | -        | -       | -                |
| 27  | CLA  | 1     | 609 | X         | -        | -       | -                |
| 27  | CLA  | 1     | 611 | X         | -        | -       | -                |
| 27  | CLA  | 1     | 612 | X         | -        | -       | -                |
| 27  | CLA  | 1     | 613 | X         | -        | -       | -                |
| 27  | CLA  | 2     | 601 | X         | -        | -       | -                |
| 27  | CLA  | 2     | 602 | X         | -        | -       | -                |
| 27  | CLA  | 2     | 603 | X         | -        | -       | -                |
| 27  | CLA  | 2     | 604 | X         | -        | -       | -                |
| 27  | CLA  | 2     | 605 | X         | -        | -       | -                |
| 27  | CLA  | 2     | 606 | X         | -        | -       | -                |
| 27  | CLA  | 2     | 607 | X         | -        | -       | -                |
| 27  | CLA  | 2     | 608 | X         | -        | -       | -                |
| 27  | CLA  | 2     | 609 | X         | -        | -       | -                |
| 27  | CLA  | 2     | 611 | X         | -        | -       | -                |
| 27  | CLA  | 2     | 612 | X         | -        | -       | -                |
| 27  | CLA  | 3     | 601 | X         | -        | -       | -                |
| 27  | CLA  | 3     | 602 | X         | -        | -       | -                |
| 27  | CLA  | 3     | 603 | X         | -        | -       | -                |
| 27  | CLA  | 3     | 604 | X         | -        | -       | -                |
| 27  | CLA  | 3     | 605 | X         | -        | -       | -                |
| 27  | CLA  | 3     | 607 | X         | -        | -       | -                |
| 27  | CLA  | 3     | 608 | X         | -        | -       | -                |
| 27  | CLA  | 3     | 609 | X         | -        | -       | -                |
| 27  | CLA  | 3     | 610 | X         | -        | -       | -                |
| 27  | CLA  | 3     | 611 | X         | -        | -       | -                |
| 27  | CLA  | 3     | 612 | X         | -        | -       | -                |
| 27  | CLA  | 4     | 601 | X         | -        | -       | -                |
| 27  | CLA  | 4     | 602 | X         | -        | -       | -                |
| 27  | CLA  | 4     | 603 | X         | -        | -       | -                |
| 27  | CLA  | 4     | 604 | X         | -        | -       | -                |
| 27  | CLA  | 4     | 606 | X         | -        | -       | -                |
| 27  | CLA  | 4     | 607 | X         | -        | -       | -                |
| 27  | CLA  | 4     | 608 | X         | -        | -       | -                |
| 27  | CLA  | 4     | 609 | X         | -        | -       | -                |
| 27  | CLA  | 4     | 610 | X         | -        | -       | -                |
| 27  | CLA  | 4     | 611 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 27  | CLA  | 5     | 601 | X         | -        | -       | -                |
| 27  | CLA  | 5     | 602 | X         | -        | -       | -                |
| 27  | CLA  | 5     | 603 | X         | -        | -       | -                |
| 27  | CLA  | 5     | 604 | X         | -        | -       | -                |
| 27  | CLA  | 5     | 605 | X         | -        | -       | -                |
| 27  | CLA  | 5     | 606 | X         | -        | -       | -                |
| 27  | CLA  | 5     | 607 | X         | -        | -       | -                |
| 27  | CLA  | 5     | 608 | X         | -        | -       | -                |
| 27  | CLA  | 5     | 609 | X         | -        | -       | -                |
| 27  | CLA  | 5     | 611 | X         | -        | -       | -                |
| 27  | CLA  | 5     | 612 | X         | -        | -       | -                |
| 27  | CLA  | 5     | 613 | X         | -        | -       | -                |
| 27  | CLA  | 6     | 601 | X         | -        | -       | -                |
| 27  | CLA  | 6     | 602 | X         | -        | -       | -                |
| 27  | CLA  | 6     | 603 | X         | -        | -       | -                |
| 27  | CLA  | 6     | 604 | X         | -        | -       | -                |
| 27  | CLA  | 6     | 605 | X         | -        | -       | -                |
| 27  | CLA  | 6     | 606 | X         | -        | -       | -                |
| 27  | CLA  | 6     | 607 | X         | -        | -       | -                |
| 27  | CLA  | 6     | 608 | X         | -        | -       | -                |
| 27  | CLA  | 6     | 609 | X         | -        | -       | -                |
| 27  | CLA  | 6     | 611 | X         | -        | -       | -                |
| 27  | CLA  | 6     | 612 | X         | -        | -       | -                |
| 27  | CLA  | 7     | 302 | X         | -        | -       | -                |
| 27  | CLA  | 7     | 303 | X         | -        | -       | -                |
| 27  | CLA  | 7     | 304 | X         | -        | -       | -                |
| 27  | CLA  | 7     | 305 | X         | -        | -       | -                |
| 27  | CLA  | 7     | 306 | X         | -        | -       | -                |
| 27  | CLA  | 7     | 308 | X         | -        | -       | -                |
| 27  | CLA  | 7     | 309 | X         | -        | -       | -                |
| 27  | CLA  | 7     | 310 | X         | -        | -       | -                |
| 27  | CLA  | 7     | 312 | X         | -        | -       | -                |
| 27  | CLA  | 7     | 313 | X         | -        | -       | -                |
| 27  | CLA  | 8     | 601 | X         | -        | -       | -                |
| 27  | CLA  | 8     | 602 | X         | -        | -       | -                |
| 27  | CLA  | 8     | 603 | X         | -        | -       | -                |
| 27  | CLA  | 8     | 604 | X         | -        | -       | -                |
| 27  | CLA  | 8     | 605 | X         | -        | -       | -                |
| 27  | CLA  | 8     | 606 | X         | -        | -       | -                |
| 27  | CLA  | 8     | 607 | X         | -        | -       | -                |
| 27  | CLA  | 8     | 608 | X         | -        | -       | -                |
| 27  | CLA  | 8     | 615 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 27  | CLA  | 9     | 601 | X         | -        | -       | -                |
| 27  | CLA  | 9     | 602 | X         | -        | -       | -                |
| 27  | CLA  | 9     | 603 | X         | -        | -       | -                |
| 27  | CLA  | 9     | 604 | X         | -        | -       | -                |
| 27  | CLA  | 9     | 605 | X         | -        | -       | -                |
| 27  | CLA  | 9     | 606 | X         | -        | -       | -                |
| 27  | CLA  | 9     | 607 | X         | -        | -       | -                |
| 27  | CLA  | 9     | 608 | X         | -        | -       | -                |
| 27  | CLA  | 9     | 609 | X         | -        | -       | -                |
| 27  | CLA  | 9     | 611 | X         | -        | -       | -                |
| 27  | CLA  | 9     | 612 | X         | -        | -       | -                |
| 27  | CLA  | 9     | 613 | X         | -        | -       | -                |
| 27  | CLA  | 9     | 614 | X         | -        | -       | -                |
| 27  | CLA  | A     | 801 | X         | -        | -       | -                |
| 27  | CLA  | A     | 802 | X         | -        | -       | -                |
| 27  | CLA  | A     | 803 | X         | -        | -       | -                |
| 27  | CLA  | A     | 804 | X         | -        | -       | -                |
| 27  | CLA  | A     | 805 | X         | -        | -       | -                |
| 27  | CLA  | A     | 806 | X         | -        | -       | -                |
| 27  | CLA  | A     | 807 | X         | -        | -       | -                |
| 27  | CLA  | A     | 808 | X         | -        | -       | -                |
| 27  | CLA  | A     | 809 | X         | -        | -       | -                |
| 27  | CLA  | A     | 810 | X         | -        | -       | -                |
| 27  | CLA  | A     | 811 | X         | -        | -       | -                |
| 27  | CLA  | A     | 812 | X         | -        | -       | -                |
| 27  | CLA  | A     | 813 | X         | -        | -       | -                |
| 27  | CLA  | A     | 814 | X         | -        | -       | -                |
| 27  | CLA  | A     | 815 | X         | -        | -       | -                |
| 27  | CLA  | A     | 816 | X         | -        | -       | -                |
| 27  | CLA  | A     | 817 | X         | -        | -       | -                |
| 27  | CLA  | A     | 818 | X         | -        | -       | -                |
| 27  | CLA  | A     | 819 | X         | -        | -       | -                |
| 27  | CLA  | A     | 820 | X         | -        | -       | -                |
| 27  | CLA  | A     | 821 | X         | -        | -       | -                |
| 27  | CLA  | A     | 822 | X         | -        | -       | -                |
| 27  | CLA  | A     | 823 | X         | -        | -       | -                |
| 27  | CLA  | A     | 824 | X         | -        | -       | -                |
| 27  | CLA  | A     | 825 | X         | -        | -       | -                |
| 27  | CLA  | A     | 826 | X         | -        | -       | -                |
| 27  | CLA  | A     | 827 | X         | -        | -       | -                |
| 27  | CLA  | A     | 828 | X         | -        | -       | -                |
| 27  | CLA  | A     | 829 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 27  | CLA  | A     | 830 | X         | -        | -       | -                |
| 27  | CLA  | A     | 831 | X         | -        | -       | -                |
| 27  | CLA  | A     | 832 | X         | -        | -       | -                |
| 27  | CLA  | A     | 833 | X         | -        | -       | -                |
| 27  | CLA  | A     | 834 | X         | -        | -       | -                |
| 27  | CLA  | A     | 835 | X         | -        | -       | -                |
| 27  | CLA  | A     | 836 | X         | -        | -       | -                |
| 27  | CLA  | A     | 837 | X         | -        | -       | -                |
| 27  | CLA  | A     | 838 | X         | -        | -       | -                |
| 27  | CLA  | A     | 839 | X         | -        | -       | -                |
| 27  | CLA  | A     | 840 | X         | -        | -       | -                |
| 27  | CLA  | A     | 841 | X         | -        | -       | -                |
| 27  | CLA  | A     | 842 | X         | -        | -       | -                |
| 27  | CLA  | A     | 843 | X         | -        | -       | -                |
| 27  | CLA  | A     | 844 | X         | -        | -       | -                |
| 27  | CLA  | B     | 801 | X         | -        | -       | -                |
| 27  | CLA  | B     | 802 | X         | -        | -       | -                |
| 27  | CLA  | B     | 803 | X         | -        | -       | -                |
| 27  | CLA  | B     | 804 | X         | -        | -       | -                |
| 27  | CLA  | B     | 805 | X         | -        | -       | -                |
| 27  | CLA  | B     | 806 | X         | -        | -       | -                |
| 27  | CLA  | B     | 807 | X         | -        | -       | -                |
| 27  | CLA  | B     | 808 | X         | -        | -       | -                |
| 27  | CLA  | B     | 809 | X         | -        | -       | -                |
| 27  | CLA  | B     | 810 | X         | -        | -       | -                |
| 27  | CLA  | B     | 811 | X         | -        | -       | -                |
| 27  | CLA  | B     | 812 | X         | -        | -       | -                |
| 27  | CLA  | B     | 813 | X         | -        | -       | -                |
| 27  | CLA  | B     | 814 | X         | -        | -       | -                |
| 27  | CLA  | B     | 815 | X         | -        | -       | -                |
| 27  | CLA  | B     | 816 | X         | -        | -       | -                |
| 27  | CLA  | B     | 817 | X         | -        | -       | -                |
| 27  | CLA  | B     | 818 | X         | -        | -       | -                |
| 27  | CLA  | B     | 819 | X         | -        | -       | -                |
| 27  | CLA  | B     | 820 | X         | -        | -       | -                |
| 27  | CLA  | B     | 821 | X         | -        | -       | -                |
| 27  | CLA  | B     | 822 | X         | -        | -       | -                |
| 27  | CLA  | B     | 823 | X         | -        | -       | -                |
| 27  | CLA  | B     | 824 | X         | -        | -       | -                |
| 27  | CLA  | B     | 825 | X         | -        | -       | -                |
| 27  | CLA  | B     | 826 | X         | -        | -       | -                |
| 27  | CLA  | B     | 827 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 27  | CLA  | B     | 828 | X         | -        | -       | -                |
| 27  | CLA  | B     | 829 | X         | -        | -       | -                |
| 27  | CLA  | B     | 830 | X         | -        | -       | -                |
| 27  | CLA  | B     | 831 | X         | -        | -       | -                |
| 27  | CLA  | B     | 832 | X         | -        | -       | -                |
| 27  | CLA  | B     | 833 | X         | -        | -       | -                |
| 27  | CLA  | B     | 834 | X         | -        | -       | -                |
| 27  | CLA  | B     | 835 | X         | -        | -       | -                |
| 27  | CLA  | B     | 836 | X         | -        | -       | -                |
| 27  | CLA  | B     | 837 | X         | -        | -       | -                |
| 27  | CLA  | B     | 838 | X         | -        | -       | -                |
| 27  | CLA  | B     | 839 | X         | -        | -       | -                |
| 27  | CLA  | B     | 840 | X         | -        | -       | -                |
| 27  | CLA  | B     | 841 | X         | -        | -       | -                |
| 27  | CLA  | F     | 202 | X         | -        | -       | -                |
| 27  | CLA  | F     | 203 | X         | -        | -       | -                |
| 27  | CLA  | F     | 204 | X         | -        | -       | -                |
| 27  | CLA  | J     | 102 | X         | -        | -       | -                |
| 27  | CLA  | K     | 101 | X         | -        | -       | -                |
| 27  | CLA  | K     | 102 | X         | -        | -       | -                |
| 27  | CLA  | L     | 201 | X         | -        | -       | -                |
| 27  | CLA  | L     | 202 | X         | -        | -       | -                |
| 27  | CLA  | L     | 203 | X         | -        | -       | -                |
| 27  | CLA  | O     | 201 | X         | -        | -       | -                |
| 27  | CLA  | O     | 202 | X         | -        | -       | -                |
| 27  | CLA  | O     | 203 | X         | -        | -       | -                |
| 27  | CLA  | O     | 204 | X         | -        | -       | -                |
| 27  | CLA  | R     | 202 | X         | -        | -       | -                |
| 27  | CLA  | Z     | 301 | X         | -        | -       | -                |
| 27  | CLA  | Z     | 304 | X         | -        | -       | -                |
| 27  | CLA  | Z     | 305 | X         | -        | -       | -                |
| 27  | CLA  | Z     | 306 | X         | -        | -       | -                |
| 27  | CLA  | Z     | 310 | X         | -        | -       | -                |
| 27  | CLA  | a     | 601 | X         | -        | -       | -                |
| 27  | CLA  | a     | 602 | X         | -        | -       | -                |
| 27  | CLA  | a     | 603 | X         | -        | -       | -                |
| 27  | CLA  | a     | 604 | X         | -        | -       | -                |
| 27  | CLA  | a     | 605 | X         | -        | -       | -                |
| 27  | CLA  | a     | 606 | X         | -        | -       | -                |
| 27  | CLA  | a     | 607 | X         | -        | -       | -                |
| 27  | CLA  | a     | 608 | X         | -        | -       | -                |
| 27  | CLA  | a     | 610 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 27  | CLA  | a     | 611 | X         | -        | -       | -                |
| 27  | CLA  | b     | 601 | X         | -        | -       | -                |
| 27  | CLA  | b     | 602 | X         | -        | -       | -                |
| 27  | CLA  | b     | 603 | X         | -        | -       | -                |
| 27  | CLA  | b     | 604 | X         | -        | -       | -                |
| 27  | CLA  | b     | 606 | X         | -        | -       | -                |
| 27  | CLA  | b     | 607 | X         | -        | -       | -                |
| 27  | CLA  | b     | 608 | X         | -        | -       | -                |
| 27  | CLA  | b     | 610 | X         | -        | -       | -                |
| 27  | CLA  | b     | 611 | X         | -        | -       | -                |

## 2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 53404 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 ACPI-1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | 1     | 179      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1338  | 861 | 227 | 242 | 8 |         |       |

- Molecule 2 is a protein called ACPI-2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | 2     | 168      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1320  | 872 | 215 | 230 | 3 |         |       |

- Molecule 3 is a protein called ACPI-3.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 3   | 3     | 180      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1362  | 875 | 231 | 246 | 10 |         |       |

- Molecule 4 is a protein called ACPI-4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | 4     | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1366  | 891 | 224 | 245 | 6 |         |       |

- Molecule 5 is a protein called ACPI-5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | 5     | 188      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1403  | 908 | 234 | 253 | 8 |         |       |

- Molecule 6 is a protein called ACPI-6.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 6   | 6     | 173      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1305  | 846 | 217 | 232 | 10 |         |       |

- Molecule 7 is a protein called ACPI-7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | 7     | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1337  | 861 | 230 | 238 | 8 |         |       |

- Molecule 8 is a protein called ACPI-8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | 8     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1298  | 842 | 217 | 235 | 4 |         |       |

- Molecule 9 is a protein called ACPI-12.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 9   | 9     | 180      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1349  | 864 | 230 | 243 | 12 |         |       |

- Molecule 10 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 10  | A     | 741      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5824  | 3804 | 992 | 1000 | 28 |         |       |

- Molecule 11 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11  | B     | 731      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5828  | 3847 | 982 | 984 | 15 |         |       |

- Molecule 12 is a protein called Photosystem I iron-sulfur center.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 12  | C     | 80       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 591   | 361 | 103 | 115 | 12 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | D     | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1070  | 685 | 184 | 198 | 3 |         |       |

- Molecule 14 is a protein called Photosystem I reaction center subunit IV.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 14  | E     | 61       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 491   | 312 | 85 | 94 |         |       |

- Molecule 15 is a protein called Photosystem I reaction center subunit III.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | F     | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1258  | 814 | 214 | 228 | 2 |         |       |

- Molecule 16 is a protein called Photosystem I reaction center subunit VIII.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 16  | I     | 33       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 258   | 180 | 34 | 42 | 2 |         |       |

- Molecule 17 is a protein called Photosystem I reaction center subunit IX.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 17  | J     | 42       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 342   | 232 | 49 | 58 | 3 |         |       |

- Molecule 18 is a protein called Photosystem I reaction center subunit Psak.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 18  | K     | 78       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 553   | 358 | 90 | 102 | 3 |         |       |

- Molecule 19 is a protein called Photosystem I reaction center subunit XI.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | L     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1119  | 730 | 180 | 207 | 2 |         |       |

- Molecule 20 is a protein called Photosystem I reaction center subunit XII.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 20  | M     | 30       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 227   | 152 | 35 | 39 | 1 |         |       |

- Molecule 21 is a protein called Psao.



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | O     | 92       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 709   | 481 | 104 | 123 | 1 |         |       |

- Molecule 22 is a protein called Psar.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | R     | 92       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 680   | 439 | 112 | 127 | 2 |         |       |

- Molecule 23 is a protein called Unk1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | X     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 725   | 435 | 145 | 145 |   |         |       |

- Molecule 24 is a protein called ACPI-S.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 24  | Z     | 153      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1130  | 721 | 188 | 211 | 10 |         |       |

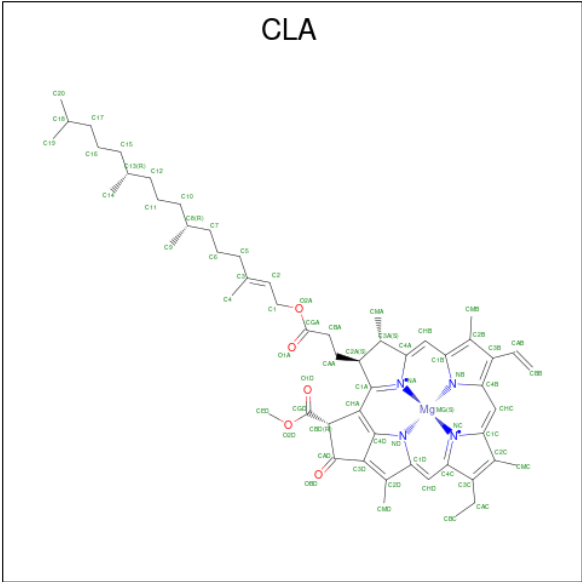
- Molecule 25 is a protein called ACPI-13.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 25  | a     | 171      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1271  | 823 | 207 | 231 | 10 |         |       |

- Molecule 26 is a protein called ACPI-14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | b     | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1368  | 891 | 224 | 244 | 9 |         |       |

- Molecule 27 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 27  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 27  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |
| 27  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |
| 27  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 27  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |
| 27  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 27  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 27  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 27  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |
| 27  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 27  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 27  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 27  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |
| 27  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 27  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 27  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 27  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 27  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 27  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 27  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 27  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |
| 27  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 27  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 27  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 27  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 27  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 27  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 27  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 27  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 27  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 27  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 27  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 27  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 27  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 27  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 27  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |
| 27  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 27  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 27  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 27  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 27  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 27  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 27  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 27  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 27  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |
| 27  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 27  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 27  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 27  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 27  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 27  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 27  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 27  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |
| 27  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 27  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 27  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 27  | 6     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 6     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 6     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 6     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 6     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 6     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 6     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 6     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 6     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 27  | 6     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 6     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 7     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 7     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 7     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 7     | 1        | Total<br>53 | C<br>43 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 7     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 7     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 7     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 7     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 27  | 7     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 7     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 27  | 8     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 8     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 8     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 8     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 8     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 8     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 8     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 27  | 8     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 8     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 9     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 9     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 9     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 9     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 9     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 9     | 1        | Total<br>64 | C<br>54 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 9     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 9     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 9     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 27  | 9     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 27  | 9     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | 9     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 27  | 9     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 27  | A     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>62 | C<br>52 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 27  | A     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 27  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>59 | C<br>49 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 27  | B     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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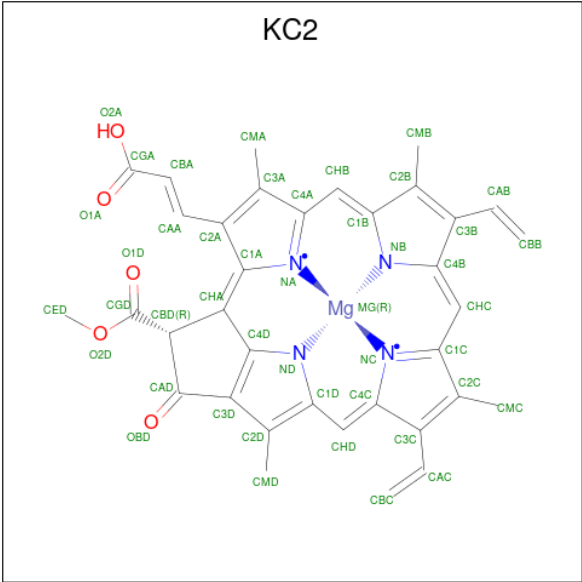
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 27  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | B     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | F     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | F     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | F     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | J     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 27  | K     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | K     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | L     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | L     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | L     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | O     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | O     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 27  | O     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | O     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | R     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | Z     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | Z     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | Z     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | Z     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 27  | Z     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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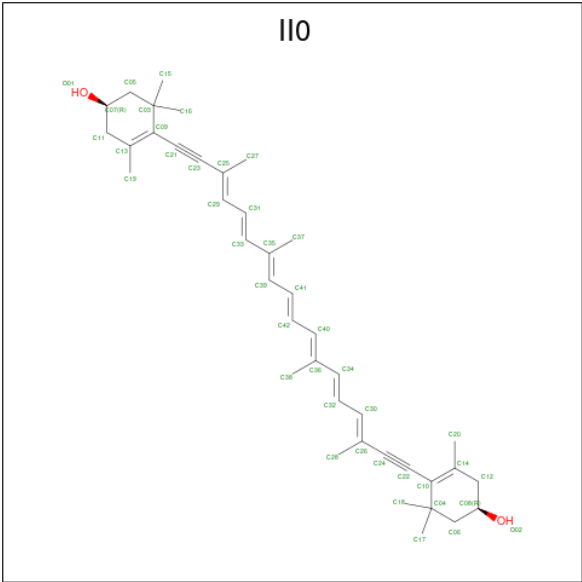
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 27  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 27  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 27  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 27  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 27  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 27  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 27  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 27  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 27  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 27  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 27  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 27  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 64    | 54 | 1  | 4 | 5 |         |
| 27  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 27  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 27  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 27  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 27  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 27  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 27  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |

- Molecule 28 is Chlorophyll c2 (CCD ID: KC2) (formula:  $C_{35}H_{28}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 28  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 28  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 28  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 28  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 28  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 28  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 28  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 28  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 28  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 28  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 28  | Z     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 28  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 28  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 28  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |

- Molecule 29 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (CCD ID: II0) (formula: C<sub>40</sub>H<sub>52</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 29  | 1     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 1     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 1     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 1     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 2     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 2     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 2     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 3     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 3     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 3     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 3     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 29  | 3     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 4     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 4     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 4     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 4     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 5     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 5     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 5     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 5     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 5     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 6     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 6     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 7     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 7     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 7     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 7     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 7     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 8     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 8     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 8     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 9     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

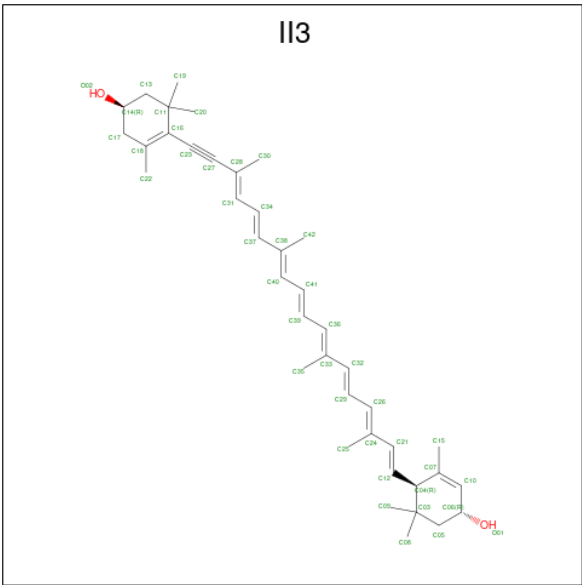
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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 29  | 9     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 9     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | 9     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | B     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | J     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | O     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | O     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | R     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | Z     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | b     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 29  | b     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

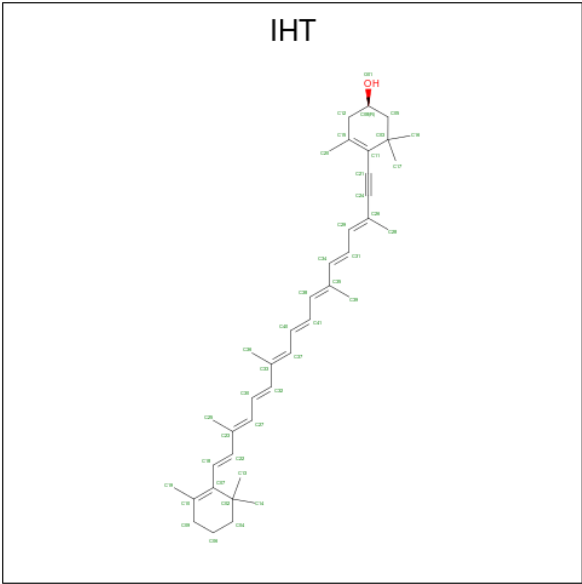
- Molecule 30 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: II3) (formula: C<sub>40</sub>H<sub>54</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).





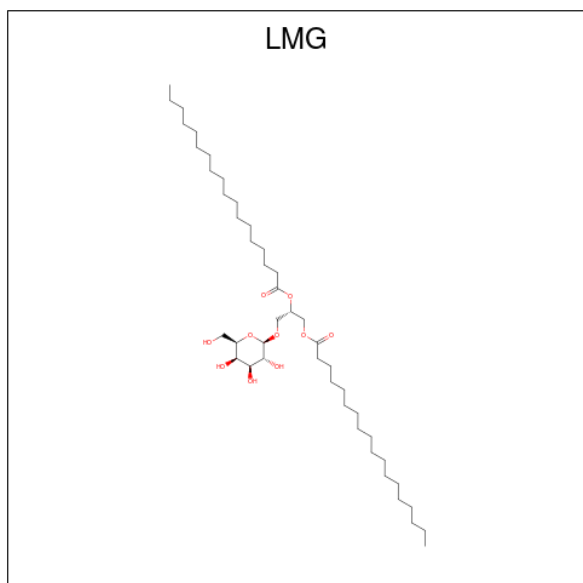
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 30  | 1     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 30  | b     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

- Molecule 31 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: IHT) (formula: C<sub>40</sub>H<sub>54</sub>O) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 31  | 1     | 1        | Total | C  | O | 0       |
|     |       |          | 41    | 40 | 1 |         |
| 31  | 2     | 1        | Total | C  | O | 0       |
|     |       |          | 41    | 40 | 1 |         |
| 31  | 5     | 1        | Total | C  | O | 0       |
|     |       |          | 41    | 40 | 1 |         |
| 31  | 6     | 1        | Total | C  | O | 0       |
|     |       |          | 41    | 40 | 1 |         |
| 31  | 8     | 1        | Total | C  | O | 0       |
|     |       |          | 41    | 40 | 1 |         |
| 31  | 9     | 1        | Total | C  | O | 0       |
|     |       |          | 41    | 40 | 1 |         |
| 31  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 41    | 40 | 1 |         |
| 31  | L     | 1        | Total | C  | O | 0       |
|     |       |          | 41    | 40 | 1 |         |
| 31  | Z     | 1        | Total | C  | O | 0       |
|     |       |          | 41    | 40 | 1 |         |
| 31  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 41    | 40 | 1 |         |

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



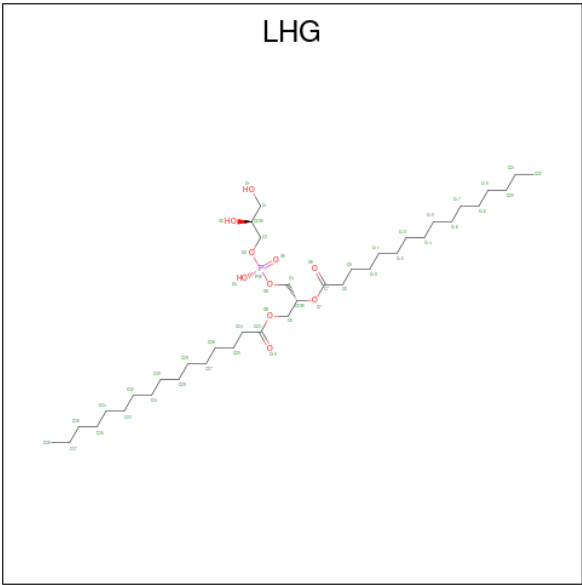
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 32  | 2     | 1        | Total | C  | O  | 0       |
|     |       |          | 36    | 26 | 10 |         |

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| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 32  | 3     | 1        | Total | C  | O  | 0       |
|     |       |          | 30    | 20 | 10 |         |
| 32  | 3     | 1        | Total | C  | O  | 0       |
|     |       |          | 32    | 22 | 10 |         |
| 32  | 6     | 1        | Total | C  | O  | 0       |
|     |       |          | 32    | 22 | 10 |         |
| 32  | 8     | 1        | Total | C  | O  | 0       |
|     |       |          | 52    | 42 | 10 |         |
| 32  | 8     | 1        | Total | C  | O  | 0       |
|     |       |          | 51    | 41 | 10 |         |
| 32  | F     | 1        | Total | C  | O  | 0       |
|     |       |          | 32    | 22 | 10 |         |

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



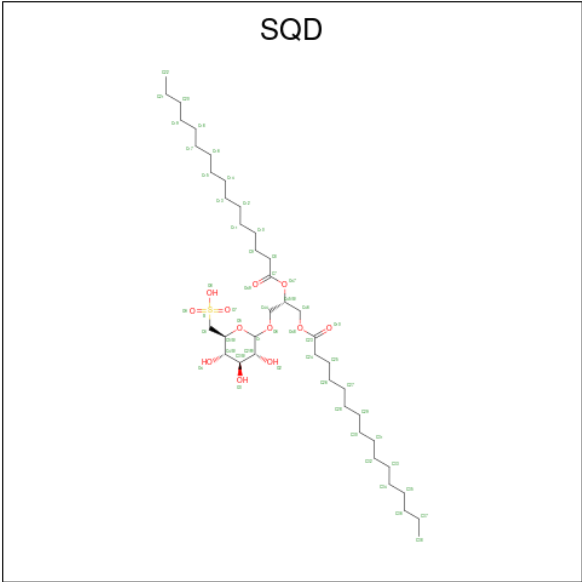
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 33  | 2     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 22    | 12 | 9  | 1 |         |
| 33  | 2     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 39    | 28 | 10 | 1 |         |
| 33  | 2     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 42    | 31 | 10 | 1 |         |
| 33  | 3     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 33  | 3     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 34    | 23 | 10 | 1 |         |

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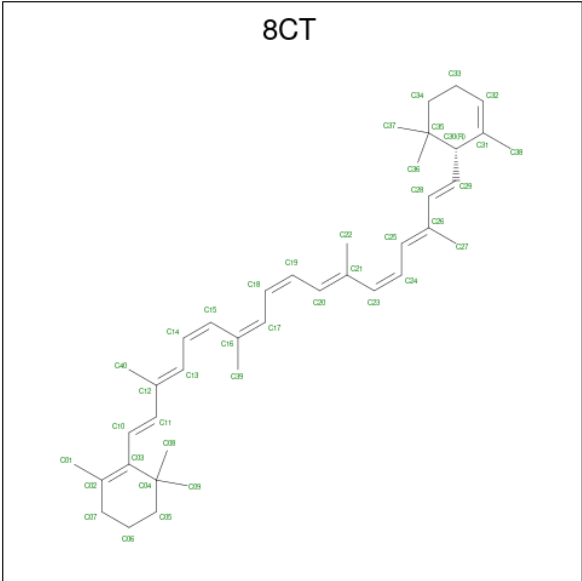
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 33  | 4     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 47    | 36 | 10 | 1 |         |
| 33  | 4     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 45    | 34 | 10 | 1 |         |
| 33  | 4     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 45    | 34 | 10 | 1 |         |
| 33  | 5     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 23    | 12 | 10 | 1 |         |
| 33  | 6     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 35    | 24 | 10 | 1 |         |
| 33  | 7     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 31    | 20 | 10 | 1 |         |
| 33  | 7     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 39    | 28 | 10 | 1 |         |
| 33  | 8     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 33    | 22 | 10 | 1 |         |
| 33  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 33  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 39    | 28 | 10 | 1 |         |
| 33  | Z     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 46    | 35 | 10 | 1 |         |
| 33  | a     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 33  | a     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 29    | 18 | 10 | 1 |         |
| 33  | b     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |

- Molecule 34 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 34  | 3     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 42    | 29 | 12 | 1 |         |
| 34  | O     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 24    | 12 | 11 | 1 |         |

- Molecule 35 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: C<sub>40</sub>H<sub>56</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 35  | 4     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |

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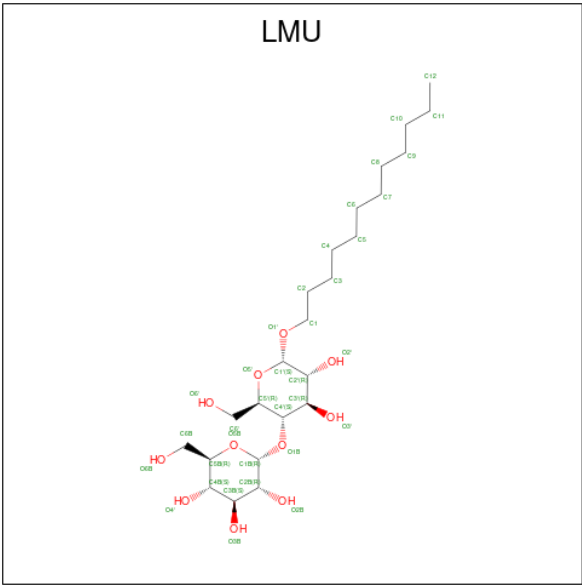
| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 35  | 7     | 1        | Total C<br>40 40 | 0       |
| 35  | A     | 1        | Total C<br>40 40 | 0       |
| 35  | A     | 1        | Total C<br>40 40 | 0       |
| 35  | A     | 1        | Total C<br>40 40 | 0       |
| 35  | A     | 1        | Total C<br>40 40 | 0       |
| 35  | A     | 1        | Total C<br>40 40 | 0       |
| 35  | B     | 1        | Total C<br>40 40 | 0       |
| 35  | B     | 1        | Total C<br>40 40 | 0       |
| 35  | B     | 1        | Total C<br>40 40 | 0       |
| 35  | B     | 1        | Total C<br>40 40 | 0       |
| 35  | B     | 1        | Total C<br>40 40 | 0       |
| 35  | B     | 1        | Total C<br>40 40 | 0       |
| 35  | B     | 1        | Total C<br>40 40 | 0       |
| 35  | F     | 1        | Total C<br>40 40 | 0       |
| 35  | I     | 1        | Total C<br>40 40 | 0       |
| 35  | J     | 1        | Total C<br>40 40 | 0       |
| 35  | K     | 1        | Total C<br>40 40 | 0       |
| 35  | L     | 1        | Total C<br>40 40 | 0       |
| 35  | M     | 1        | Total C<br>40 40 | 0       |
| 35  | R     | 1        | Total C<br>40 40 | 0       |
| 35  | R     | 1        | Total C<br>40 40 | 0       |
| 35  | Z     | 1        | Total C<br>40 40 | 0       |

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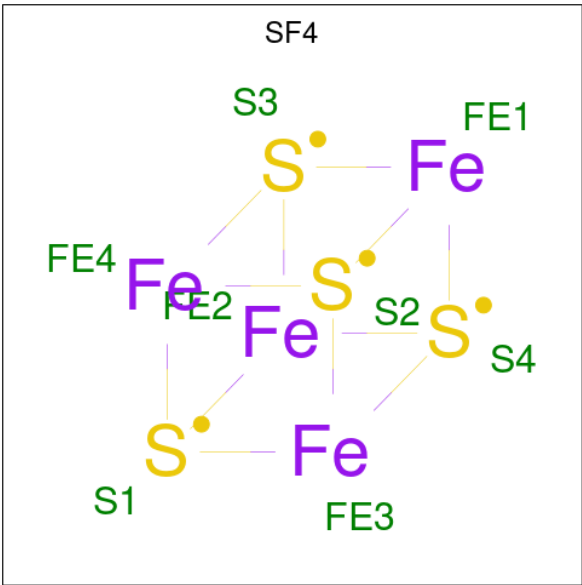
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 35  | Z     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 35  | b     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |

- Molecule 36 is DODECYL-ALPHA-D-MALTOSE (CCD ID: LMU) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



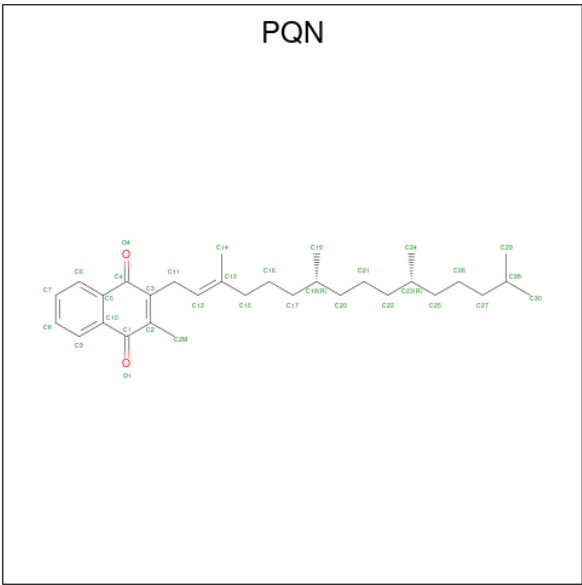
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 36  | 4     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 36  | 7     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 36  | J     | 1        | Total | C  | O  | 0       |
|     |       |          | 31    | 20 | 11 |         |

- Molecule 37 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 37  | A     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 37  | C     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 37  | C     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

- Molecule 38 is PHYLLOQUINONE (CCD ID: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 38  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |

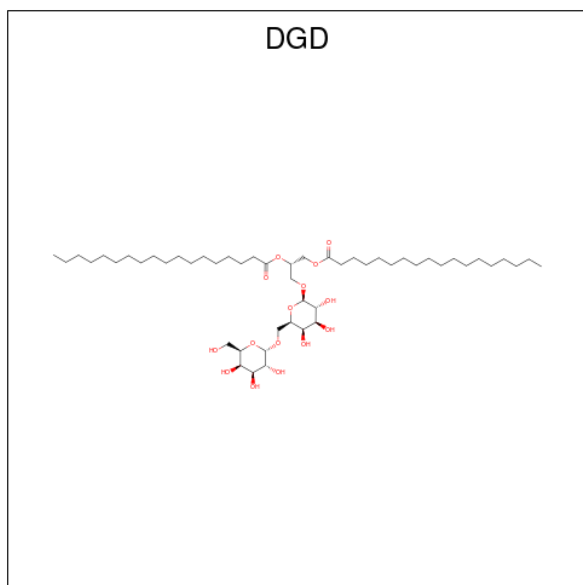
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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 38  | B     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |

- Molecule 39 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).

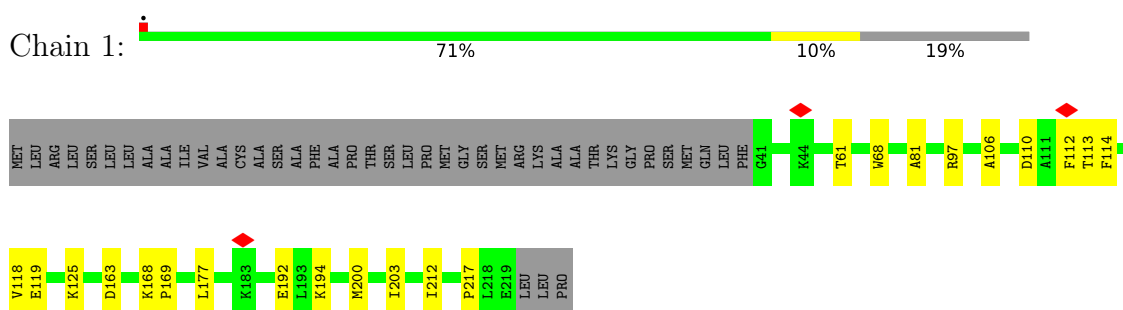


| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 39  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 59    | 44 | 15 |         |
| 39  | Z     | 1        | Total | C  | O  | 0       |
|     |       |          | 60    | 45 | 15 |         |

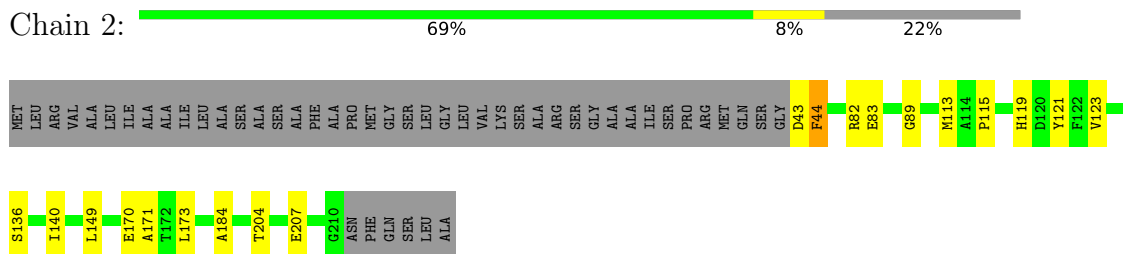
### 3 Residue-property plots

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

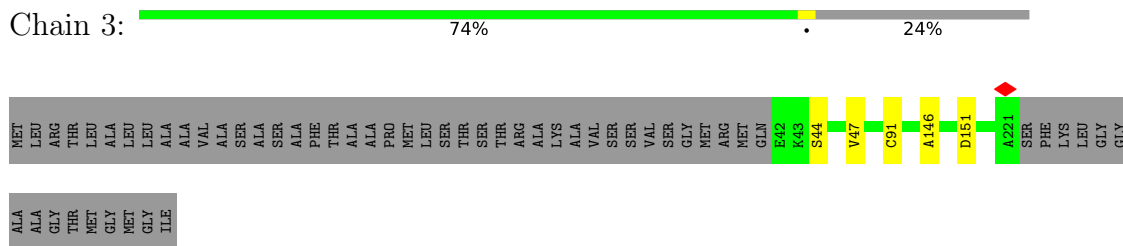
#### • Molecule 1: ACPI-1



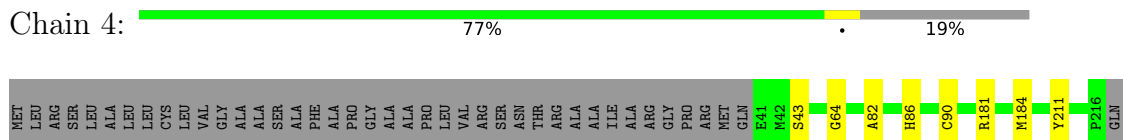
#### • Molecule 2: ACPI-2



#### • Molecule 3: ACPI-3

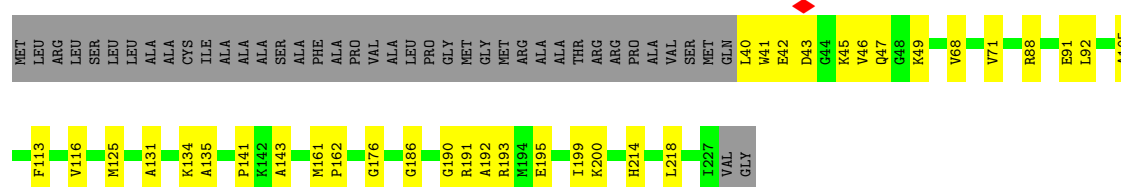


#### • Molecule 4: ACPI-4



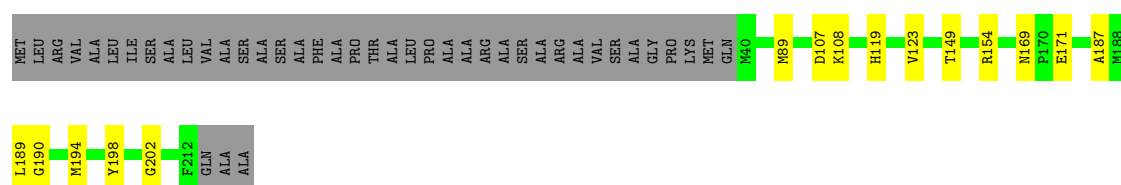
- Molecule 5: ACPI-5

Chain 5:  67% 15% 18%



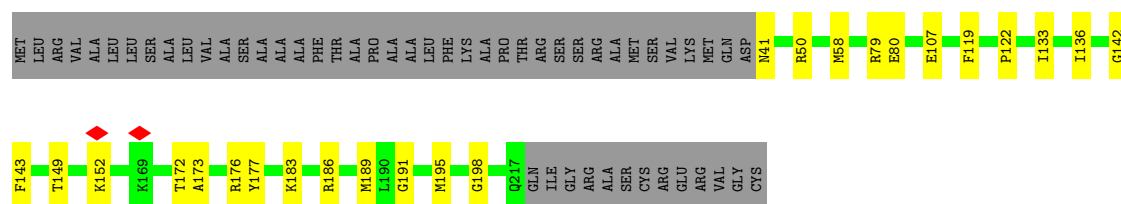
- Molecule 6: ACPI-6

Chain 6:  73% 7% 20%



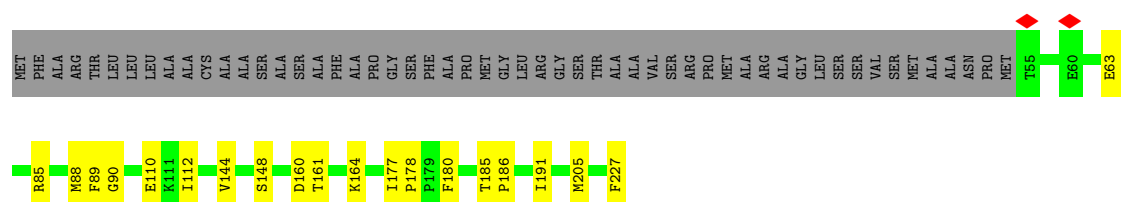
- Molecule 7: ACPI-7

Chain 7:  67% 10% 23%



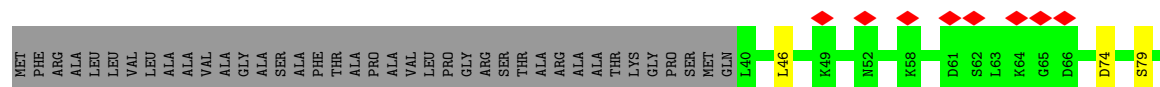
- Molecule 8: ACPI-8

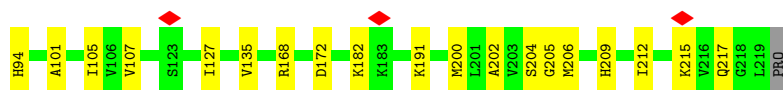
Chain 8:  67% 9% 24%



- Molecule 9: ACPI-12

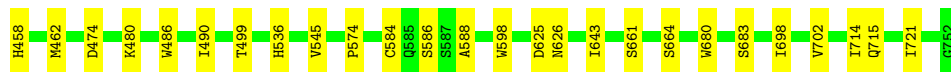
Chain 9:  5% 72% 10% 18%





- Molecule 10: Photosystem I P700 chlorophyll a apoprotein A1

Chain A: 92% 7%



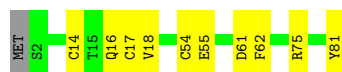
- Molecule 11: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 90% 9%



- Molecule 12: Photosystem I iron-sulfur center

Chain C: 86% 12%



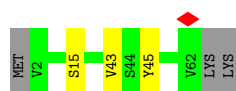
- Molecule 13: Photosystem I reaction center subunit II

Chain D: 89% 9%



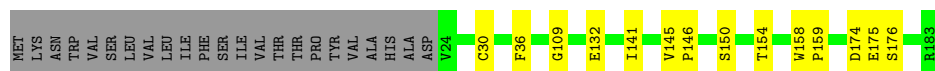
- Molecule 14: Photosystem I reaction center subunit IV

Chain E: 91% 5% 5%



- Molecule 15: Photosystem I reaction center subunit III

Chain F:  80% 8% 13%

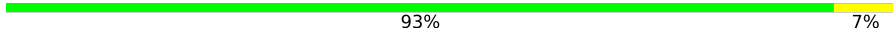


- Molecule 16: Photosystem I reaction center subunit VIII

Chain I:  86% 6% 8%



- Molecule 17: Photosystem I reaction center subunit IX

Chain J:  93% 7%



- Molecule 18: Photosystem I reaction center subunit PsaK

Chain K:  82% 8% 10%



- Molecule 19: Photosystem I reaction center subunit XI

Chain L:  7% 88% 8%



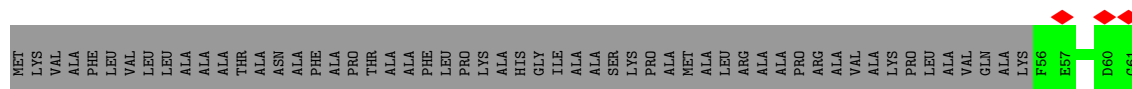
- Molecule 20: Photosystem I reaction center subunit XII

Chain M:  90% 10%

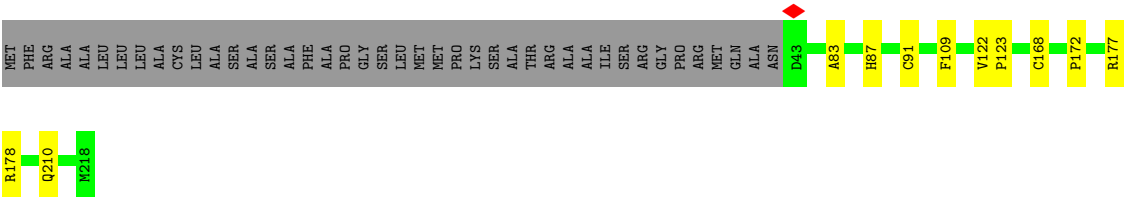


- Molecule 21: PsaO

Chain O:  14% 56% 40%







## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 118810                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 1000                                    | Depositor |
| Maximum defocus (nm)                 | 1800                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 1.988                                   | Depositor |
| Minimum map value                    | -0.065                                  | Depositor |
| Average map value                    | 0.033                                   | Depositor |
| Map value standard deviation         | 0.057                                   | Depositor |
| Recommended contour level            | 0.3                                     | Depositor |
| Map size (Å)                         | 423.99997, 423.99997, 423.99997         | wwPDB     |
| Map dimensions                       | 400, 400, 400                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.06, 1.06, 1.06                        | Depositor |



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: II3, LMU, IHT, SQD, LMG, LHG, SF4, DGD, CLA, II0, 8CT, PQN, KC2

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   | 1     | 0.37         | 0/1371         | 0.63        | 0/1854          |
| 2   | 2     | 0.18         | 0/1356         | 0.33        | 0/1835          |
| 3   | 3     | 0.19         | 0/1392         | 0.32        | 0/1883          |
| 4   | 4     | 0.18         | 0/1406         | 0.29        | 0/1900          |
| 5   | 5     | 0.37         | 0/1438         | 0.57        | 1/1940 (0.1%)   |
| 6   | 6     | 0.18         | 0/1334         | 0.32        | 0/1796          |
| 7   | 7     | 0.33         | 1/1373 (0.1%)  | 0.47        | 0/1858          |
| 8   | 8     | 0.23         | 0/1326         | 0.35        | 0/1804          |
| 9   | 9     | 0.20         | 0/1376         | 0.34        | 0/1846          |
| 10  | A     | 0.24         | 3/6019 (0.0%)  | 0.35        | 0/8204          |
| 11  | B     | 0.30         | 3/6046 (0.0%)  | 0.45        | 3/8254 (0.0%)   |
| 12  | C     | 0.27         | 0/600          | 0.42        | 0/812           |
| 13  | D     | 0.24         | 0/1094         | 0.43        | 0/1476          |
| 14  | E     | 0.33         | 0/499          | 0.54        | 0/677           |
| 15  | F     | 0.21         | 0/1290         | 0.35        | 0/1745          |
| 16  | I     | 0.17         | 0/266          | 0.30        | 0/362           |
| 17  | J     | 0.21         | 0/353          | 0.32        | 0/481           |
| 18  | K     | 0.41         | 0/563          | 0.40        | 0/768           |
| 19  | L     | 0.41         | 0/1147         | 0.55        | 4/1561 (0.3%)   |
| 20  | M     | 0.17         | 0/228          | 0.22        | 0/310           |
| 21  | O     | 0.27         | 0/737          | 0.50        | 0/1011          |
| 22  | R     | 0.35         | 0/700          | 0.46        | 2/963 (0.2%)    |
| 24  | Z     | 0.20         | 0/1163         | 0.35        | 0/1572          |
| 25  | a     | 0.40         | 2/1299 (0.2%)  | 0.52        | 2/1747 (0.1%)   |
| 26  | b     | 0.24         | 0/1404         | 0.41        | 3/1902 (0.2%)   |
| All | All   | 0.28         | 9/35780 (0.0%) | 0.42        | 15/48561 (0.0%) |

The worst 5 of 9 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 25  | a     | 172 | ASN  | C-N   | -7.75 | 1.23        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 25  | a     | 171 | LYS  | C-N   | -7.27 | 1.23        | 1.33     |
| 11  | B     | 683 | GLU  | C-N   | -6.88 | 1.23        | 1.33     |
| 10  | A     | 196 | SER  | C-N   | 6.42  | 1.42        | 1.34     |
| 11  | B     | 583 | MET  | C-O   | -6.42 | 1.16        | 1.24     |

The worst 5 of 15 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 19  | L     | 80  | PHE  | CA-C-O | -6.55 | 113.48      | 120.42   |
| 5   | 5     | 141 | PRO  | N-CA-C | -6.41 | 99.26       | 112.47   |
| 11  | B     | 546 | LEU  | CA-C-O | -5.99 | 114.53      | 120.70   |
| 25  | a     | 172 | ASN  | CA-C-N | 5.87  | 128.62      | 120.29   |
| 25  | a     | 172 | ASN  | C-N-CA | 5.87  | 128.62      | 120.29   |

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   | 1     | 1338  | 0        | 1329     | 18      | 0            |
| 2   | 2     | 1320  | 0        | 1309     | 12      | 0            |
| 3   | 3     | 1362  | 0        | 1389     | 4       | 0            |
| 4   | 4     | 1366  | 0        | 1349     | 5       | 0            |
| 5   | 5     | 1403  | 0        | 1398     | 33      | 0            |
| 6   | 6     | 1305  | 0        | 1324     | 8       | 0            |
| 7   | 7     | 1337  | 0        | 1317     | 16      | 0            |
| 8   | 8     | 1298  | 0        | 1322     | 16      | 0            |
| 9   | 9     | 1349  | 0        | 1358     | 20      | 0            |
| 10  | A     | 5824  | 0        | 5672     | 38      | 0            |
| 11  | B     | 5828  | 0        | 5626     | 44      | 0            |
| 12  | C     | 591   | 0        | 568      | 9       | 0            |
| 13  | D     | 1070  | 0        | 1076     | 10      | 0            |
| 14  | E     | 491   | 0        | 491      | 3       | 0            |
| 15  | F     | 1258  | 0        | 1266     | 11      | 0            |
| 16  | I     | 258   | 0        | 268      | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 17  | J     | 342   | 0        | 344      | 2       | 0            |
| 18  | K     | 553   | 0        | 581      | 8       | 0            |
| 19  | L     | 1119  | 0        | 1117     | 7       | 0            |
| 20  | M     | 227   | 0        | 257      | 3       | 0            |
| 21  | O     | 709   | 0        | 691      | 4       | 0            |
| 22  | R     | 680   | 0        | 674      | 7       | 0            |
| 23  | X     | 725   | 0        | 151      | 12      | 0            |
| 24  | Z     | 1130  | 0        | 1088     | 6       | 0            |
| 25  | a     | 1271  | 0        | 1281     | 15      | 0            |
| 26  | b     | 1368  | 0        | 1346     | 6       | 0            |
| 27  | 1     | 584   | 0        | 476      | 5       | 0            |
| 27  | 2     | 547   | 0        | 456      | 1       | 0            |
| 27  | 3     | 625   | 0        | 596      | 0       | 0            |
| 27  | 4     | 598   | 0        | 597      | 1       | 0            |
| 27  | 5     | 563   | 0        | 442      | 7       | 0            |
| 27  | 6     | 581   | 0        | 514      | 2       | 0            |
| 27  | 7     | 509   | 0        | 431      | 4       | 0            |
| 27  | 8     | 496   | 0        | 471      | 4       | 0            |
| 27  | 9     | 642   | 0        | 539      | 6       | 0            |
| 27  | A     | 2679  | 0        | 2767     | 18      | 0            |
| 27  | B     | 2471  | 0        | 2530     | 20      | 0            |
| 27  | F     | 160   | 0        | 141      | 0       | 0            |
| 27  | J     | 41    | 0        | 29       | 0       | 0            |
| 27  | K     | 120   | 0        | 121      | 1       | 0            |
| 27  | L     | 161   | 0        | 139      | 2       | 0            |
| 27  | O     | 206   | 0        | 176      | 1       | 0            |
| 27  | R     | 55    | 0        | 49       | 1       | 0            |
| 27  | Z     | 290   | 0        | 278      | 1       | 0            |
| 27  | a     | 580   | 0        | 560      | 5       | 0            |
| 27  | b     | 530   | 0        | 525      | 1       | 0            |
| 28  | 1     | 45    | 0        | 0        | 0       | 0            |
| 28  | 2     | 45    | 0        | 0        | 0       | 0            |
| 28  | 3     | 45    | 0        | 0        | 0       | 0            |
| 28  | 4     | 45    | 0        | 0        | 0       | 0            |
| 28  | 5     | 45    | 0        | 0        | 0       | 0            |
| 28  | 6     | 90    | 0        | 0        | 0       | 0            |
| 28  | 7     | 90    | 0        | 0        | 2       | 0            |
| 28  | 9     | 45    | 0        | 0        | 1       | 0            |
| 28  | Z     | 45    | 0        | 0        | 0       | 0            |
| 28  | a     | 45    | 0        | 0        | 0       | 0            |
| 28  | b     | 90    | 0        | 0        | 1       | 0            |
| 29  | 1     | 168   | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 29  | 2     | 126   | 0        | 0        | 1       | 0            |
| 29  | 3     | 210   | 0        | 0        | 1       | 0            |
| 29  | 4     | 168   | 0        | 0        | 1       | 0            |
| 29  | 5     | 210   | 0        | 0        | 1       | 0            |
| 29  | 6     | 84    | 0        | 0        | 0       | 0            |
| 29  | 7     | 210   | 0        | 0        | 0       | 0            |
| 29  | 8     | 126   | 0        | 0        | 1       | 0            |
| 29  | 9     | 168   | 0        | 0        | 0       | 0            |
| 29  | B     | 42    | 0        | 0        | 0       | 0            |
| 29  | J     | 42    | 0        | 0        | 0       | 0            |
| 29  | O     | 84    | 0        | 0        | 0       | 0            |
| 29  | R     | 42    | 0        | 0        | 0       | 0            |
| 29  | Z     | 42    | 0        | 0        | 0       | 0            |
| 29  | a     | 168   | 0        | 0        | 1       | 0            |
| 29  | b     | 84    | 0        | 0        | 0       | 0            |
| 30  | 1     | 42    | 0        | 0        | 0       | 0            |
| 30  | b     | 42    | 0        | 0        | 1       | 0            |
| 31  | 1     | 41    | 0        | 0        | 0       | 0            |
| 31  | 2     | 41    | 0        | 0        | 1       | 0            |
| 31  | 5     | 41    | 0        | 0        | 0       | 0            |
| 31  | 6     | 41    | 0        | 0        | 1       | 0            |
| 31  | 8     | 41    | 0        | 0        | 0       | 0            |
| 31  | 9     | 41    | 0        | 0        | 1       | 0            |
| 31  | A     | 41    | 0        | 0        | 1       | 0            |
| 31  | L     | 41    | 0        | 0        | 0       | 0            |
| 31  | Z     | 41    | 0        | 0        | 0       | 0            |
| 31  | a     | 41    | 0        | 0        | 1       | 0            |
| 32  | 2     | 36    | 0        | 42       | 0       | 0            |
| 32  | 3     | 62    | 0        | 64       | 0       | 0            |
| 32  | 6     | 32    | 0        | 34       | 0       | 0            |
| 32  | 8     | 103   | 0        | 152      | 0       | 0            |
| 32  | F     | 32    | 0        | 34       | 0       | 0            |
| 33  | 2     | 103   | 0        | 125      | 1       | 0            |
| 33  | 3     | 83    | 0        | 112      | 0       | 0            |
| 33  | 4     | 137   | 0        | 190      | 0       | 0            |
| 33  | 5     | 23    | 0        | 16       | 0       | 0            |
| 33  | 6     | 35    | 0        | 40       | 1       | 0            |
| 33  | 7     | 70    | 0        | 83       | 0       | 0            |
| 33  | 8     | 33    | 0        | 36       | 0       | 0            |
| 33  | A     | 88    | 0        | 122      | 0       | 0            |
| 33  | Z     | 46    | 0        | 65       | 0       | 0            |
| 33  | a     | 78    | 0        | 102      | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 33  | b     | 49    | 0        | 74       | 0       | 0            |
| 34  | 3     | 42    | 0        | 48       | 0       | 0            |
| 34  | O     | 24    | 0        | 18       | 0       | 0            |
| 35  | 4     | 40    | 0        | 0        | 1       | 0            |
| 35  | 7     | 40    | 0        | 0        | 1       | 0            |
| 35  | A     | 200   | 0        | 0        | 0       | 0            |
| 35  | B     | 240   | 0        | 0        | 0       | 0            |
| 35  | F     | 40    | 0        | 0        | 0       | 0            |
| 35  | I     | 40    | 0        | 0        | 0       | 0            |
| 35  | J     | 40    | 0        | 0        | 0       | 0            |
| 35  | K     | 40    | 0        | 0        | 0       | 0            |
| 35  | L     | 40    | 0        | 0        | 0       | 0            |
| 35  | M     | 40    | 0        | 0        | 1       | 0            |
| 35  | R     | 80    | 0        | 0        | 0       | 0            |
| 35  | Z     | 80    | 0        | 0        | 0       | 0            |
| 35  | b     | 40    | 0        | 0        | 0       | 0            |
| 36  | 4     | 35    | 0        | 46       | 2       | 0            |
| 36  | 7     | 35    | 0        | 46       | 1       | 0            |
| 36  | J     | 31    | 0        | 35       | 1       | 0            |
| 37  | A     | 8     | 0        | 0        | 0       | 0            |
| 37  | C     | 16    | 0        | 0        | 1       | 0            |
| 38  | A     | 33    | 0        | 46       | 0       | 0            |
| 38  | B     | 33    | 0        | 46       | 0       | 0            |
| 39  | B     | 59    | 0        | 79       | 0       | 0            |
| 39  | Z     | 60    | 0        | 78       | 1       | 0            |
| All | All   | 53404 | 0        | 48162    | 332     | 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 3.

The worst 5 of 332 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) |
|------------------|------------------|--------------------------|-------------------|
| 5:5:41:TRP:HB2   | 5:5:192:ALA:HB1  | 1.44                     | 0.99              |
| 13:D:99:HIS:HB3  | 13:D:100:PRO:HD3 | 1.55                     | 0.88              |
| 5:5:42:GLU:HB3   | 5:5:45:LYS:HB2   | 1.58                     | 0.84              |
| 22:R:74:VAL:O    | 22:R:128:GLN:NE2 | 2.13                     | 0.81              |
| 26:b:177:ARG:NH2 | 28:b:609:KC2:O1A | 2.14                     | 0.80              |

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   | 1     | 177/222 (80%)   | 167 (94%)  | 10 (6%) | 0        | 100         | 100 |
| 2   | 2     | 158/216 (73%)   | 154 (98%)  | 3 (2%)  | 1 (1%)   | 21          | 42  |
| 3   | 3     | 121/236 (51%)   | 119 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 4   | 4     | 121/217 (56%)   | 120 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 5   | 5     | 186/229 (81%)   | 176 (95%)  | 10 (5%) | 0        | 100         | 100 |
| 6   | 6     | 82/215 (38%)    | 80 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 7   | 7     | 158/230 (69%)   | 154 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 8   | 8     | 171/227 (75%)   | 168 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 9   | 9     | 178/220 (81%)   | 175 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 10  | A     | 739/752 (98%)   | 714 (97%)  | 25 (3%) | 0        | 100         | 100 |
| 11  | B     | 157/734 (21%)   | 153 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 13  | D     | 9/141 (6%)      | 9 (100%)   | 0       | 0        | 100         | 100 |
| 14  | E     | 44/64 (69%)     | 44 (100%)  | 0       | 0        | 100         | 100 |
| 15  | F     | 14/183 (8%)     | 14 (100%)  | 0       | 0        | 100         | 100 |
| 16  | I     | 20/36 (56%)     | 18 (90%)   | 2 (10%) | 0        | 100         | 100 |
| 17  | J     | 40/42 (95%)     | 40 (100%)  | 0       | 0        | 100         | 100 |
| 18  | K     | 52/87 (60%)     | 51 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 25  | a     | 87/215 (40%)    | 85 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 26  | b     | 174/218 (80%)   | 171 (98%)  | 2 (1%)  | 1 (1%)   | 21          | 42  |
| All | All   | 2688/4484 (60%) | 2612 (97%) | 74 (3%) | 2 (0%)   | 49          | 72  |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2     | 44  | PHE  |
| 26  | b     | 172 | PRO  |

### 5.3.2 Protein sidechains [i](#)

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

357 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 | $\# Z  > 2$ |
| 27  | CLA  | B     | 802 | -    | 69,73,73     | 1.73 | 9 (13%)     | 82,113,113  | 1.24 | 9 (10%)     |
| 27  | CLA  | 6     | 604 | -    | 64,68,73     | 1.79 | 9 (14%)     | 76,107,113  | 1.35 | 8 (10%)     |
| 27  | CLA  | A     | 813 | -    | 46,50,73     | 2.11 | 9 (19%)     | 53,85,113   | 1.62 | 9 (16%)     |
| 27  | CLA  | A     | 823 | -    | 69,73,73     | 1.72 | 9 (13%)     | 82,113,113  | 1.25 | 9 (10%)     |
| 31  | IHT  | 2     | 616 | -    | 40,42,42     | 2.62 | 3 (7%)      | 52,58,58    | 2.21 | 16 (30%)    |
| 35  | 8CT  | M     | 101 | -    | 40,41,41     | 0.14 | 0           | 51,56,56    | 0.79 | 1 (1%)      |
| 27  | CLA  | 2     | 612 | -    | 49,53,73     | 2.03 | 9 (18%)     | 58,89,113   | 1.53 | 8 (13%)     |
| 27  | CLA  | B     | 836 | -    | 51,55,73     | 1.97 | 9 (17%)     | 60,91,113   | 1.47 | 8 (13%)     |
| 27  | CLA  | 1     | 604 | 1    | 49,53,73     | 2.09 | 9 (18%)     | 58,89,113   | 1.51 | 7 (12%)     |
| 31  | IHT  | A     | 854 | -    | 40,42,42     | 2.70 | 4 (10%)     | 52,58,58    | 1.97 | 17 (32%)    |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 27  | CLA  | b     | 604 | -    | 69,73,73     | 1.73 | 9 (13%)  | 82,113,113  | 1.28 | 9 (10%)  |
| 29  | II0  | 8     | 610 | -    | 39,43,43     | 2.05 | 2 (5%)   | 48,60,60    | 1.32 | 6 (12%)  |
| 27  | CLA  | a     | 602 | 25   | 59,63,73     | 1.86 | 9 (15%)  | 70,101,113  | 1.49 | 10 (14%) |
| 27  | CLA  | 8     | 606 | 8    | 59,63,73     | 1.87 | 9 (15%)  | 70,101,113  | 1.38 | 8 (11%)  |
| 27  | CLA  | a     | 601 | 25   | 49,53,73     | 2.03 | 9 (18%)  | 58,89,113   | 1.51 | 8 (13%)  |
| 27  | CLA  | 4     | 602 | 4    | 63,67,73     | 1.79 | 9 (14%)  | 74,105,113  | 1.40 | 9 (12%)  |
| 28  | KC2  | 6     | 613 | 6    | 49,53,53     | 1.81 | 4 (8%)   | 60,89,89    | 1.12 | 4 (6%)   |
| 35  | 8CT  | K     | 103 | -    | 40,41,41     | 0.15 | 0        | 51,56,56    | 0.34 | 0        |
| 27  | CLA  | 6     | 609 | 33   | 45,49,73     | 2.21 | 10 (22%) | 54,84,113   | 1.61 | 8 (14%)  |
| 27  | CLA  | 4     | 608 | 33   | 69,73,73     | 1.71 | 9 (13%)  | 82,113,113  | 1.30 | 9 (10%)  |
| 27  | CLA  | A     | 808 | -    | 59,63,73     | 1.86 | 9 (15%)  | 70,101,113  | 1.40 | 8 (11%)  |
| 27  | CLA  | B     | 809 | -    | 69,73,73     | 1.73 | 9 (13%)  | 82,113,113  | 1.33 | 9 (10%)  |
| 27  | CLA  | B     | 822 | -    | 69,73,73     | 1.69 | 9 (13%)  | 82,113,113  | 1.29 | 8 (9%)   |
| 27  | CLA  | K     | 102 | -    | 59,63,73     | 1.88 | 9 (15%)  | 70,101,113  | 1.41 | 8 (11%)  |
| 27  | CLA  | 2     | 604 | 2    | 59,63,73     | 1.87 | 9 (15%)  | 70,101,113  | 1.41 | 7 (10%)  |
| 27  | CLA  | A     | 805 | -    | 54,58,73     | 1.94 | 9 (16%)  | 64,95,113   | 1.49 | 8 (12%)  |
| 33  | LHG  | 4     | 620 | -    | 44,44,48     | 0.66 | 2 (4%)   | 47,50,54    | 1.22 | 4 (8%)   |
| 27  | CLA  | Z     | 310 | -    | 69,73,73     | 1.69 | 9 (13%)  | 82,113,113  | 1.30 | 8 (9%)   |
| 35  | 8CT  | Z     | 309 | -    | 40,41,41     | 0.22 | 0        | 51,56,56    | 0.63 | 1 (1%)   |
| 27  | CLA  | b     | 602 | 26   | 68,72,73     | 1.75 | 9 (13%)  | 80,111,113  | 1.39 | 9 (11%)  |
| 27  | CLA  | 1     | 611 | -    | 49,53,73     | 2.08 | 9 (18%)  | 58,89,113   | 1.54 | 8 (13%)  |
| 27  | CLA  | A     | 816 | -    | 64,68,73     | 1.75 | 9 (14%)  | 76,107,113  | 1.37 | 8 (10%)  |
| 29  | II0  | 5     | 617 | -    | 39,43,43     | 2.03 | 2 (5%)   | 48,60,60    | 1.38 | 8 (16%)  |
| 27  | CLA  | 5     | 609 | -    | 45,49,73     | 2.20 | 10 (22%) | 54,84,113   | 1.61 | 8 (14%)  |
| 27  | CLA  | F     | 204 | 15   | 59,63,73     | 1.83 | 9 (15%)  | 70,101,113  | 1.37 | 9 (12%)  |
| 35  | 8CT  | 7     | 318 | -    | 40,41,41     | 0.41 | 1 (2%)   | 51,56,56    | 0.60 | 0        |
| 35  | 8CT  | R     | 203 | -    | 40,41,41     | 0.16 | 0        | 51,56,56    | 0.48 | 1 (1%)   |
| 27  | CLA  | 3     | 609 | -    | 69,73,73     | 1.72 | 9 (13%)  | 82,113,113  | 1.28 | 8 (9%)   |
| 27  | CLA  | 9     | 613 | 9    | 49,53,73     | 2.06 | 9 (18%)  | 58,89,113   | 1.50 | 8 (13%)  |
| 31  | IHT  | Z     | 302 | -    | 40,42,42     | 2.61 | 3 (7%)   | 52,58,58    | 2.15 | 12 (23%) |
| 27  | CLA  | 9     | 601 | 9    | 49,53,73     | 2.03 | 9 (18%)  | 58,89,113   | 1.53 | 9 (15%)  |
| 29  | II0  | b     | 612 | -    | 39,43,43     | 1.99 | 2 (5%)   | 48,60,60    | 1.35 | 5 (10%)  |
| 27  | CLA  | B     | 827 | -    | 69,73,73     | 1.71 | 9 (13%)  | 82,113,113  | 1.29 | 8 (9%)   |
| 27  | CLA  | B     | 839 | 33   | 69,73,73     | 1.75 | 9 (13%)  | 82,113,113  | 1.32 | 9 (10%)  |
| 27  | CLA  | B     | 805 | -    | 69,73,73     | 1.72 | 9 (13%)  | 82,113,113  | 1.30 | 7 (8%)   |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 27  | CLA  | B     | 829 | -    | 49,53,73     | 2.07 | 9 (18%)  | 58,89,113   | 1.60 | 8 (13%)  |
| 27  | CLA  | b     | 608 | -    | 69,73,73     | 1.72 | 9 (13%)  | 82,113,113  | 1.28 | 9 (10%)  |
| 33  | LHG  | 3     | 622 | 28   | 33,33,48     | 0.74 | 1 (3%)   | 36,39,54    | 1.31 | 3 (8%)   |
| 27  | CLA  | 7     | 309 | 7    | 59,63,73     | 1.84 | 9 (15%)  | 70,101,113  | 1.46 | 9 (12%)  |
| 27  | CLA  | A     | 839 | -    | 69,73,73     | 1.71 | 9 (13%)  | 82,113,113  | 1.33 | 8 (9%)   |
| 27  | CLA  | b     | 606 | 26   | 69,73,73     | 1.71 | 9 (13%)  | 82,113,113  | 1.26 | 8 (9%)   |
| 27  | CLA  | A     | 836 | -    | 59,63,73     | 1.86 | 9 (15%)  | 70,101,113  | 1.41 | 8 (11%)  |
| 27  | CLA  | B     | 806 | -    | 69,73,73     | 1.67 | 9 (13%)  | 82,113,113  | 1.32 | 9 (10%)  |
| 29  | II0  | O     | 205 | -    | 39,43,43     | 2.03 | 2 (5%)   | 48,60,60    | 1.33 | 6 (12%)  |
| 29  | II0  | 5     | 620 | -    | 39,43,43     | 2.04 | 2 (5%)   | 48,60,60    | 1.37 | 5 (10%)  |
| 29  | II0  | 2     | 615 | -    | 39,43,43     | 2.04 | 2 (5%)   | 48,60,60    | 1.34 | 7 (14%)  |
| 27  | CLA  | 3     | 611 | 3    | 54,58,73     | 1.97 | 9 (16%)  | 64,95,113   | 1.44 | 8 (12%)  |
| 27  | CLA  | A     | 826 | -    | 69,73,73     | 1.68 | 9 (13%)  | 82,113,113  | 1.24 | 9 (10%)  |
| 29  | II0  | 1     | 617 | -    | 39,43,43     | 2.02 | 2 (5%)   | 48,60,60    | 1.35 | 7 (14%)  |
| 27  | CLA  | J     | 102 | -    | 45,49,73     | 2.21 | 10 (22%) | 54,84,113   | 1.64 | 9 (16%)  |
| 35  | 8CT  | A     | 847 | -    | 40,41,41     | 0.22 | 0        | 51,56,56    | 0.79 | 1 (1%)   |
| 33  | LHG  | Z     | 311 | -    | 45,45,48     | 0.64 | 1 (2%)   | 48,51,54    | 1.23 | 4 (8%)   |
| 27  | CLA  | A     | 814 | -    | 49,53,73     | 2.06 | 9 (18%)  | 58,89,113   | 1.53 | 8 (13%)  |
| 27  | CLA  | 6     | 608 | 6    | 64,68,73     | 1.78 | 9 (14%)  | 76,107,113  | 1.37 | 8 (10%)  |
| 35  | 8CT  | A     | 845 | -    | 40,41,41     | 0.24 | 0        | 51,56,56    | 0.36 | 0        |
| 27  | CLA  | A     | 829 | -    | 54,58,73     | 1.94 | 9 (16%)  | 64,95,113   | 1.52 | 8 (12%)  |
| 29  | II0  | 6     | 615 | -    | 39,43,43     | 2.00 | 2 (5%)   | 48,60,60    | 1.32 | 5 (10%)  |
| 33  | LHG  | 7     | 319 | -    | 30,30,48     | 0.76 | 1 (3%)   | 33,36,54    | 1.23 | 3 (9%)   |
| 27  | CLA  | 9     | 606 | -    | 68,72,73     | 1.71 | 9 (13%)  | 80,111,113  | 1.30 | 9 (11%)  |
| 27  | CLA  | B     | 820 | -    | 64,68,73     | 1.80 | 9 (14%)  | 76,107,113  | 1.35 | 8 (10%)  |
| 27  | CLA  | A     | 827 | -    | 69,73,73     | 1.68 | 9 (13%)  | 82,113,113  | 1.28 | 9 (10%)  |
| 29  | II0  | Z     | 312 | -    | 39,43,43     | 2.00 | 2 (5%)   | 48,60,60    | 1.31 | 6 (12%)  |
| 28  | KC2  | 7     | 307 | -    | 49,53,53     | 1.83 | 4 (8%)   | 60,89,89    | 1.17 | 4 (6%)   |
| 33  | LHG  | 7     | 320 | 27   | 38,38,48     | 0.66 | 0        | 41,44,54    | 1.20 | 3 (7%)   |
| 27  | CLA  | 3     | 605 | 3    | 59,63,73     | 1.85 | 9 (15%)  | 70,101,113  | 1.44 | 7 (10%)  |
| 27  | CLA  | Z     | 306 | 24   | 64,68,73     | 1.77 | 9 (14%)  | 76,107,113  | 1.35 | 8 (10%)  |
| 27  | CLA  | B     | 821 | -    | 64,68,73     | 1.76 | 9 (14%)  | 76,107,113  | 1.39 | 9 (11%)  |
| 29  | II0  | 4     | 614 | -    | 39,43,43     | 2.00 | 2 (5%)   | 48,60,60    | 1.30 | 6 (12%)  |
| 36  | LMU  | J     | 104 | -    | 32,32,36     | 0.46 | 0        | 43,43,47    | 1.05 | 2 (4%)   |
| 27  | CLA  | A     | 819 | -    | 69,73,73     | 1.74 | 9 (13%)  | 82,113,113  | 1.32 | 9 (10%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 28  | KC2  | Z     | 307 | -    | 49,53,53     | 1.78 | 4 (8%)   | 60,89,89    | 1.13 | 4 (6%)   |
| 27  | CLA  | 8     | 615 | -    | 69,73,73     | 1.73 | 9 (13%)  | 82,113,113  | 1.31 | 8 (9%)   |
| 27  | CLA  | A     | 802 | 27   | 59,63,73     | 1.82 | 9 (15%)  | 70,101,113  | 1.38 | 8 (11%)  |
| 35  | 8CT  | A     | 848 | -    | 40,41,41     | 0.37 | 0        | 51,56,56    | 0.55 | 0        |
| 29  | II0  | 3     | 617 | -    | 39,43,43     | 2.02 | 2 (5%)   | 48,60,60    | 1.31 | 6 (12%)  |
| 27  | CLA  | 2     | 611 | -    | 49,53,73     | 2.04 | 9 (18%)  | 58,89,113   | 1.50 | 9 (15%)  |
| 27  | CLA  | B     | 803 | -    | 49,53,73     | 2.02 | 9 (18%)  | 58,89,113   | 1.45 | 8 (13%)  |
| 27  | CLA  | 4     | 611 | -    | 69,73,73     | 1.70 | 9 (13%)  | 82,113,113  | 1.27 | 9 (10%)  |
| 27  | CLA  | 7     | 302 | 7    | 49,53,73     | 2.03 | 9 (18%)  | 58,89,113   | 1.49 | 8 (13%)  |
| 27  | CLA  | 7     | 312 | -    | 59,63,73     | 1.86 | 9 (15%)  | 70,101,113  | 1.40 | 8 (11%)  |
| 27  | CLA  | 9     | 609 | -    | 45,49,73     | 2.18 | 10 (22%) | 54,84,113   | 1.62 | 9 (16%)  |
| 27  | CLA  | A     | 837 | -    | 69,73,73     | 1.68 | 9 (13%)  | 82,113,113  | 1.26 | 8 (9%)   |
| 27  | CLA  | A     | 801 | -    | 69,73,73     | 1.69 | 8 (11%)  | 82,113,113  | 1.24 | 10 (12%) |
| 27  | CLA  | B     | 813 | -    | 65,69,73     | 1.73 | 9 (13%)  | 77,108,113  | 1.34 | 9 (11%)  |
| 33  | LHG  | 6     | 617 | 27   | 34,34,48     | 0.76 | 1 (2%)   | 37,40,54    | 1.22 | 3 (8%)   |
| 27  | CLA  | O     | 204 | -    | 59,63,73     | 1.90 | 9 (15%)  | 70,101,113  | 1.48 | 9 (12%)  |
| 27  | CLA  | 8     | 601 | 8    | 49,53,73     | 2.04 | 9 (18%)  | 58,89,113   | 1.51 | 8 (13%)  |
| 28  | KC2  | 6     | 610 | 6    | 49,53,53     | 1.81 | 4 (8%)   | 60,89,89    | 1.11 | 3 (5%)   |
| 27  | CLA  | 7     | 303 | 7    | 69,73,73     | 1.73 | 9 (13%)  | 82,113,113  | 1.34 | 10 (12%) |
| 27  | CLA  | 2     | 609 | -    | 45,49,73     | 2.21 | 10 (22%) | 54,84,113   | 1.64 | 8 (14%)  |
| 27  | CLA  | O     | 201 | -    | 59,63,73     | 1.84 | 9 (15%)  | 70,101,113  | 1.43 | 10 (14%) |
| 27  | CLA  | a     | 605 | -    | 59,63,73     | 1.83 | 9 (15%)  | 70,101,113  | 1.42 | 9 (12%)  |
| 29  | II0  | 2     | 614 | -    | 39,43,43     | 2.01 | 2 (5%)   | 48,60,60    | 1.33 | 6 (12%)  |
| 27  | CLA  | 7     | 308 | 7    | 49,53,73     | 2.05 | 9 (18%)  | 58,89,113   | 1.56 | 7 (12%)  |
| 27  | CLA  | 2     | 607 | 2    | 49,53,73     | 2.03 | 9 (18%)  | 58,89,113   | 1.55 | 8 (13%)  |
| 27  | CLA  | 5     | 613 | 5    | 45,49,73     | 2.21 | 10 (22%) | 54,84,113   | 1.60 | 9 (16%)  |
| 27  | CLA  | F     | 203 | -    | 49,53,73     | 2.03 | 9 (18%)  | 58,89,113   | 1.49 | 8 (13%)  |
| 33  | LHG  | 4     | 619 | 27   | 44,44,48     | 0.66 | 1 (2%)   | 47,50,54    | 1.23 | 5 (10%)  |
| 27  | CLA  | B     | 840 | -    | 69,73,73     | 1.68 | 9 (13%)  | 82,113,113  | 1.28 | 8 (9%)   |
| 35  | 8CT  | Z     | 308 | -    | 40,41,41     | 0.15 | 0        | 51,56,56    | 0.31 | 0        |
| 35  | 8CT  | B     | 850 | -    | 40,41,41     | 0.20 | 0        | 51,56,56    | 0.45 | 0        |
| 29  | II0  | 1     | 616 | -    | 39,43,43     | 2.00 | 2 (5%)   | 48,60,60    | 1.36 | 6 (12%)  |
| 27  | CLA  | A     | 843 | -    | 69,73,73     | 1.74 | 9 (13%)  | 82,113,113  | 1.38 | 7 (8%)   |
| 27  | CLA  | B     | 808 | 11   | 69,73,73     | 1.69 | 9 (13%)  | 82,113,113  | 1.26 | 9 (10%)  |
| 27  | CLA  | 5     | 611 | -    | 49,53,73     | 2.04 | 9 (18%)  | 58,89,113   | 1.48 | 8 (13%)  |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 37  | SF4  | C     | 102 | 12    | 0,12,12      | -    | -        | -           |      |          |
| 27  | CLA  | 9     | 602 | 9     | 59,63,73     | 1.88 | 9 (15%)  | 70,101,113  | 1.46 | 8 (11%)  |
| 29  | II0  | 1     | 619 | -     | 39,43,43     | 2.10 | 2 (5%)   | 48,60,60    | 1.40 | 9 (18%)  |
| 37  | SF4  | A     | 849 | 10,11 | 0,12,12      | -    | -        | -           |      |          |
| 27  | CLA  | b     | 603 | -     | 64,68,73     | 1.78 | 9 (14%)  | 76,107,113  | 1.36 | 9 (11%)  |
| 27  | CLA  | a     | 610 | -     | 59,63,73     | 1.87 | 9 (15%)  | 70,101,113  | 1.38 | 8 (11%)  |
| 35  | 8CT  | B     | 849 | -     | 40,41,41     | 0.33 | 0        | 51,56,56    | 0.74 | 1 (1%)   |
| 38  | PQN  | B     | 842 | -     | 34,34,34     | 0.37 | 0        | 43,45,45    | 0.63 | 1 (2%)   |
| 27  | CLA  | A     | 835 | -     | 64,68,73     | 1.76 | 9 (14%)  | 76,107,113  | 1.32 | 8 (10%)  |
| 28  | KC2  | 4     | 605 | 4     | 49,53,53     | 1.80 | 4 (8%)   | 60,89,89    | 1.10 | 3 (5%)   |
| 29  | II0  | 7     | 315 | -     | 39,43,43     | 2.00 | 2 (5%)   | 48,60,60    | 1.39 | 6 (12%)  |
| 27  | CLA  | B     | 825 | -     | 69,73,73     | 1.70 | 9 (13%)  | 82,113,113  | 1.27 | 10 (12%) |
| 27  | CLA  | L     | 202 | -     | 64,68,73     | 1.81 | 9 (14%)  | 76,107,113  | 1.35 | 8 (10%)  |
| 29  | II0  | 3     | 615 | -     | 39,43,43     | 2.04 | 2 (5%)   | 48,60,60    | 1.28 | 5 (10%)  |
| 33  | LHG  | A     | 852 | -     | 38,38,48     | 0.71 | 1 (2%)   | 41,44,54    | 1.29 | 3 (7%)   |
| 27  | CLA  | B     | 817 | -     | 64,68,73     | 1.75 | 9 (14%)  | 76,107,113  | 1.34 | 8 (10%)  |
| 29  | II0  | 9     | 617 | -     | 39,43,43     | 2.03 | 2 (5%)   | 48,60,60    | 1.35 | 6 (12%)  |
| 29  | II0  | 4     | 612 | -     | 39,43,43     | 2.02 | 2 (5%)   | 48,60,60    | 1.27 | 5 (10%)  |
| 27  | CLA  | 9     | 603 | -     | 49,53,73     | 2.07 | 9 (18%)  | 58,89,113   | 1.53 | 8 (13%)  |
| 27  | CLA  | A     | 818 | -     | 69,73,73     | 1.72 | 9 (13%)  | 82,113,113  | 1.32 | 8 (9%)   |
| 27  | CLA  | 4     | 603 | -     | 58,62,73     | 1.88 | 9 (15%)  | 68,99,113   | 1.44 | 8 (11%)  |
| 27  | CLA  | 5     | 608 | 5     | 64,68,73     | 1.79 | 9 (14%)  | 76,107,113  | 1.52 | 8 (10%)  |
| 29  | II0  | B     | 843 | -     | 39,43,43     | 2.04 | 2 (5%)   | 48,60,60    | 1.34 | 5 (10%)  |
| 27  | CLA  | 4     | 607 | 4     | 64,68,73     | 1.78 | 9 (14%)  | 76,107,113  | 1.38 | 9 (11%)  |
| 27  | CLA  | A     | 817 | -     | 69,73,73     | 1.72 | 9 (13%)  | 82,113,113  | 1.42 | 8 (9%)   |
| 27  | CLA  | A     | 824 | -     | 69,73,73     | 1.74 | 9 (13%)  | 82,113,113  | 1.30 | 7 (8%)   |
| 27  | CLA  | 5     | 605 | 5     | 49,53,73     | 2.04 | 9 (18%)  | 58,89,113   | 1.51 | 8 (13%)  |
| 29  | II0  | a     | 615 | -     | 39,43,43     | 2.02 | 2 (5%)   | 48,60,60    | 1.35 | 10 (20%) |
| 27  | CLA  | B     | 841 | -     | 56,60,73     | 1.88 | 9 (16%)  | 65,97,113   | 1.45 | 8 (12%)  |
| 33  | LHG  | a     | 618 | -     | 28,28,48     | 0.83 | 1 (3%)   | 31,34,54    | 1.36 | 3 (9%)   |
| 27  | CLA  | Z     | 305 | -     | 54,58,73     | 1.92 | 9 (16%)  | 64,95,113   | 1.48 | 9 (14%)  |
| 29  | II0  | a     | 612 | -     | 39,43,43     | 2.04 | 2 (5%)   | 48,60,60    | 1.36 | 6 (12%)  |
| 27  | CLA  | b     | 601 | 26    | 49,53,73     | 2.04 | 9 (18%)  | 58,89,113   | 1.53 | 8 (13%)  |
| 29  | II0  | 3     | 616 | -     | 39,43,43     | 2.01 | 2 (5%)   | 48,60,60    | 1.33 | 4 (8%)   |
| 28  | KC2  | a     | 609 | -     | 49,53,53     | 1.81 | 4 (8%)   | 60,89,89    | 1.14 | 4 (6%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 27  | CLA  | A     | 841 | -    | 69,73,73     | 1.72 | 9 (13%)  | 82,113,113  | 1.29 | 8 (9%)   |
| 27  | CLA  | B     | 834 | -    | 59,63,73     | 1.84 | 9 (15%)  | 70,101,113  | 1.41 | 8 (11%)  |
| 27  | CLA  | a     | 608 | -    | 64,68,73     | 1.77 | 9 (14%)  | 76,107,113  | 1.38 | 9 (11%)  |
| 27  | CLA  | b     | 607 | 26   | 64,68,73     | 1.80 | 9 (14%)  | 76,107,113  | 1.35 | 8 (10%)  |
| 27  | CLA  | 2     | 608 | 2    | 64,68,73     | 1.79 | 9 (14%)  | 76,107,113  | 1.37 | 9 (11%)  |
| 35  | 8CT  | I     | 101 | -    | 40,41,41     | 0.24 | 0        | 51,56,56    | 0.40 | 0        |
| 27  | CLA  | 6     | 605 | 6    | 59,63,73     | 1.83 | 9 (15%)  | 70,101,113  | 1.38 | 9 (12%)  |
| 30  | II3  | b     | 613 | -    | 40,43,43     | 1.54 | 2 (5%)   | 47,60,60    | 1.82 | 13 (27%) |
| 27  | CLA  | B     | 811 | -    | 59,63,73     | 1.86 | 9 (15%)  | 70,101,113  | 1.42 | 8 (11%)  |
| 27  | CLA  | B     | 826 | -    | 69,73,73     | 1.69 | 9 (13%)  | 82,113,113  | 1.27 | 8 (9%)   |
| 27  | CLA  | 1     | 605 | -    | 45,50,73     | 2.10 | 9 (20%)  | 52,85,113   | 1.56 | 8 (15%)  |
| 29  | II0  | 4     | 613 | -    | 39,43,43     | 2.01 | 2 (5%)   | 48,60,60    | 1.28 | 5 (10%)  |
| 27  | CLA  | A     | 810 | -    | 69,73,73     | 1.69 | 9 (13%)  | 82,113,113  | 1.27 | 10 (12%) |
| 28  | KC2  | b     | 605 | 26   | 49,53,53     | 1.80 | 4 (8%)   | 60,89,89    | 1.15 | 4 (6%)   |
| 27  | CLA  | 7     | 305 | 7    | 57,61,73     | 1.89 | 9 (15%)  | 67,98,113   | 1.45 | 9 (13%)  |
| 37  | SF4  | C     | 101 | 12   | 0,12,12      | -    | -        | -           | -    | -        |
| 29  | II0  | 9     | 618 | -    | 39,43,43     | 1.99 | 2 (5%)   | 48,60,60    | 1.34 | 5 (10%)  |
| 29  | II0  | a     | 613 | -    | 39,43,43     | 2.00 | 2 (5%)   | 48,60,60    | 1.35 | 5 (10%)  |
| 27  | CLA  | A     | 825 | -    | 69,73,73     | 1.72 | 9 (13%)  | 82,113,113  | 1.29 | 8 (9%)   |
| 33  | LHG  | 8     | 613 | -    | 32,32,48     | 0.77 | 2 (6%)   | 35,38,54    | 1.24 | 2 (5%)   |
| 29  | II0  | 4     | 615 | -    | 39,43,43     | 2.01 | 2 (5%)   | 48,60,60    | 1.34 | 6 (12%)  |
| 38  | PQN  | A     | 850 | -    | 34,34,34     | 0.36 | 0        | 43,45,45    | 0.75 | 1 (2%)   |
| 32  | LMG  | 2     | 617 | -    | 36,36,55     | 0.85 | 1 (2%)   | 44,44,63    | 1.24 | 5 (11%)  |
| 27  | CLA  | A     | 803 | -    | 69,73,73     | 1.71 | 9 (13%)  | 82,113,113  | 1.36 | 9 (10%)  |
| 27  | CLA  | 5     | 606 | -    | 49,53,73     | 2.04 | 9 (18%)  | 58,89,113   | 1.54 | 9 (15%)  |
| 27  | CLA  | 9     | 608 | 9    | 59,63,73     | 1.84 | 9 (15%)  | 70,101,113  | 1.44 | 8 (11%)  |
| 27  | CLA  | O     | 202 | -    | 45,49,73     | 2.22 | 10 (22%) | 54,84,113   | 1.66 | 7 (12%)  |
| 33  | LHG  | a     | 617 | -    | 48,48,48     | 0.61 | 1 (2%)   | 51,54,54    | 1.22 | 5 (9%)   |
| 32  | LMG  | 8     | 616 | -    | 51,51,55     | 0.73 | 0        | 59,59,63    | 1.30 | 6 (10%)  |
| 27  | CLA  | B     | 815 | -    | 69,73,73     | 1.75 | 9 (13%)  | 82,113,113  | 1.33 | 8 (9%)   |
| 36  | LMU  | 4     | 618 | -    | 36,36,36     | 0.48 | 1 (2%)   | 47,47,47    | 0.93 | 2 (4%)   |
| 27  | CLA  | b     | 610 | 26   | 55,59,73     | 1.94 | 9 (16%)  | 64,96,113   | 1.49 | 9 (14%)  |
| 35  | 8CT  | J     | 103 | -    | 40,41,41     | 0.16 | 0        | 51,56,56    | 0.41 | 0        |
| 32  | LMG  | 3     | 618 | -    | 30,30,55     | 0.96 | 1 (3%)   | 38,38,63    | 1.22 | 5 (13%)  |
| 29  | II0  | 9     | 615 | -    | 39,43,43     | 2.01 | 2 (5%)   | 48,60,60    | 1.40 | 7 (14%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 27  | CLA  | 2     | 606 | -    | 49,53,73     | 2.02 | 9 (18%)  | 58,89,113   | 1.50 | 8 (13%)  |
| 27  | CLA  | B     | 804 | -    | 69,73,73     | 1.69 | 9 (13%)  | 82,113,113  | 1.29 | 9 (10%)  |
| 34  | SQD  | O     | 207 | -    | 22,24,54     | 1.47 | 3 (13%)  | 31,34,65    | 1.27 | 4 (12%)  |
| 35  | 8CT  | B     | 847 | -    | 40,41,41     | 0.15 | 0        | 51,56,56    | 0.46 | 0        |
| 27  | CLA  | B     | 814 | -    | 46,50,73     | 2.12 | 9 (19%)  | 53,85,113   | 1.61 | 9 (16%)  |
| 27  | CLA  | A     | 806 | 10   | 69,73,73     | 1.71 | 9 (13%)  | 82,113,113  | 1.25 | 9 (10%)  |
| 33  | LHG  | A     | 851 | -    | 48,48,48     | 0.60 | 0        | 51,54,54    | 1.19 | 4 (7%)   |
| 27  | CLA  | 8     | 604 | -    | 69,73,73     | 1.73 | 9 (13%)  | 82,113,113  | 1.33 | 10 (12%) |
| 27  | CLA  | B     | 833 | -    | 49,53,73     | 2.03 | 9 (18%)  | 58,89,113   | 1.49 | 8 (13%)  |
| 27  | CLA  | 4     | 606 | 4    | 64,68,73     | 1.80 | 9 (14%)  | 76,107,113  | 1.34 | 9 (11%)  |
| 27  | CLA  | 6     | 602 | 6    | 69,73,73     | 1.77 | 9 (13%)  | 82,113,113  | 1.38 | 7 (8%)   |
| 27  | CLA  | 1     | 608 | 1    | 64,68,73     | 1.77 | 9 (14%)  | 76,107,113  | 1.37 | 8 (10%)  |
| 28  | KC2  | 1     | 610 | -    | 49,53,53     | 1.82 | 4 (8%)   | 60,89,89    | 1.10 | 3 (5%)   |
| 27  | CLA  | a     | 611 | -    | 69,73,73     | 1.67 | 9 (13%)  | 82,113,113  | 1.27 | 8 (9%)   |
| 29  | II0  | 7     | 317 | -    | 39,43,43     | 2.02 | 2 (5%)   | 48,60,60    | 1.43 | 8 (16%)  |
| 30  | II3  | 1     | 615 | -    | 40,43,43     | 1.57 | 2 (5%)   | 47,60,60    | 1.67 | 10 (21%) |
| 27  | CLA  | 3     | 610 | -    | 69,73,73     | 1.72 | 9 (13%)  | 82,113,113  | 1.32 | 9 (10%)  |
| 27  | CLA  | A     | 820 | -    | 69,73,73     | 1.74 | 9 (13%)  | 82,113,113  | 1.30 | 8 (9%)   |
| 33  | LHG  | 5     | 619 | -    | 22,22,48     | 0.88 | 1 (4%)   | 25,28,54    | 1.35 | 3 (12%)  |
| 27  | CLA  | 9     | 605 | -    | 49,53,73     | 2.04 | 9 (18%)  | 58,89,113   | 1.54 | 8 (13%)  |
| 27  | CLA  | A     | 842 | -    | 69,73,73     | 1.72 | 9 (13%)  | 82,113,113  | 1.31 | 8 (9%)   |
| 27  | CLA  | 8     | 602 | 8    | 49,53,73     | 2.06 | 9 (18%)  | 58,89,113   | 1.44 | 6 (10%)  |
| 32  | LMG  | 8     | 614 | -    | 52,52,55     | 0.81 | 2 (3%)   | 60,60,63    | 1.30 | 6 (10%)  |
| 27  | CLA  | 8     | 608 | -    | 69,73,73     | 1.73 | 9 (13%)  | 82,113,113  | 1.28 | 8 (9%)   |
| 27  | CLA  | 3     | 603 | -    | 64,68,73     | 1.77 | 9 (14%)  | 76,107,113  | 1.33 | 7 (9%)   |
| 27  | CLA  | A     | 830 | -    | 64,68,73     | 1.79 | 9 (14%)  | 76,107,113  | 1.37 | 8 (10%)  |
| 27  | CLA  | A     | 822 | -    | 69,73,73     | 1.72 | 9 (13%)  | 82,113,113  | 1.29 | 8 (9%)   |
| 27  | CLA  | 9     | 607 | 9    | 69,73,73     | 1.67 | 9 (13%)  | 82,113,113  | 1.27 | 8 (9%)   |
| 27  | CLA  | A     | 833 | -    | 69,73,73     | 1.72 | 9 (13%)  | 82,113,113  | 1.32 | 9 (10%)  |
| 29  | II0  | 7     | 301 | -    | 39,43,43     | 2.05 | 2 (5%)   | 48,60,60    | 1.53 | 11 (22%) |
| 27  | CLA  | B     | 835 | -    | 69,73,73     | 1.75 | 9 (13%)  | 82,113,113  | 1.42 | 9 (10%)  |
| 29  | II0  | 2     | 613 | -    | 39,43,43     | 2.07 | 2 (5%)   | 48,60,60    | 1.36 | 8 (16%)  |
| 27  | CLA  | B     | 812 | -    | 69,73,73     | 1.71 | 9 (13%)  | 82,113,113  | 1.33 | 9 (10%)  |
| 28  | KC2  | 9     | 610 | -    | 49,53,53     | 1.81 | 4 (8%)   | 60,89,89    | 1.13 | 4 (6%)   |
| 28  | KC2  | 3     | 606 | 33   | 49,53,53     | 1.81 | 4 (8%)   | 60,89,89    | 1.15 | 5 (8%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 27  | CLA  | A     | 812 | -    | 59,63,73     | 1.87 | 9 (15%)  | 70,101,113  | 1.46 | 9 (12%)  |
| 27  | CLA  | 2     | 602 | 2    | 63,67,73     | 1.81 | 9 (14%)  | 74,105,113  | 1.50 | 10 (13%) |
| 35  | 8CT  | A     | 853 | -    | 40,41,41     | 0.23 | 0        | 51,56,56    | 0.64 | 1 (1%)   |
| 27  | CLA  | 5     | 602 | 5    | 59,63,73     | 1.87 | 9 (15%)  | 70,101,113  | 1.41 | 9 (12%)  |
| 39  | DGD  | B     | 848 | -    | 60,60,67     | 0.88 | 2 (3%)   | 74,74,81    | 1.33 | 8 (10%)  |
| 29  | II0  | 3     | 613 | -    | 39,43,43     | 2.02 | 2 (5%)   | 48,60,60    | 1.36 | 8 (16%)  |
| 27  | CLA  | 3     | 602 | 3    | 59,63,73     | 1.85 | 9 (15%)  | 70,101,113  | 1.43 | 8 (11%)  |
| 27  | CLA  | 3     | 601 | 3    | 49,53,73     | 2.05 | 9 (18%)  | 58,89,113   | 1.48 | 8 (13%)  |
| 35  | 8CT  | A     | 846 | -    | 40,41,41     | 0.18 | 0        | 51,56,56    | 0.35 | 0        |
| 27  | CLA  | B     | 832 | -    | 69,73,73     | 1.72 | 9 (13%)  | 82,113,113  | 1.29 | 9 (10%)  |
| 35  | 8CT  | B     | 845 | -    | 40,41,41     | 0.34 | 0        | 51,56,56    | 0.56 | 1 (1%)   |
| 35  | 8CT  | R     | 201 | -    | 40,41,41     | 0.19 | 0        | 51,56,56    | 0.41 | 0        |
| 35  | 8CT  | L     | 205 | -    | 40,41,41     | 0.16 | 0        | 51,56,56    | 0.36 | 0        |
| 27  | CLA  | 3     | 608 | 3    | 64,68,73     | 1.79 | 9 (14%)  | 76,107,113  | 1.36 | 8 (10%)  |
| 27  | CLA  | a     | 603 | -    | 64,68,73     | 1.79 | 9 (14%)  | 76,107,113  | 1.33 | 8 (10%)  |
| 27  | CLA  | 6     | 611 | -    | 59,63,73     | 1.86 | 9 (15%)  | 70,101,113  | 1.47 | 9 (12%)  |
| 27  | CLA  | R     | 202 | -    | 59,63,73     | 1.88 | 9 (15%)  | 70,101,113  | 1.57 | 10 (14%) |
| 33  | LHG  | 4     | 617 | 27   | 46,46,48     | 0.62 | 1 (2%)   | 49,52,54    | 1.23 | 6 (12%)  |
| 27  | CLA  | A     | 840 | -    | 59,63,73     | 1.82 | 9 (15%)  | 70,101,113  | 1.40 | 7 (10%)  |
| 31  | IHT  | L     | 204 | -    | 40,42,42     | 2.58 | 4 (10%)  | 52,58,58    | 2.29 | 16 (30%) |
| 29  | II0  | 7     | 314 | -    | 39,43,43     | 2.02 | 2 (5%)   | 48,60,60    | 1.32 | 6 (12%)  |
| 27  | CLA  | 5     | 604 | -    | 59,63,73     | 1.91 | 9 (15%)  | 70,101,113  | 1.43 | 7 (10%)  |
| 29  | II0  | O     | 206 | -    | 39,43,43     | 2.03 | 2 (5%)   | 48,60,60    | 1.25 | 5 (10%)  |
| 29  | II0  | 1     | 614 | -    | 39,43,43     | 2.02 | 2 (5%)   | 48,60,60    | 1.32 | 5 (10%)  |
| 27  | CLA  | 5     | 601 | 5    | 45,49,73     | 2.24 | 10 (22%) | 54,84,113   | 1.70 | 8 (14%)  |
| 27  | CLA  | B     | 818 | -    | 64,68,73     | 1.78 | 9 (14%)  | 76,107,113  | 1.37 | 9 (11%)  |
| 29  | II0  | 5     | 615 | -    | 39,43,43     | 2.03 | 2 (5%)   | 48,60,60    | 1.40 | 6 (12%)  |
| 27  | CLA  | B     | 824 | -    | 64,68,73     | 1.79 | 9 (14%)  | 76,107,113  | 1.40 | 7 (9%)   |
| 29  | II0  | a     | 614 | -    | 39,43,43     | 2.04 | 2 (5%)   | 48,60,60    | 1.30 | 7 (14%)  |
| 34  | SQD  | 3     | 621 | -    | 40,42,54     | 1.26 | 3 (7%)   | 50,53,65    | 1.07 | 4 (8%)   |
| 29  | II0  | R     | 204 | -    | 39,43,43     | 2.03 | 2 (5%)   | 48,60,60    | 1.29 | 8 (16%)  |
| 27  | CLA  | 9     | 612 | -    | 49,53,73     | 2.02 | 9 (18%)  | 58,89,113   | 1.49 | 8 (13%)  |
| 35  | 8CT  | b     | 615 | -    | 40,41,41     | 0.21 | 0        | 51,56,56    | 0.32 | 0        |
| 27  | CLA  | B     | 816 | -    | 63,67,73     | 1.79 | 9 (14%)  | 74,105,113  | 1.37 | 9 (12%)  |
| 36  | LMU  | 7     | 321 | -    | 36,36,36     | 0.40 | 0        | 47,47,47    | 0.73 | 1 (2%)   |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 27  | CLA  | B     | 838 | -    | 69,73,73     | 1.73 | 9 (13%)  | 82,113,113  | 1.31 | 9 (10%)  |
| 27  | CLA  | a     | 606 | 25   | 69,73,73     | 1.72 | 9 (13%)  | 82,113,113  | 1.27 | 8 (9%)   |
| 27  | CLA  | 1     | 602 | 1    | 63,67,73     | 1.79 | 9 (14%)  | 74,105,113  | 1.39 | 9 (12%)  |
| 27  | CLA  | B     | 807 | -    | 69,73,73     | 1.69 | 9 (13%)  | 82,113,113  | 1.27 | 9 (10%)  |
| 27  | CLA  | B     | 837 | -    | 69,73,73     | 1.73 | 9 (13%)  | 82,113,113  | 1.28 | 8 (9%)   |
| 27  | CLA  | A     | 838 | -    | 69,73,73     | 1.71 | 9 (13%)  | 82,113,113  | 1.27 | 9 (10%)  |
| 33  | LHG  | 2     | 619 | -    | 38,38,48     | 0.70 | 1 (2%)   | 41,44,54    | 1.28 | 4 (9%)   |
| 27  | CLA  | a     | 607 | 25   | 64,68,73     | 1.78 | 9 (14%)  | 76,107,113  | 1.38 | 8 (10%)  |
| 27  | CLA  | 9     | 604 | -    | 59,63,73     | 1.87 | 9 (15%)  | 70,101,113  | 1.41 | 8 (11%)  |
| 27  | CLA  | B     | 801 | -    | 69,73,73     | 1.67 | 9 (13%)  | 82,113,113  | 1.24 | 10 (12%) |
| 29  | II0  | 8     | 612 | -    | 39,43,43     | 2.03 | 2 (5%)   | 48,60,60    | 1.37 | 5 (10%)  |
| 27  | CLA  | 4     | 604 | -    | 59,63,73     | 1.86 | 9 (15%)  | 70,101,113  | 1.39 | 9 (12%)  |
| 27  | CLA  | B     | 810 | -    | 64,68,73     | 1.76 | 9 (14%)  | 76,107,113  | 1.35 | 8 (10%)  |
| 28  | KC2  | b     | 609 | -    | 49,53,53     | 1.82 | 4 (8%)   | 60,89,89    | 1.16 | 4 (6%)   |
| 35  | 8CT  | F     | 201 | -    | 40,41,41     | 0.43 | 1 (2%)   | 51,56,56    | 0.40 | 0        |
| 27  | CLA  | 4     | 601 | 4    | 59,63,73     | 1.83 | 9 (15%)  | 70,101,113  | 1.37 | 8 (11%)  |
| 32  | LMG  | F     | 205 | -    | 32,32,55     | 0.85 | 0        | 40,40,63    | 1.30 | 6 (15%)  |
| 27  | CLA  | 7     | 313 | -    | 54,58,73     | 1.95 | 9 (16%)  | 64,95,113   | 1.49 | 9 (14%)  |
| 31  | IHT  | 6     | 616 | -    | 40,42,42     | 2.56 | 3 (7%)   | 52,58,58    | 2.20 | 16 (30%) |
| 27  | CLA  | 7     | 306 | 7    | 49,53,73     | 2.07 | 9 (18%)  | 58,89,113   | 1.51 | 8 (13%)  |
| 29  | II0  | 5     | 616 | -    | 39,43,43     | 2.04 | 2 (5%)   | 48,60,60    | 1.37 | 6 (12%)  |
| 27  | CLA  | B     | 828 | -    | 69,73,73     | 1.72 | 9 (13%)  | 82,113,113  | 1.27 | 8 (9%)   |
| 27  | CLA  | 2     | 605 | -    | 64,68,73     | 1.77 | 9 (14%)  | 76,107,113  | 1.33 | 7 (9%)   |
| 27  | CLA  | 6     | 603 | -    | 49,53,73     | 2.09 | 9 (18%)  | 58,89,113   | 1.54 | 8 (13%)  |
| 27  | CLA  | 3     | 612 | -    | 49,53,73     | 2.03 | 9 (18%)  | 58,89,113   | 1.51 | 8 (13%)  |
| 33  | LHG  | 3     | 619 | -    | 48,48,48     | 0.62 | 1 (2%)   | 51,54,54    | 1.25 | 6 (11%)  |
| 32  | LMG  | 6     | 618 | -    | 32,32,55     | 0.98 | 2 (6%)   | 40,40,63    | 1.24 | 5 (12%)  |
| 29  | II0  | 9     | 616 | -    | 39,43,43     | 2.01 | 2 (5%)   | 48,60,60    | 1.30 | 7 (14%)  |
| 27  | CLA  | B     | 819 | -    | 64,68,73     | 1.79 | 9 (14%)  | 76,107,113  | 1.42 | 9 (11%)  |
| 27  | CLA  | 1     | 603 | -    | 56,60,73     | 1.90 | 9 (16%)  | 65,97,113   | 1.44 | 8 (12%)  |
| 27  | CLA  | A     | 828 | -    | 69,73,73     | 1.73 | 9 (13%)  | 82,113,113  | 1.27 | 9 (10%)  |
| 29  | II0  | J     | 101 | -    | 39,43,43     | 2.03 | 2 (5%)   | 48,60,60    | 1.39 | 7 (14%)  |
| 35  | 8CT  | 4     | 616 | -    | 40,41,41     | 0.17 | 0        | 51,56,56    | 0.28 | 0        |
| 27  | CLA  | 6     | 612 | -    | 49,53,73     | 2.01 | 9 (18%)  | 58,89,113   | 1.53 | 9 (15%)  |
| 27  | CLA  | B     | 831 | -    | 59,63,73     | 1.88 | 9 (15%)  | 70,101,113  | 1.46 | 8 (11%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 29  | II0  | 7     | 316 | -    | 39,43,43     | 2.05 | 2 (5%)   | 48,60,60    | 1.32 | 7 (14%)  |
| 27  | CLA  | L     | 203 | -    | 54,58,73     | 1.91 | 9 (16%)  | 64,95,113   | 1.52 | 10 (15%) |
| 27  | CLA  | 3     | 604 | -    | 69,73,73     | 1.71 | 9 (13%)  | 82,113,113  | 1.30 | 8 (9%)   |
| 27  | CLA  | 8     | 603 | -    | 69,73,73     | 1.73 | 9 (13%)  | 82,113,113  | 1.30 | 8 (9%)   |
| 27  | CLA  | 5     | 603 | -    | 49,53,73     | 2.06 | 9 (18%)  | 58,89,113   | 1.54 | 9 (15%)  |
| 29  | II0  | 6     | 614 | -    | 39,43,43     | 1.99 | 2 (5%)   | 48,60,60    | 1.29 | 5 (10%)  |
| 27  | CLA  | 1     | 613 | -    | 49,53,73     | 2.10 | 9 (18%)  | 58,89,113   | 1.57 | 9 (15%)  |
| 27  | CLA  | 5     | 612 | -    | 49,53,73     | 2.03 | 9 (18%)  | 58,89,113   | 1.53 | 8 (13%)  |
| 27  | CLA  | 5     | 607 | 5    | 49,53,73     | 2.01 | 9 (18%)  | 58,89,113   | 1.52 | 8 (13%)  |
| 27  | CLA  | B     | 823 | -    | 69,73,73     | 1.72 | 9 (13%)  | 82,113,113  | 1.28 | 10 (12%) |
| 27  | CLA  | K     | 101 | -    | 69,73,73     | 1.72 | 9 (13%)  | 82,113,113  | 1.25 | 8 (9%)   |
| 27  | CLA  | L     | 201 | 19   | 55,59,73     | 1.93 | 9 (16%)  | 64,96,113   | 1.47 | 8 (12%)  |
| 31  | IHT  | 5     | 618 | -    | 40,42,42     | 2.57 | 4 (10%)  | 52,58,58    | 2.28 | 15 (28%) |
| 27  | CLA  | 4     | 609 | 4    | 64,68,73     | 1.78 | 9 (14%)  | 76,107,113  | 1.33 | 8 (10%)  |
| 27  | CLA  | B     | 830 | -    | 64,68,73     | 1.80 | 9 (14%)  | 76,107,113  | 1.37 | 8 (10%)  |
| 27  | CLA  | 1     | 612 | -    | 64,68,73     | 1.75 | 9 (14%)  | 76,107,113  | 1.30 | 9 (11%)  |
| 27  | CLA  | 6     | 601 | 6    | 49,53,73     | 2.02 | 9 (18%)  | 58,89,113   | 1.54 | 9 (15%)  |
| 27  | CLA  | Z     | 304 | 24   | 59,63,73     | 1.85 | 9 (15%)  | 70,101,113  | 1.37 | 8 (11%)  |
| 27  | CLA  | 4     | 610 | -    | 69,73,73     | 1.70 | 9 (13%)  | 82,113,113  | 1.29 | 8 (9%)   |
| 27  | CLA  | 7     | 304 | -    | 59,63,73     | 1.88 | 9 (15%)  | 70,101,113  | 1.43 | 9 (12%)  |
| 35  | 8CT  | B     | 844 | -    | 40,41,41     | 0.18 | 0        | 51,56,56    | 0.57 | 0        |
| 27  | CLA  | 6     | 607 | 6    | 59,63,73     | 1.84 | 9 (15%)  | 70,101,113  | 1.39 | 8 (11%)  |
| 27  | CLA  | b     | 611 | -    | 59,63,73     | 1.83 | 9 (15%)  | 70,101,113  | 1.37 | 9 (12%)  |
| 28  | KC2  | 7     | 311 | 7    | 49,53,53     | 1.81 | 4 (8%)   | 60,89,89    | 1.16 | 4 (6%)   |
| 27  | CLA  | 2     | 601 | 2    | 46,50,73     | 2.13 | 9 (19%)  | 53,85,113   | 1.66 | 9 (16%)  |
| 29  | II0  | 5     | 614 | -    | 39,43,43     | 2.00 | 2 (5%)   | 48,60,60    | 1.34 | 6 (12%)  |
| 27  | CLA  | A     | 844 | -    | 69,73,73     | 1.65 | 9 (13%)  | 82,113,113  | 1.32 | 10 (12%) |
| 27  | CLA  | 8     | 607 | 8    | 45,49,73     | 2.19 | 10 (22%) | 54,84,113   | 1.63 | 9 (16%)  |
| 29  | II0  | b     | 614 | -    | 39,43,43     | 2.03 | 2 (5%)   | 48,60,60    | 1.33 | 7 (14%)  |
| 27  | CLA  | a     | 604 | -    | 64,68,73     | 1.81 | 9 (14%)  | 76,107,113  | 1.37 | 7 (9%)   |
| 27  | CLA  | Z     | 301 | -    | 64,68,73     | 1.80 | 9 (14%)  | 76,107,113  | 1.35 | 7 (9%)   |
| 27  | CLA  | A     | 815 | -    | 66,70,73     | 1.79 | 9 (13%)  | 78,109,113  | 1.32 | 8 (10%)  |
| 35  | 8CT  | B     | 846 | -    | 40,41,41     | 0.09 | 0        | 51,56,56    | 0.47 | 0        |
| 27  | CLA  | 9     | 614 | -    | 45,49,73     | 2.23 | 10 (22%) | 54,84,113   | 1.68 | 9 (16%)  |
| 33  | LHG  | 2     | 620 | -    | 41,41,48     | 0.66 | 1 (2%)   | 44,47,54    | 1.24 | 5 (11%)  |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 27  | CLA  | 1     | 607 | 1    | 49,53,73     | 2.05 | 9 (18%)  | 58,89,113   | 1.53 | 8 (13%)  |
| 27  | CLA  | 1     | 601 | 1    | 49,53,73     | 2.10 | 9 (18%)  | 58,89,113   | 1.59 | 9 (15%)  |
| 28  | KC2  | 2     | 610 | -    | 49,53,53     | 1.83 | 4 (8%)   | 60,89,89    | 1.12 | 4 (6%)   |
| 31  | IHT  | 8     | 609 | -    | 40,42,42     | 2.56 | 3 (7%)   | 52,58,58    | 2.38 | 16 (30%) |
| 27  | CLA  | A     | 834 | 10   | 59,63,73     | 1.85 | 9 (15%)  | 70,101,113  | 1.42 | 10 (14%) |
| 27  | CLA  | 6     | 606 | -    | 59,63,73     | 1.89 | 9 (15%)  | 70,101,113  | 1.46 | 10 (14%) |
| 27  | CLA  | A     | 809 | 27   | 64,68,73     | 1.83 | 9 (14%)  | 76,107,113  | 1.45 | 8 (10%)  |
| 27  | CLA  | A     | 811 | -    | 69,73,73     | 1.72 | 9 (13%)  | 82,113,113  | 1.36 | 6 (7%)   |
| 27  | CLA  | A     | 807 | 10   | 54,58,73     | 1.95 | 9 (16%)  | 64,95,113   | 1.49 | 9 (14%)  |
| 27  | CLA  | 9     | 611 | -    | 45,49,73     | 2.17 | 10 (22%) | 54,84,113   | 1.63 | 9 (16%)  |
| 27  | CLA  | O     | 203 | -    | 59,63,73     | 1.86 | 9 (15%)  | 70,101,113  | 1.39 | 8 (11%)  |
| 32  | LMG  | 3     | 620 | -    | 32,32,55     | 0.91 | 1 (3%)   | 40,40,63    | 1.28 | 6 (15%)  |
| 27  | CLA  | A     | 821 | -    | 59,63,73     | 1.84 | 9 (15%)  | 70,101,113  | 1.46 | 8 (11%)  |
| 27  | CLA  | 8     | 605 | 8    | 54,58,73     | 1.95 | 9 (16%)  | 64,95,113   | 1.49 | 9 (14%)  |
| 29  | II0  | 3     | 614 | -    | 39,43,43     | 2.01 | 2 (5%)   | 48,60,60    | 1.39 | 6 (12%)  |
| 31  | IHT  | a     | 616 | -    | 40,42,42     | 2.57 | 3 (7%)   | 52,58,58    | 2.35 | 15 (28%) |
| 27  | CLA  | A     | 804 | 10   | 69,73,73     | 1.71 | 9 (13%)  | 82,113,113  | 1.29 | 9 (10%)  |
| 29  | II0  | 8     | 611 | -    | 39,43,43     | 2.04 | 2 (5%)   | 48,60,60    | 1.24 | 4 (8%)   |
| 27  | CLA  | 7     | 310 | 33   | 45,49,73     | 2.20 | 10 (22%) | 54,84,113   | 1.62 | 8 (14%)  |
| 33  | LHG  | 2     | 618 | -    | 21,21,48     | 0.76 | 0        | 23,26,54    | 1.29 | 2 (8%)   |
| 33  | LHG  | b     | 616 | -    | 48,48,48     | 0.58 | 1 (2%)   | 51,54,54    | 1.18 | 4 (7%)   |
| 27  | CLA  | F     | 202 | -    | 64,68,73     | 1.79 | 9 (14%)  | 76,107,113  | 1.34 | 8 (10%)  |
| 27  | CLA  | 3     | 607 | 3    | 64,68,73     | 1.77 | 9 (14%)  | 76,107,113  | 1.32 | 8 (10%)  |
| 27  | CLA  | 1     | 606 | -    | 49,53,73     | 2.04 | 9 (18%)  | 58,89,113   | 1.54 | 8 (13%)  |
| 31  | IHT  | 9     | 619 | -    | 40,42,42     | 2.58 | 4 (10%)  | 52,58,58    | 2.43 | 13 (25%) |
| 27  | CLA  | 1     | 609 | -    | 45,49,73     | 2.20 | 10 (22%) | 54,84,113   | 1.64 | 8 (14%)  |
| 39  | DGD  | Z     | 303 | -    | 61,61,67     | 0.94 | 3 (4%)   | 75,75,81    | 1.36 | 7 (9%)   |
| 28  | KC2  | 5     | 610 | 5    | 49,53,53     | 1.82 | 4 (8%)   | 60,89,89    | 1.11 | 4 (6%)   |
| 31  | IHT  | 1     | 618 | -    | 40,42,42     | 2.60 | 4 (10%)  | 52,58,58    | 2.07 | 13 (25%) |
| 27  | CLA  | A     | 832 | -    | 69,73,73     | 1.71 | 9 (13%)  | 82,113,113  | 1.26 | 8 (9%)   |
| 27  | CLA  | A     | 831 | -    | 69,73,73     | 1.70 | 9 (13%)  | 82,113,113  | 1.25 | 8 (9%)   |
| 27  | CLA  | 2     | 603 | -    | 54,58,73     | 1.96 | 9 (16%)  | 64,95,113   | 1.45 | 8 (12%)  |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.  
'-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 27  | CLA  | B     | 802 | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 27  | CLA  | 6     | 604 | -    | 1/1/14/20 | 6/33/109/115  | -       |
| 27  | CLA  | A     | 813 | -    | 1/1/10/20 | 0/12/88/115   | -       |
| 27  | CLA  | A     | 823 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 31  | IHT  | 2     | 616 | -    | -         | 2/25/65/65    | 0/2/2/2 |
| 35  | 8CT  | M     | 101 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 27  | CLA  | 2     | 612 | -    | 1/1/11/20 | 5/15/91/115   | -       |
| 27  | CLA  | B     | 836 | -    | 1/1/11/20 | 3/18/94/115   | -       |
| 27  | CLA  | 1     | 604 | 1    | 1/1/11/20 | 3/15/91/115   | -       |
| 31  | IHT  | A     | 854 | -    | -         | 1/25/65/65    | 0/2/2/2 |
| 27  | CLA  | b     | 604 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 29  | II0  | 8     | 610 | -    | -         | 2/21/67/67    | 0/2/2/2 |
| 27  | CLA  | a     | 602 | 25   | 1/1/13/20 | 8/27/103/115  | -       |
| 27  | CLA  | 8     | 606 | 8    | 1/1/13/20 | 3/27/103/115  | -       |
| 27  | CLA  | a     | 601 | 25   | 1/1/11/20 | 3/15/91/115   | -       |
| 27  | CLA  | 4     | 602 | 4    | 1/1/13/20 | 5/32/108/115  | -       |
| 28  | KC2  | 6     | 613 | 6    | -         | 8/15/71/71    | -       |
| 35  | 8CT  | K     | 103 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 27  | CLA  | 6     | 609 | 33   | 1/1/10/20 | 2/10/86/115   | -       |
| 27  | CLA  | 4     | 608 | 33   | 1/1/15/20 | 4/39/115/115  | -       |
| 27  | CLA  | A     | 808 | -    | 1/1/13/20 | 1/27/103/115  | -       |
| 27  | CLA  | B     | 809 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 27  | CLA  | B     | 822 | -    | 1/1/15/20 | 5/39/115/115  | -       |
| 27  | CLA  | K     | 102 | -    | 1/1/13/20 | 2/27/103/115  | -       |
| 27  | CLA  | 2     | 604 | 2    | 1/1/13/20 | 1/27/103/115  | -       |
| 27  | CLA  | A     | 805 | -    | 1/1/12/20 | 3/21/97/115   | -       |
| 33  | LHG  | 4     | 620 | -    | -         | 16/49/49/53   | -       |
| 27  | CLA  | Z     | 310 | -    | 1/1/15/20 | 7/39/115/115  | -       |
| 35  | 8CT  | Z     | 309 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 27  | CLA  | b     | 602 | 26   | 1/1/14/20 | 14/38/114/115 | -       |
| 27  | CLA  | 1     | 611 | -    | 1/1/11/20 | 2/15/91/115   | -       |
| 27  | CLA  | A     | 816 | -    | 1/1/14/20 | 9/33/109/115  | -       |
| 29  | II0  | 5     | 617 | -    | -         | 2/21/67/67    | 0/2/2/2 |
| 27  | CLA  | 5     | 609 | -    | 1/1/10/20 | 2/10/86/115   | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 27  | CLA  | F     | 204 | 15   | 1/1/13/20 | 6/27/103/115  | -       |
| 35  | 8CT  | 7     | 318 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 35  | 8CT  | R     | 203 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 27  | CLA  | 3     | 609 | -    | 1/1/15/20 | 2/39/115/115  | -       |
| 27  | CLA  | 9     | 613 | 9    | 1/1/11/20 | 3/15/91/115   | -       |
| 31  | IHT  | Z     | 302 | -    | -         | 2/25/65/65    | 0/2/2/2 |
| 27  | CLA  | 9     | 601 | 9    | 1/1/11/20 | 6/15/91/115   | -       |
| 29  | II0  | b     | 612 | -    | -         | 1/21/67/67    | 0/2/2/2 |
| 27  | CLA  | B     | 827 | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 27  | CLA  | B     | 839 | 33   | 1/1/15/20 | 4/39/115/115  | -       |
| 27  | CLA  | B     | 805 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 27  | CLA  | B     | 829 | -    | 1/1/11/20 | 2/15/91/115   | -       |
| 27  | CLA  | b     | 608 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 33  | LHG  | 3     | 622 | 28   | -         | 13/38/38/53   | -       |
| 27  | CLA  | 7     | 309 | 7    | 1/1/13/20 | 10/27/103/115 | -       |
| 27  | CLA  | A     | 839 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 27  | CLA  | b     | 606 | 26   | 1/1/15/20 | 4/39/115/115  | -       |
| 27  | CLA  | A     | 836 | -    | 1/1/13/20 | 2/27/103/115  | -       |
| 27  | CLA  | B     | 806 | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 29  | II0  | O     | 205 | -    | -         | 2/21/67/67    | 0/2/2/2 |
| 29  | II0  | 5     | 620 | -    | -         | 1/21/67/67    | 0/2/2/2 |
| 29  | II0  | 2     | 615 | -    | -         | 2/21/67/67    | 0/2/2/2 |
| 27  | CLA  | 3     | 611 | 3    | 1/1/12/20 | 2/21/97/115   | -       |
| 27  | CLA  | A     | 826 | -    | 1/1/15/20 | 4/39/115/115  | -       |
| 29  | II0  | 1     | 617 | -    | -         | 2/21/67/67    | 0/2/2/2 |
| 27  | CLA  | J     | 102 | -    | 1/1/10/20 | 2/10/86/115   | -       |
| 35  | 8CT  | A     | 847 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 33  | LHG  | Z     | 311 | -    | -         | 23/50/50/53   | -       |
| 27  | CLA  | A     | 814 | -    | 1/1/11/20 | 3/15/91/115   | -       |
| 27  | CLA  | 6     | 608 | 6    | 1/1/14/20 | 7/33/109/115  | -       |
| 35  | 8CT  | A     | 845 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 27  | CLA  | A     | 829 | -    | 1/1/12/20 | 5/21/97/115   | -       |
| 29  | II0  | 6     | 615 | -    | -         | 1/21/67/67    | 0/2/2/2 |
| 33  | LHG  | 7     | 319 | -    | -         | 9/35/35/53    | -       |
| 27  | CLA  | 9     | 606 | -    | 1/1/14/20 | 10/38/114/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 27  | CLA  | B     | 820 | -    | 1/1/14/20 | 7/33/109/115  | -       |
| 27  | CLA  | A     | 827 | -    | 1/1/15/20 | 5/39/115/115  | -       |
| 29  | II0  | Z     | 312 | -    | -         | 1/21/67/67    | 0/2/2/2 |
| 28  | KC2  | 7     | 307 | -    | -         | 5/15/71/71    | -       |
| 33  | LHG  | 7     | 320 | 27   | -         | 20/43/43/53   | -       |
| 27  | CLA  | 3     | 605 | 3    | 1/1/13/20 | 4/27/103/115  | -       |
| 27  | CLA  | Z     | 306 | 24   | 1/1/14/20 | 12/33/109/115 | -       |
| 27  | CLA  | B     | 821 | -    | 1/1/14/20 | 9/33/109/115  | -       |
| 29  | II0  | 4     | 614 | -    | -         | 2/21/67/67    | 0/2/2/2 |
| 36  | LMU  | J     | 104 | -    | -         | 8/17/57/61    | 0/2/2/2 |
| 27  | CLA  | A     | 819 | -    | 1/1/15/20 | 5/39/115/115  | -       |
| 28  | KC2  | Z     | 307 | -    | -         | 9/15/71/71    | -       |
| 27  | CLA  | 8     | 615 | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 27  | CLA  | A     | 802 | 27   | 1/1/13/20 | 3/27/103/115  | -       |
| 35  | 8CT  | A     | 848 | -    | -         | 1/29/63/63    | 0/2/2/2 |
| 29  | II0  | 3     | 617 | -    | -         | 1/21/67/67    | 0/2/2/2 |
| 27  | CLA  | 2     | 611 | -    | 1/1/11/20 | 0/15/91/115   | -       |
| 27  | CLA  | B     | 803 | -    | 1/1/11/20 | 3/15/91/115   | -       |
| 27  | CLA  | 4     | 611 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 27  | CLA  | 7     | 302 | 7    | 1/1/11/20 | 2/15/91/115   | -       |
| 27  | CLA  | 7     | 312 | -    | 1/1/13/20 | 4/27/103/115  | -       |
| 27  | CLA  | 9     | 609 | -    | 1/1/10/20 | 1/10/86/115   | -       |
| 27  | CLA  | A     | 837 | -    | 1/1/15/20 | 7/39/115/115  | -       |
| 27  | CLA  | A     | 801 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 27  | CLA  | B     | 813 | -    | 1/1/14/20 | 11/35/111/115 | -       |
| 33  | LHG  | 6     | 617 | 27   | -         | 16/39/39/53   | -       |
| 27  | CLA  | O     | 204 | -    | 1/1/13/20 | 6/27/103/115  | -       |
| 27  | CLA  | 8     | 601 | 8    | 1/1/11/20 | 3/15/91/115   | -       |
| 28  | KC2  | 6     | 610 | 6    | -         | 6/15/71/71    | -       |
| 27  | CLA  | 7     | 303 | 7    | 1/1/15/20 | 4/39/115/115  | -       |
| 27  | CLA  | 2     | 609 | -    | 1/1/10/20 | 2/10/86/115   | -       |
| 27  | CLA  | O     | 201 | -    | 1/1/13/20 | 2/27/103/115  | -       |
| 27  | CLA  | a     | 605 | -    | 1/1/13/20 | 9/27/103/115  | -       |
| 29  | II0  | 2     | 614 | -    | -         | 0/21/67/67    | 0/2/2/2 |
| 27  | CLA  | 7     | 308 | 7    | 1/1/11/20 | 1/15/91/115   | -       |

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| Mol | Type | Chain | Res | Link  | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|-------|-----------|---------------|---------|
| 27  | CLA  | 2     | 607 | 2     | 1/1/11/20 | 2/15/91/115   | -       |
| 27  | CLA  | 5     | 613 | 5     | 1/1/10/20 | 4/10/86/115   | -       |
| 27  | CLA  | F     | 203 | -     | 1/1/11/20 | 5/15/91/115   | -       |
| 33  | LHG  | 4     | 619 | 27    | -         | 17/49/49/53   | -       |
| 27  | CLA  | B     | 840 | -     | 1/1/15/20 | 0/39/115/115  | -       |
| 35  | 8CT  | Z     | 308 | -     | -         | 6/29/63/63    | 0/2/2/2 |
| 35  | 8CT  | B     | 850 | -     | -         | 9/29/63/63    | 0/2/2/2 |
| 29  | II0  | 1     | 616 | -     | -         | 2/21/67/67    | 0/2/2/2 |
| 27  | CLA  | A     | 843 | -     | 1/1/15/20 | 8/39/115/115  | -       |
| 27  | CLA  | B     | 808 | 11    | 1/1/15/20 | 8/39/115/115  | -       |
| 27  | CLA  | 5     | 611 | -     | 1/1/11/20 | 6/15/91/115   | -       |
| 37  | SF4  | C     | 102 | 12    | -         | -             | 0/6/5/5 |
| 27  | CLA  | 9     | 602 | 9     | 1/1/13/20 | 10/27/103/115 | -       |
| 29  | II0  | 1     | 619 | -     | -         | 1/21/67/67    | 0/2/2/2 |
| 37  | SF4  | A     | 849 | 10,11 | -         | -             | 0/6/5/5 |
| 27  | CLA  | b     | 603 | -     | 1/1/14/20 | 8/33/109/115  | -       |
| 27  | CLA  | a     | 610 | -     | 1/1/13/20 | 6/27/103/115  | -       |
| 35  | 8CT  | B     | 849 | -     | -         | 4/29/63/63    | 0/2/2/2 |
| 38  | PQN  | B     | 842 | -     | -         | 5/23/43/43    | 0/2/2/2 |
| 27  | CLA  | A     | 835 | -     | 1/1/14/20 | 5/33/109/115  | -       |
| 28  | KC2  | 4     | 605 | 4     | -         | 6/15/71/71    | -       |
| 29  | II0  | 7     | 315 | -     | -         | 1/21/67/67    | 0/2/2/2 |
| 27  | CLA  | B     | 825 | -     | 1/1/15/20 | 3/39/115/115  | -       |
| 27  | CLA  | L     | 202 | -     | 1/1/14/20 | 10/33/109/115 | -       |
| 29  | II0  | 3     | 615 | -     | -         | 1/21/67/67    | 0/2/2/2 |
| 33  | LHG  | A     | 852 | -     | -         | 19/43/43/53   | -       |
| 27  | CLA  | B     | 817 | -     | 1/1/14/20 | 1/33/109/115  | -       |
| 29  | II0  | 9     | 617 | -     | -         | 2/21/67/67    | 0/2/2/2 |
| 29  | II0  | 4     | 612 | -     | -         | 2/21/67/67    | 0/2/2/2 |
| 27  | CLA  | 9     | 603 | -     | 1/1/11/20 | 4/15/91/115   | -       |
| 27  | CLA  | A     | 818 | -     | 1/1/15/20 | 7/39/115/115  | -       |
| 27  | CLA  | 4     | 603 | -     | 1/1/12/20 | 4/26/102/115  | -       |
| 27  | CLA  | 5     | 608 | 5     | 1/1/14/20 | 11/33/109/115 | -       |
| 29  | II0  | B     | 843 | -     | -         | 2/21/67/67    | 0/2/2/2 |
| 27  | CLA  | 4     | 607 | 4     | 1/1/14/20 | 8/33/109/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 27  | CLA  | A     | 817 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 27  | CLA  | A     | 824 | -    | 1/1/15/20 | 4/39/115/115  | -       |
| 27  | CLA  | 5     | 605 | 5    | 1/1/11/20 | 2/15/91/115   | -       |
| 29  | II0  | a     | 615 | -    | -         | 1/21/67/67    | 0/2/2/2 |
| 27  | CLA  | B     | 841 | -    | 1/1/12/20 | 7/24/100/115  | -       |
| 33  | LHG  | a     | 618 | -    | -         | 16/33/33/53   | -       |
| 27  | CLA  | Z     | 305 | -    | 1/1/12/20 | 2/21/97/115   | -       |
| 29  | II0  | a     | 612 | -    | -         | 2/21/67/67    | 0/2/2/2 |
| 27  | CLA  | b     | 601 | 26   | 1/1/11/20 | 4/15/91/115   | -       |
| 29  | II0  | 3     | 616 | -    | -         | 2/21/67/67    | 0/2/2/2 |
| 28  | KC2  | a     | 609 | -    | -         | 4/15/71/71    | -       |
| 27  | CLA  | A     | 841 | -    | 1/1/15/20 | 4/39/115/115  | -       |
| 27  | CLA  | B     | 834 | -    | 1/1/13/20 | 2/27/103/115  | -       |
| 27  | CLA  | a     | 608 | -    | 1/1/14/20 | 9/33/109/115  | -       |
| 27  | CLA  | b     | 607 | 26   | 1/1/14/20 | 3/33/109/115  | -       |
| 27  | CLA  | 2     | 608 | 2    | 1/1/14/20 | 4/33/109/115  | -       |
| 35  | 8CT  | I     | 101 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 27  | CLA  | 6     | 605 | 6    | 1/1/13/20 | 7/27/103/115  | -       |
| 30  | II3  | b     | 613 | -    | -         | 1/25/67/67    | 0/2/2/2 |
| 27  | CLA  | B     | 811 | -    | 1/1/13/20 | 8/27/103/115  | -       |
| 27  | CLA  | B     | 826 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 27  | CLA  | 1     | 605 | -    | 1/1/10/20 | 3/11/87/115   | -       |
| 29  | II0  | 4     | 613 | -    | -         | 1/21/67/67    | 0/2/2/2 |
| 27  | CLA  | A     | 810 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 28  | KC2  | b     | 605 | 26   | -         | 6/15/71/71    | -       |
| 27  | CLA  | 7     | 305 | 7    | 1/1/12/20 | 7/25/101/115  | -       |
| 37  | SF4  | C     | 101 | 12   | -         | -             | 0/6/5/5 |
| 29  | II0  | 9     | 618 | -    | -         | 2/21/67/67    | 0/2/2/2 |
| 29  | II0  | a     | 613 | -    | -         | 2/21/67/67    | 0/2/2/2 |
| 27  | CLA  | A     | 825 | -    | 1/1/15/20 | 5/39/115/115  | -       |
| 33  | LHG  | 8     | 613 | -    | -         | 21/37/37/53   | -       |
| 29  | II0  | 4     | 615 | -    | -         | 0/21/67/67    | 0/2/2/2 |
| 38  | PQN  | A     | 850 | -    | -         | 10/23/43/43   | 0/2/2/2 |
| 32  | LMG  | 2     | 617 | -    | -         | 8/31/51/70    | 0/1/1/1 |
| 27  | CLA  | A     | 803 | -    | 1/1/15/20 | 6/39/115/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 27  | CLA  | 5     | 606 | -    | 1/1/11/20 | 4/15/91/115   | -       |
| 27  | CLA  | 9     | 608 | 9    | 1/1/13/20 | 11/27/103/115 | -       |
| 27  | CLA  | O     | 202 | -    | 1/1/10/20 | 4/10/86/115   | -       |
| 33  | LHG  | a     | 617 | -    | -         | 24/53/53/53   | -       |
| 32  | LMG  | 8     | 616 | -    | -         | 24/46/66/70   | 0/1/1/1 |
| 27  | CLA  | B     | 815 | -    | 1/1/15/20 | 7/39/115/115  | -       |
| 36  | LMU  | 4     | 618 | -    | -         | 11/21/61/61   | 0/2/2/2 |
| 27  | CLA  | b     | 610 | 26   | 1/1/12/20 | 8/23/99/115   | -       |
| 35  | 8CT  | J     | 103 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 32  | LMG  | 3     | 618 | -    | -         | 9/25/45/70    | 0/1/1/1 |
| 29  | II0  | 9     | 615 | -    | -         | 1/21/67/67    | 0/2/2/2 |
| 27  | CLA  | 2     | 606 | -    | 1/1/11/20 | 2/15/91/115   | -       |
| 27  | CLA  | B     | 804 | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 34  | SQD  | O     | 207 | -    | -         | 7/18/38/69    | 0/1/1/1 |
| 35  | 8CT  | B     | 847 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 27  | CLA  | B     | 814 | -    | 1/1/10/20 | 4/12/88/115   | -       |
| 27  | CLA  | A     | 806 | 10   | 1/1/15/20 | 7/39/115/115  | -       |
| 33  | LHG  | A     | 851 | -    | -         | 23/53/53/53   | -       |
| 27  | CLA  | 8     | 604 | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 27  | CLA  | B     | 833 | -    | 1/1/11/20 | 1/15/91/115   | -       |
| 27  | CLA  | 4     | 606 | 4    | 1/1/14/20 | 3/33/109/115  | -       |
| 27  | CLA  | 6     | 602 | 6    | 1/1/15/20 | 5/39/115/115  | -       |
| 27  | CLA  | 1     | 608 | 1    | 1/1/14/20 | 4/33/109/115  | -       |
| 28  | KC2  | 1     | 610 | -    | -         | 8/15/71/71    | -       |
| 27  | CLA  | a     | 611 | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 29  | II0  | 7     | 317 | -    | -         | 0/21/67/67    | 0/2/2/2 |
| 30  | II3  | 1     | 615 | -    | -         | 1/25/67/67    | 0/2/2/2 |
| 27  | CLA  | 3     | 610 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 27  | CLA  | A     | 820 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 33  | LHG  | 5     | 619 | -    | -         | 13/26/26/53   | -       |
| 27  | CLA  | 9     | 605 | -    | 1/1/11/20 | 2/15/91/115   | -       |
| 27  | CLA  | A     | 842 | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 27  | CLA  | 8     | 602 | 8    | 1/1/11/20 | 3/15/91/115   | -       |
| 32  | LMG  | 8     | 614 | -    | -         | 23/47/67/70   | 0/1/1/1 |
| 27  | CLA  | 8     | 608 | -    | 1/1/15/20 | 6/39/115/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 27  | CLA  | 3     | 603 | -    | 1/1/14/20 | 3/33/109/115  | -       |
| 27  | CLA  | A     | 830 | -    | 1/1/14/20 | 4/33/109/115  | -       |
| 27  | CLA  | A     | 822 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 27  | CLA  | 9     | 607 | 9    | 1/1/15/20 | 9/39/115/115  | -       |
| 27  | CLA  | A     | 833 | -    | 1/1/15/20 | 5/39/115/115  | -       |
| 29  | II0  | 7     | 301 | -    | -         | 2/21/67/67    | 0/2/2/2 |
| 27  | CLA  | B     | 835 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 29  | II0  | 2     | 613 | -    | -         | 1/21/67/67    | 0/2/2/2 |
| 27  | CLA  | B     | 812 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 28  | KC2  | 9     | 610 | -    | -         | 6/15/71/71    | -       |
| 28  | KC2  | 3     | 606 | 33   | -         | 8/15/71/71    | -       |
| 27  | CLA  | A     | 812 | -    | 1/1/13/20 | 2/27/103/115  | -       |
| 27  | CLA  | 2     | 602 | 2    | 1/1/13/20 | 12/32/108/115 | -       |
| 35  | 8CT  | A     | 853 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 27  | CLA  | 5     | 602 | 5    | 1/1/13/20 | 4/27/103/115  | -       |
| 39  | DGD  | B     | 848 | -    | -         | 15/48/88/95   | 0/2/2/2 |
| 29  | II0  | 3     | 613 | -    | -         | 2/21/67/67    | 0/2/2/2 |
| 27  | CLA  | 3     | 602 | 3    | 1/1/13/20 | 2/27/103/115  | -       |
| 27  | CLA  | 3     | 601 | 3    | 1/1/11/20 | 6/15/91/115   | -       |
| 35  | 8CT  | A     | 846 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 27  | CLA  | B     | 832 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 35  | 8CT  | B     | 845 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 35  | 8CT  | R     | 201 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 35  | 8CT  | L     | 205 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 27  | CLA  | 3     | 608 | 3    | 1/1/14/20 | 6/33/109/115  | -       |
| 27  | CLA  | a     | 603 | -    | 1/1/14/20 | 6/33/109/115  | -       |
| 27  | CLA  | 6     | 611 | -    | 1/1/13/20 | 2/27/103/115  | -       |
| 27  | CLA  | R     | 202 | -    | 1/1/13/20 | 8/27/103/115  | -       |
| 33  | LHG  | 4     | 617 | 27   | -         | 18/51/51/53   | -       |
| 27  | CLA  | A     | 840 | -    | 1/1/13/20 | 4/27/103/115  | -       |
| 31  | IHT  | L     | 204 | -    | -         | 2/25/65/65    | 0/2/2/2 |
| 29  | II0  | 7     | 314 | -    | -         | 0/21/67/67    | 0/2/2/2 |
| 27  | CLA  | 5     | 604 | -    | 1/1/13/20 | 8/27/103/115  | -       |
| 29  | II0  | O     | 206 | -    | -         | 1/21/67/67    | 0/2/2/2 |
| 29  | II0  | 1     | 614 | -    | -         | 2/21/67/67    | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 27  | CLA  | 5     | 601 | 5    | 1/1/10/20 | 2/10/86/115   | -       |
| 27  | CLA  | B     | 818 | -    | 1/1/14/20 | 3/33/109/115  | -       |
| 29  | II0  | 5     | 615 | -    | -         | 1/21/67/67    | 0/2/2/2 |
| 27  | CLA  | B     | 824 | -    | 1/1/14/20 | 3/33/109/115  | -       |
| 29  | II0  | a     | 614 | -    | -         | 2/21/67/67    | 0/2/2/2 |
| 34  | SQD  | 3     | 621 | -    | -         | 15/37/57/69   | 0/1/1/1 |
| 29  | II0  | R     | 204 | -    | -         | 2/21/67/67    | 0/2/2/2 |
| 27  | CLA  | 9     | 612 | -    | 1/1/11/20 | 4/15/91/115   | -       |
| 35  | 8CT  | b     | 615 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 27  | CLA  | B     | 816 | -    | 1/1/13/20 | 14/32/108/115 | -       |
| 36  | LMU  | 7     | 321 | -    | -         | 8/21/61/61    | 0/2/2/2 |
| 27  | CLA  | B     | 838 | -    | 1/1/15/20 | 4/39/115/115  | -       |
| 27  | CLA  | a     | 606 | 25   | 1/1/15/20 | 5/39/115/115  | -       |
| 27  | CLA  | 1     | 602 | 1    | 1/1/13/20 | 4/32/108/115  | -       |
| 27  | CLA  | B     | 807 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 27  | CLA  | B     | 837 | -    | 1/1/15/20 | 4/39/115/115  | -       |
| 27  | CLA  | A     | 838 | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 33  | LHG  | 2     | 619 | -    | -         | 16/43/43/53   | -       |
| 27  | CLA  | a     | 607 | 25   | 1/1/14/20 | 1/33/109/115  | -       |
| 27  | CLA  | 9     | 604 | -    | 1/1/13/20 | 1/27/103/115  | -       |
| 27  | CLA  | B     | 801 | -    | 1/1/15/20 | 5/39/115/115  | -       |
| 29  | II0  | 8     | 612 | -    | -         | 1/21/67/67    | 0/2/2/2 |
| 27  | CLA  | 4     | 604 | -    | 1/1/13/20 | 9/27/103/115  | -       |
| 27  | CLA  | B     | 810 | -    | 1/1/14/20 | 3/33/109/115  | -       |
| 28  | KC2  | b     | 609 | -    | -         | 3/15/71/71    | -       |
| 35  | 8CT  | F     | 201 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 27  | CLA  | 4     | 601 | 4    | 1/1/13/20 | 5/27/103/115  | -       |
| 32  | LMG  | F     | 205 | -    | -         | 11/27/47/70   | 0/1/1/1 |
| 27  | CLA  | 7     | 313 | -    | 1/1/12/20 | 6/21/97/115   | -       |
| 31  | IHT  | 6     | 616 | -    | -         | 3/25/65/65    | 0/2/2/2 |
| 27  | CLA  | 7     | 306 | 7    | 1/1/11/20 | 6/15/91/115   | -       |
| 29  | II0  | 5     | 616 | -    | -         | 1/21/67/67    | 0/2/2/2 |
| 27  | CLA  | B     | 828 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 27  | CLA  | 2     | 605 | -    | 1/1/14/20 | 6/33/109/115  | -       |
| 27  | CLA  | 6     | 603 | -    | 1/1/11/20 | 7/15/91/115   | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 27  | CLA  | 3     | 612 | -    | 1/1/11/20 | 2/15/91/115   | -       |
| 33  | LHG  | 3     | 619 | -    | -         | 24/53/53/53   | -       |
| 32  | LMG  | 6     | 618 | -    | -         | 5/27/47/70    | 0/1/1/1 |
| 29  | II0  | 9     | 616 | -    | -         | 2/21/67/67    | 0/2/2/2 |
| 27  | CLA  | B     | 819 | -    | 1/1/14/20 | 7/33/109/115  | -       |
| 27  | CLA  | 1     | 603 | -    | 1/1/12/20 | 4/24/100/115  | -       |
| 27  | CLA  | A     | 828 | -    | 1/1/15/20 | 7/39/115/115  | -       |
| 29  | II0  | J     | 101 | -    | -         | 1/21/67/67    | 0/2/2/2 |
| 35  | 8CT  | 4     | 616 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 27  | CLA  | 6     | 612 | -    | 1/1/11/20 | 4/15/91/115   | -       |
| 27  | CLA  | B     | 831 | -    | 1/1/13/20 | 10/27/103/115 | -       |
| 29  | II0  | 7     | 316 | -    | -         | 2/21/67/67    | 0/2/2/2 |
| 27  | CLA  | L     | 203 | -    | 1/1/12/20 | 5/21/97/115   | -       |
| 27  | CLA  | 3     | 604 | -    | 1/1/15/20 | 2/39/115/115  | -       |
| 27  | CLA  | 8     | 603 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 27  | CLA  | 5     | 603 | -    | 1/1/11/20 | 2/15/91/115   | -       |
| 29  | II0  | 6     | 614 | -    | -         | 1/21/67/67    | 0/2/2/2 |
| 27  | CLA  | 1     | 613 | -    | 1/1/11/20 | 0/15/91/115   | -       |
| 27  | CLA  | 5     | 612 | -    | 1/1/11/20 | 3/15/91/115   | -       |
| 27  | CLA  | 5     | 607 | 5    | 1/1/11/20 | 2/15/91/115   | -       |
| 27  | CLA  | B     | 823 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 27  | CLA  | K     | 101 | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 27  | CLA  | L     | 201 | 19   | 1/1/12/20 | 0/23/99/115   | -       |
| 31  | IHT  | 5     | 618 | -    | -         | 1/25/65/65    | 0/2/2/2 |
| 27  | CLA  | 4     | 609 | 4    | 1/1/14/20 | 3/33/109/115  | -       |
| 27  | CLA  | B     | 830 | -    | 1/1/14/20 | 1/33/109/115  | -       |
| 27  | CLA  | 1     | 612 | -    | 1/1/14/20 | 7/33/109/115  | -       |
| 27  | CLA  | 6     | 601 | 6    | 1/1/11/20 | 4/15/91/115   | -       |
| 27  | CLA  | Z     | 304 | 24   | 1/1/13/20 | 3/27/103/115  | -       |
| 27  | CLA  | 4     | 610 | -    | 1/1/15/20 | 5/39/115/115  | -       |
| 27  | CLA  | 7     | 304 | -    | 1/1/13/20 | 1/27/103/115  | -       |
| 35  | 8CT  | B     | 844 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 27  | CLA  | 6     | 607 | 6    | 1/1/13/20 | 2/27/103/115  | -       |
| 27  | CLA  | b     | 611 | -    | 1/1/13/20 | 4/27/103/115  | -       |
| 28  | KC2  | 7     | 311 | 7    | -         | 7/15/71/71    | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 27  | CLA  | 2     | 601 | 2    | 1/1/10/20 | 3/12/88/115   | -       |
| 29  | II0  | 5     | 614 | -    | -         | 2/21/67/67    | 0/2/2/2 |
| 27  | CLA  | A     | 844 | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 27  | CLA  | 8     | 607 | 8    | 1/1/10/20 | 4/10/86/115   | -       |
| 29  | II0  | b     | 614 | -    | -         | 0/21/67/67    | 0/2/2/2 |
| 27  | CLA  | a     | 604 | -    | 1/1/14/20 | 10/33/109/115 | -       |
| 27  | CLA  | Z     | 301 | -    | 1/1/14/20 | 12/33/109/115 | -       |
| 27  | CLA  | A     | 815 | -    | 1/1/14/20 | 2/36/112/115  | -       |
| 35  | 8CT  | B     | 846 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 27  | CLA  | 9     | 614 | -    | 1/1/10/20 | 2/10/86/115   | -       |
| 33  | LHG  | 2     | 620 | -    | -         | 15/46/46/53   | -       |
| 27  | CLA  | 1     | 607 | 1    | 1/1/11/20 | 0/15/91/115   | -       |
| 27  | CLA  | 1     | 601 | 1    | 1/1/11/20 | 3/15/91/115   | -       |
| 28  | KC2  | 2     | 610 | -    | -         | 8/15/71/71    | -       |
| 31  | IHT  | 8     | 609 | -    | -         | 1/25/65/65    | 0/2/2/2 |
| 27  | CLA  | A     | 834 | 10   | 1/1/13/20 | 5/27/103/115  | -       |
| 27  | CLA  | 6     | 606 | -    | 1/1/13/20 | 8/27/103/115  | -       |
| 27  | CLA  | A     | 809 | 27   | 1/1/14/20 | 5/33/109/115  | -       |
| 27  | CLA  | A     | 811 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 27  | CLA  | A     | 807 | 10   | 1/1/12/20 | 1/21/97/115   | -       |
| 27  | CLA  | 9     | 611 | -    | 1/1/10/20 | 2/10/86/115   | -       |
| 27  | CLA  | O     | 203 | -    | 1/1/13/20 | 5/27/103/115  | -       |
| 32  | LMG  | 3     | 620 | -    | -         | 12/27/47/70   | 0/1/1/1 |
| 27  | CLA  | A     | 821 | -    | 1/1/13/20 | 2/27/103/115  | -       |
| 27  | CLA  | 8     | 605 | 8    | 1/1/12/20 | 2/21/97/115   | -       |
| 29  | II0  | 3     | 614 | -    | -         | 0/21/67/67    | 0/2/2/2 |
| 31  | IHT  | a     | 616 | -    | -         | 6/25/65/65    | 0/2/2/2 |
| 27  | CLA  | A     | 804 | 10   | 1/1/15/20 | 15/39/115/115 | -       |
| 29  | II0  | 8     | 611 | -    | -         | 2/21/67/67    | 0/2/2/2 |
| 27  | CLA  | 7     | 310 | 33   | 1/1/10/20 | 2/10/86/115   | -       |
| 33  | LHG  | 2     | 618 | -    | -         | 8/24/24/53    | -       |
| 33  | LHG  | b     | 616 | -    | -         | 25/53/53/53   | -       |
| 27  | CLA  | F     | 202 | -    | 1/1/14/20 | 10/33/109/115 | -       |
| 27  | CLA  | 3     | 607 | 3    | 1/1/14/20 | 5/33/109/115  | -       |
| 27  | CLA  | 1     | 606 | -    | 1/1/11/20 | 0/15/91/115   | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 31  | IHT  | 9     | 619 | -    | -         | 3/25/65/65    | 0/2/2/2 |
| 27  | CLA  | 1     | 609 | -    | 1/1/10/20 | 2/10/86/115   | -       |
| 39  | DGD  | Z     | 303 | -    | -         | 26/49/89/95   | 0/2/2/2 |
| 28  | KC2  | 5     | 610 | 5    | -         | 4/15/71/71    | -       |
| 31  | IHT  | 1     | 618 | -    | -         | 2/25/65/65    | 0/2/2/2 |
| 27  | CLA  | A     | 832 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 27  | CLA  | A     | 831 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 27  | CLA  | 2     | 603 | -    | 1/1/12/20 | 3/21/97/115   | -       |

The worst 5 of 2238 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 31  | A     | 854 | IHT  | C10-C07 | 10.50  | 1.52        | 1.34     |
| 31  | 1     | 618 | IHT  | C10-C07 | 10.14  | 1.51        | 1.34     |
| 28  | 2     | 610 | KC2  | MG-ND   | -10.00 | 1.86        | 2.05     |
| 28  | 7     | 307 | KC2  | MG-ND   | -9.99  | 1.86        | 2.05     |
| 31  | Z     | 302 | IHT  | C10-C07 | 9.99   | 1.51        | 1.34     |

The worst 5 of 2530 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 31  | 8     | 609 | IHT  | C02-C07-C10 | -10.48 | 108.32      | 122.64   |
| 31  | 9     | 619 | IHT  | C02-C07-C10 | -10.45 | 108.35      | 122.64   |
| 31  | L     | 204 | IHT  | C02-C07-C10 | -9.51  | 109.64      | 122.64   |
| 31  | 5     | 618 | IHT  | C02-C07-C10 | -9.25  | 110.00      | 122.64   |
| 31  | 6     | 616 | IHT  | C02-C07-C10 | -8.34  | 111.24      | 122.64   |

5 of 222 chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 27  | 1     | 601 | CLA  | ND   |
| 27  | 1     | 602 | CLA  | ND   |
| 27  | 1     | 603 | CLA  | ND   |
| 27  | 1     | 604 | CLA  | ND   |
| 27  | 1     | 605 | CLA  | ND   |

5 of 2021 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | 1     | 603 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | 1     | 605 | CLA  | C2B-C3B-CAB-CBB |
| 27  | 1     | 605 | CLA  | C4B-C3B-CAB-CBB |
| 27  | 2     | 601 | CLA  | C3A-C2A-CAA-CBA |
| 27  | 2     | 602 | CLA  | C3A-C2A-CAA-CBA |

There are no ring outliers.

82 monomers are involved in 98 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 27  | B     | 802 | CLA  | 2       | 0            |
| 27  | A     | 823 | CLA  | 2       | 0            |
| 31  | 2     | 616 | IHT  | 1       | 0            |
| 35  | M     | 101 | 8CT  | 1       | 0            |
| 27  | 2     | 612 | CLA  | 1       | 0            |
| 27  | 1     | 604 | CLA  | 2       | 0            |
| 31  | A     | 854 | IHT  | 1       | 0            |
| 29  | 8     | 610 | II0  | 1       | 0            |
| 27  | 6     | 609 | CLA  | 1       | 0            |
| 27  | A     | 808 | CLA  | 1       | 0            |
| 27  | B     | 809 | CLA  | 1       | 0            |
| 27  | K     | 102 | CLA  | 1       | 0            |
| 27  | 1     | 611 | CLA  | 2       | 0            |
| 27  | 5     | 609 | CLA  | 2       | 0            |
| 35  | 7     | 318 | 8CT  | 1       | 0            |
| 27  | B     | 839 | CLA  | 1       | 0            |
| 27  | A     | 836 | CLA  | 2       | 0            |
| 29  | 5     | 620 | II0  | 1       | 0            |
| 27  | A     | 826 | CLA  | 2       | 0            |
| 27  | 9     | 606 | CLA  | 1       | 0            |
| 36  | J     | 104 | LMU  | 1       | 0            |
| 27  | A     | 819 | CLA  | 1       | 0            |
| 27  | 4     | 611 | CLA  | 1       | 0            |
| 27  | 9     | 609 | CLA  | 1       | 0            |
| 33  | 6     | 617 | LHG  | 1       | 0            |
| 27  | O     | 201 | CLA  | 1       | 0            |
| 29  | 2     | 614 | II0  | 1       | 0            |
| 27  | 7     | 308 | CLA  | 1       | 0            |
| 27  | B     | 840 | CLA  | 2       | 0            |
| 27  | 5     | 611 | CLA  | 1       | 0            |
| 37  | C     | 102 | SF4  | 1       | 0            |
| 27  | B     | 825 | CLA  | 1       | 0            |
| 27  | A     | 818 | CLA  | 3       | 0            |

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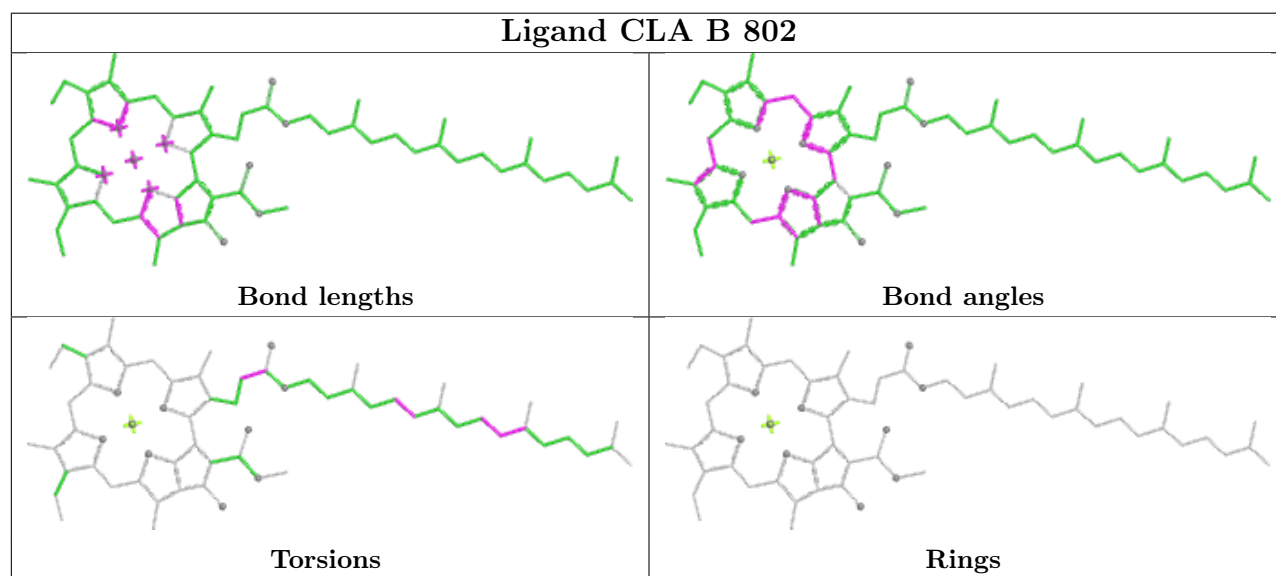
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 27  | 5     | 608 | CLA  | 2       | 0            |
| 27  | B     | 834 | CLA  | 2       | 0            |
| 30  | b     | 613 | II3  | 1       | 0            |
| 27  | B     | 826 | CLA  | 1       | 0            |
| 29  | 4     | 613 | II0  | 1       | 0            |
| 27  | A     | 810 | CLA  | 3       | 0            |
| 27  | B     | 815 | CLA  | 1       | 0            |
| 36  | 4     | 618 | LMU  | 2       | 0            |
| 27  | b     | 610 | CLA  | 1       | 0            |
| 27  | a     | 611 | CLA  | 3       | 0            |
| 27  | A     | 842 | CLA  | 1       | 0            |
| 27  | 8     | 608 | CLA  | 1       | 0            |
| 27  | B     | 835 | CLA  | 1       | 0            |
| 28  | 9     | 610 | KC2  | 1       | 0            |
| 27  | B     | 832 | CLA  | 1       | 0            |
| 27  | a     | 603 | CLA  | 2       | 0            |
| 27  | R     | 202 | CLA  | 1       | 0            |
| 27  | 5     | 604 | CLA  | 1       | 0            |
| 27  | B     | 818 | CLA  | 2       | 0            |
| 29  | a     | 614 | II0  | 1       | 0            |
| 27  | B     | 816 | CLA  | 2       | 0            |
| 36  | 7     | 321 | LMU  | 1       | 0            |
| 27  | B     | 807 | CLA  | 1       | 0            |
| 33  | 2     | 619 | LHG  | 1       | 0            |
| 27  | 9     | 604 | CLA  | 2       | 0            |
| 27  | B     | 801 | CLA  | 2       | 0            |
| 28  | b     | 609 | KC2  | 1       | 0            |
| 27  | 7     | 313 | CLA  | 2       | 0            |
| 31  | 6     | 616 | IHT  | 1       | 0            |
| 35  | 4     | 616 | 8CT  | 1       | 0            |
| 27  | 6     | 612 | CLA  | 1       | 0            |
| 27  | B     | 831 | CLA  | 1       | 0            |
| 27  | L     | 203 | CLA  | 1       | 0            |
| 27  | 8     | 603 | CLA  | 1       | 0            |
| 27  | 5     | 612 | CLA  | 1       | 0            |
| 27  | B     | 823 | CLA  | 1       | 0            |
| 27  | L     | 201 | CLA  | 1       | 0            |
| 27  | Z     | 304 | CLA  | 1       | 0            |
| 28  | 7     | 311 | KC2  | 2       | 0            |
| 27  | A     | 844 | CLA  | 3       | 0            |
| 27  | A     | 834 | CLA  | 1       | 0            |
| 27  | 9     | 611 | CLA  | 2       | 0            |

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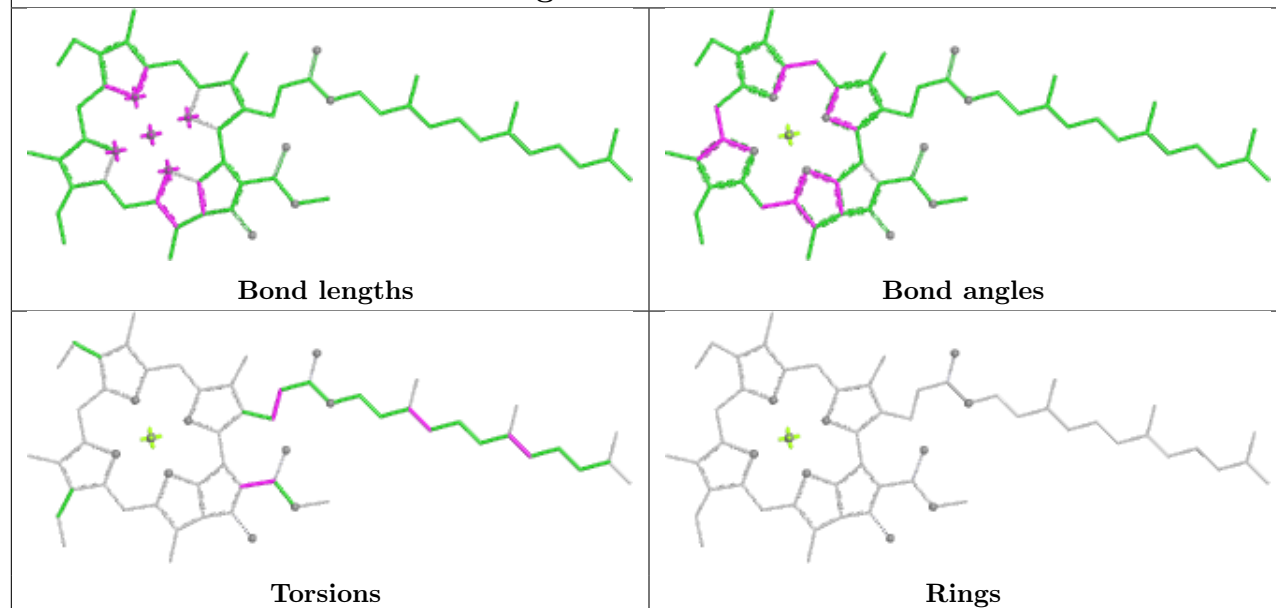
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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 27  | 8     | 605 | CLA  | 2       | 0            |
| 29  | 3     | 614 | II0  | 1       | 0            |
| 31  | a     | 616 | IHT  | 1       | 0            |
| 27  | 7     | 310 | CLA  | 1       | 0            |
| 31  | 9     | 619 | IHT  | 1       | 0            |
| 27  | 1     | 609 | CLA  | 1       | 0            |
| 39  | Z     | 303 | DGD  | 1       | 0            |

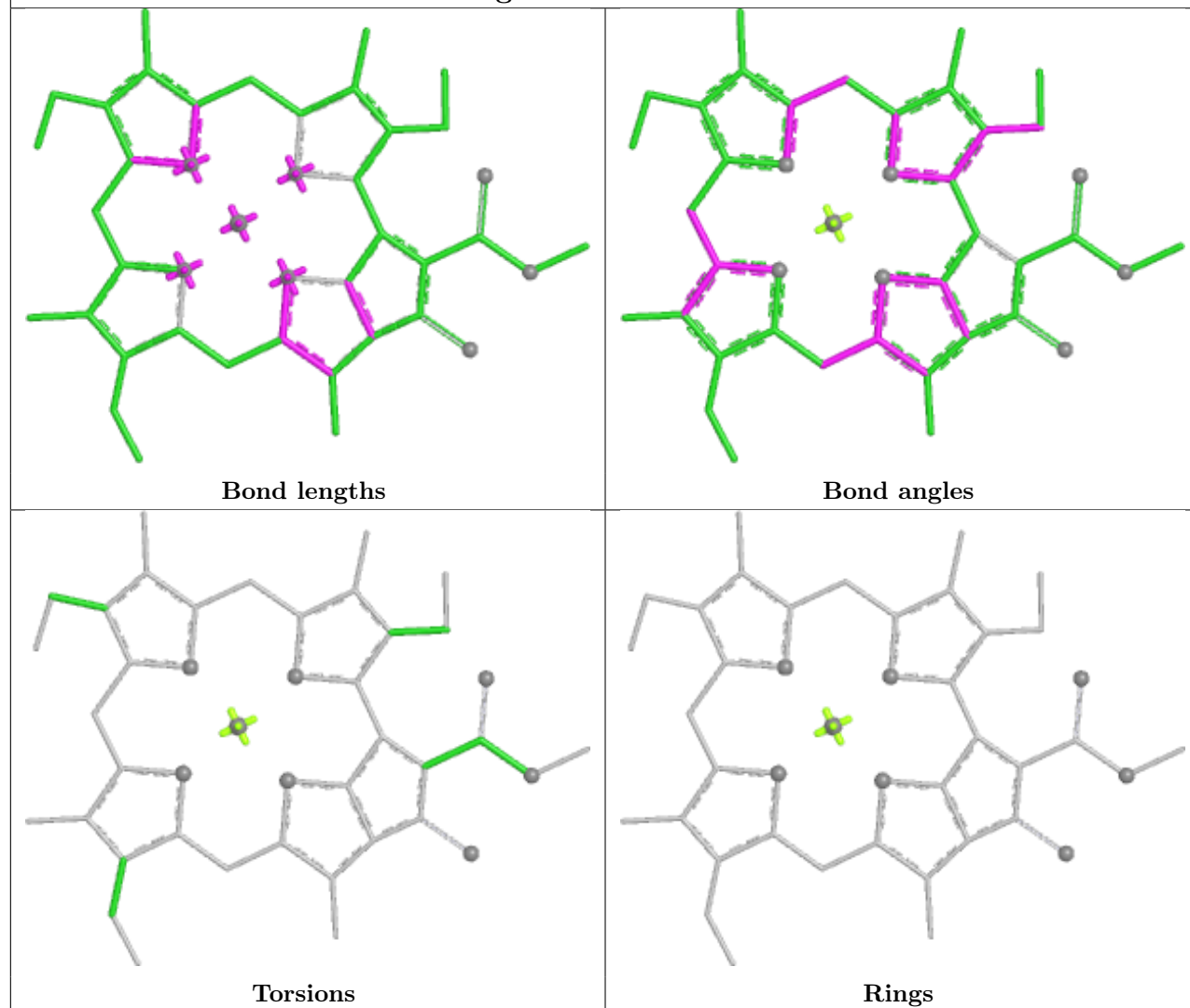
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



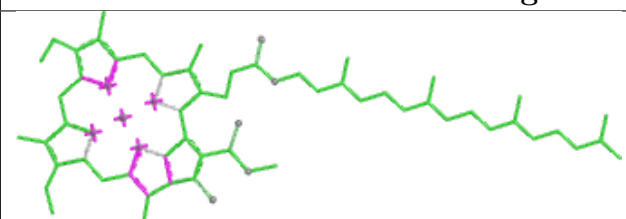
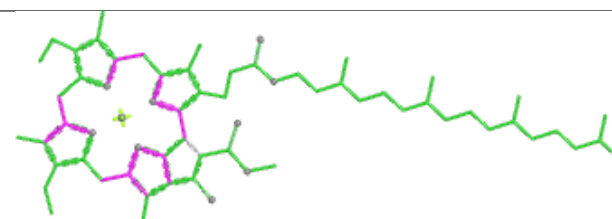
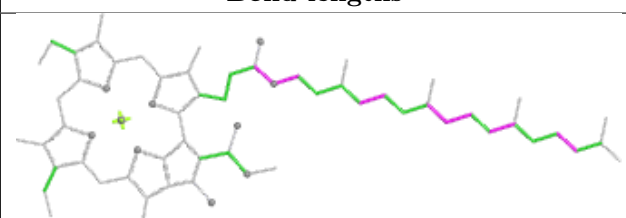
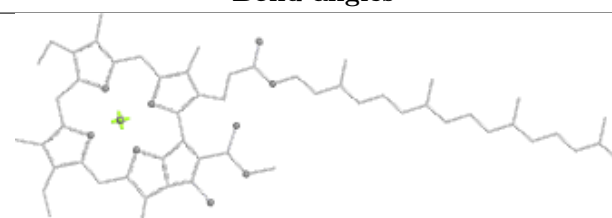
## Ligand CLA 6 604

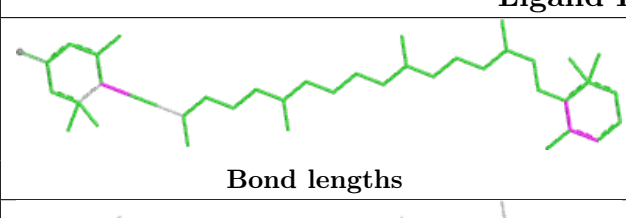
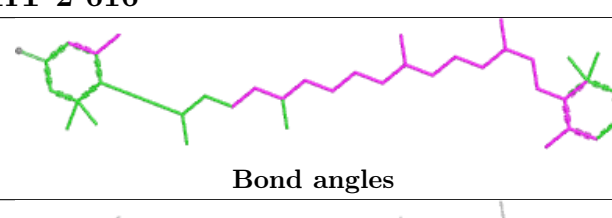
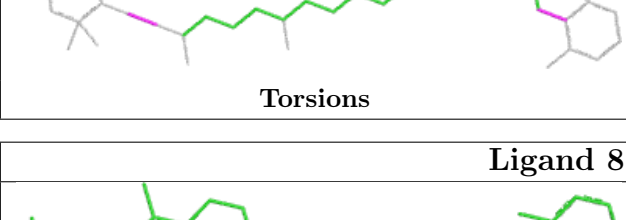


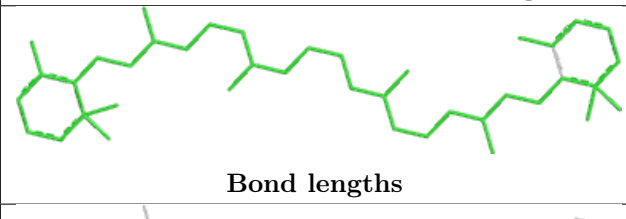
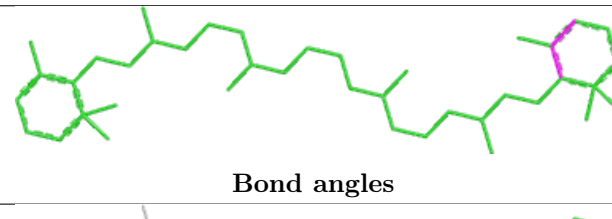
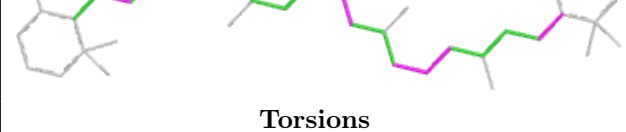
## Ligand CLA A 813



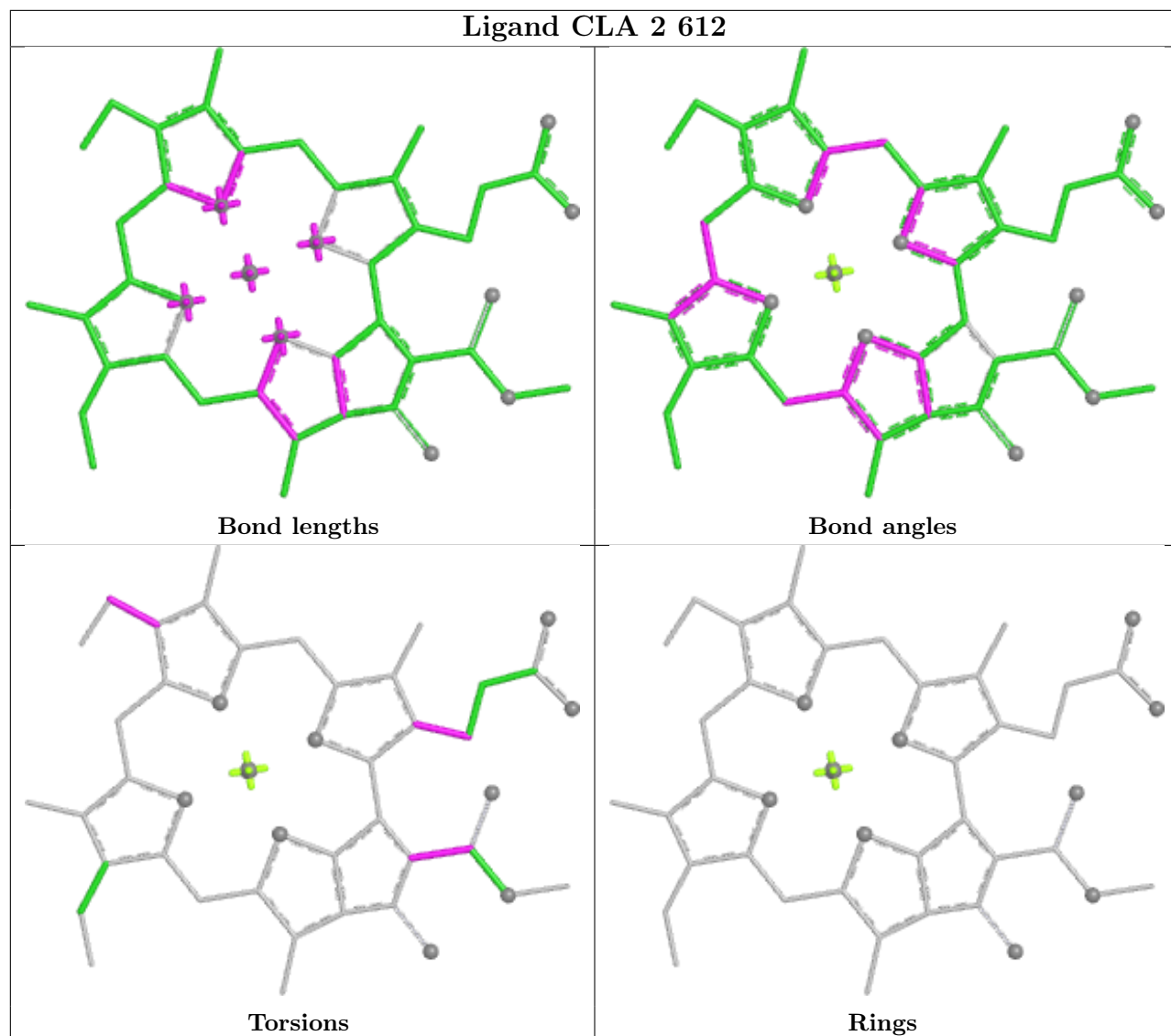


| Ligand CLA A 823                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

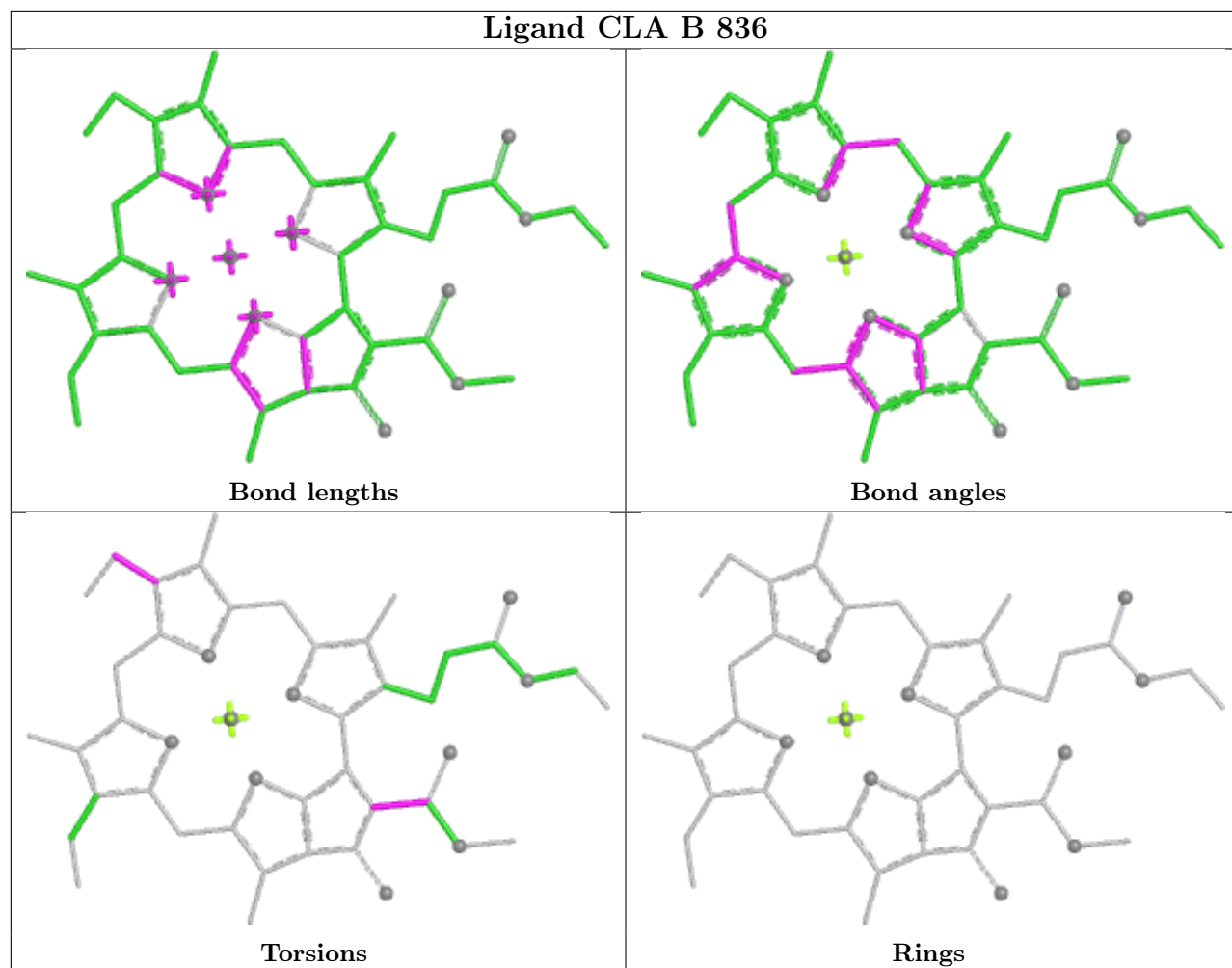
| Ligand IHT 2 616                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|    |    |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

| Ligand 8CT M 101                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

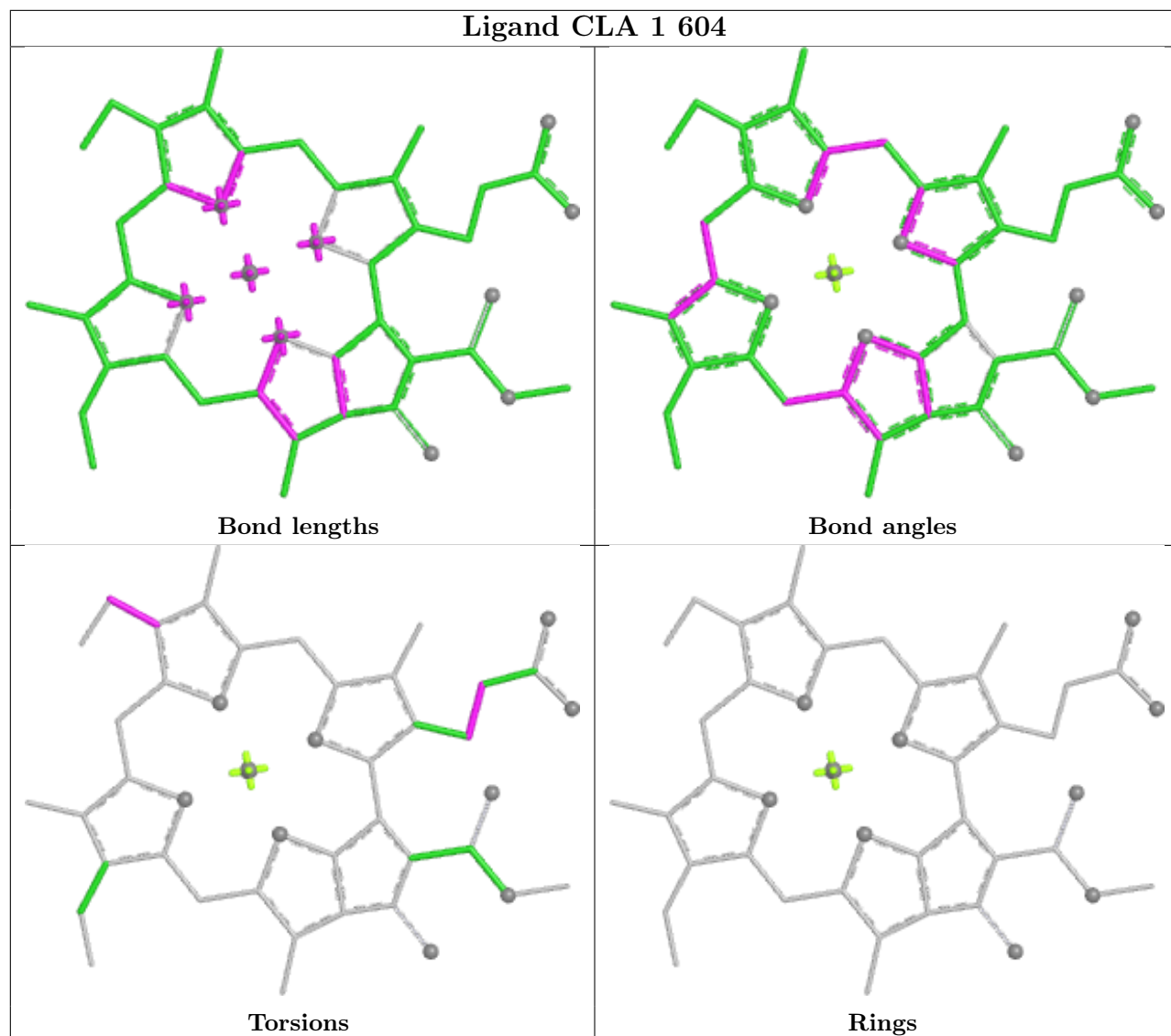
## Ligand CLA 2 612



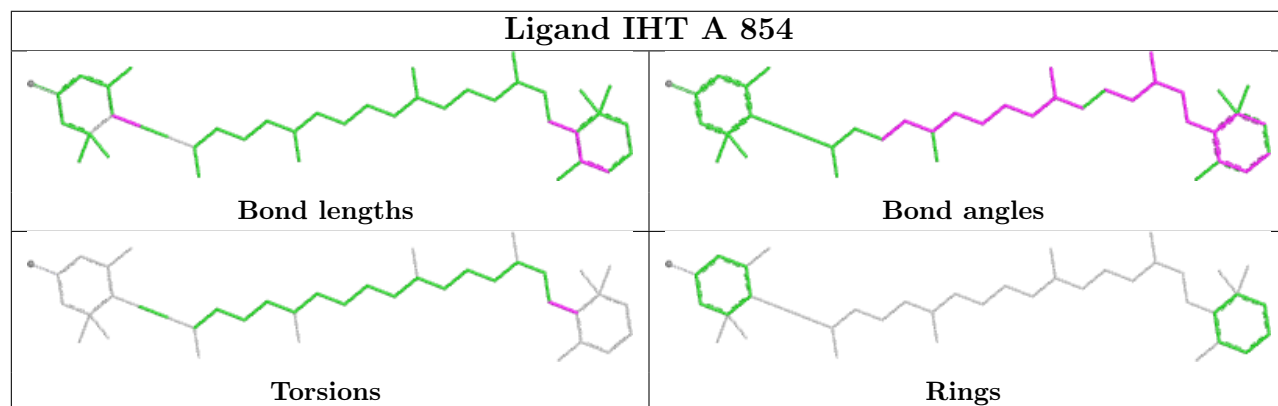
## Ligand CLA B 836

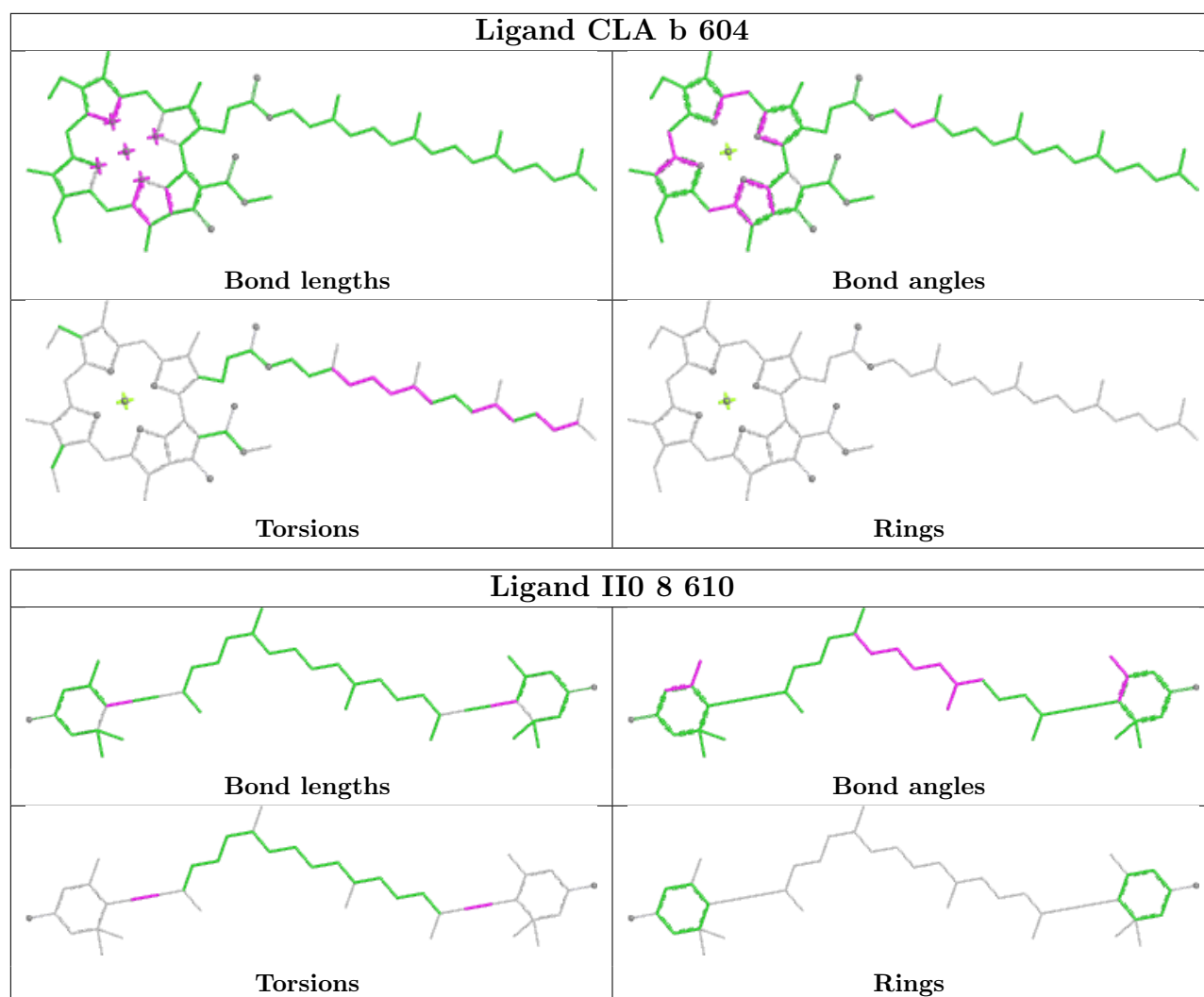


## Ligand CLA 1 604

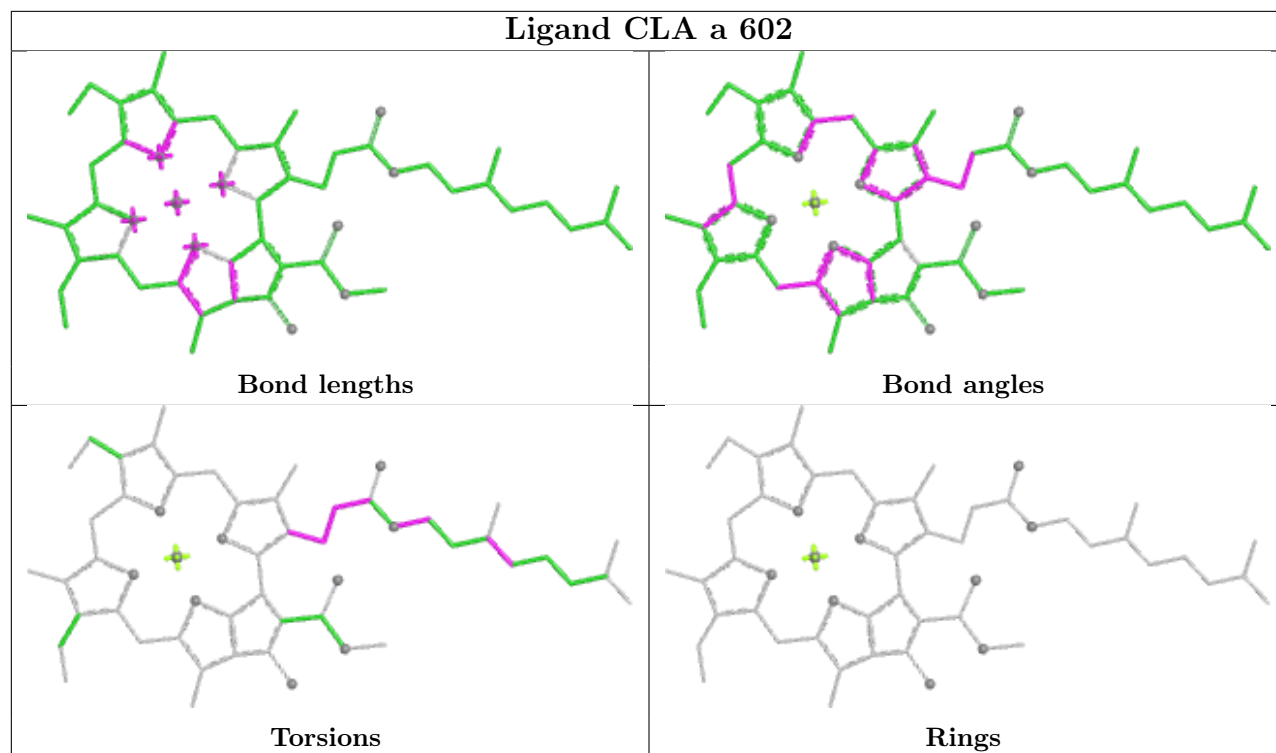


## Ligand IHT A 854

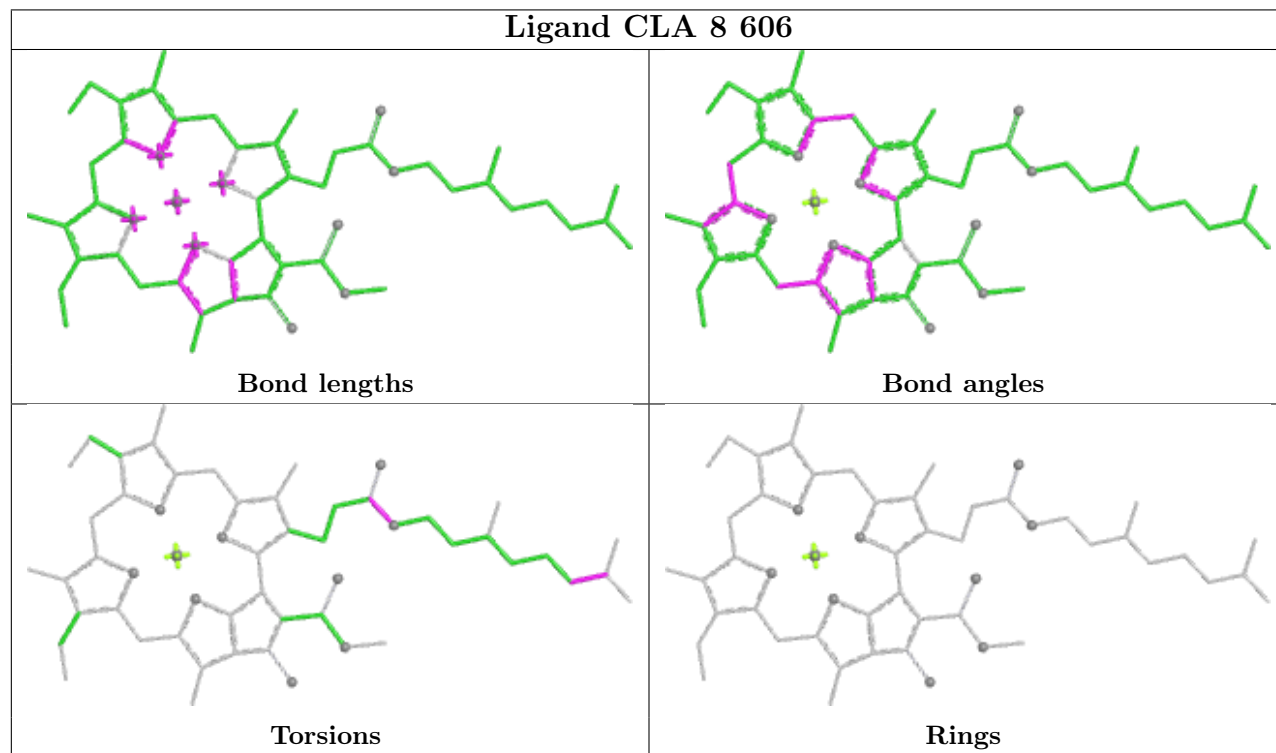




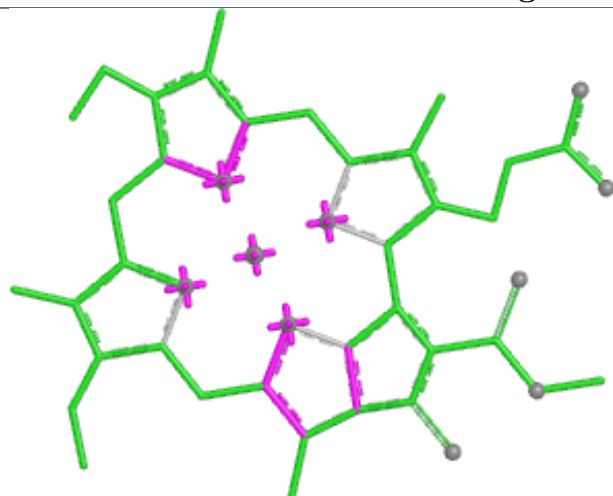
## Ligand CLA a 602



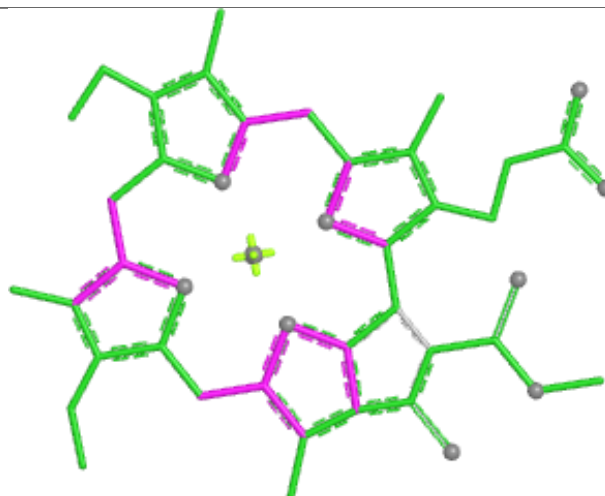
## Ligand CLA 8 606



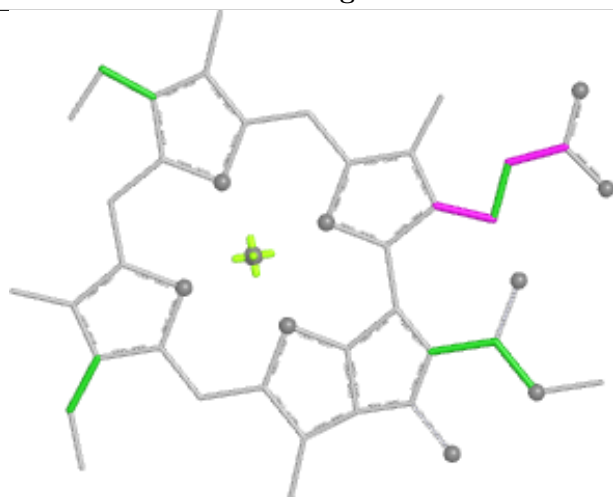
## Ligand CLA a 601



Bond lengths



Bond angles

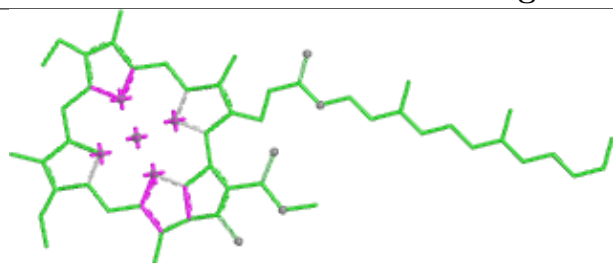


Torsions

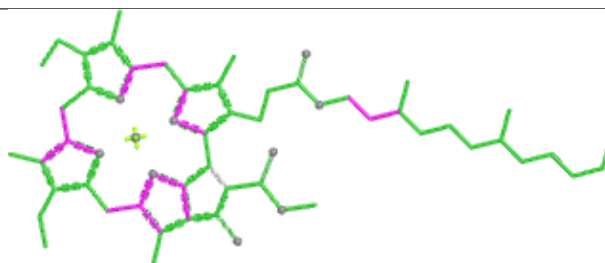


Rings

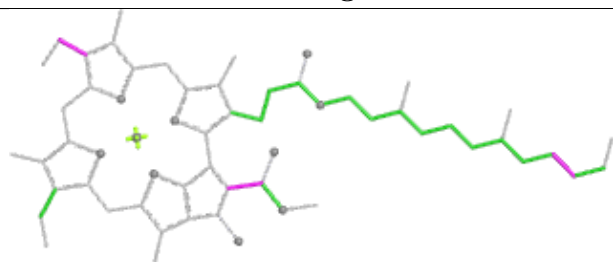
## Ligand CLA 4 602



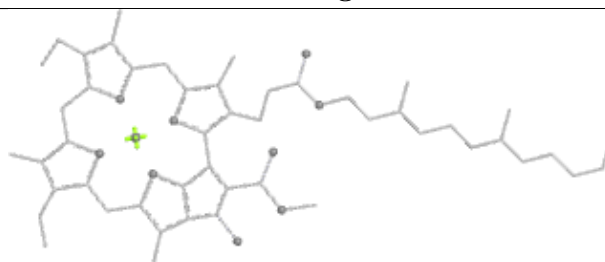
Bond lengths



Bond angles

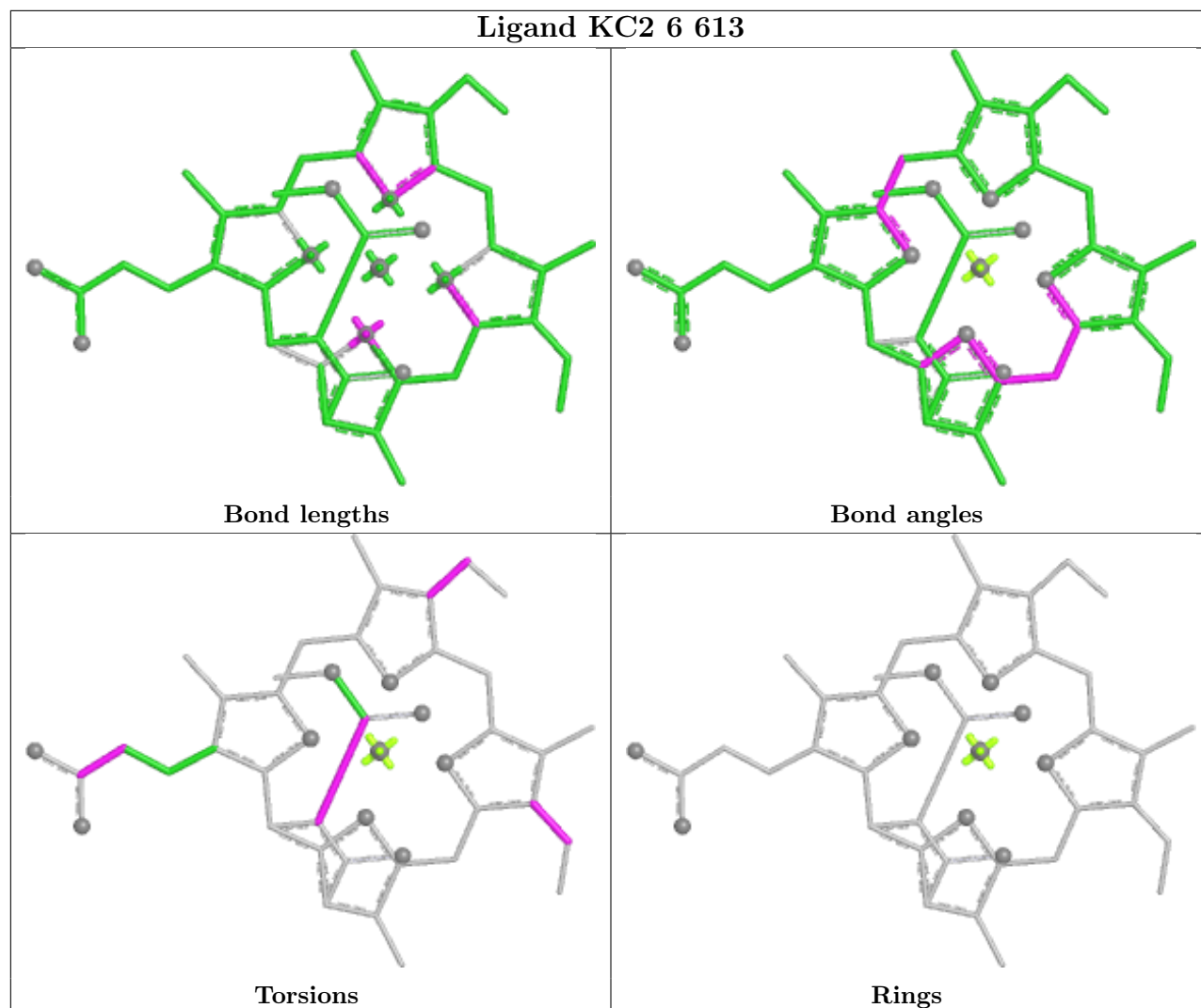


Torsions

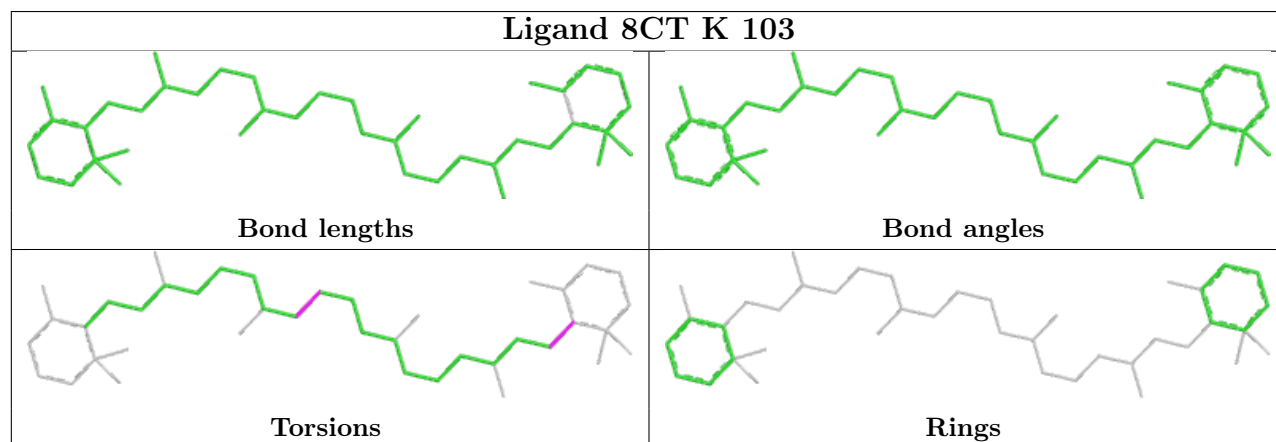


Rings

## Ligand KC2 6 613

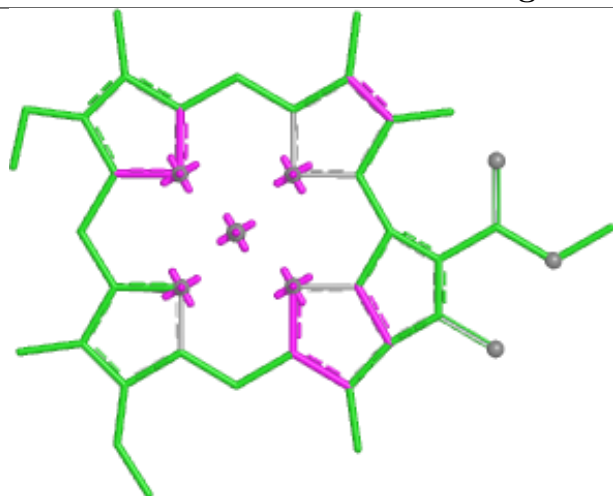


## Ligand 8CT K 103

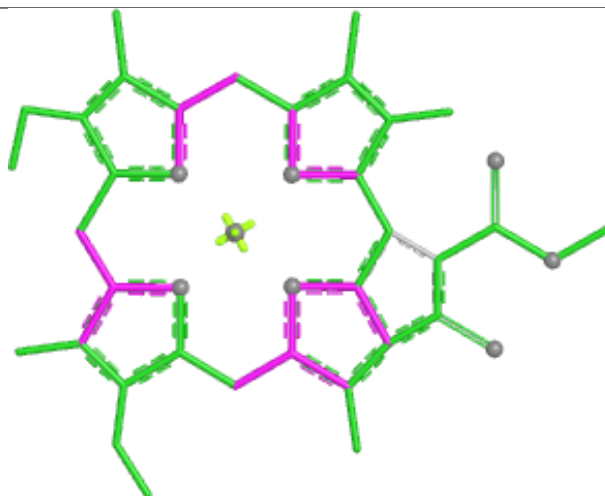




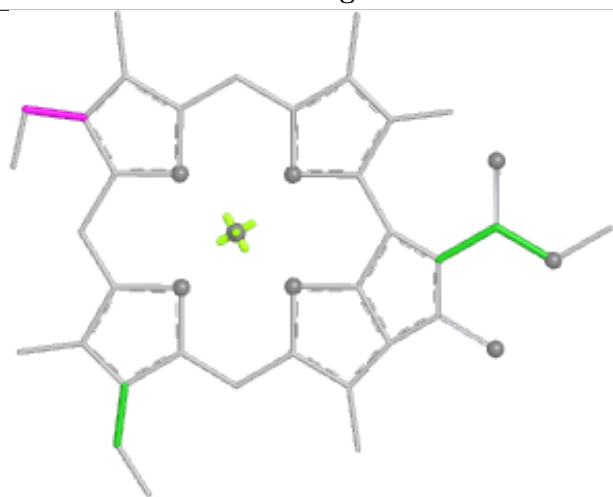
## Ligand CLA 6 609



Bond lengths



Bond angles

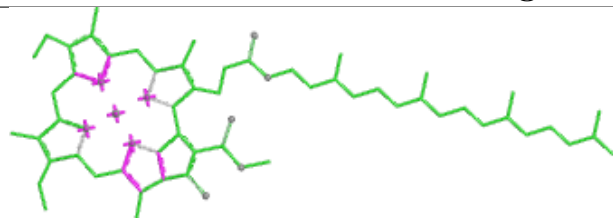


Torsions

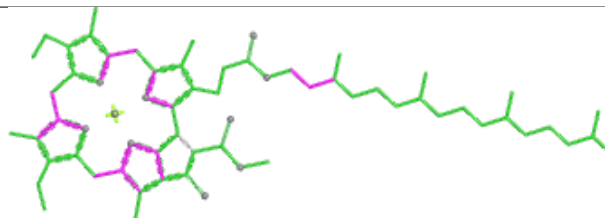


Rings

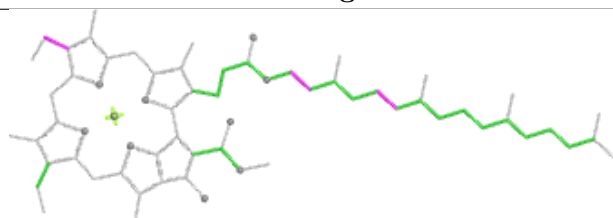
## Ligand CLA 4 608



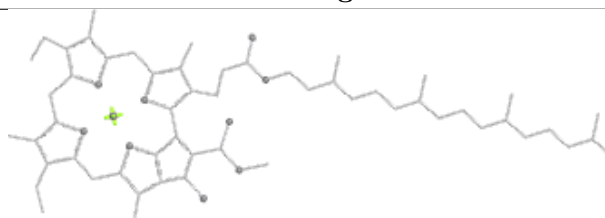
Bond lengths



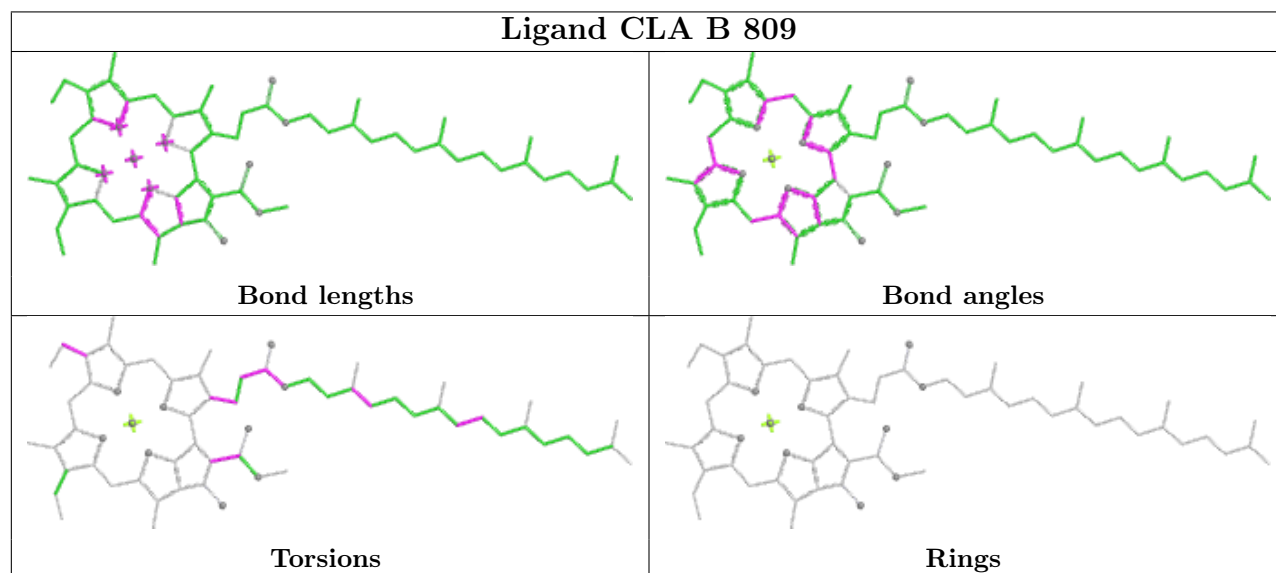
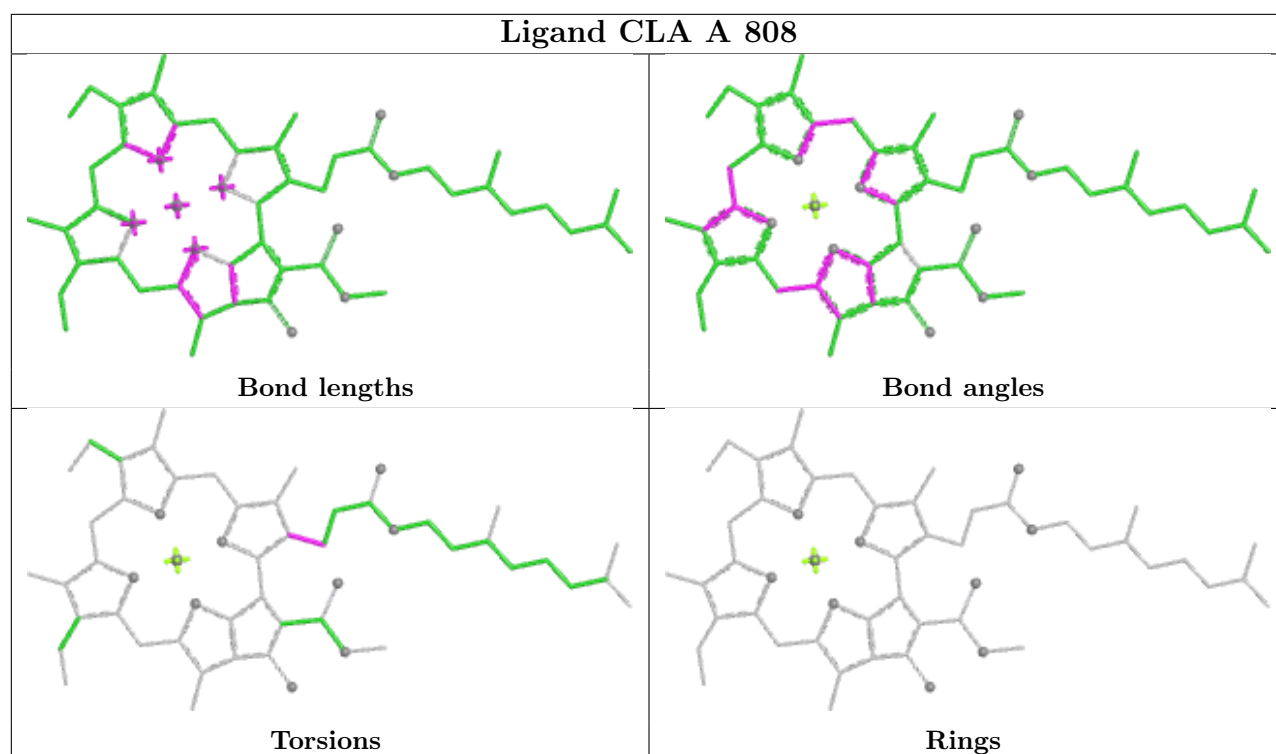
Bond angles

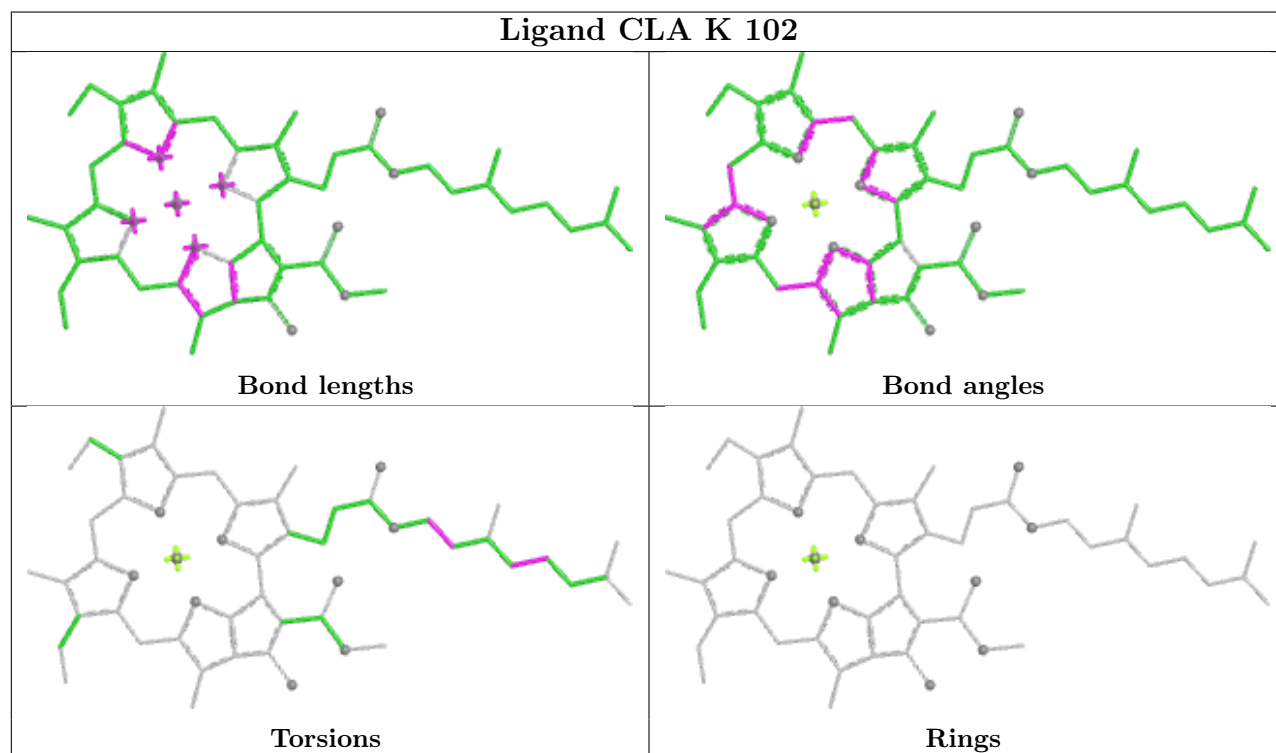
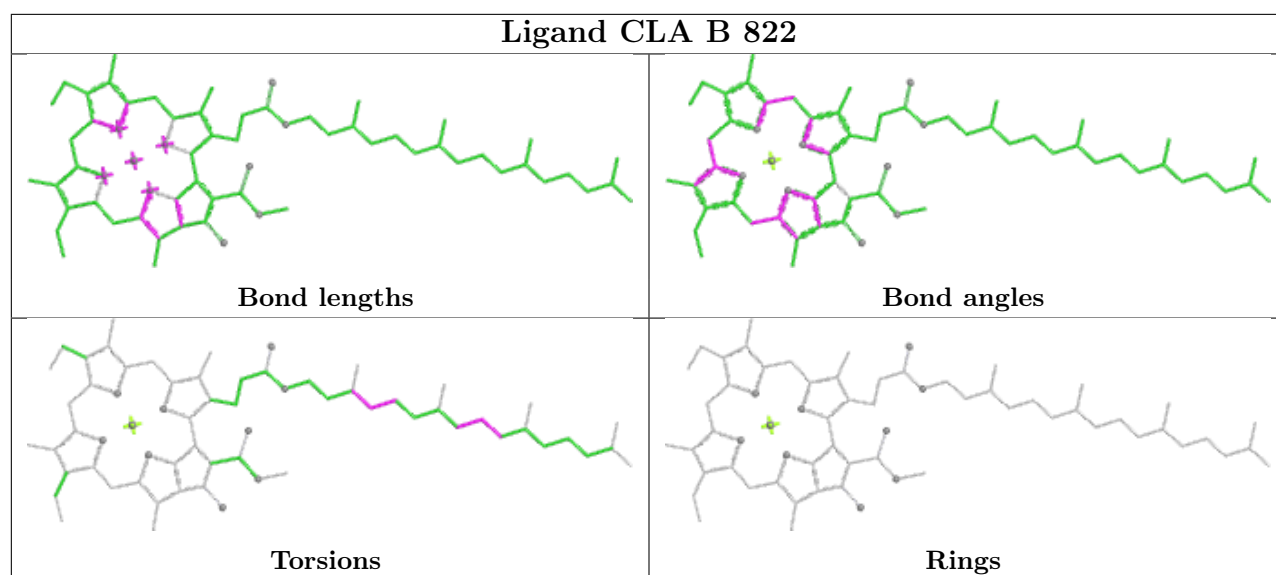


Torsions

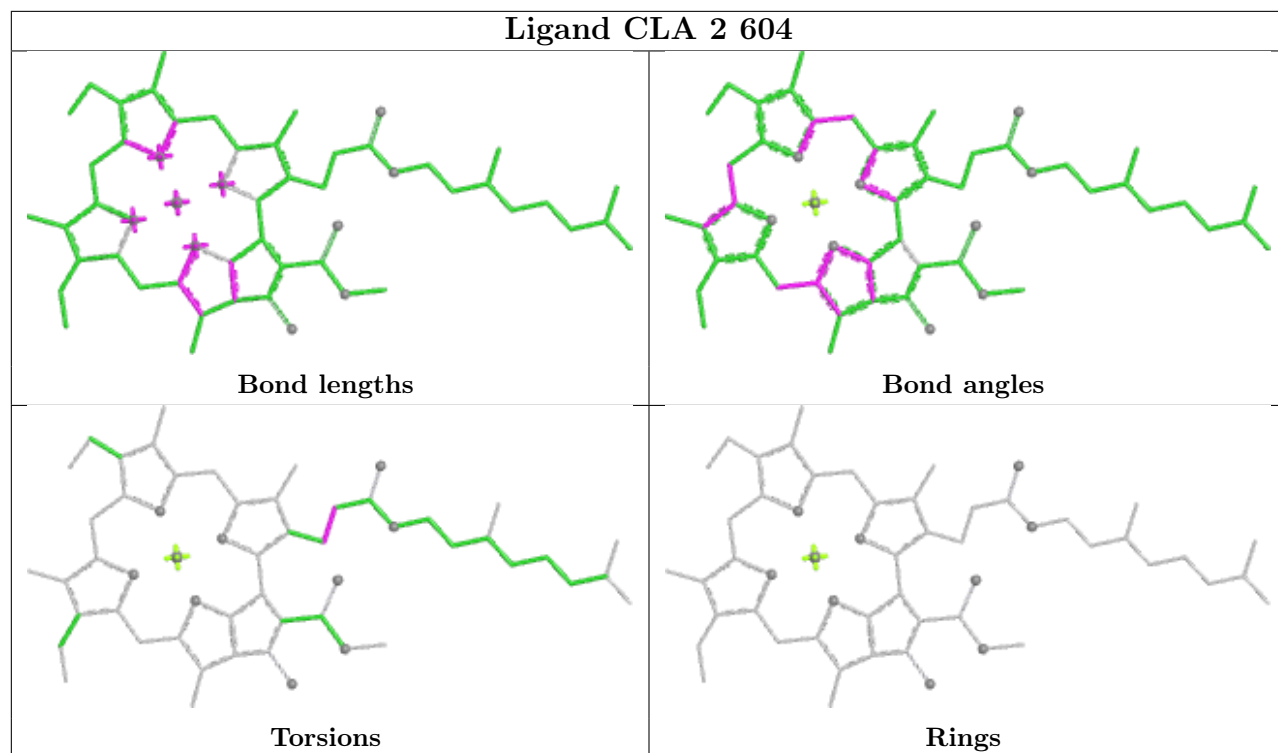


Rings

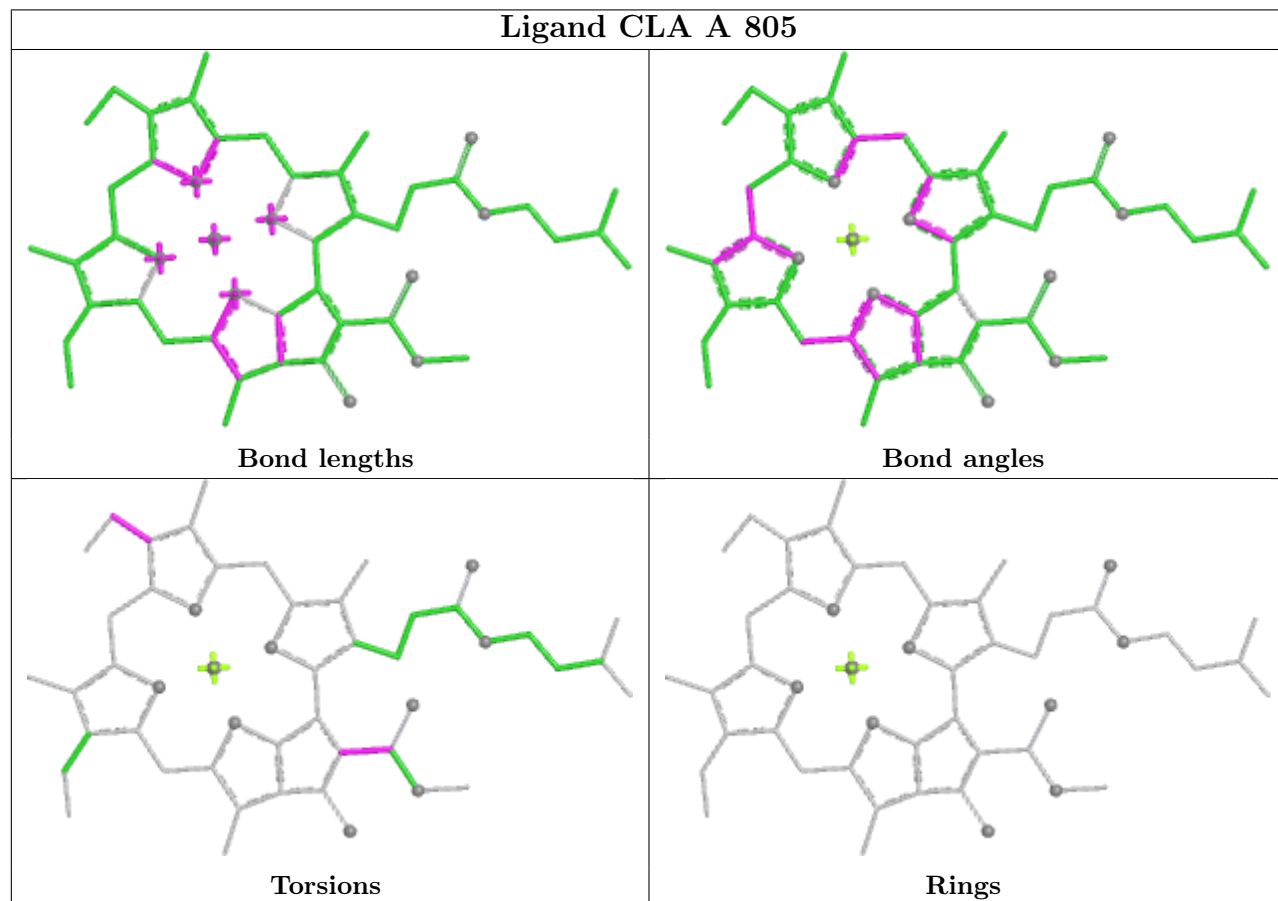


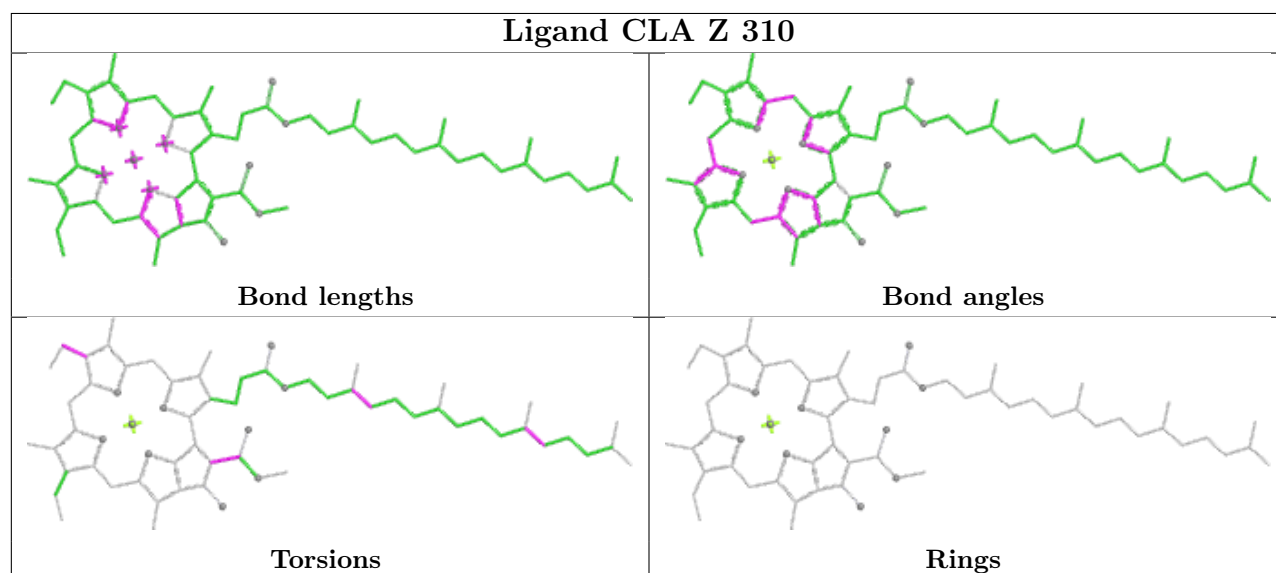
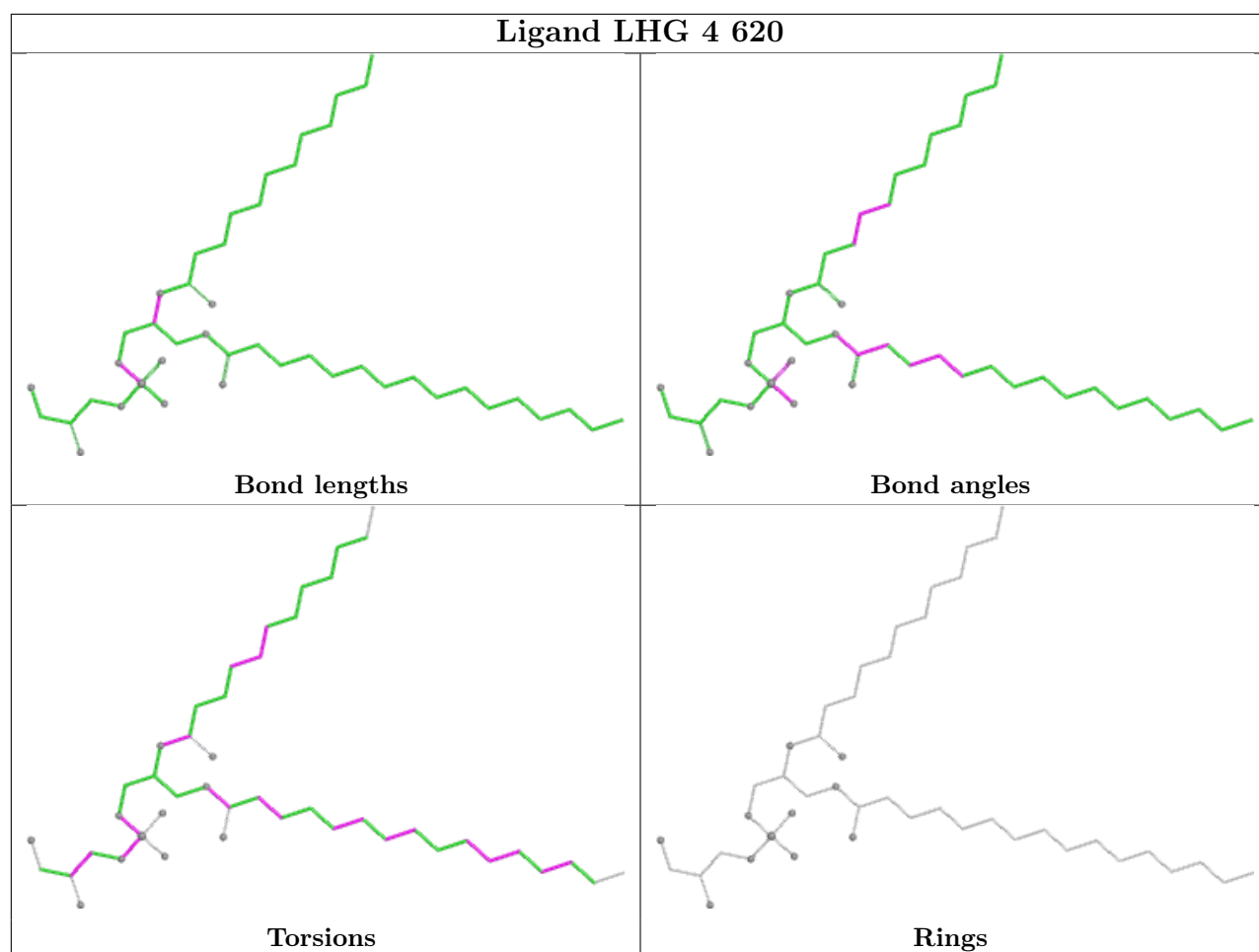


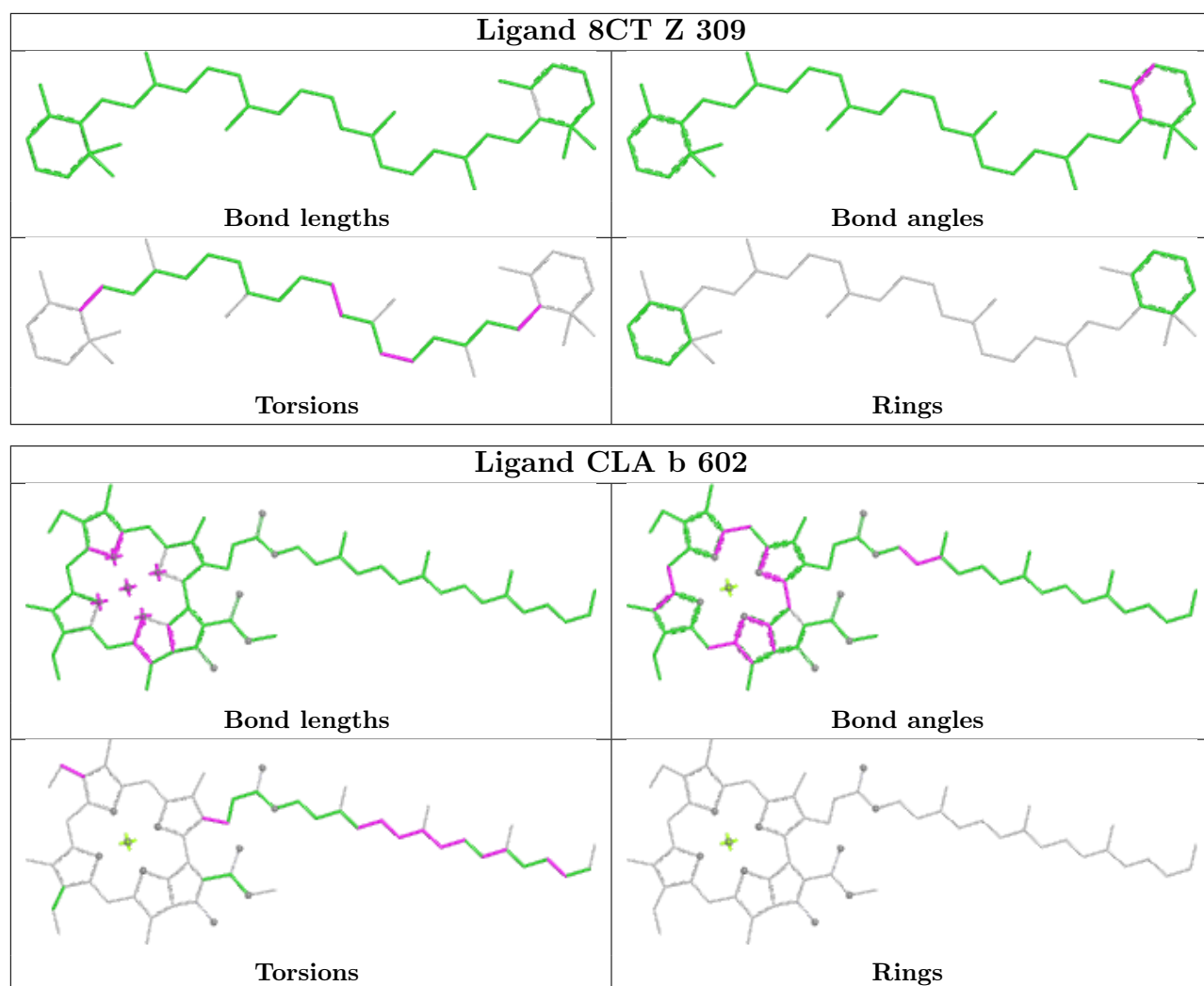
## Ligand CLA 2 604



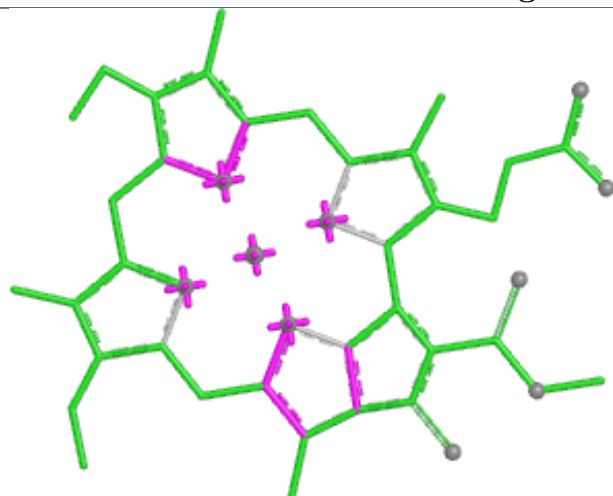
## Ligand CLA A 805



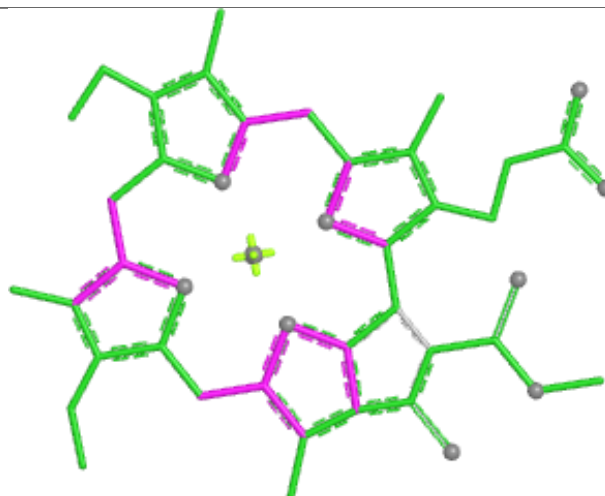




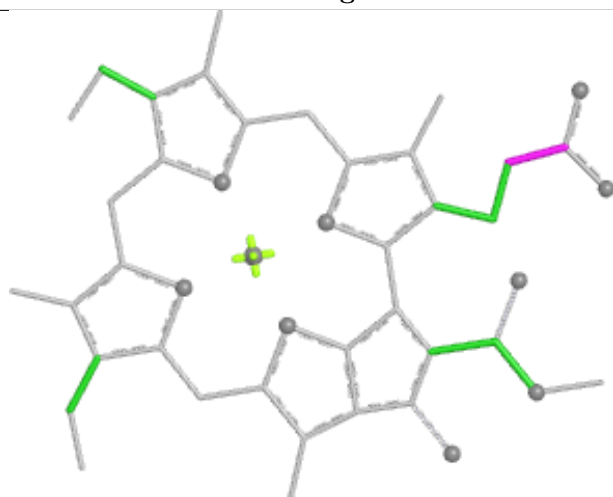
## Ligand CLA 1 611



Bond lengths



Bond angles

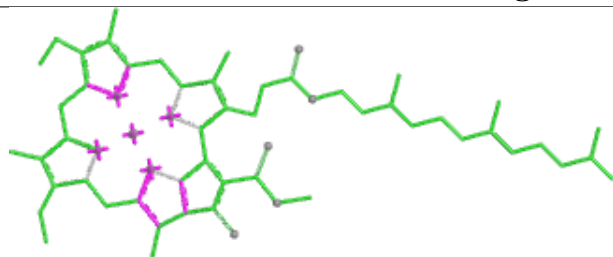


Torsions

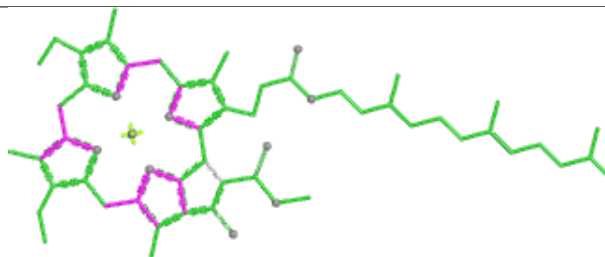


Rings

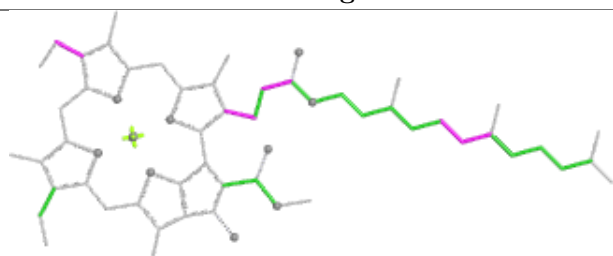
## Ligand CLA A 816



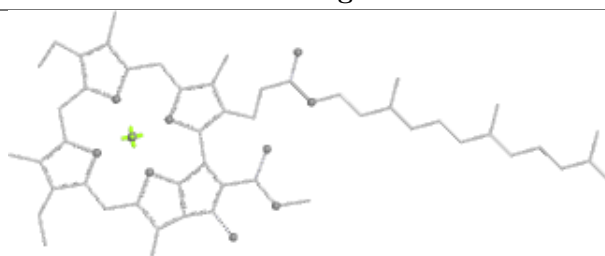
Bond lengths



Bond angles

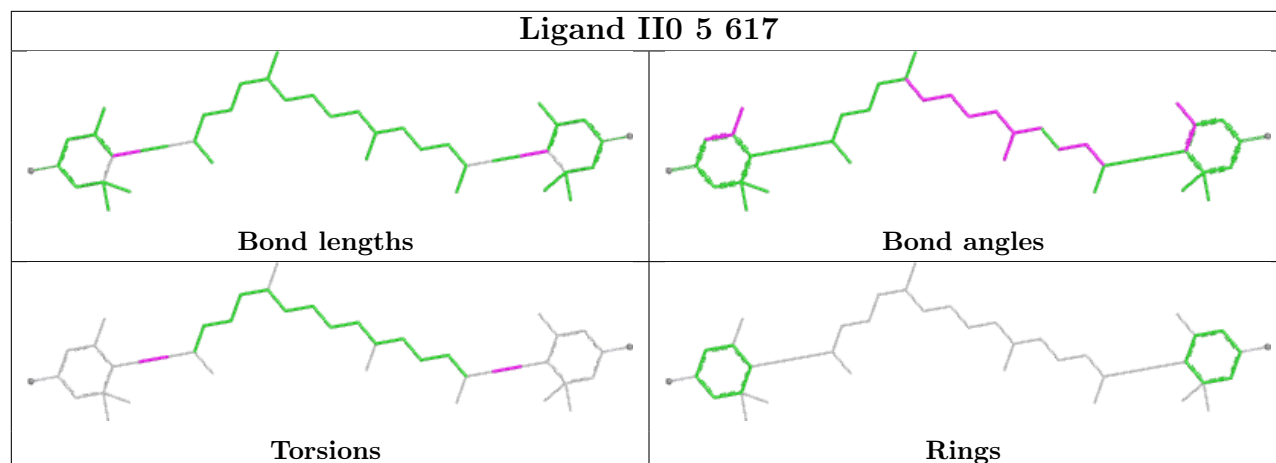


Torsions

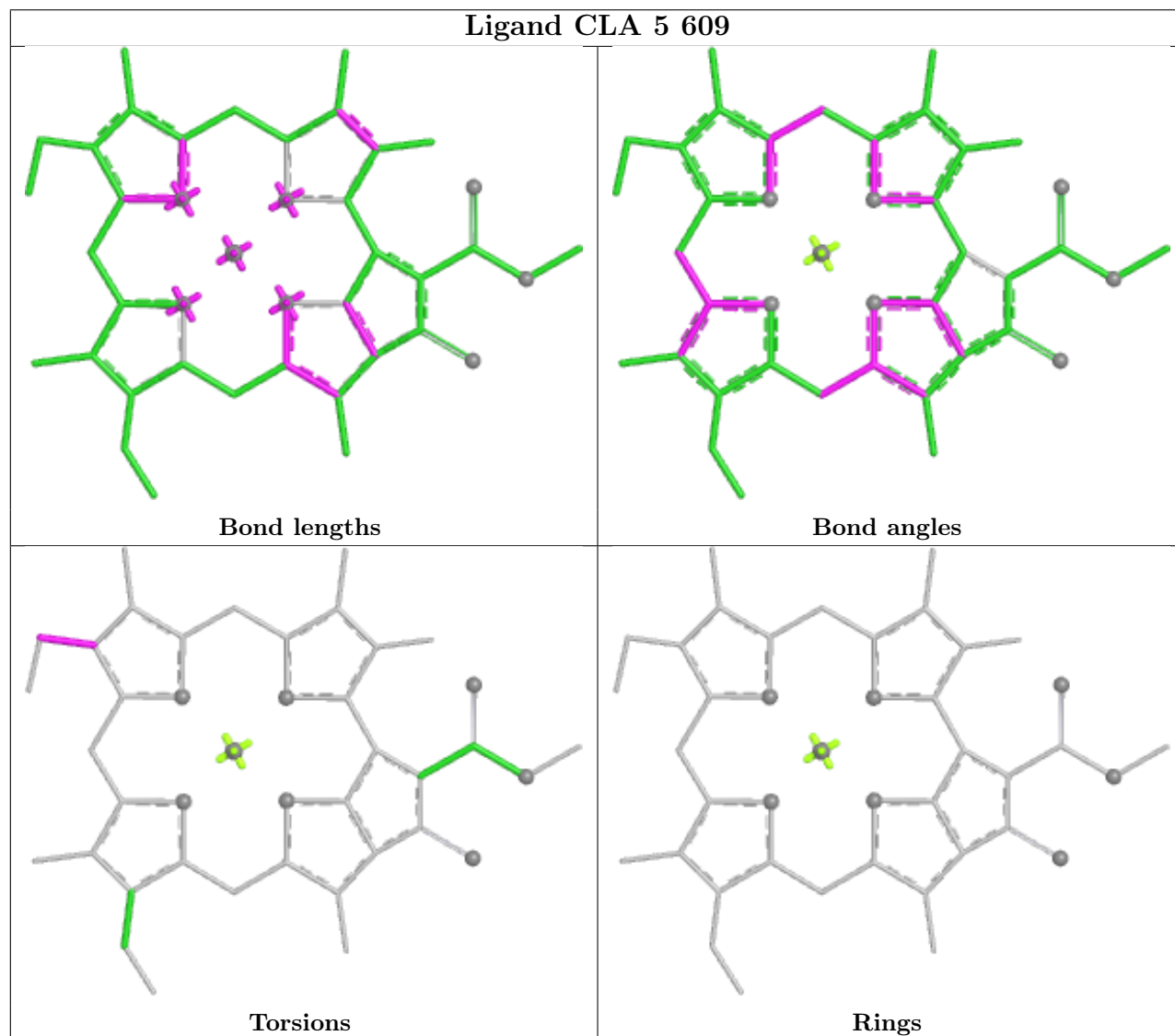


Rings

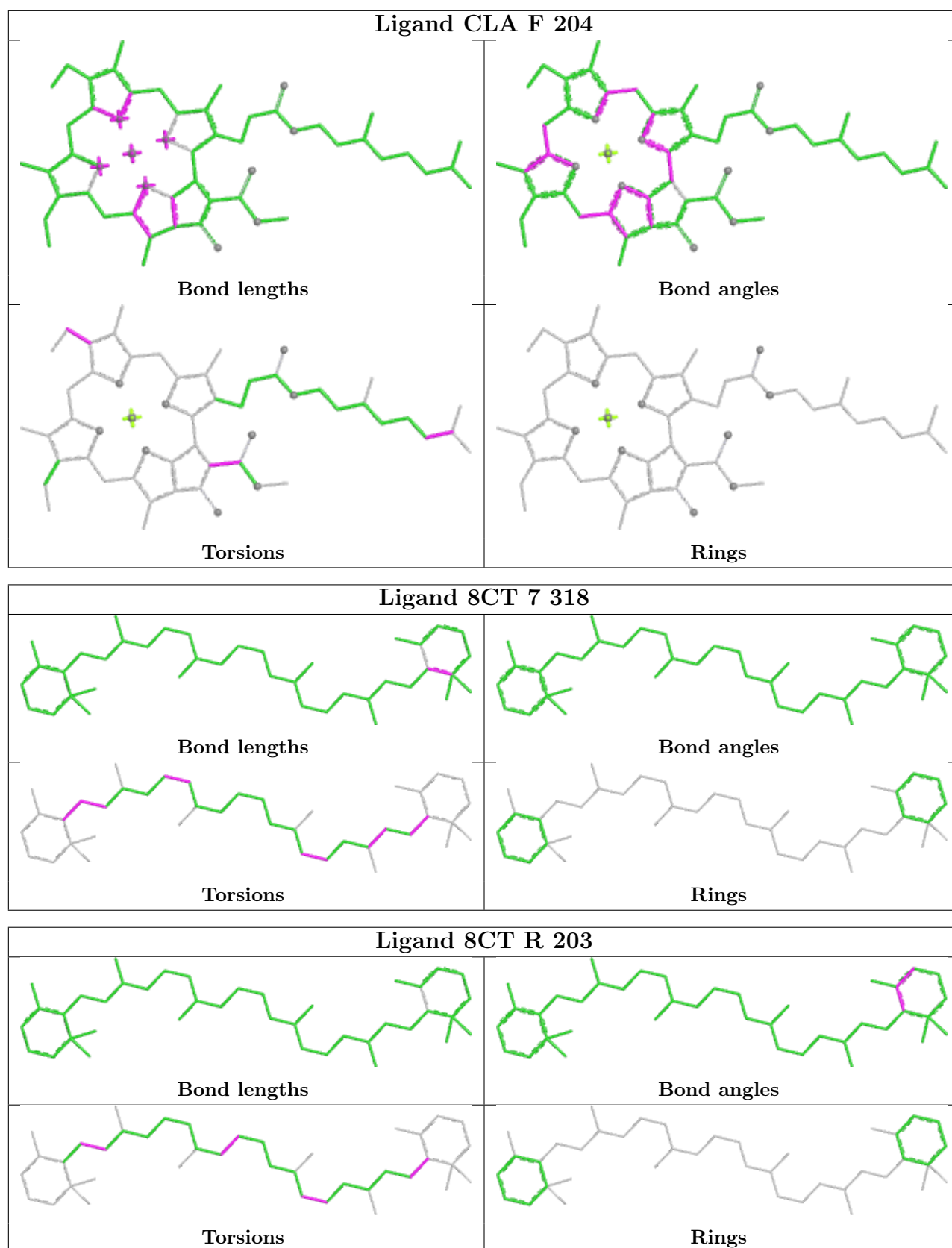
## Ligand II0 5 617

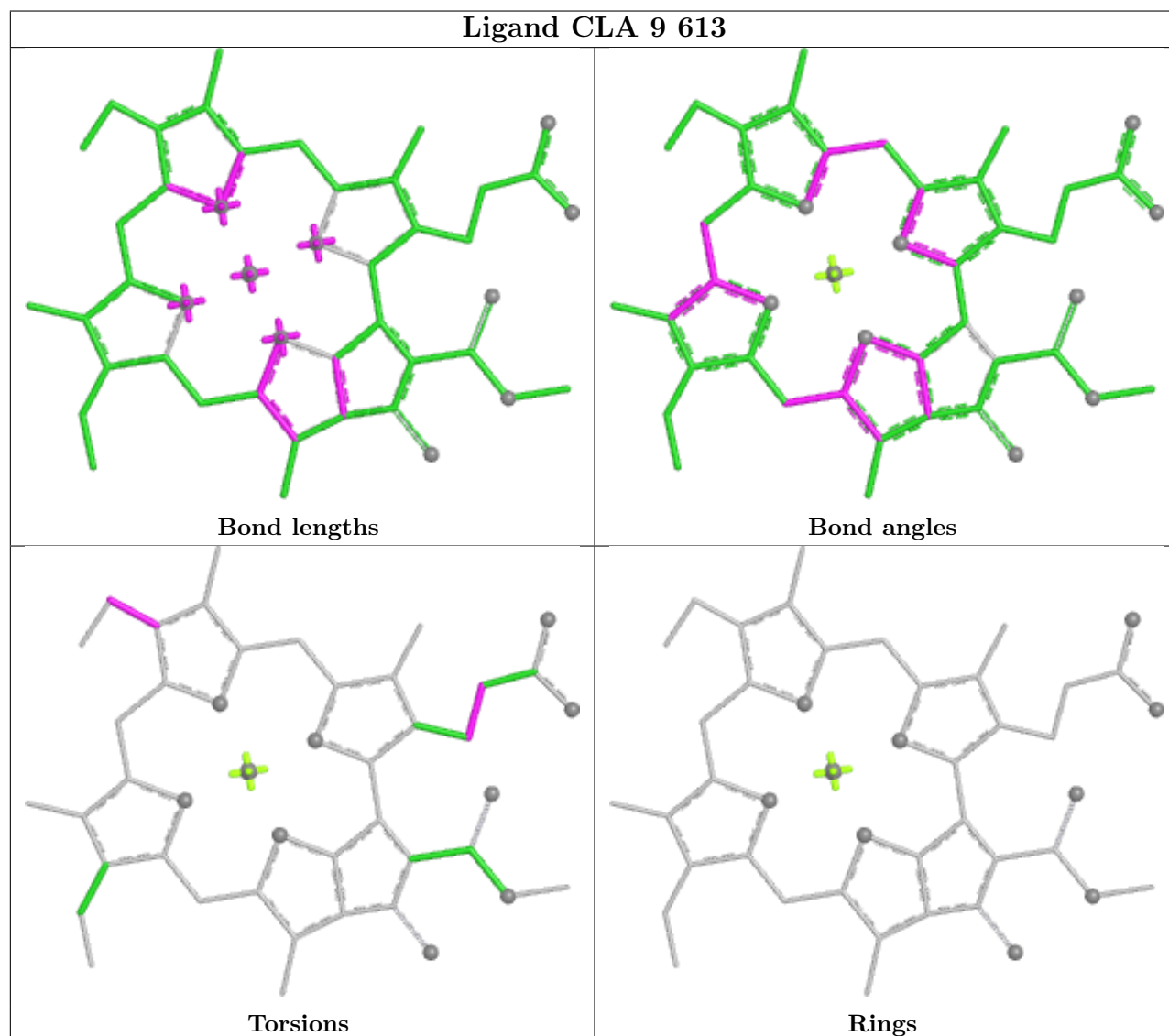
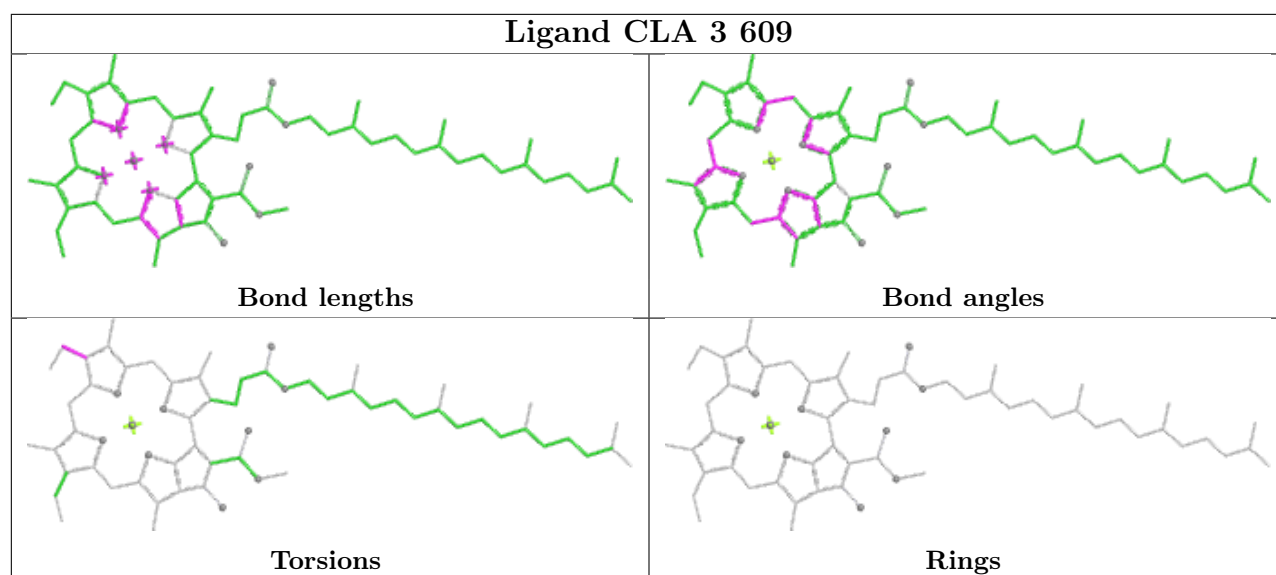


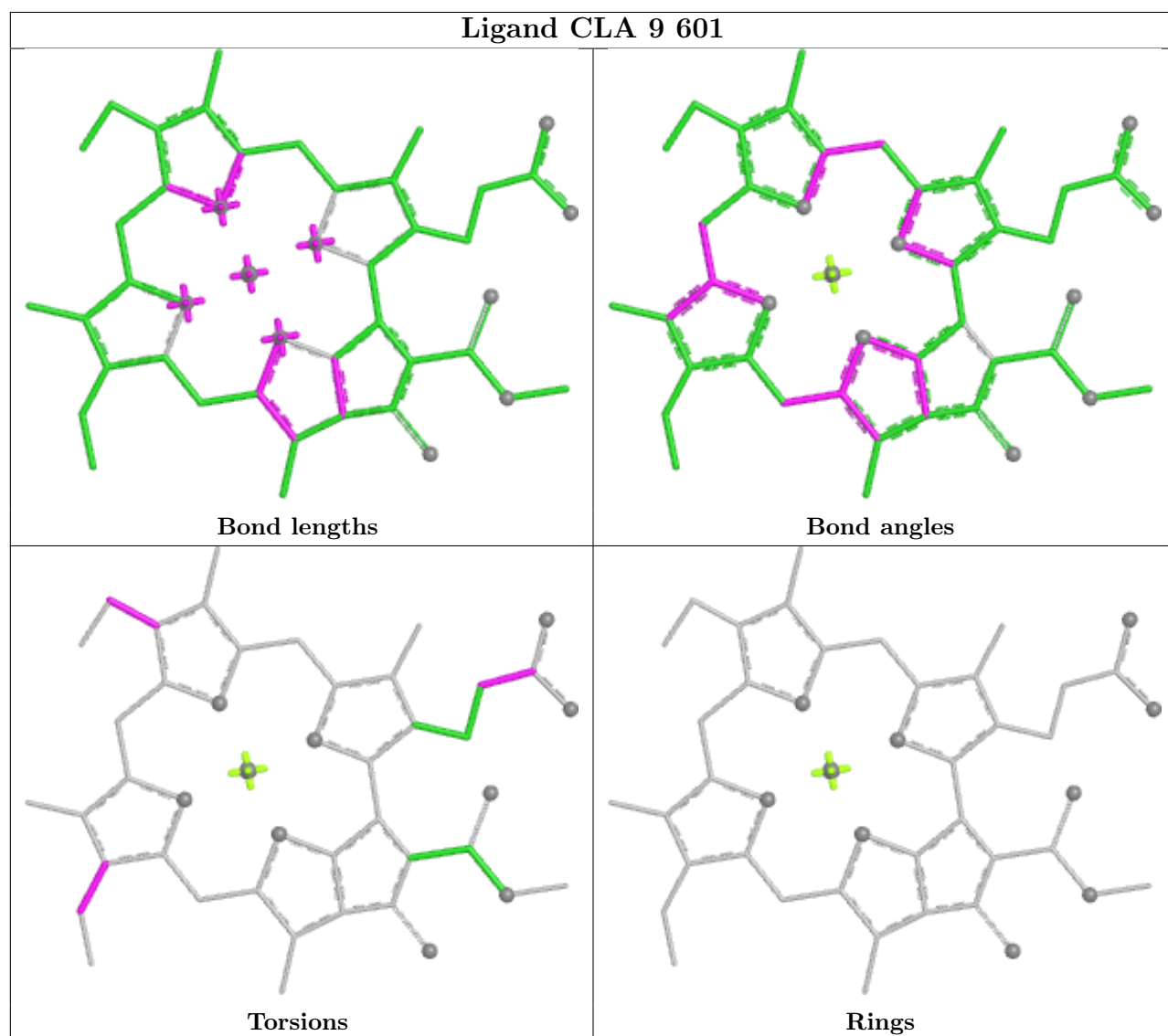
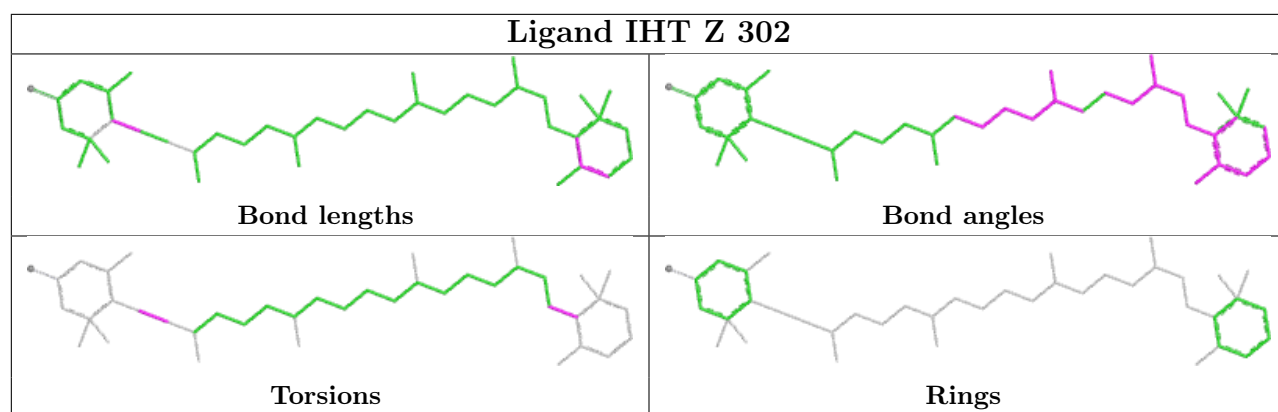
## Ligand CLA 5 609

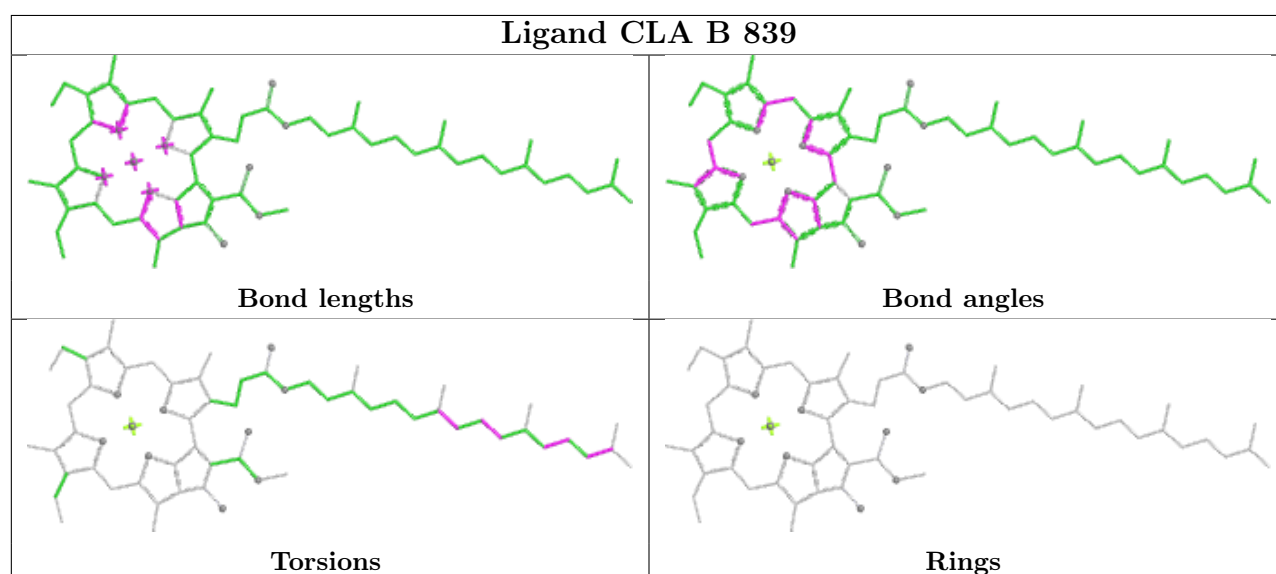
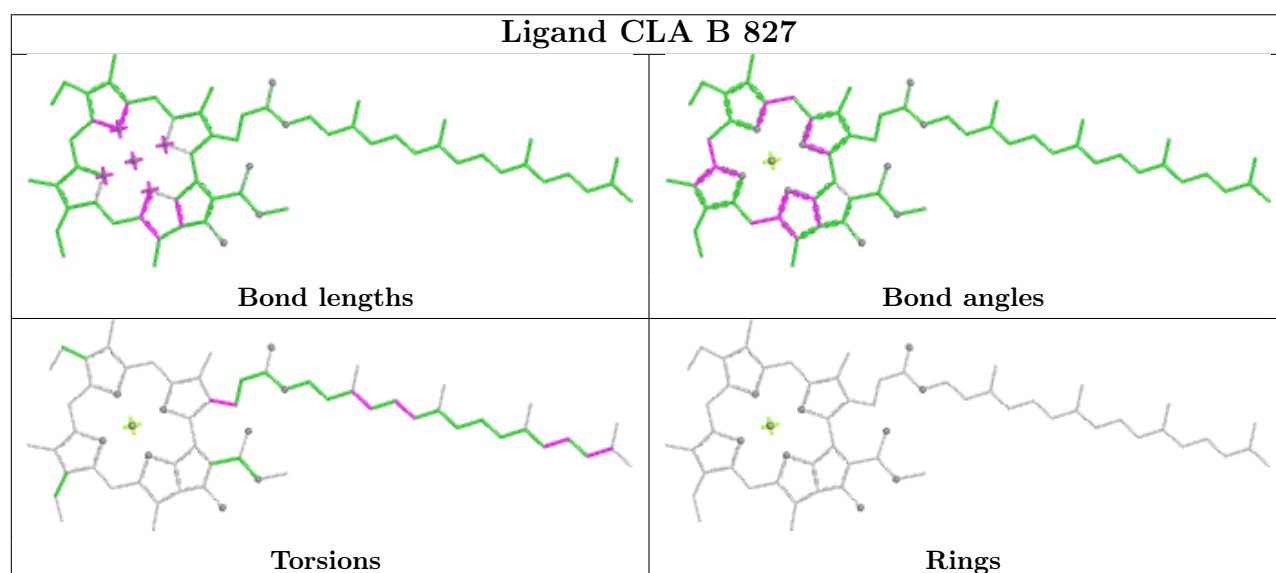
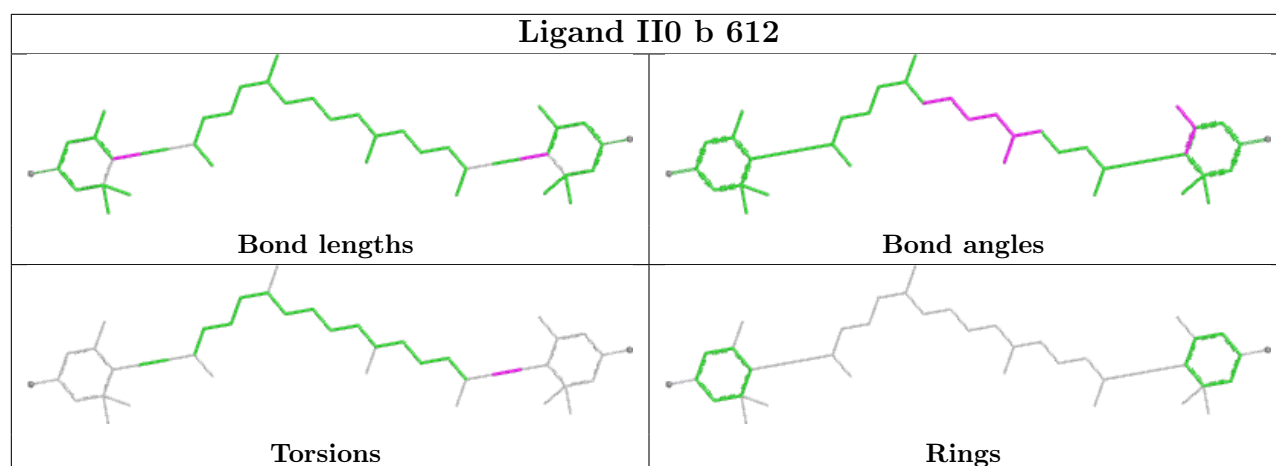


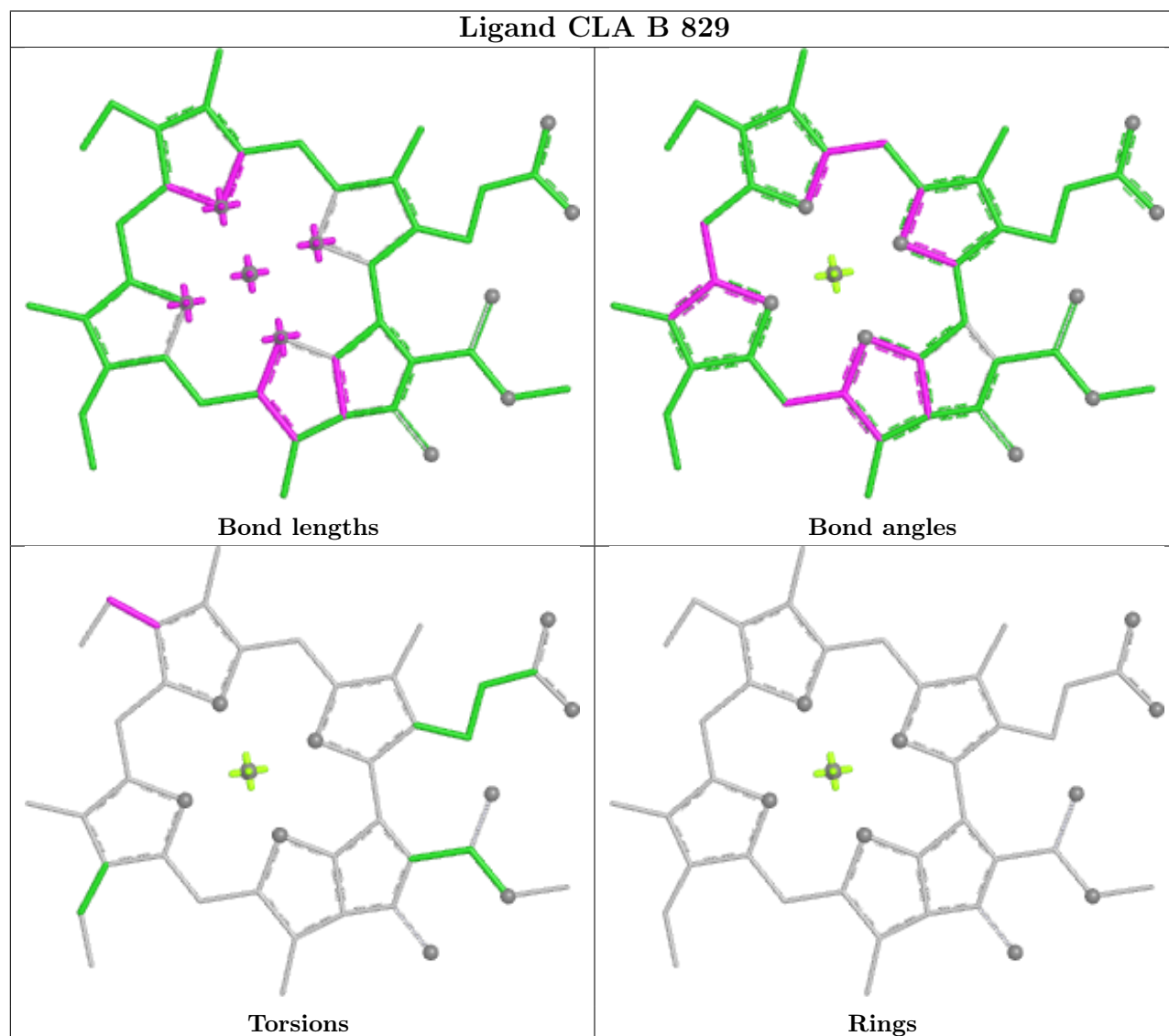
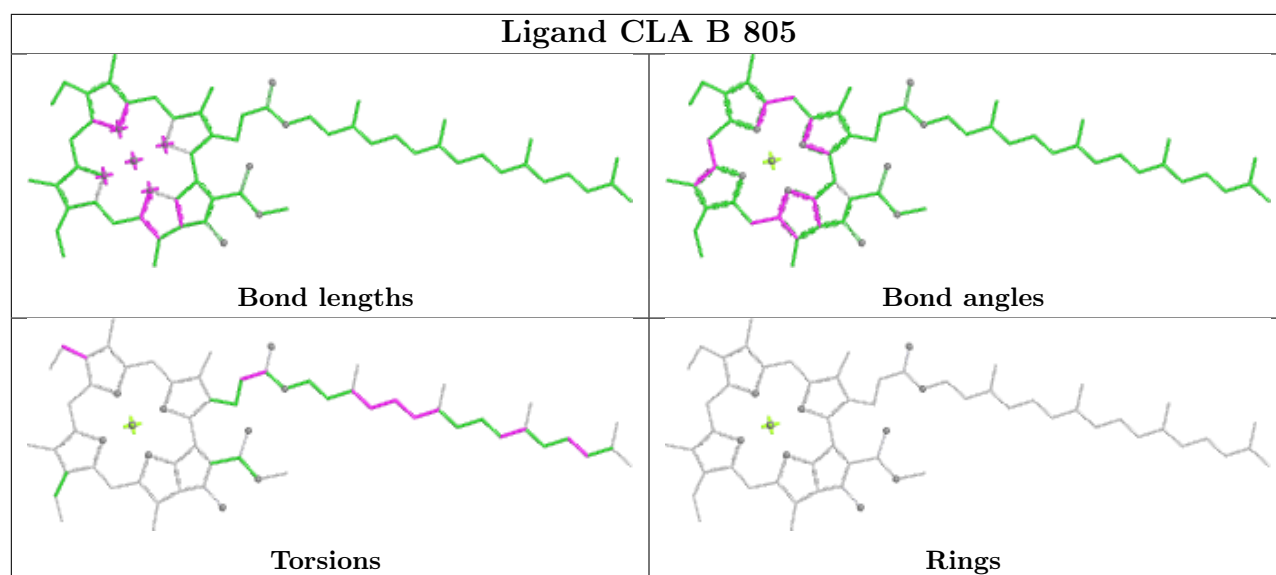


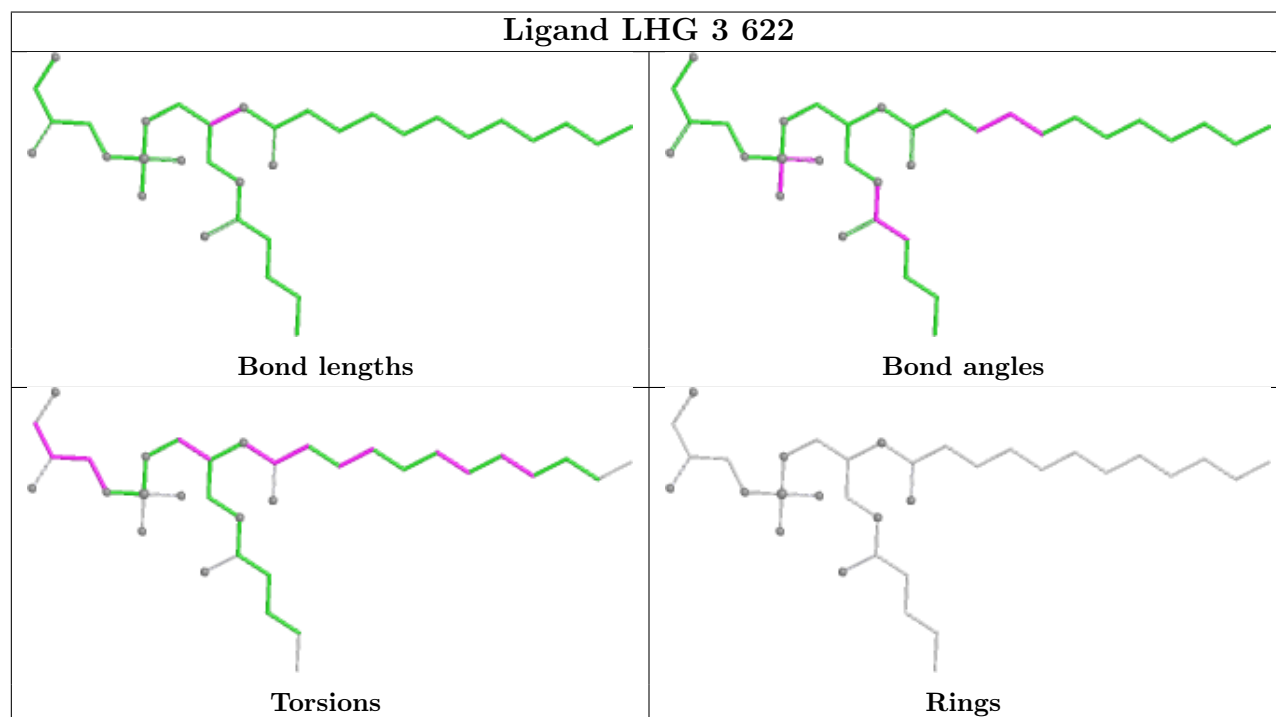
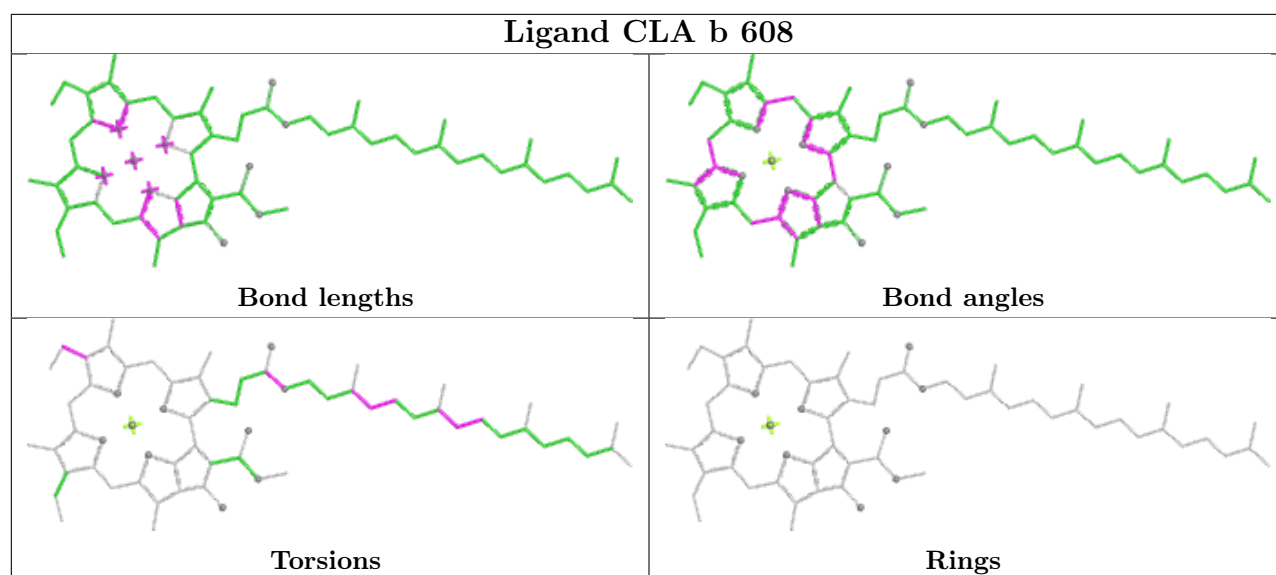


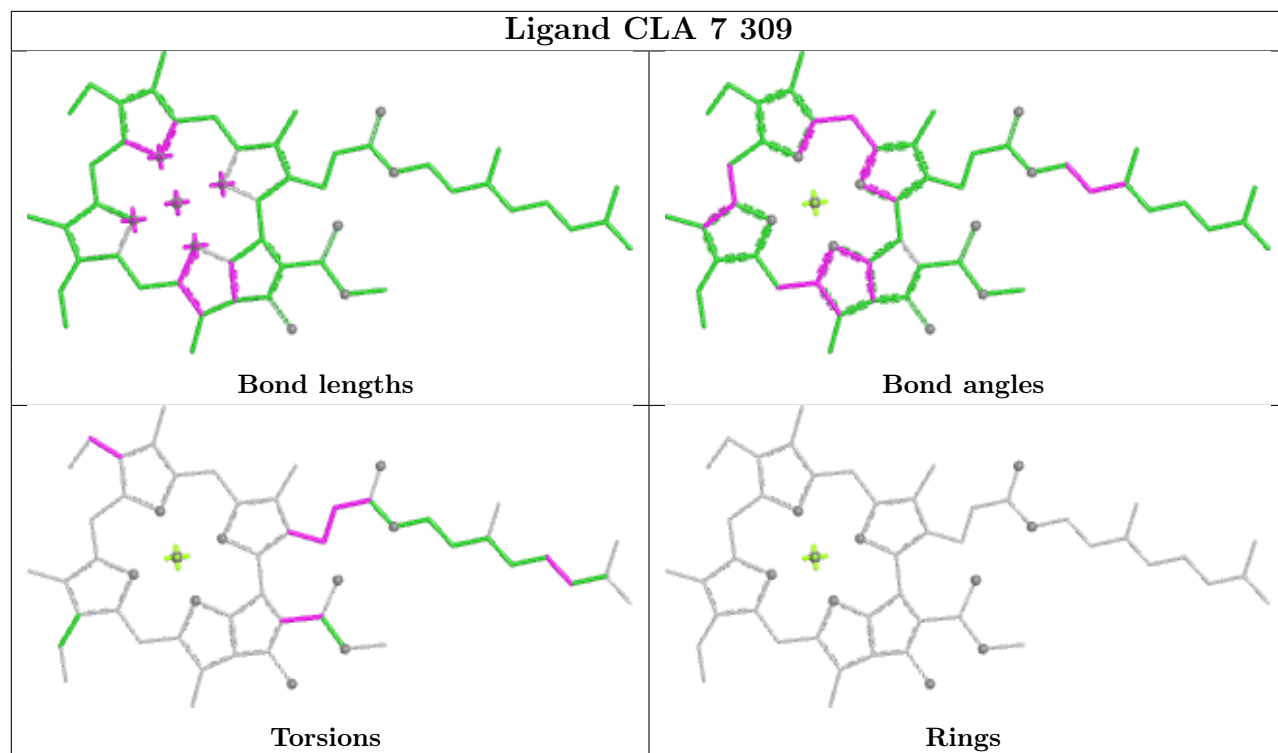
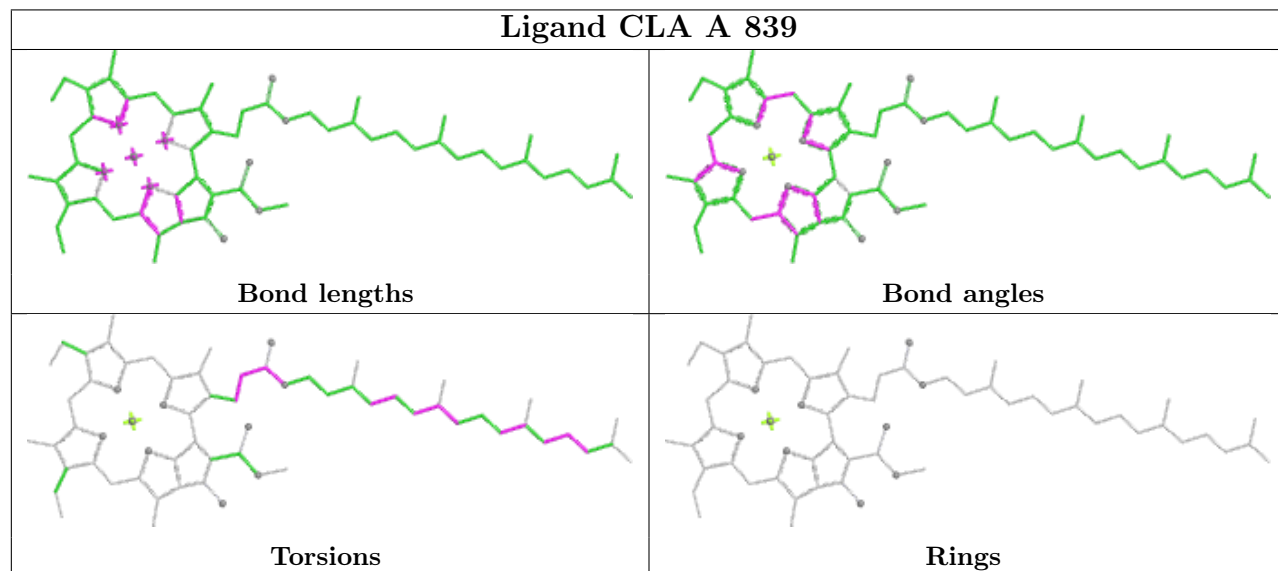


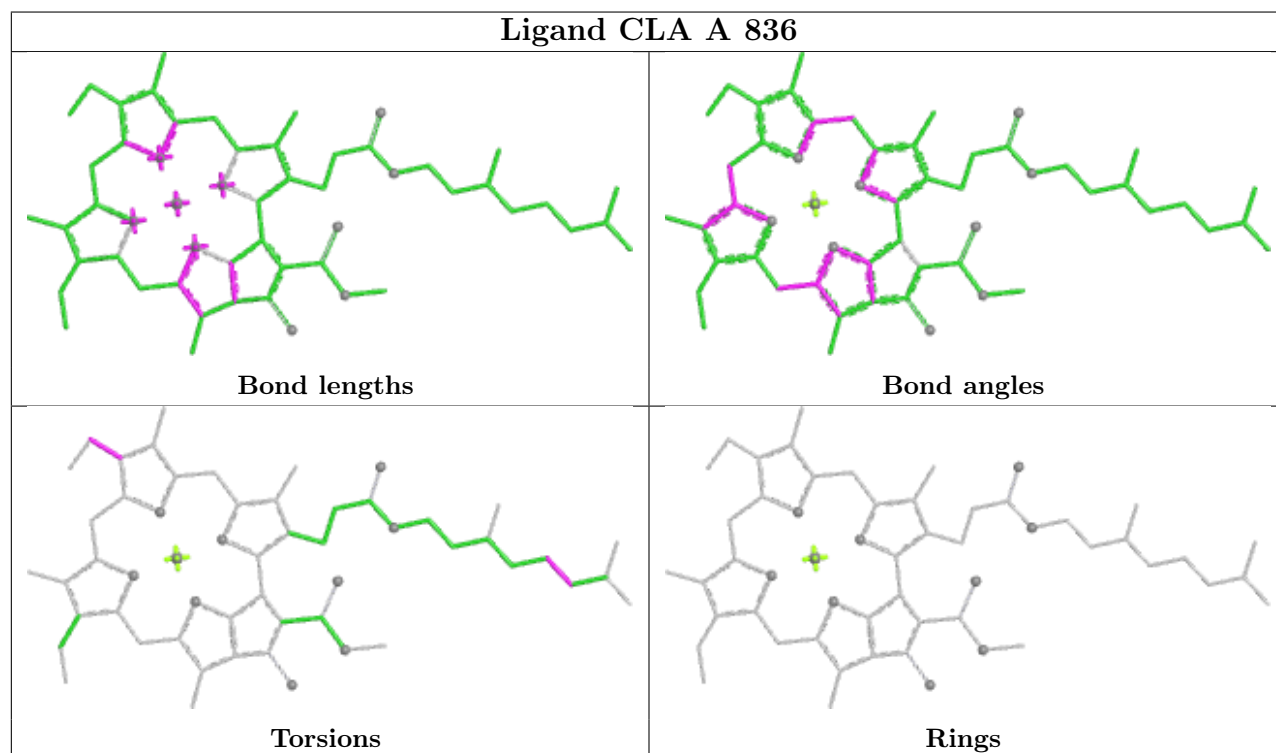
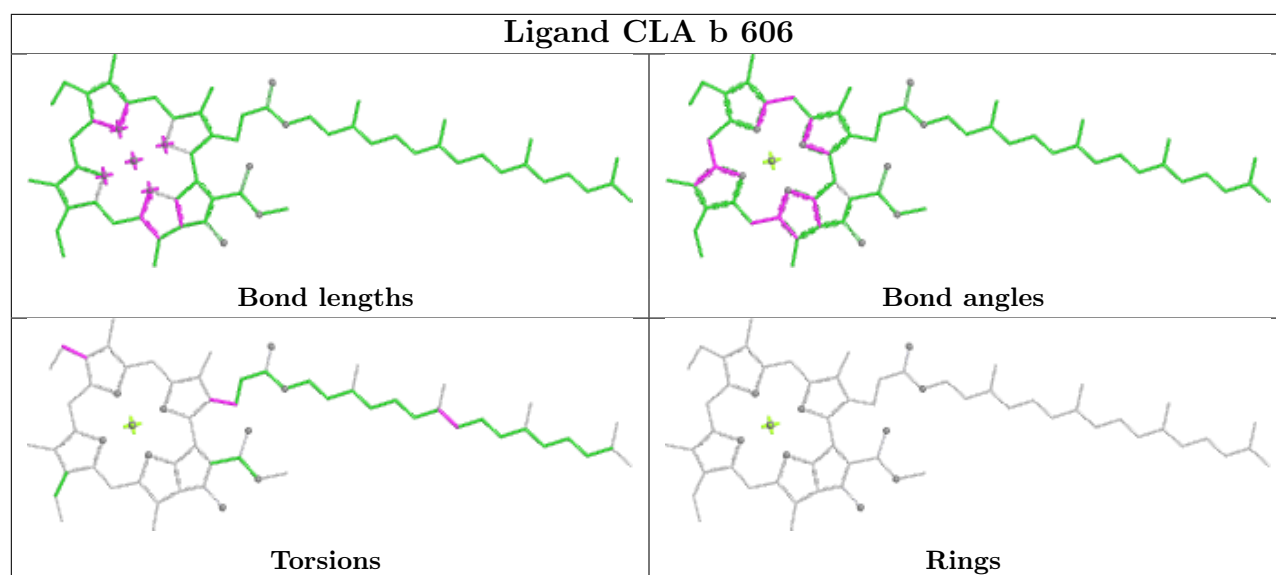




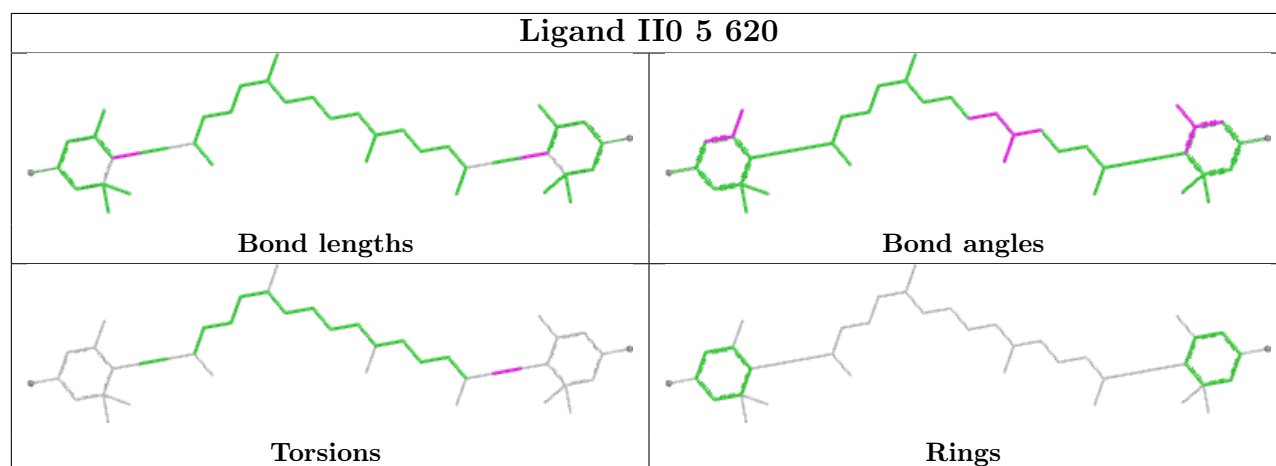
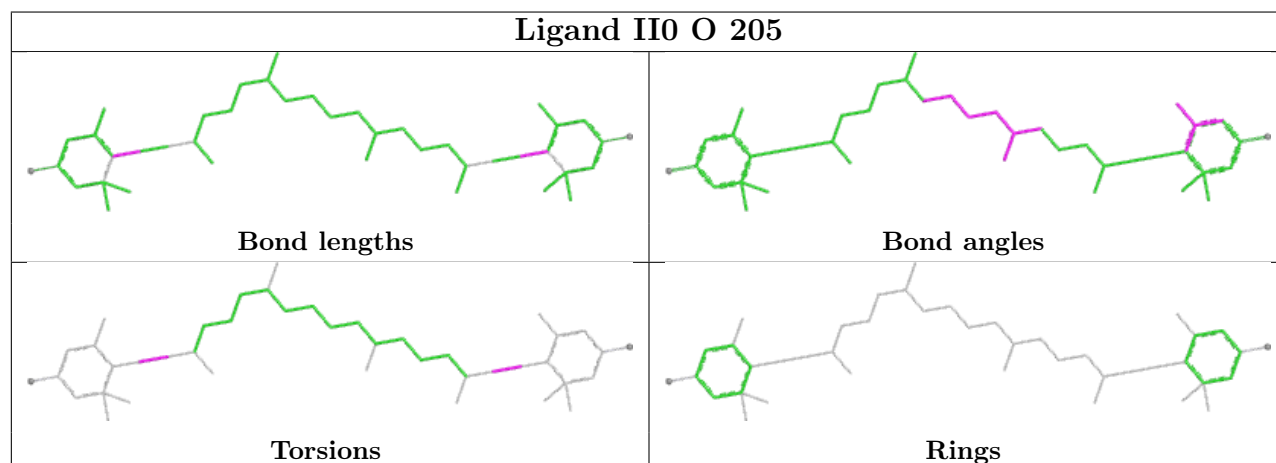
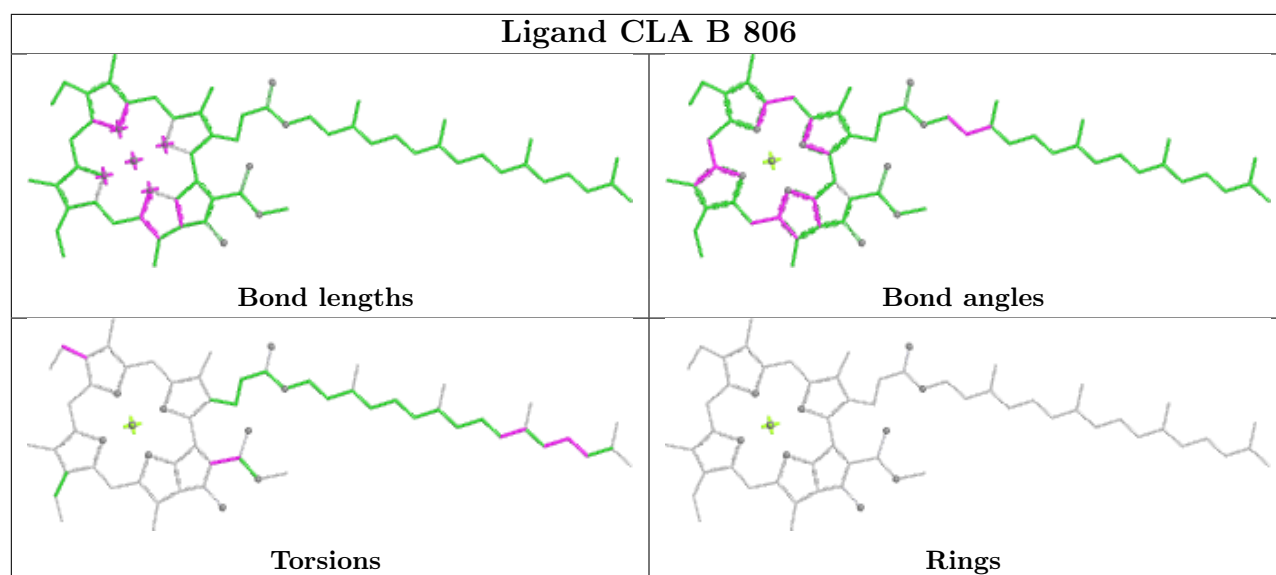


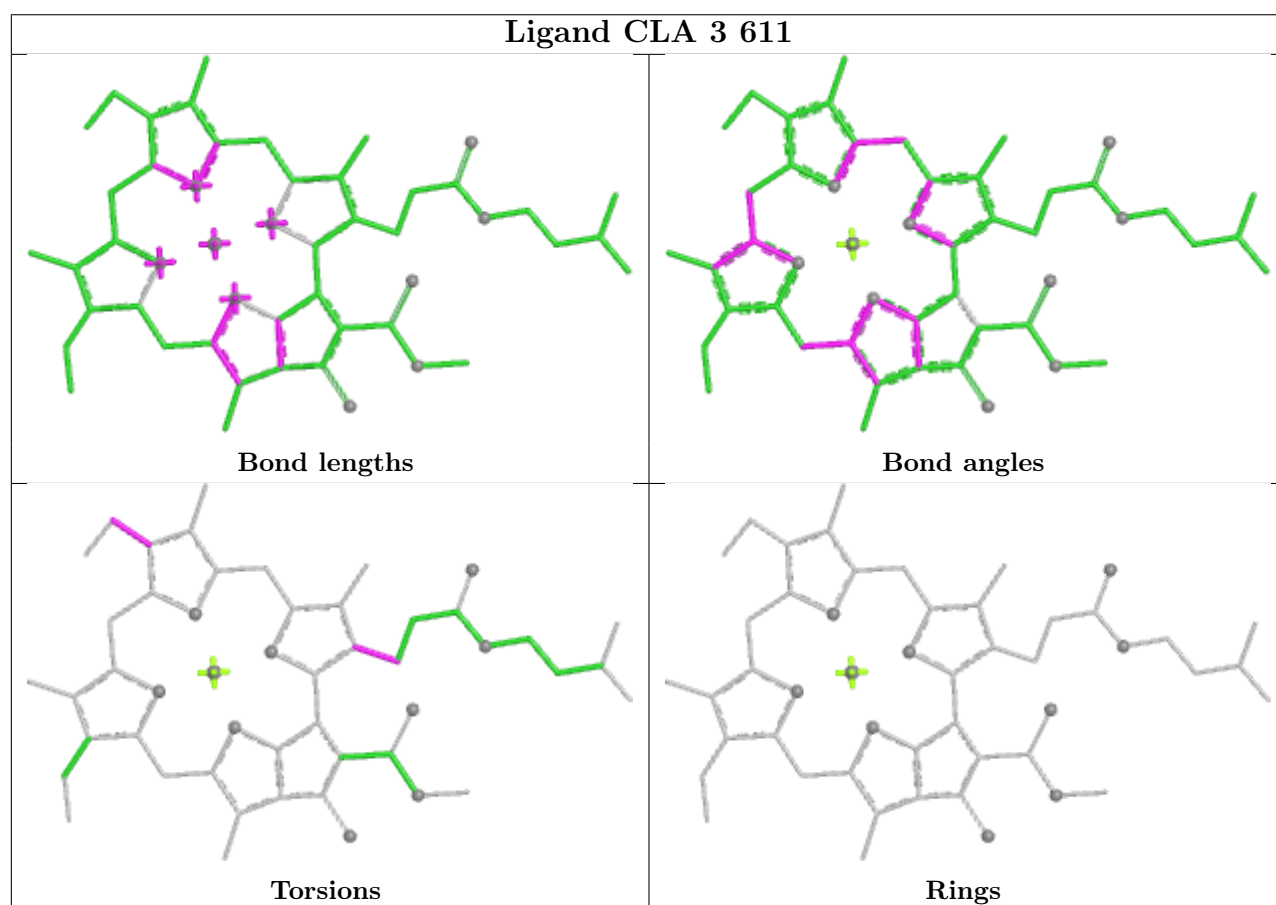
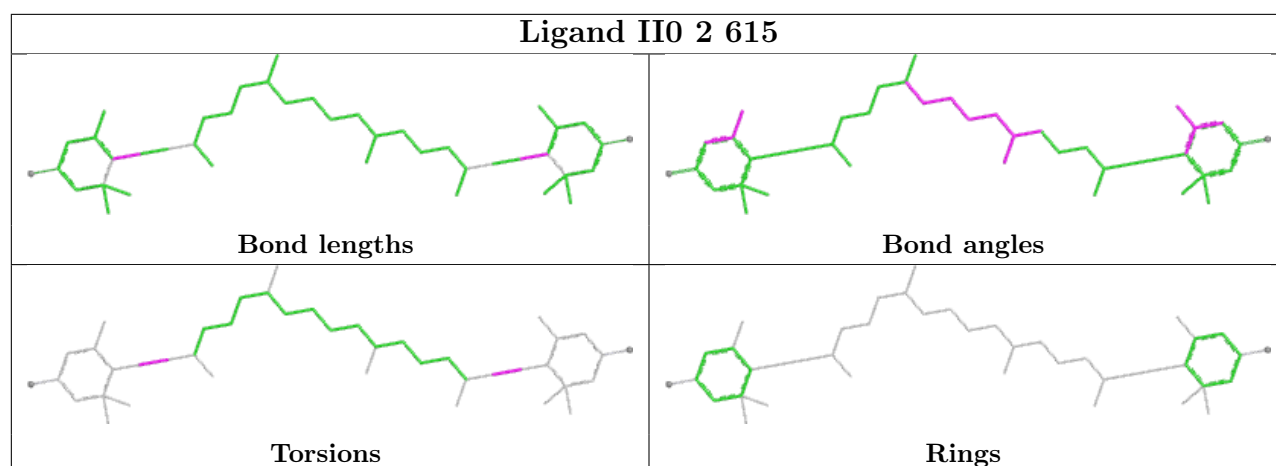


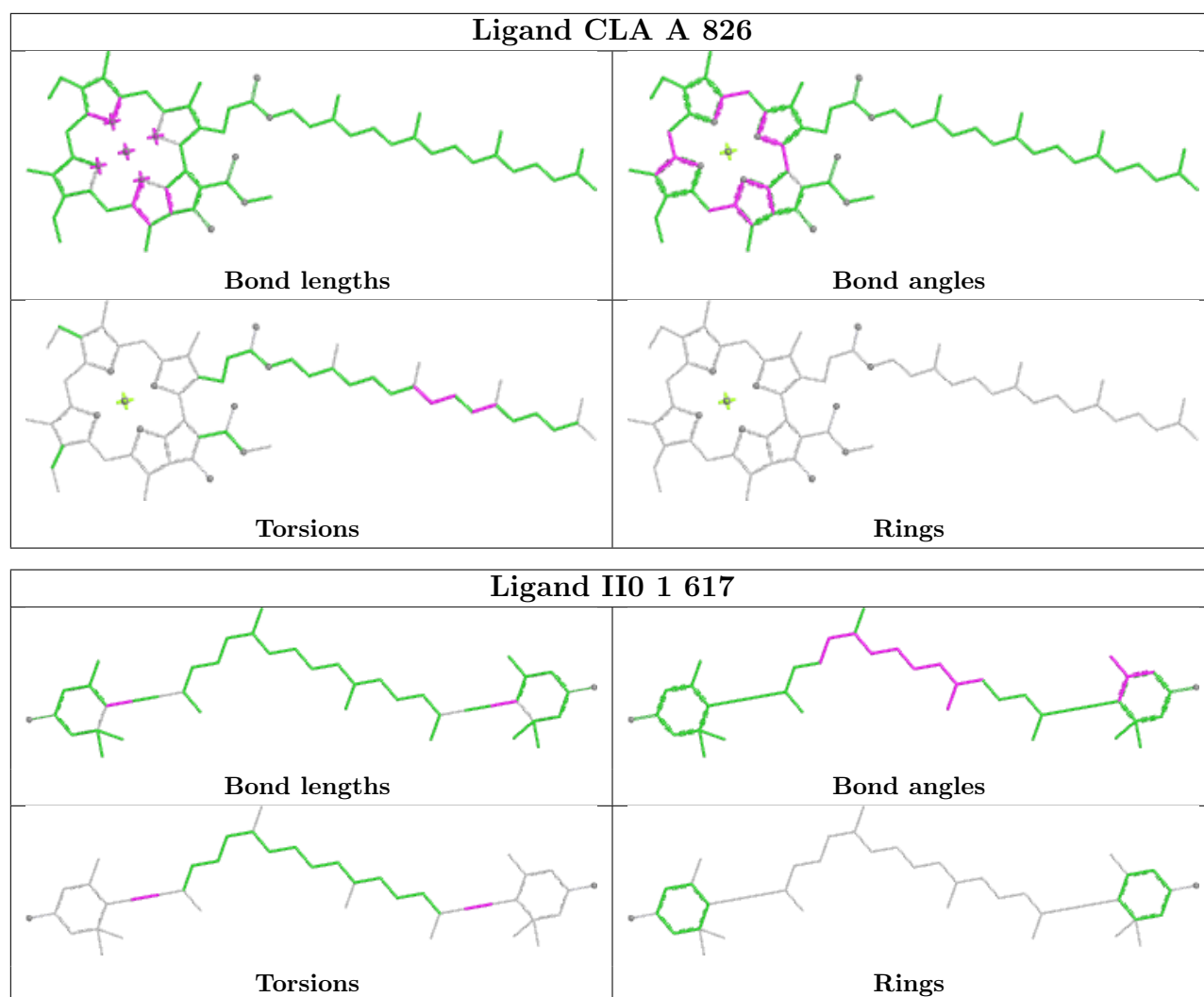
**Ligand CLA 7 309****Ligand CLA A 839**



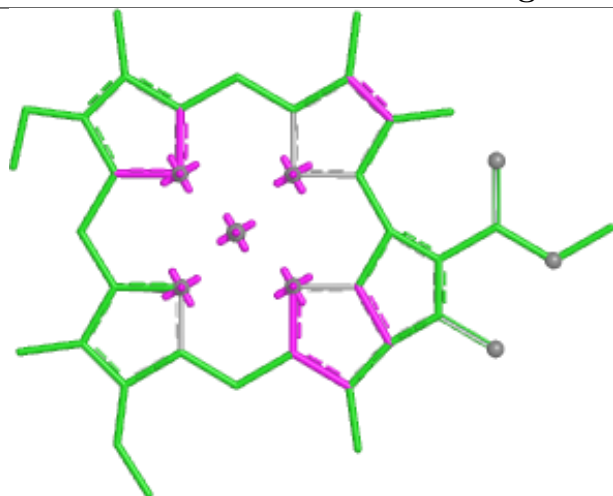




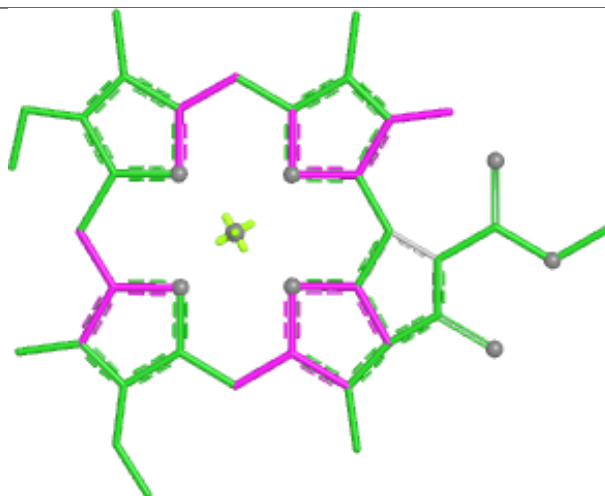




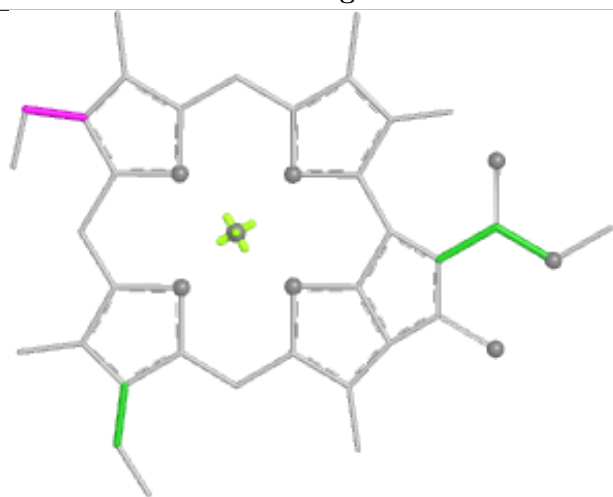
## Ligand CLA J 102



Bond lengths



Bond angles

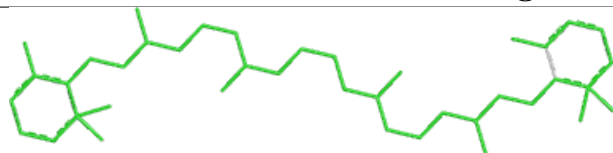


Torsions

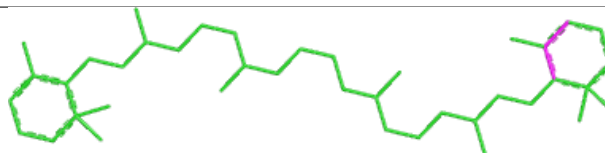


Rings

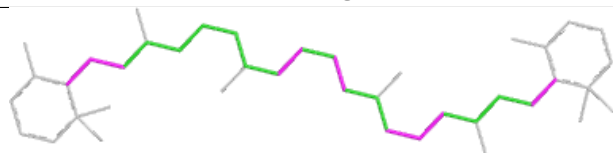
## Ligand 8CT A 847



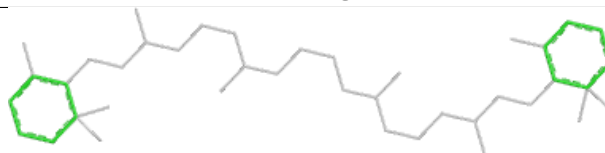
Bond lengths



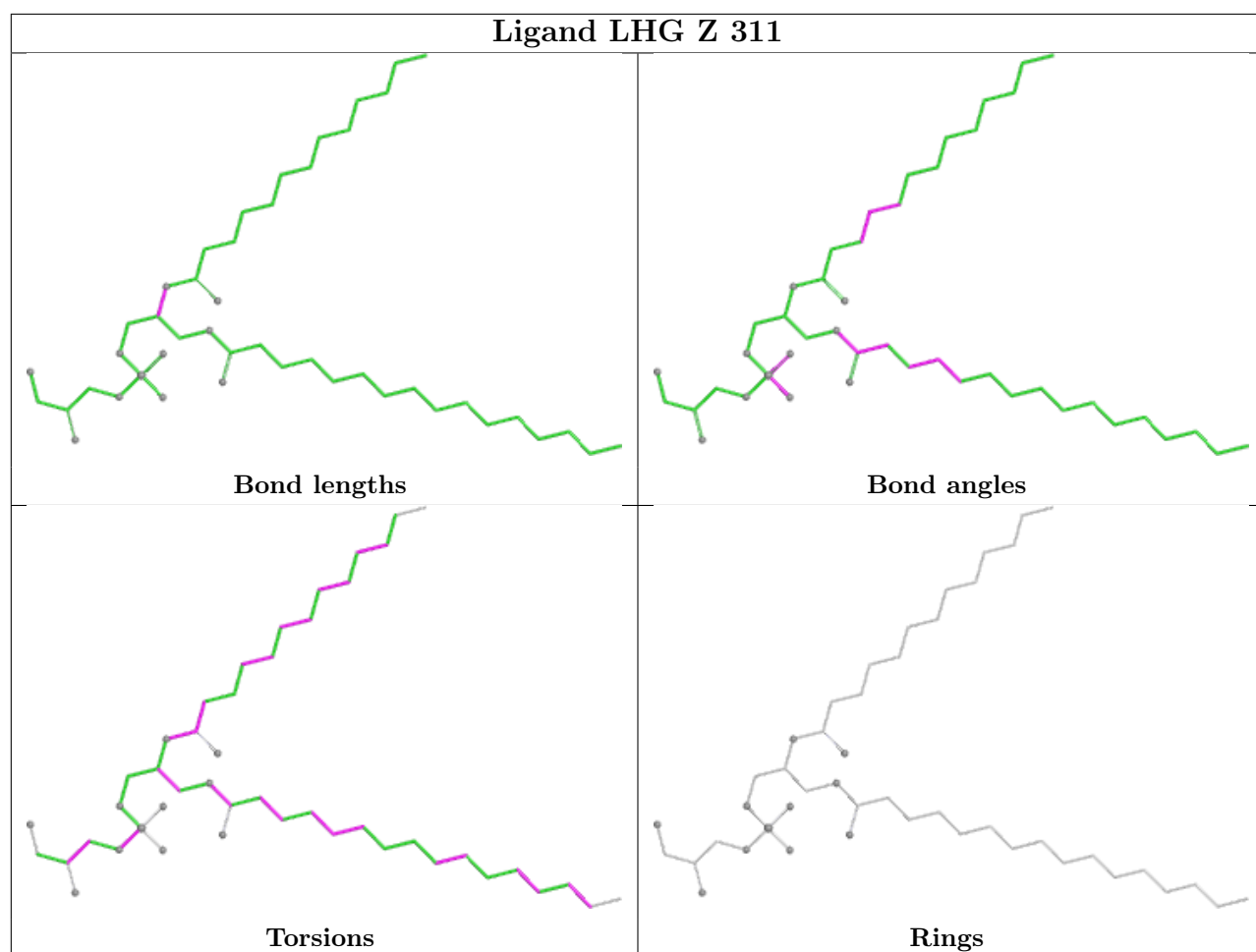
Bond angles



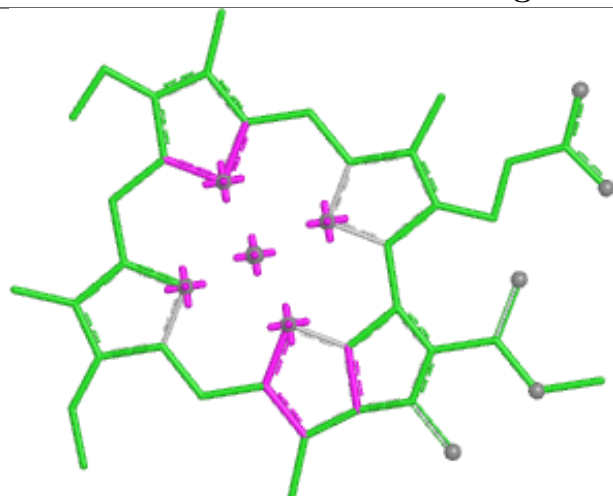
Torsions



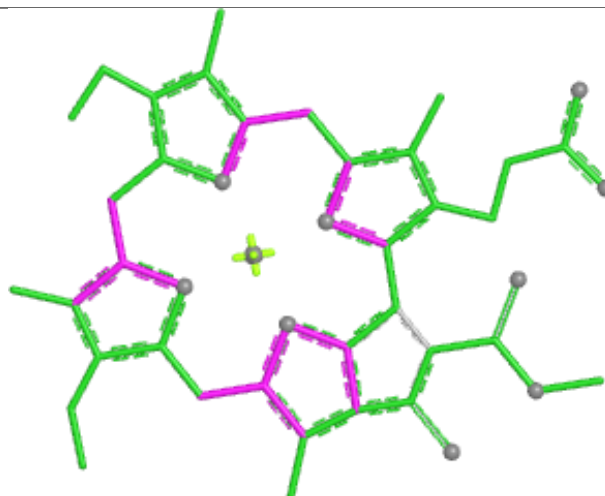
Rings



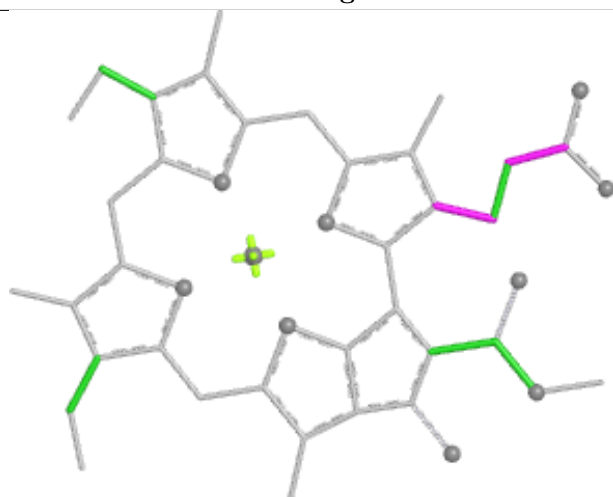
## Ligand CLA A 814



Bond lengths



Bond angles

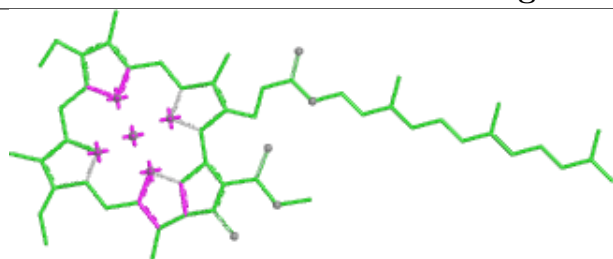


Torsions

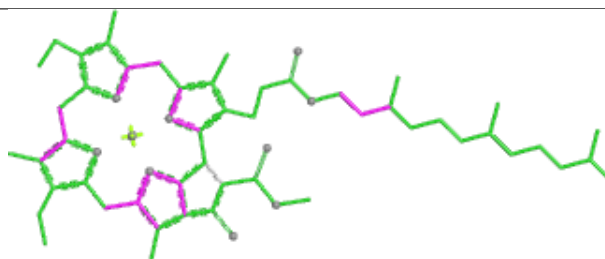


Rings

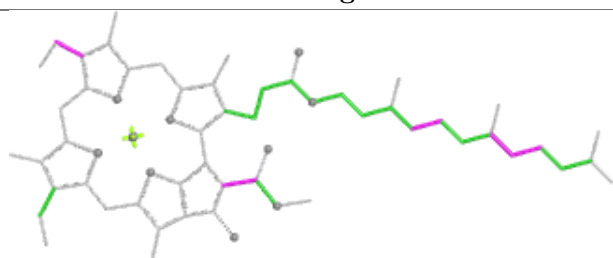
## Ligand CLA 6 608



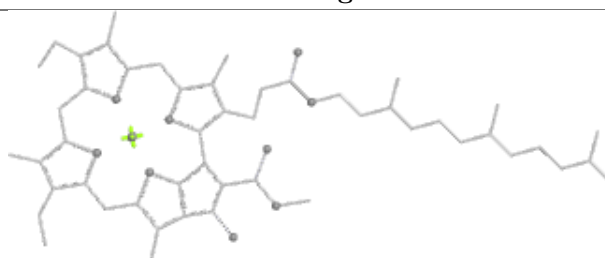
Bond lengths



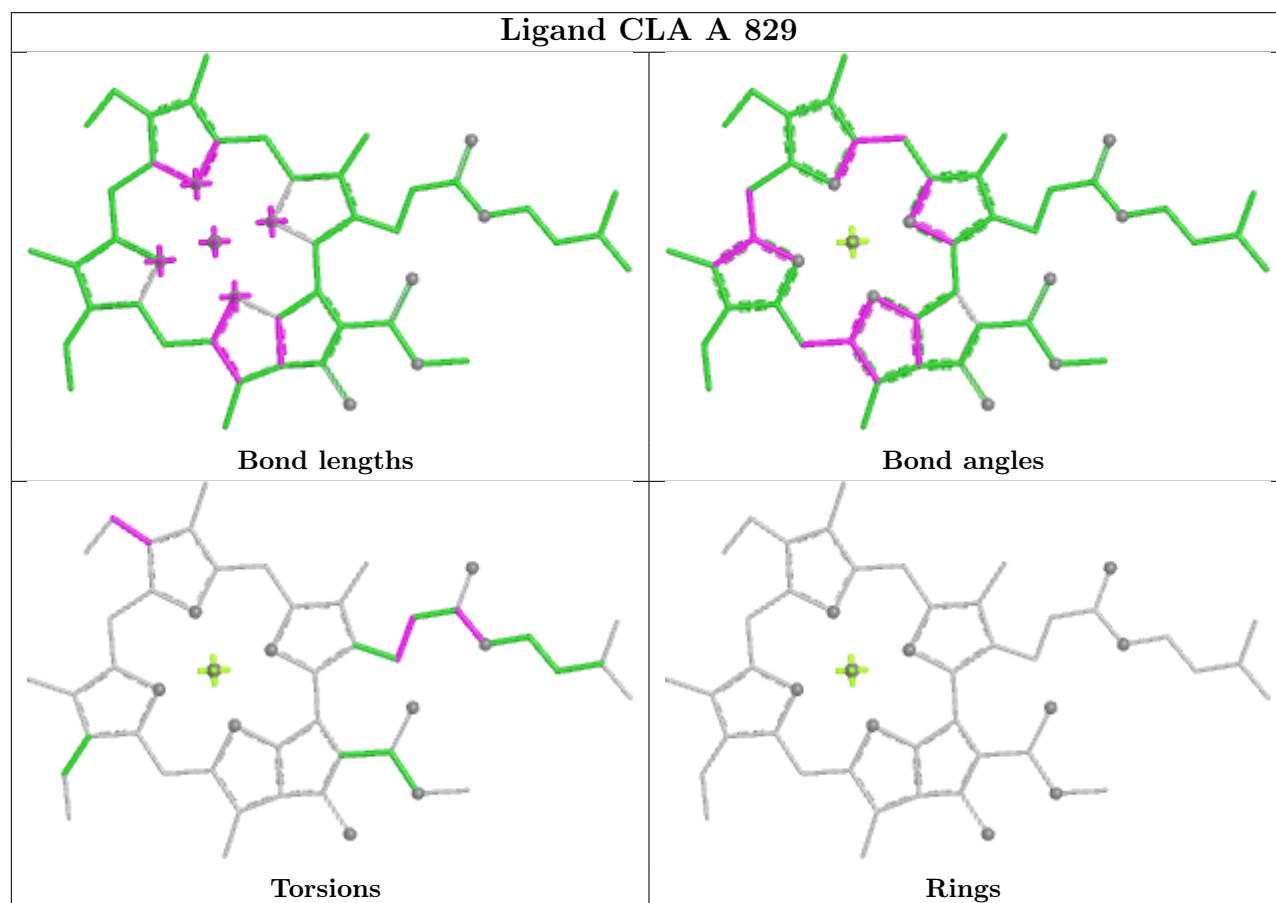
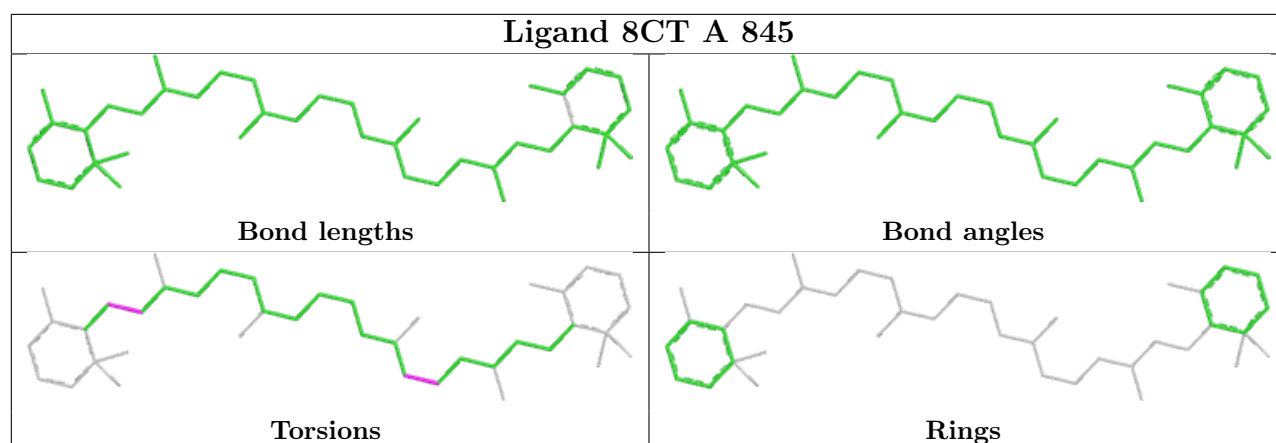
Bond angles

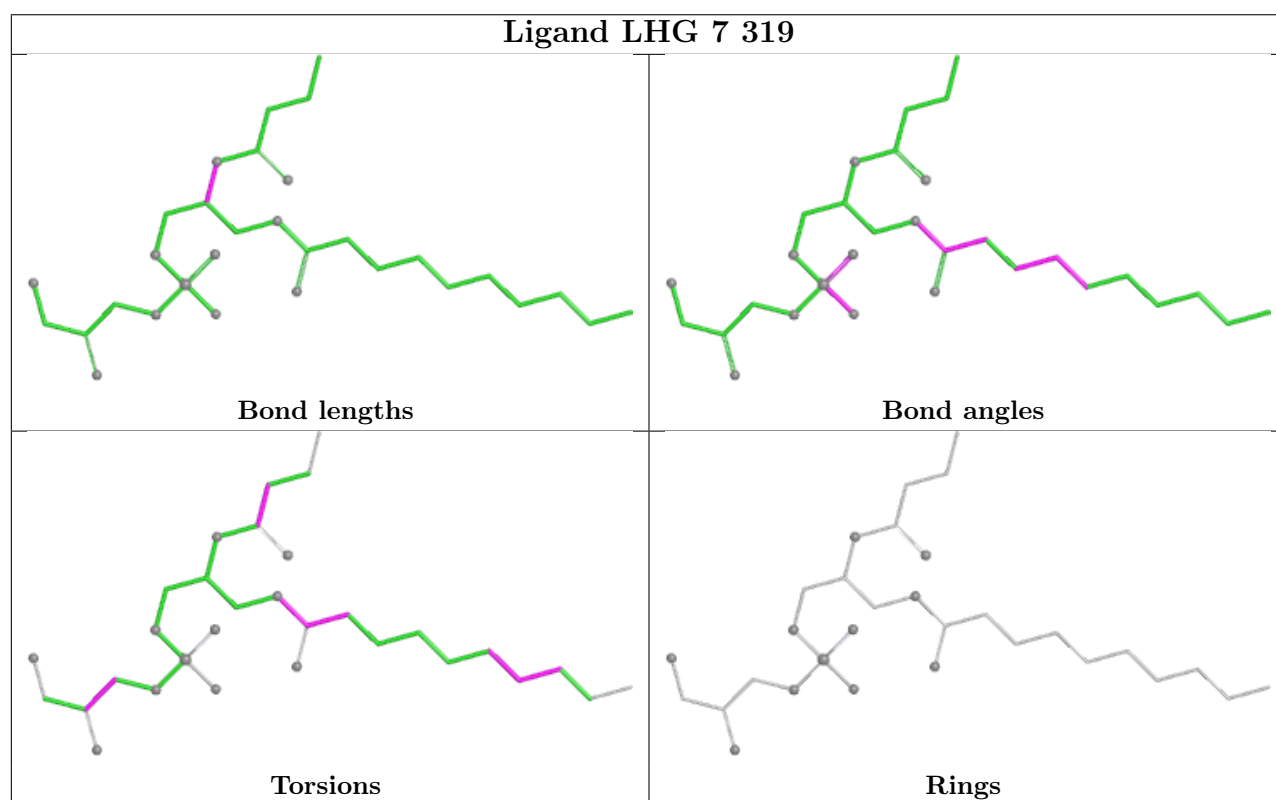
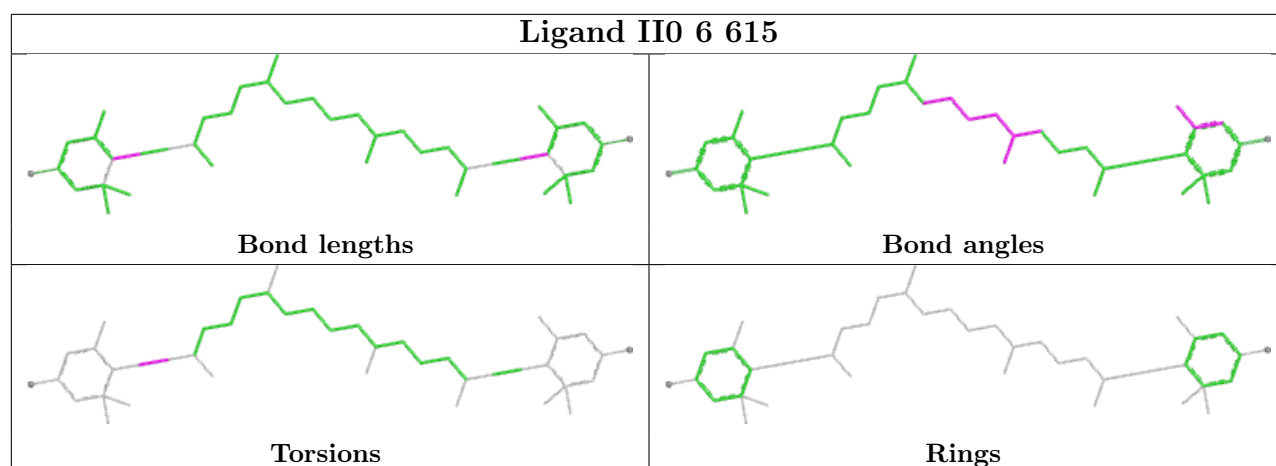


Torsions

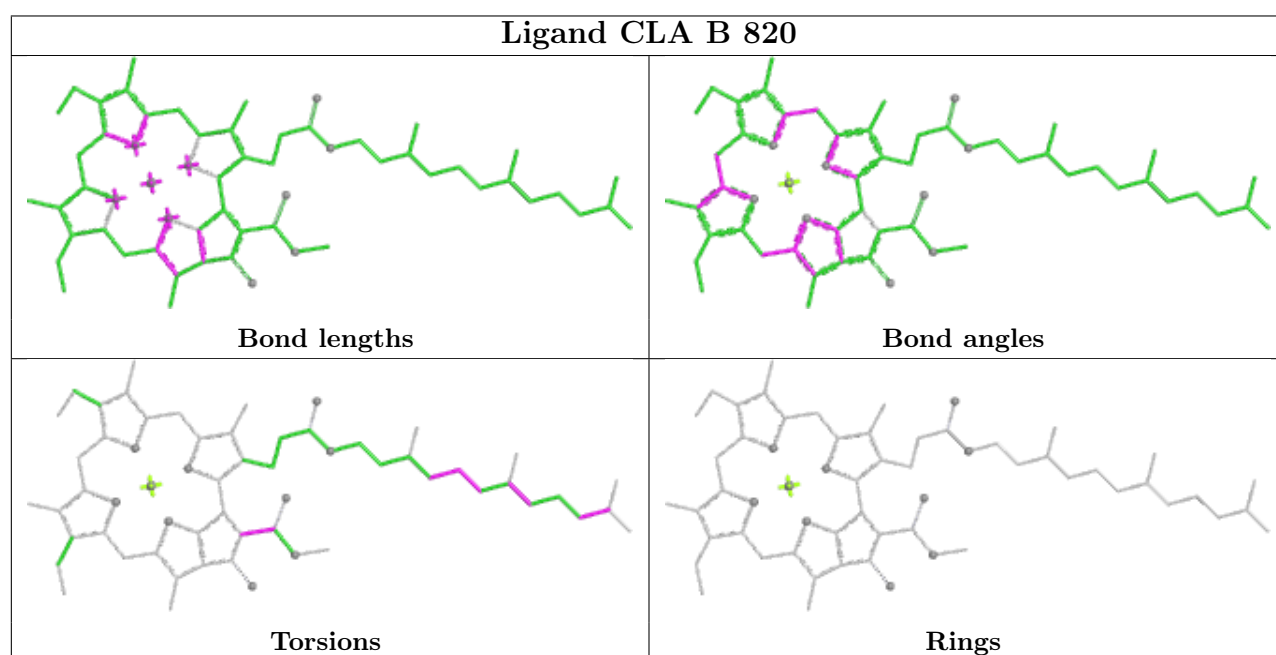
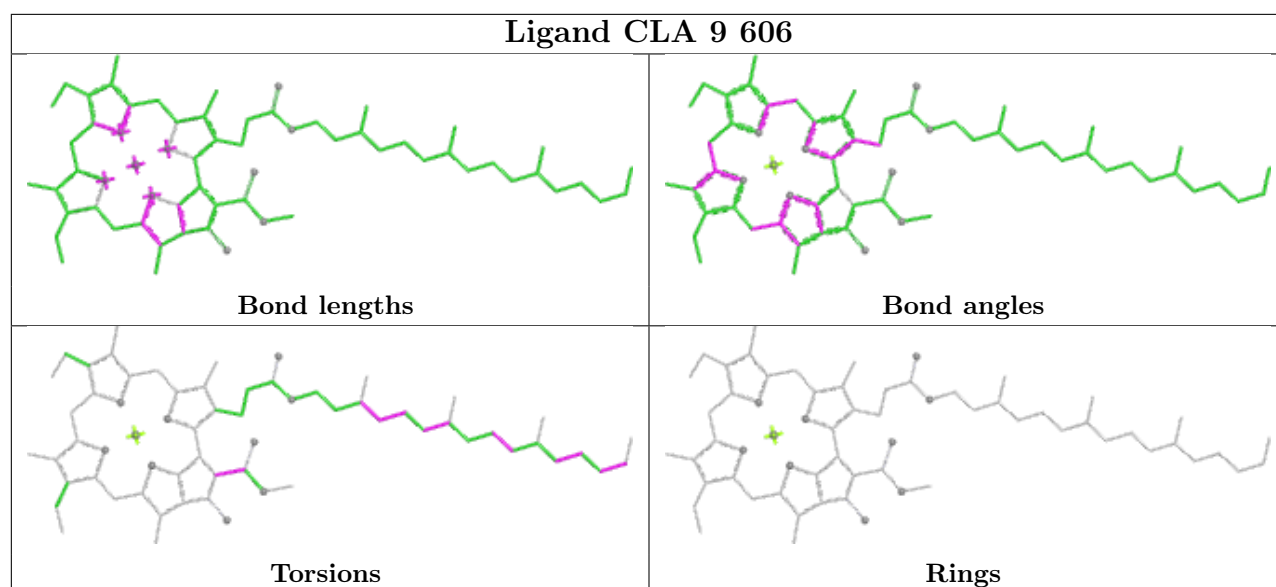


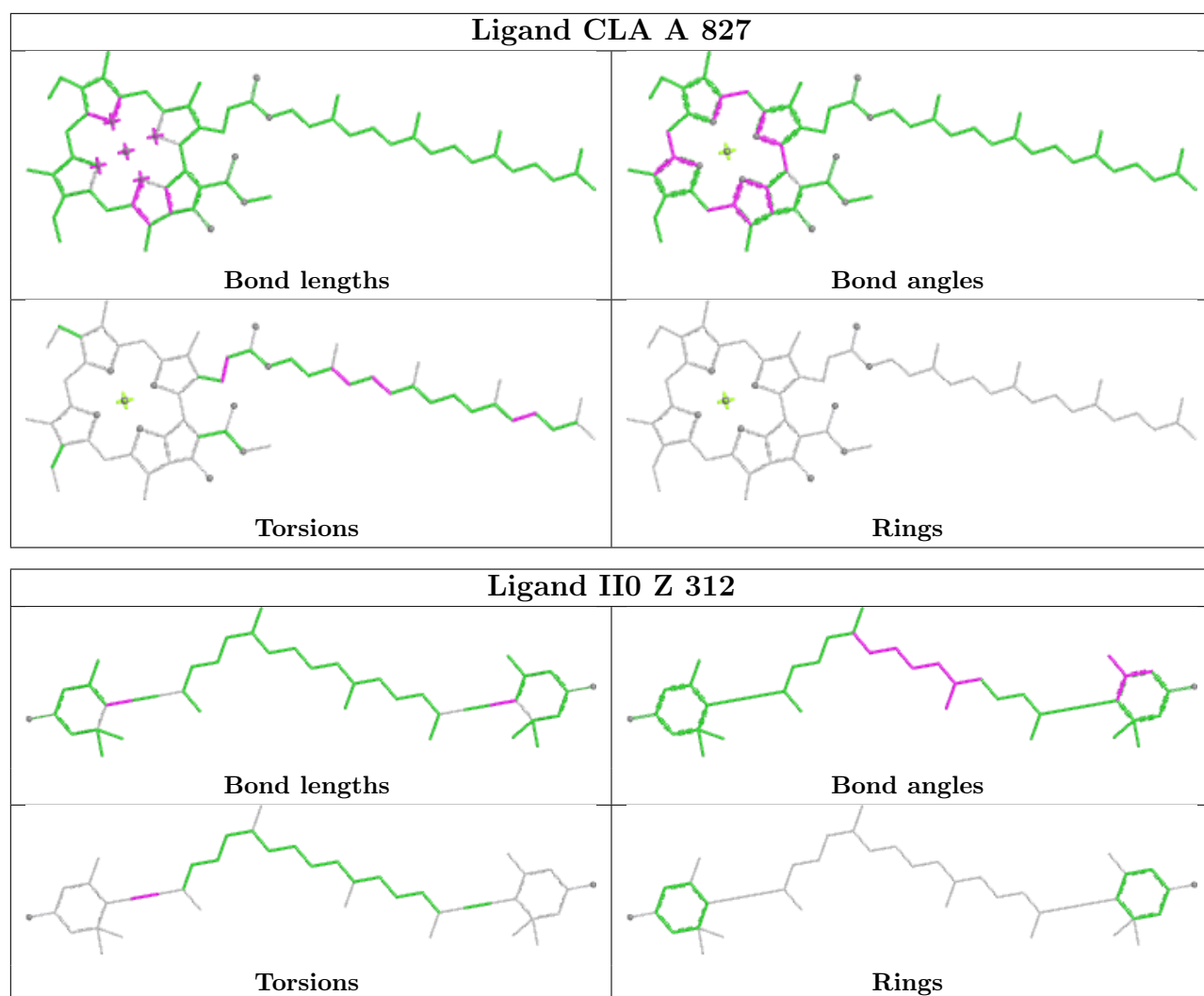
Rings



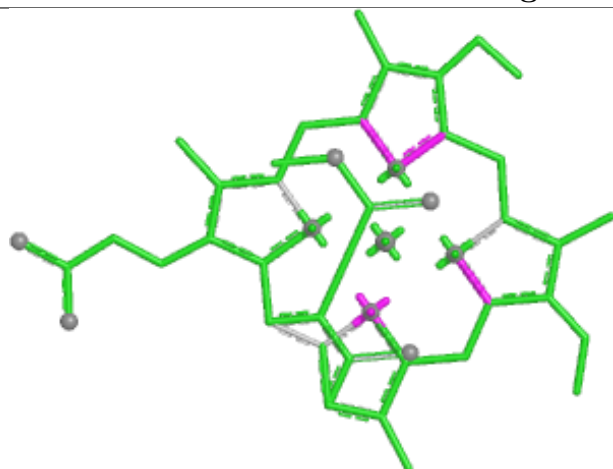




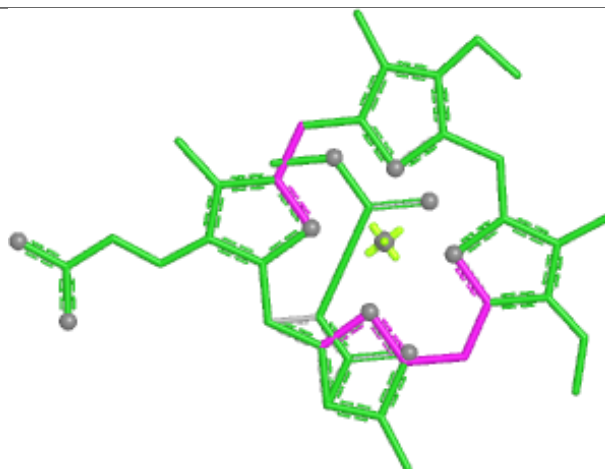




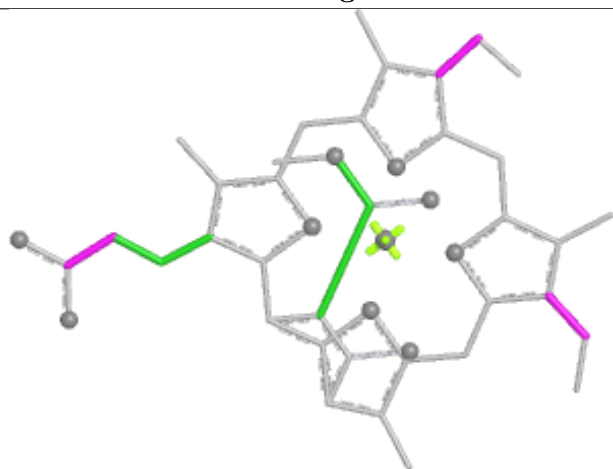
## Ligand KC2 7 307



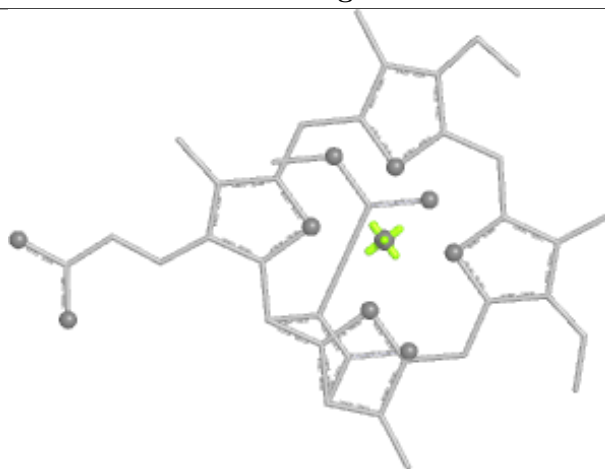
Bond lengths



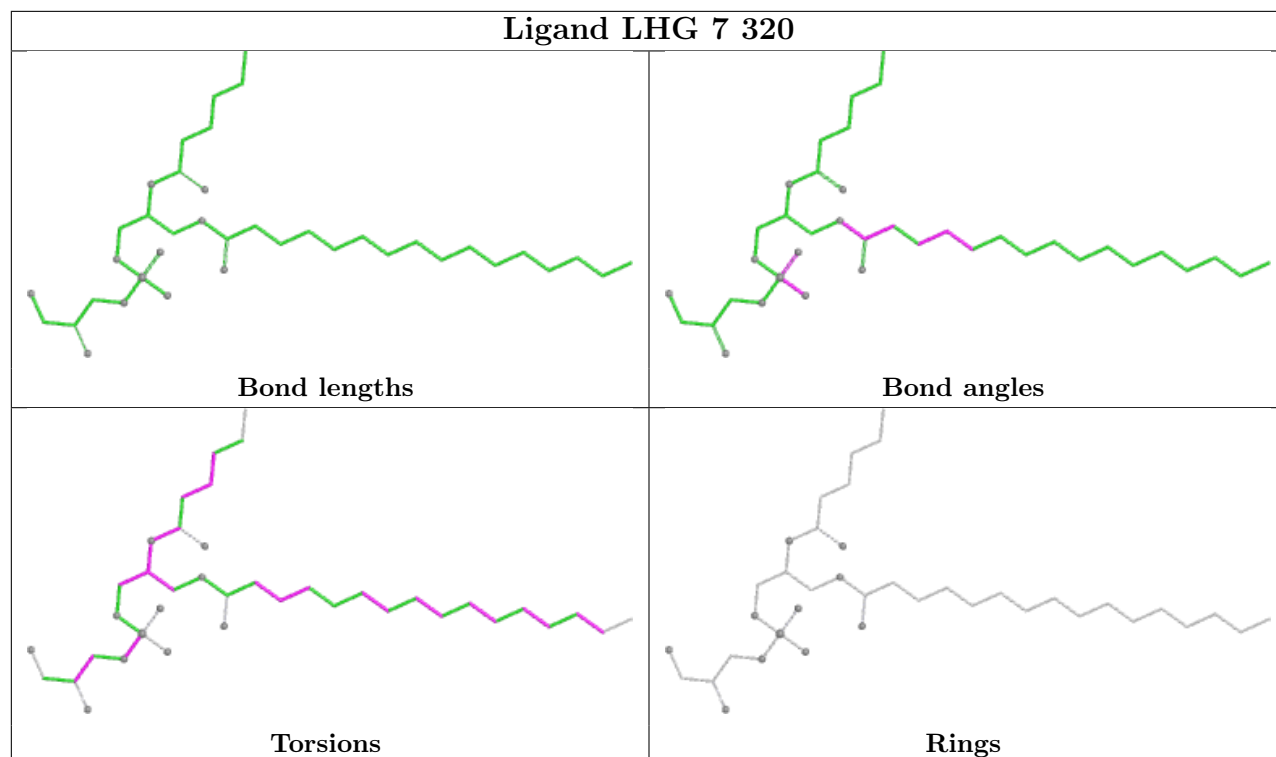
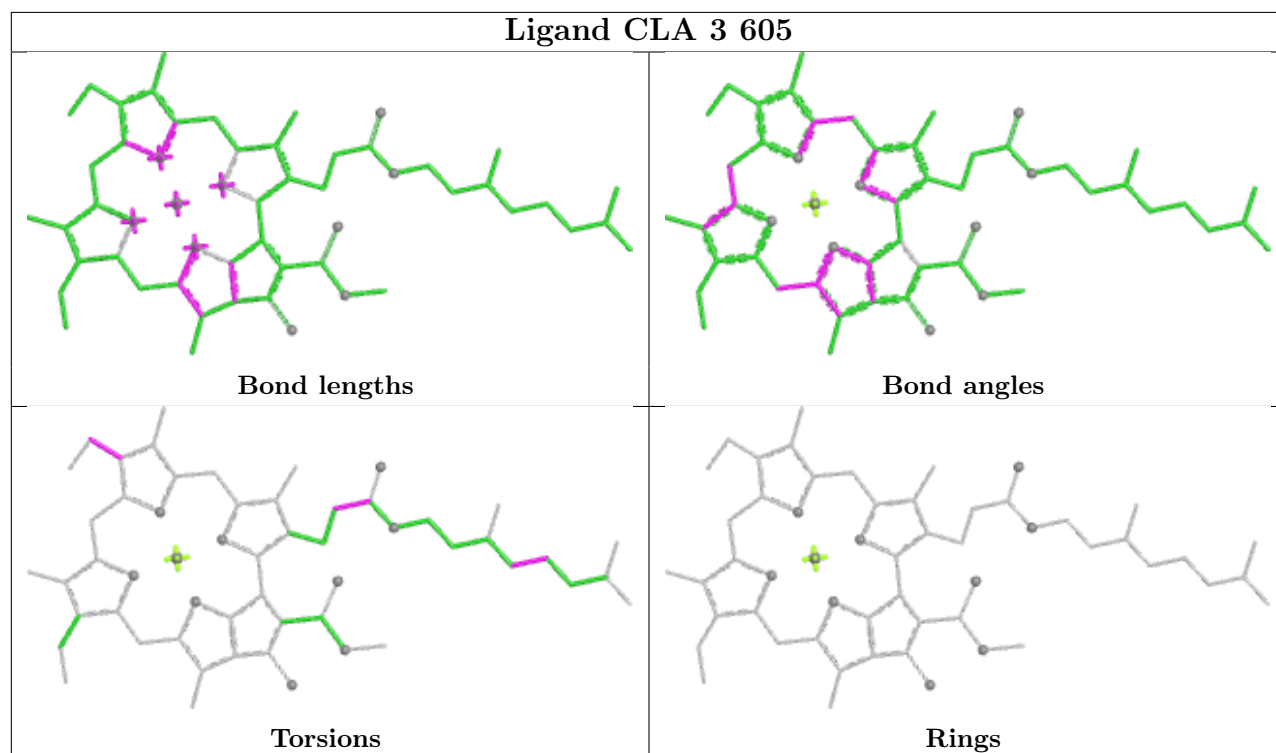
Bond angles

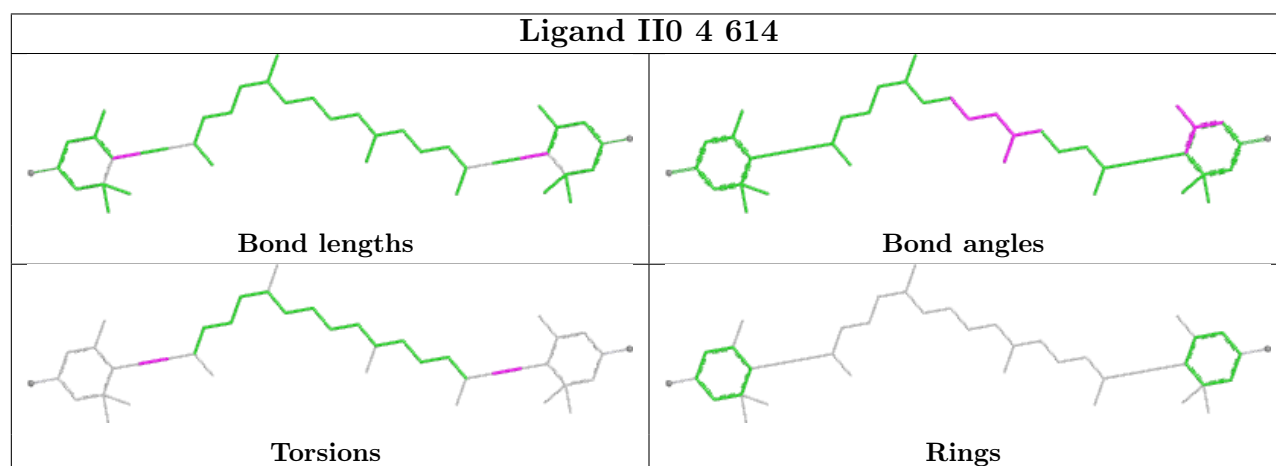
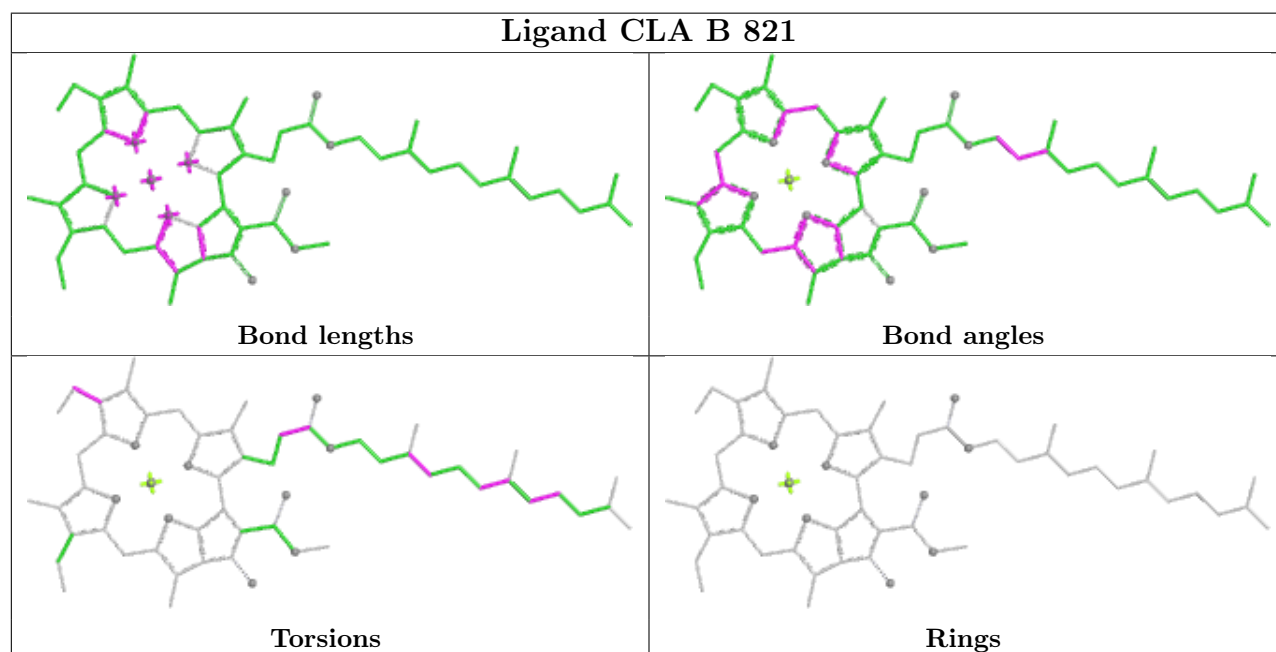
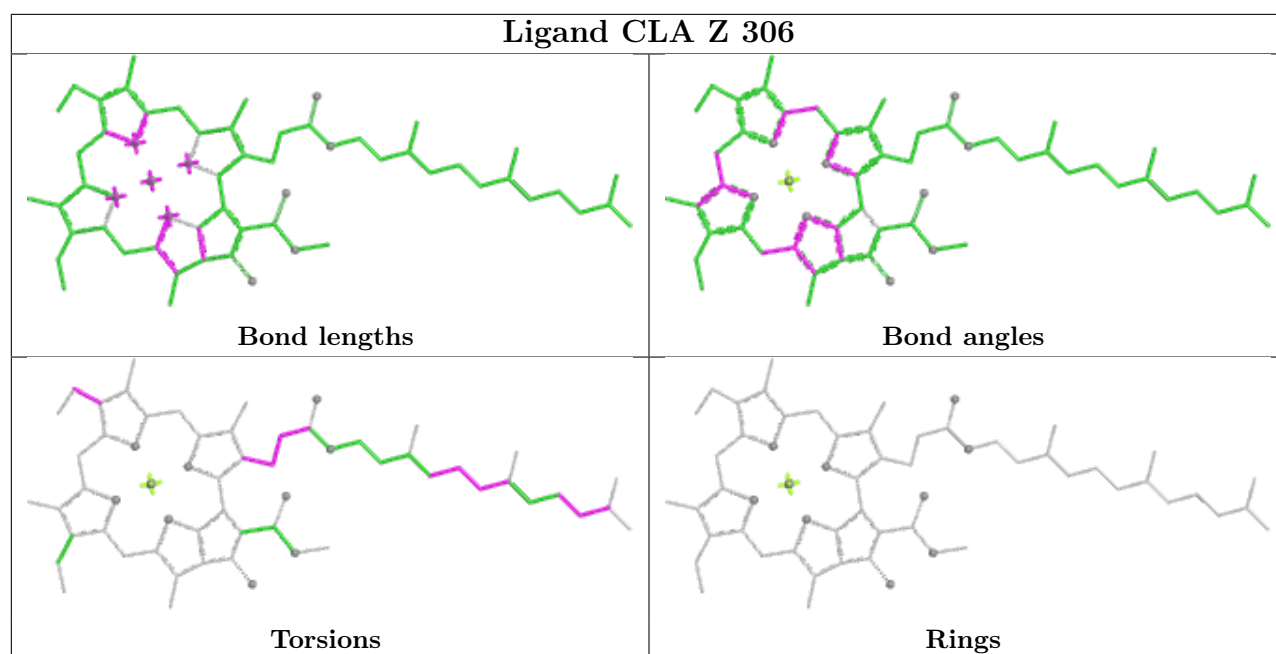


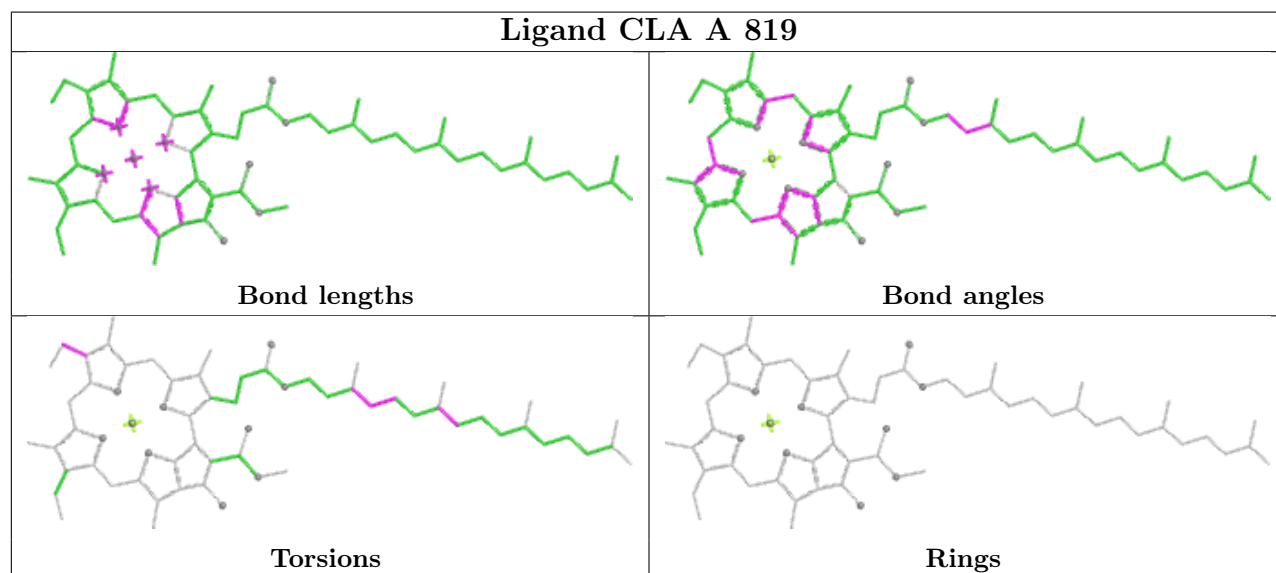
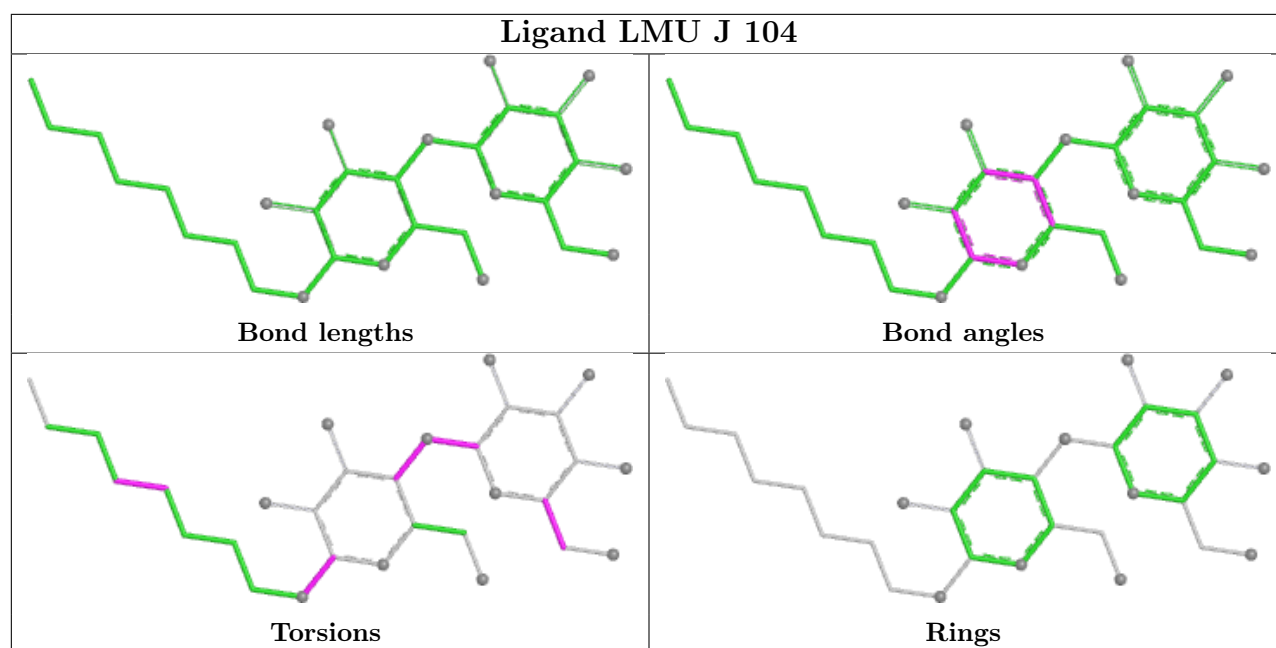
Torsions



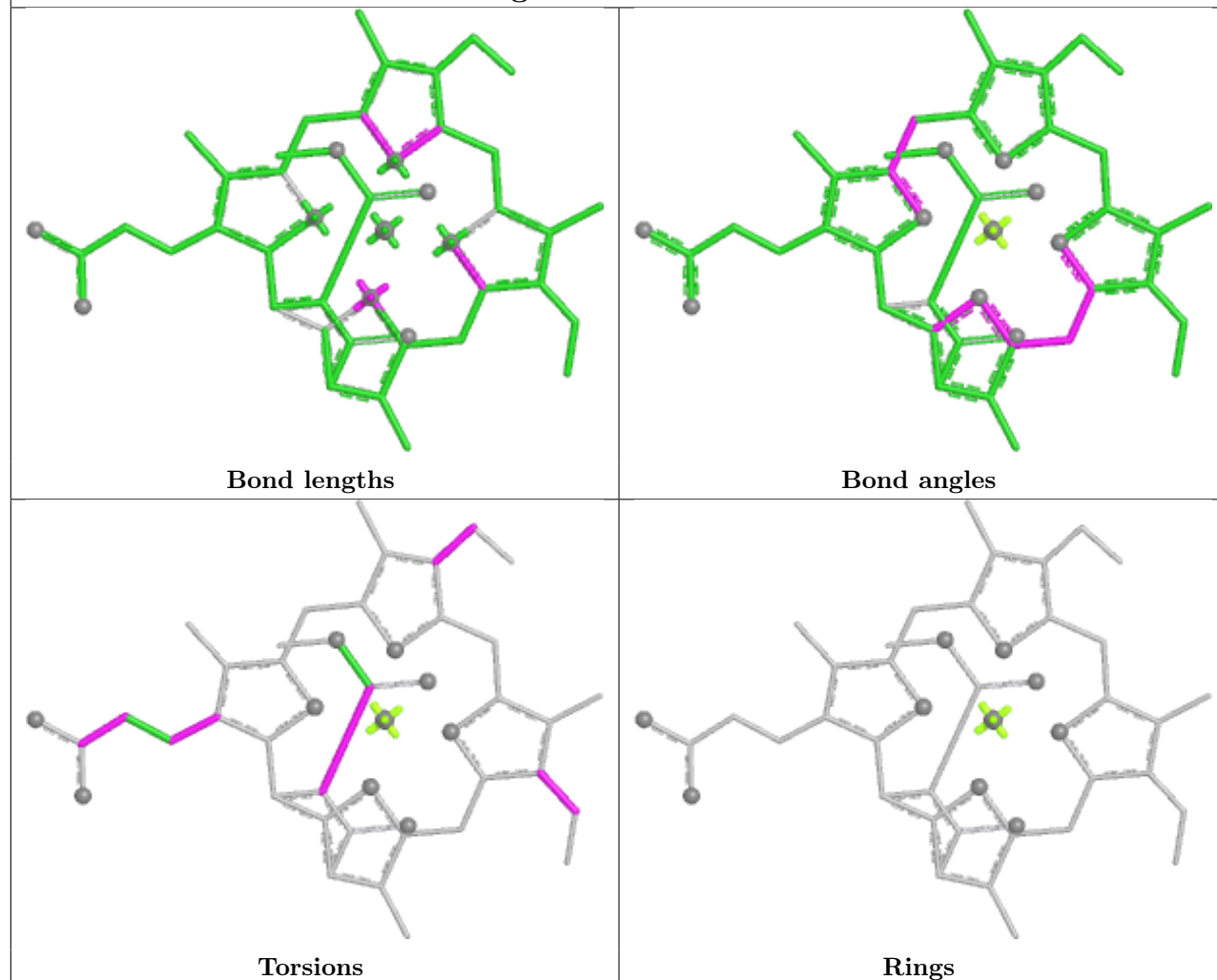
Rings

**Ligand LHG 7 320****Ligand CLA 3 605**

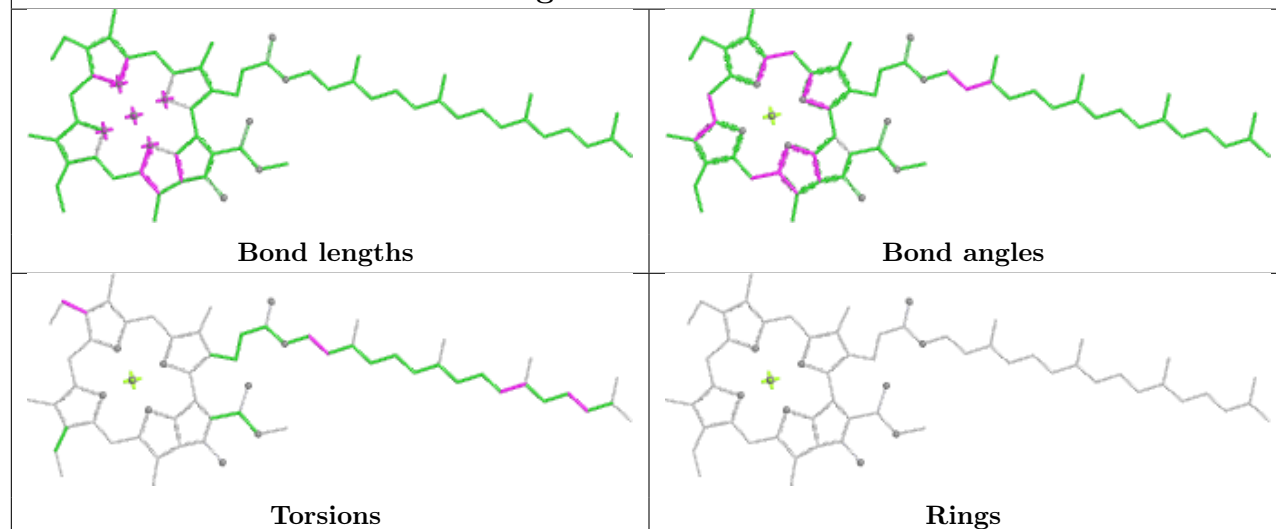


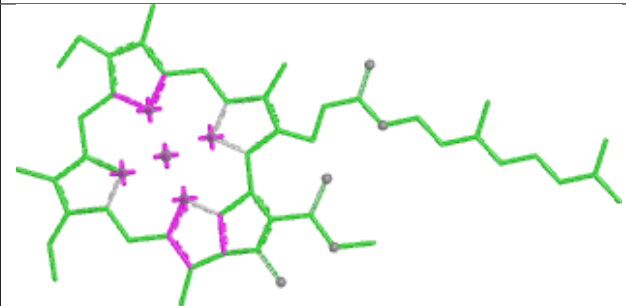
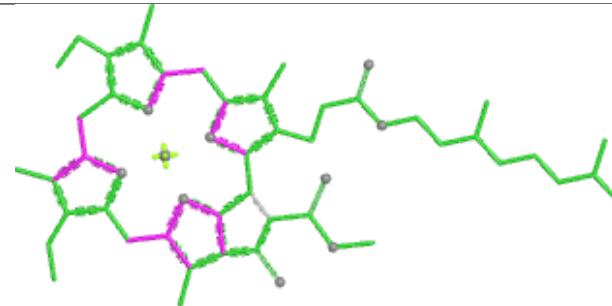
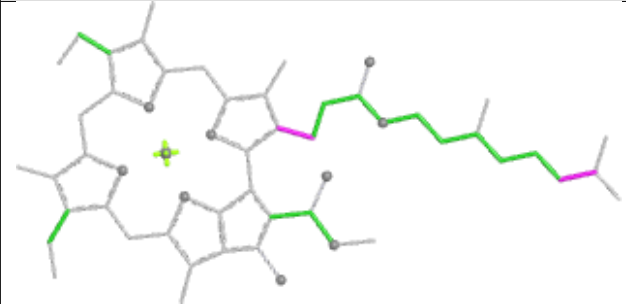
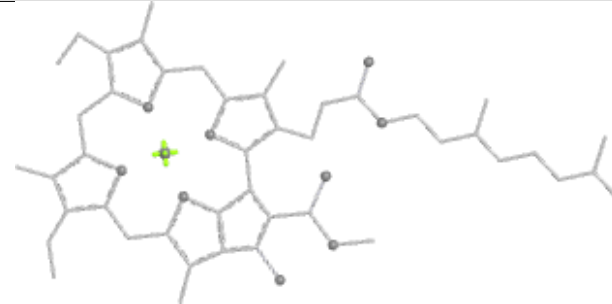


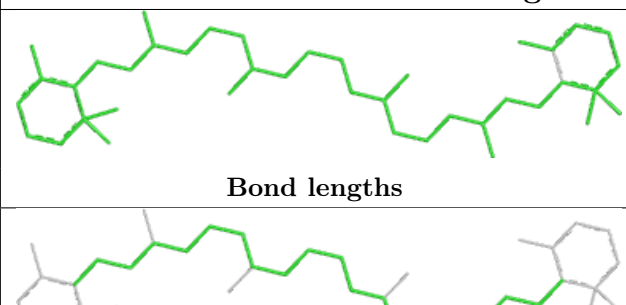
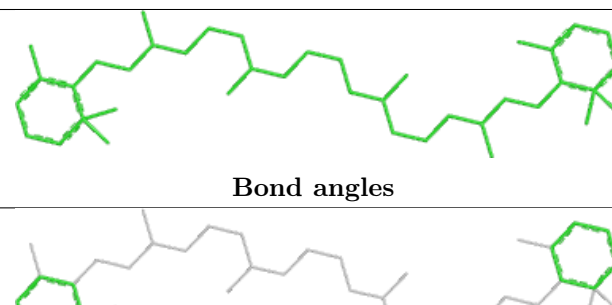
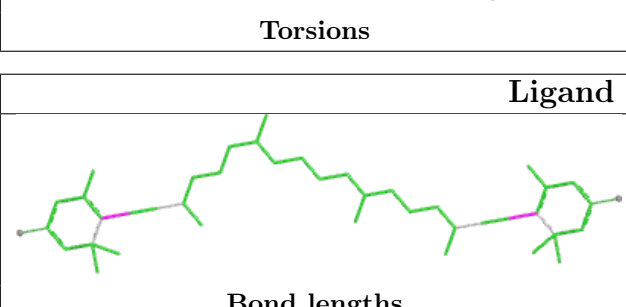
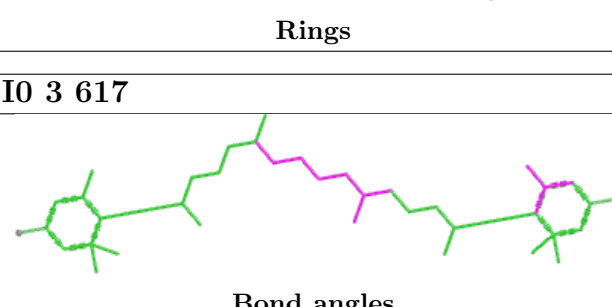
## Ligand KC2 Z 307

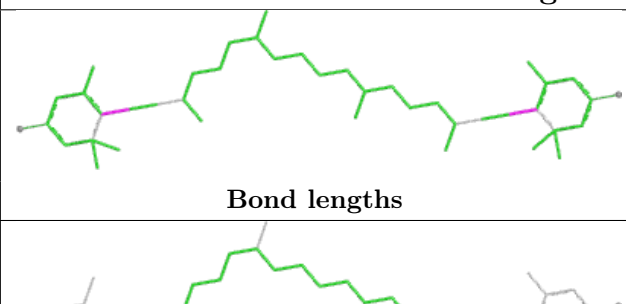
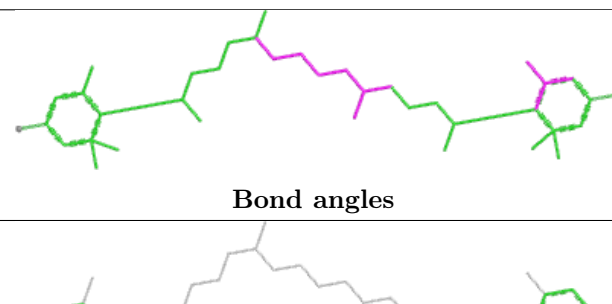


## Ligand CLA 8 615



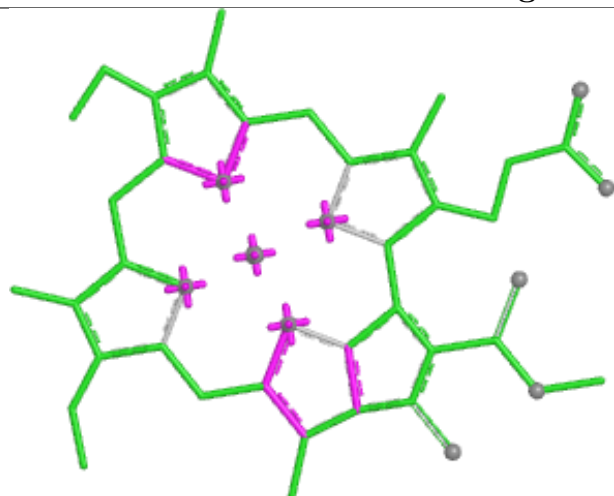
| Ligand CLA A 802                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand 8CT A 848                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

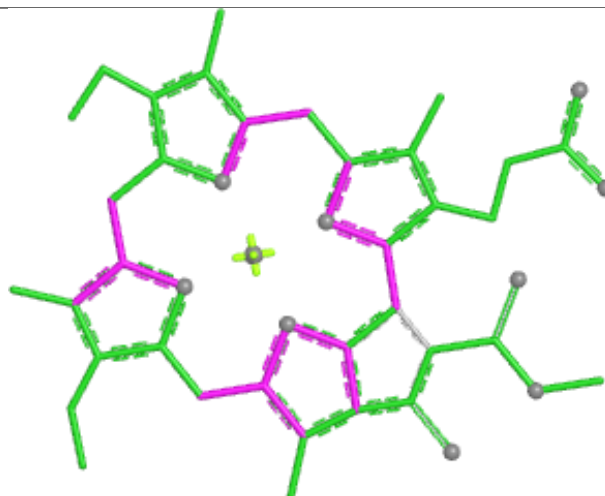
| Ligand II0 3 617                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |



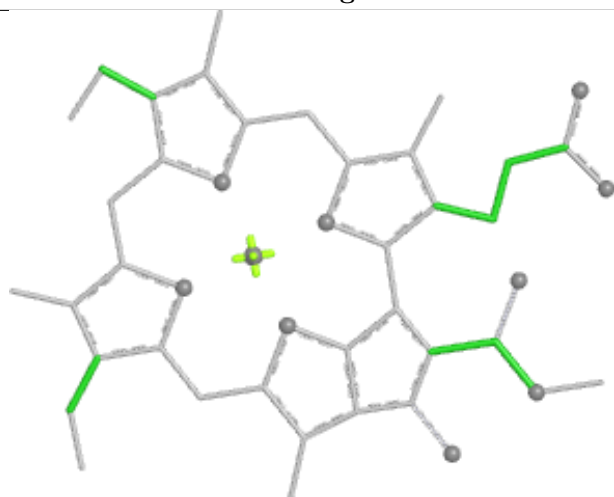
## Ligand CLA 2 611



Bond lengths



Bond angles

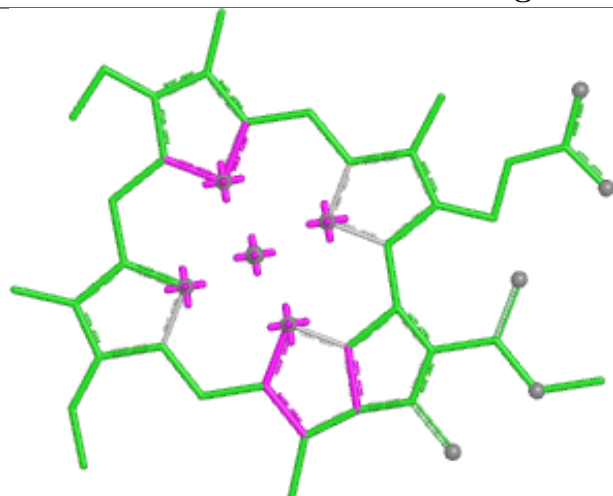


Torsions

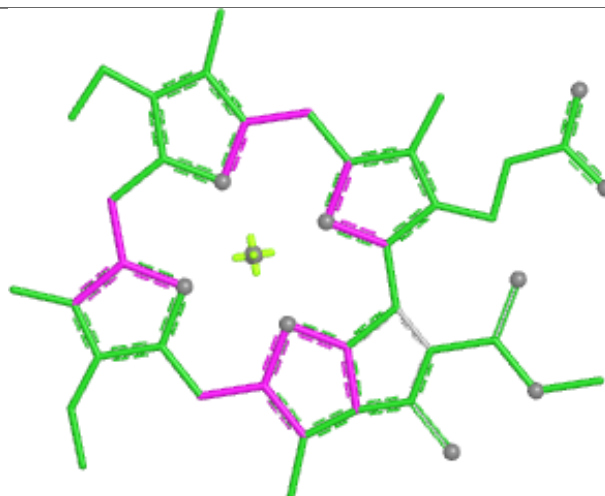


Rings

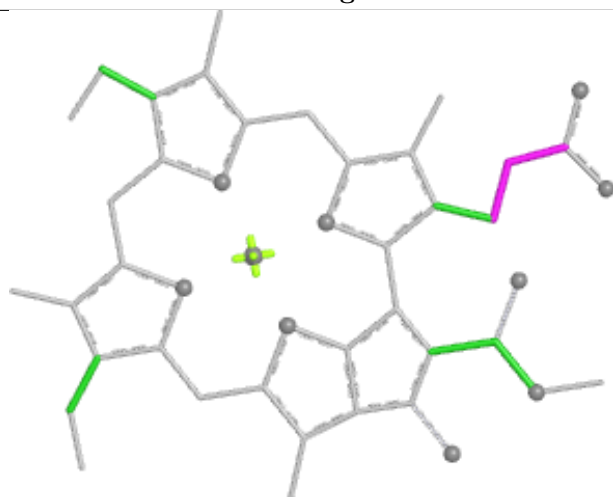
## Ligand CLA B 803



Bond lengths



Bond angles

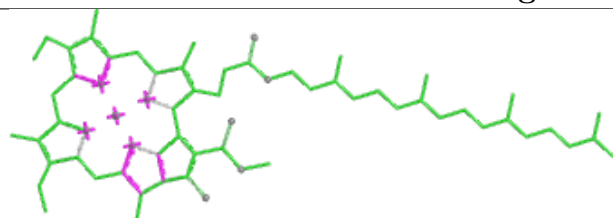


Torsions

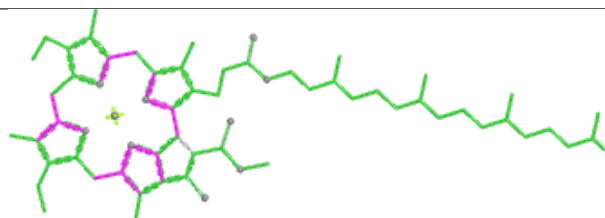


Rings

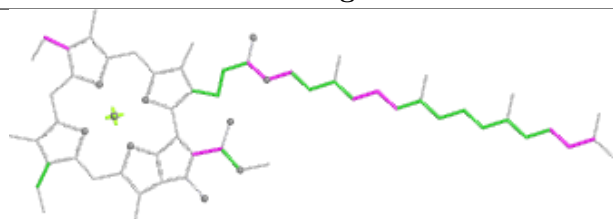
## Ligand CLA 4 611



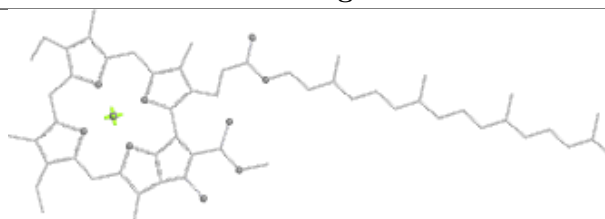
Bond lengths



Bond angles

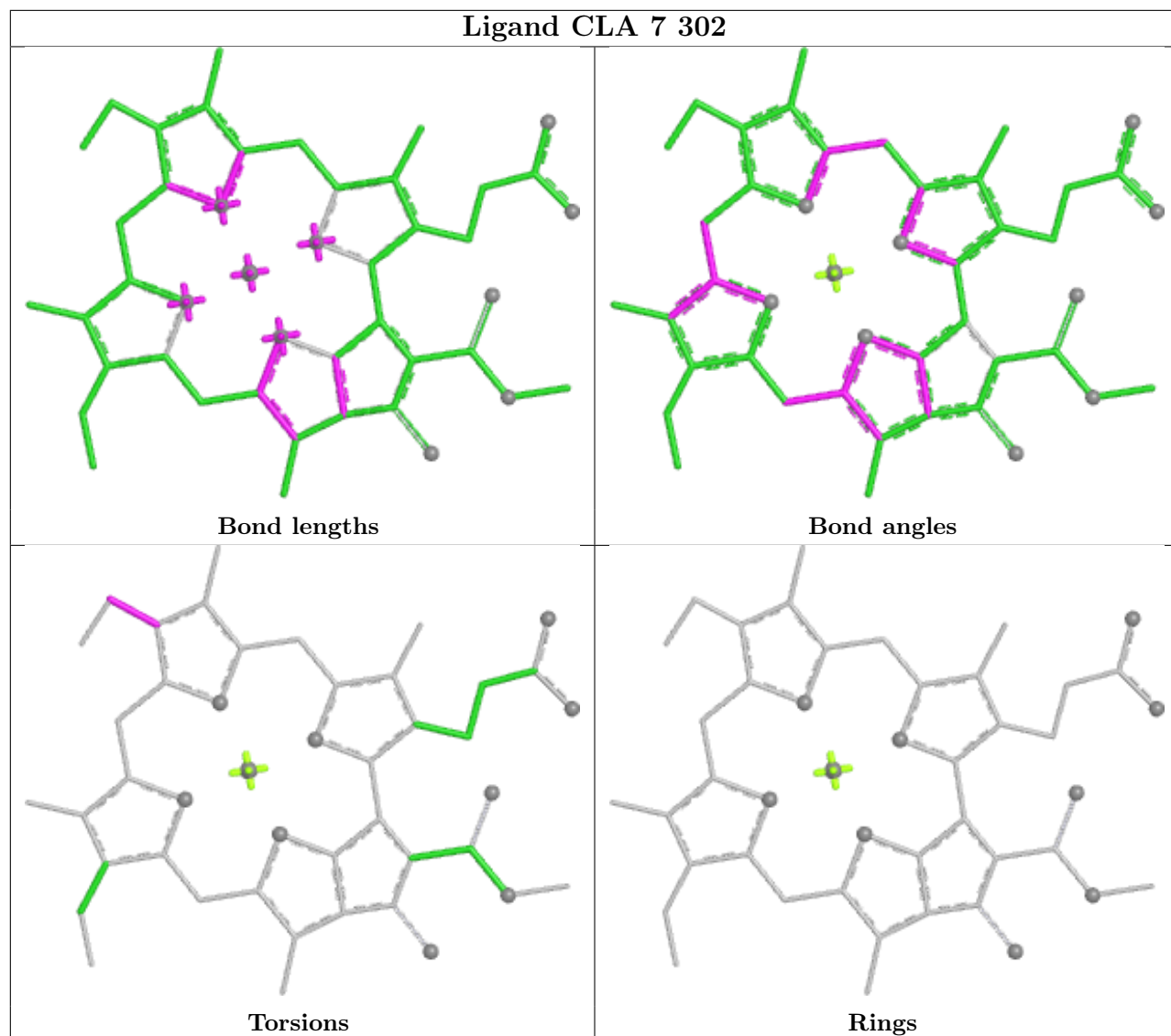


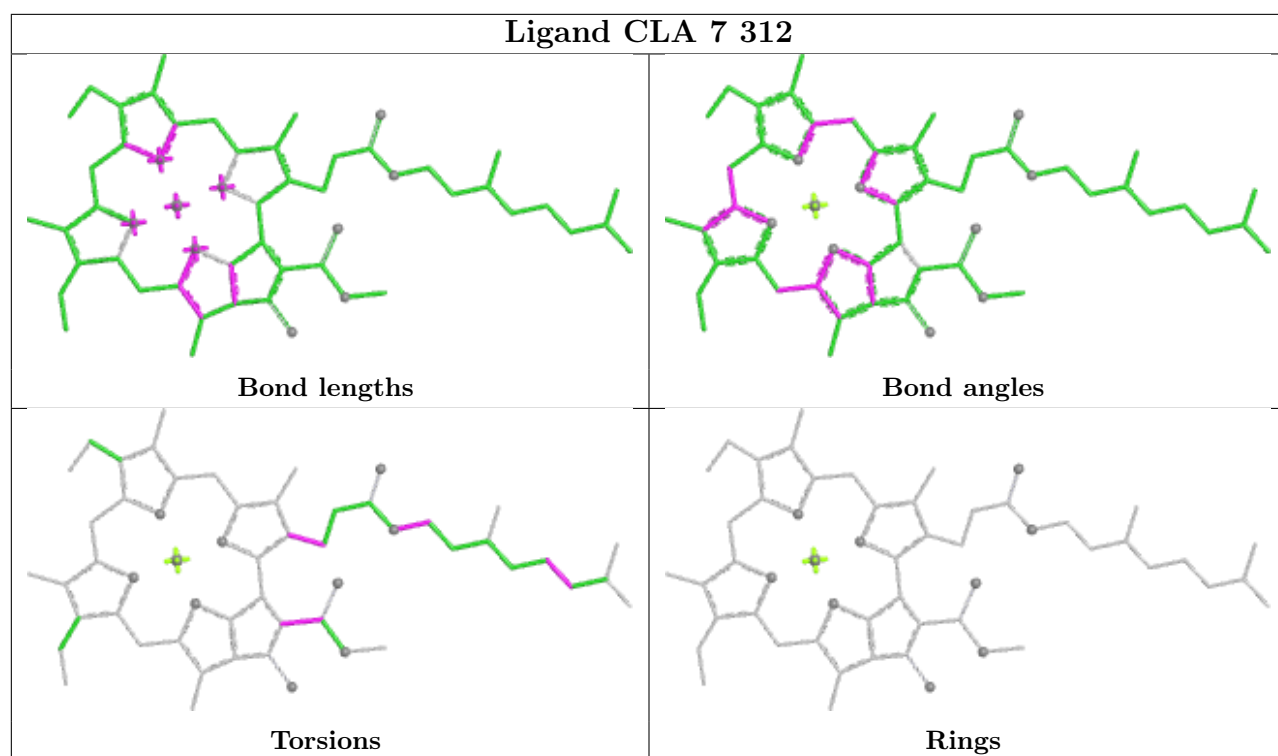
Torsions



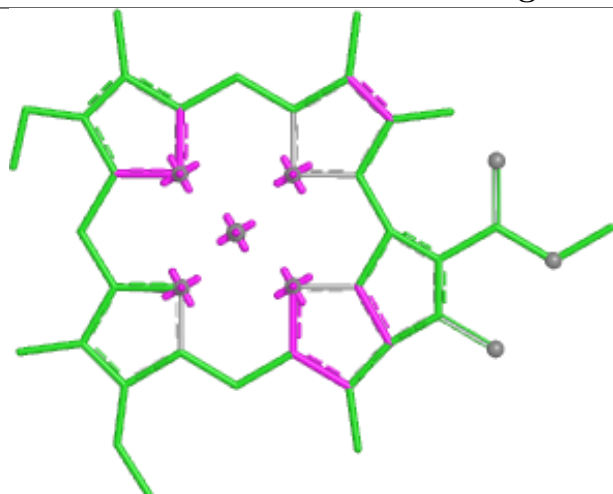
Rings

## Ligand CLA 7 302

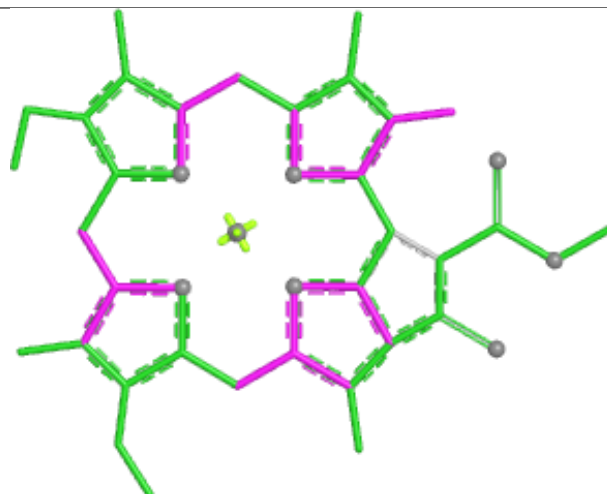




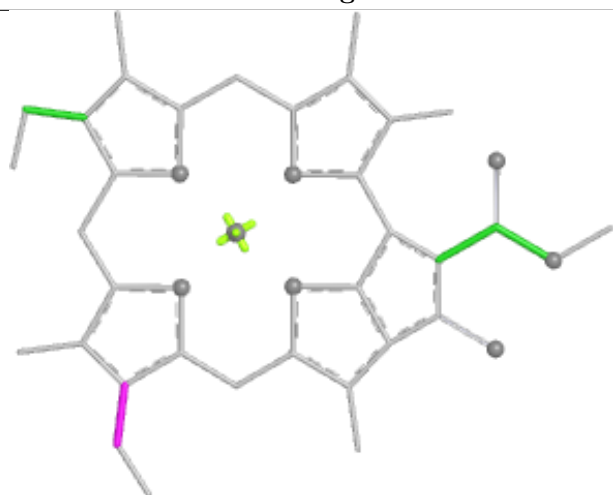
## Ligand CLA 9 609



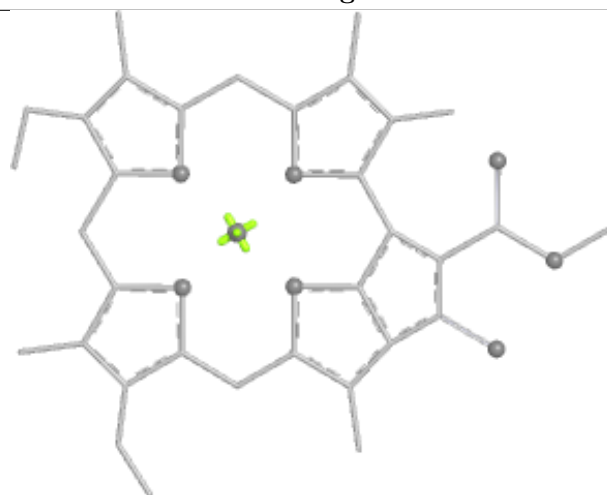
Bond lengths



Bond angles

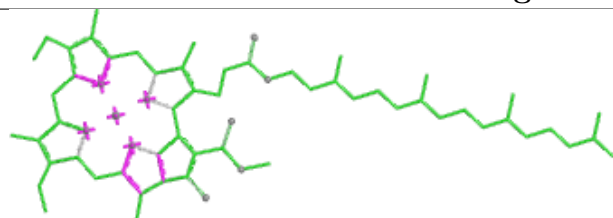


Torsions

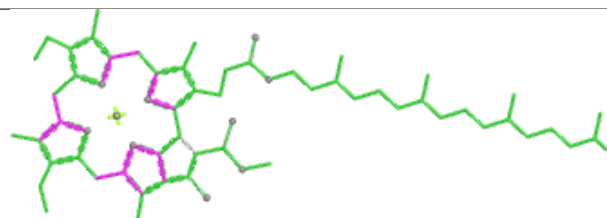


Rings

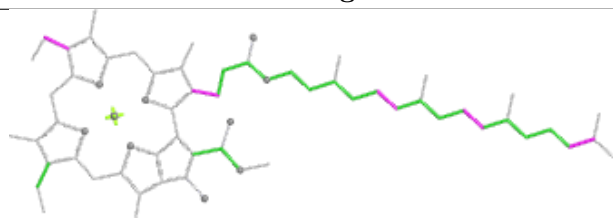
## Ligand CLA A 837



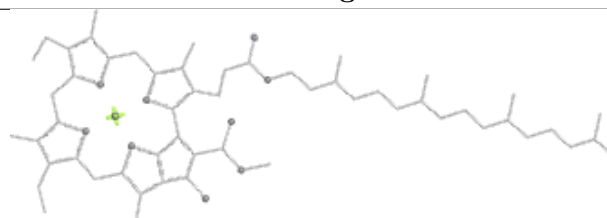
Bond lengths



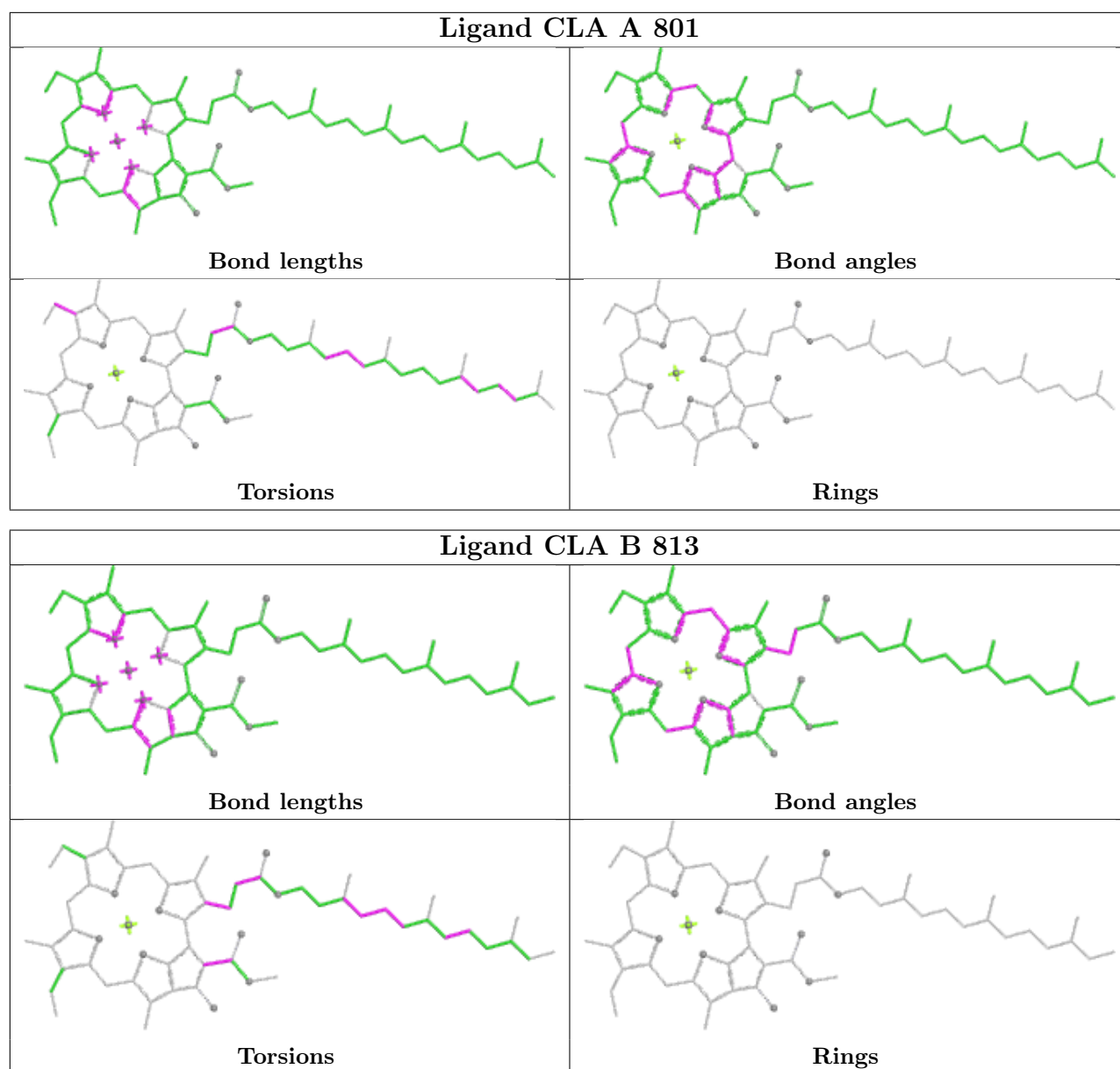
Bond angles

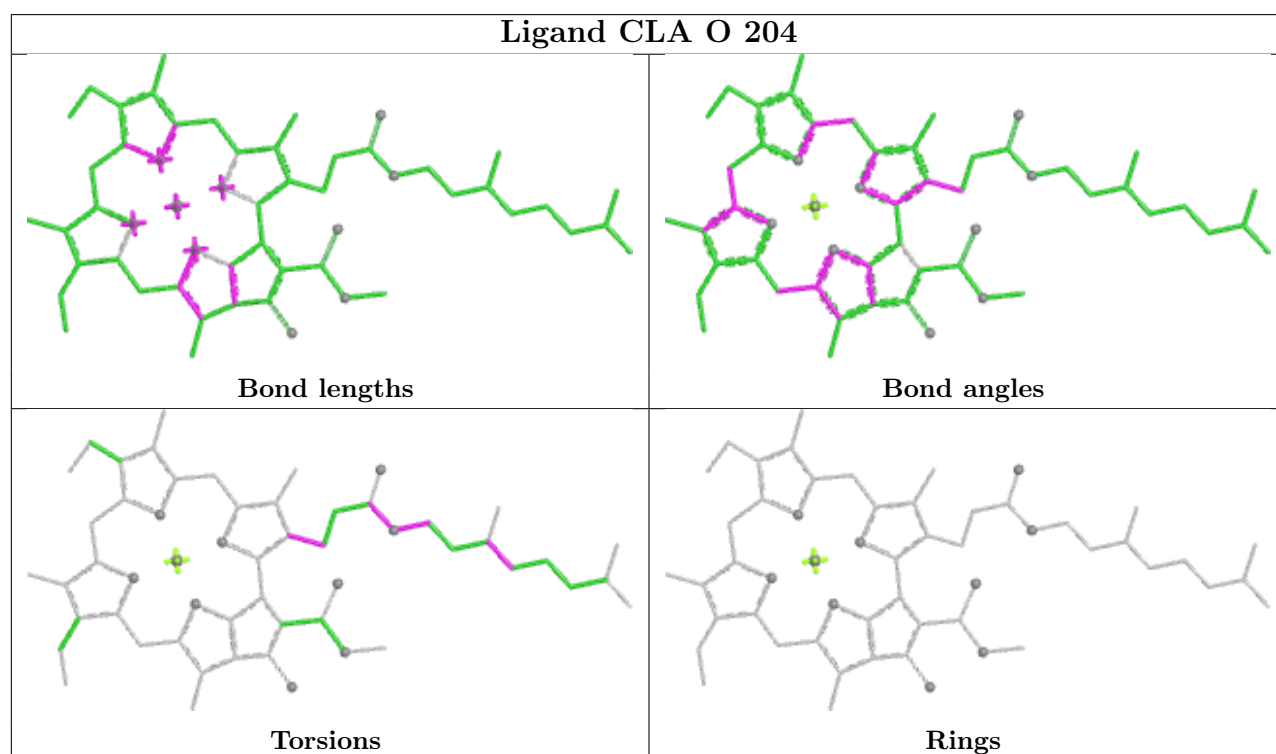
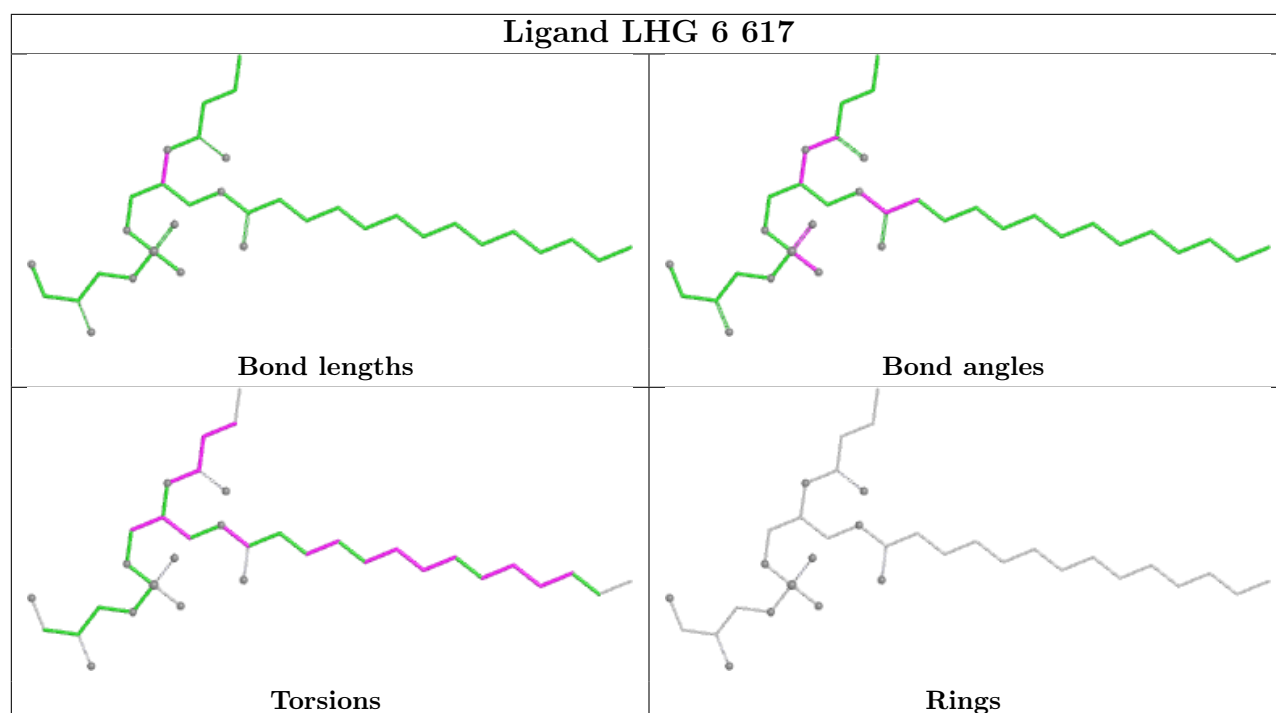


Torsions

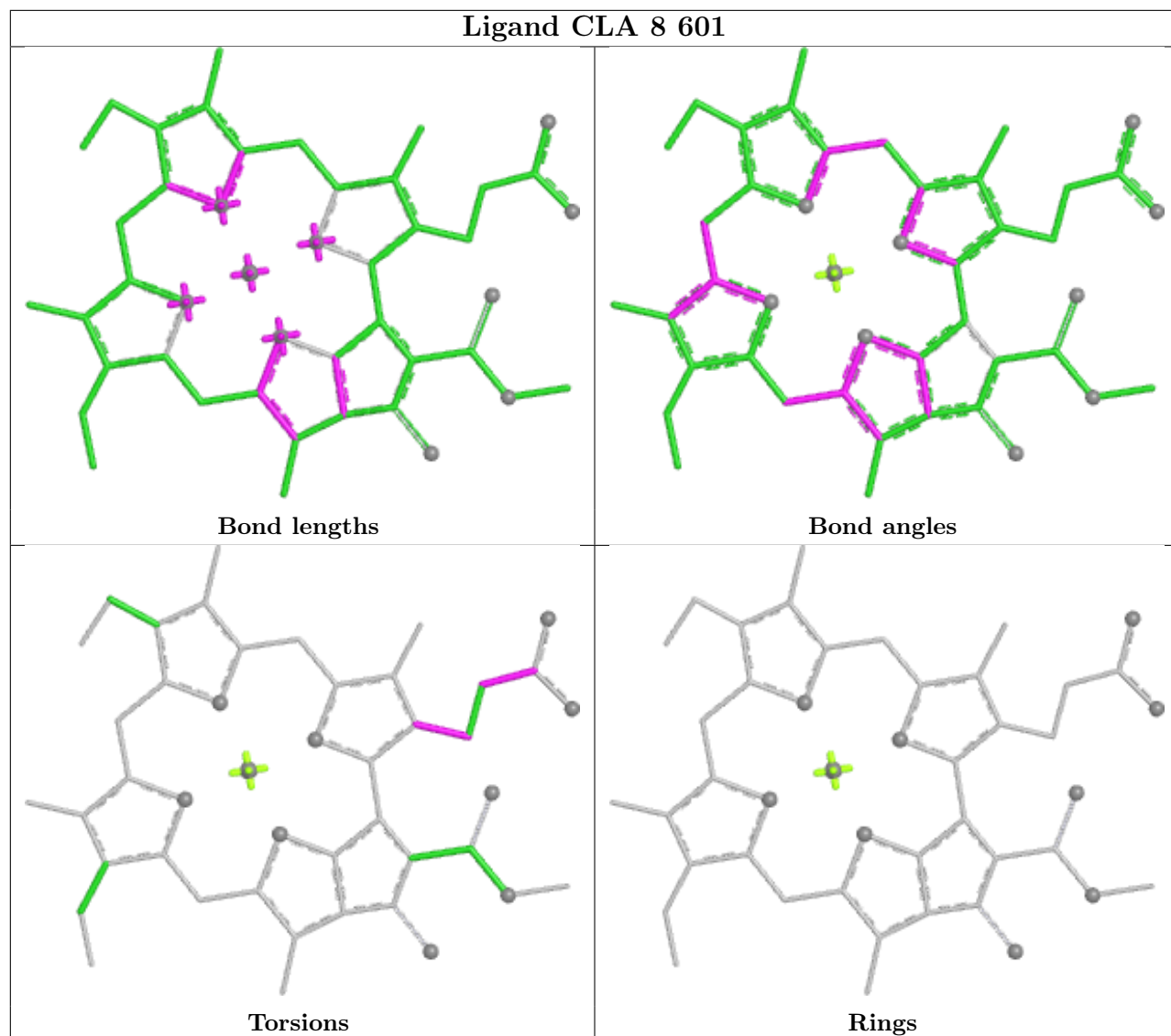


Rings



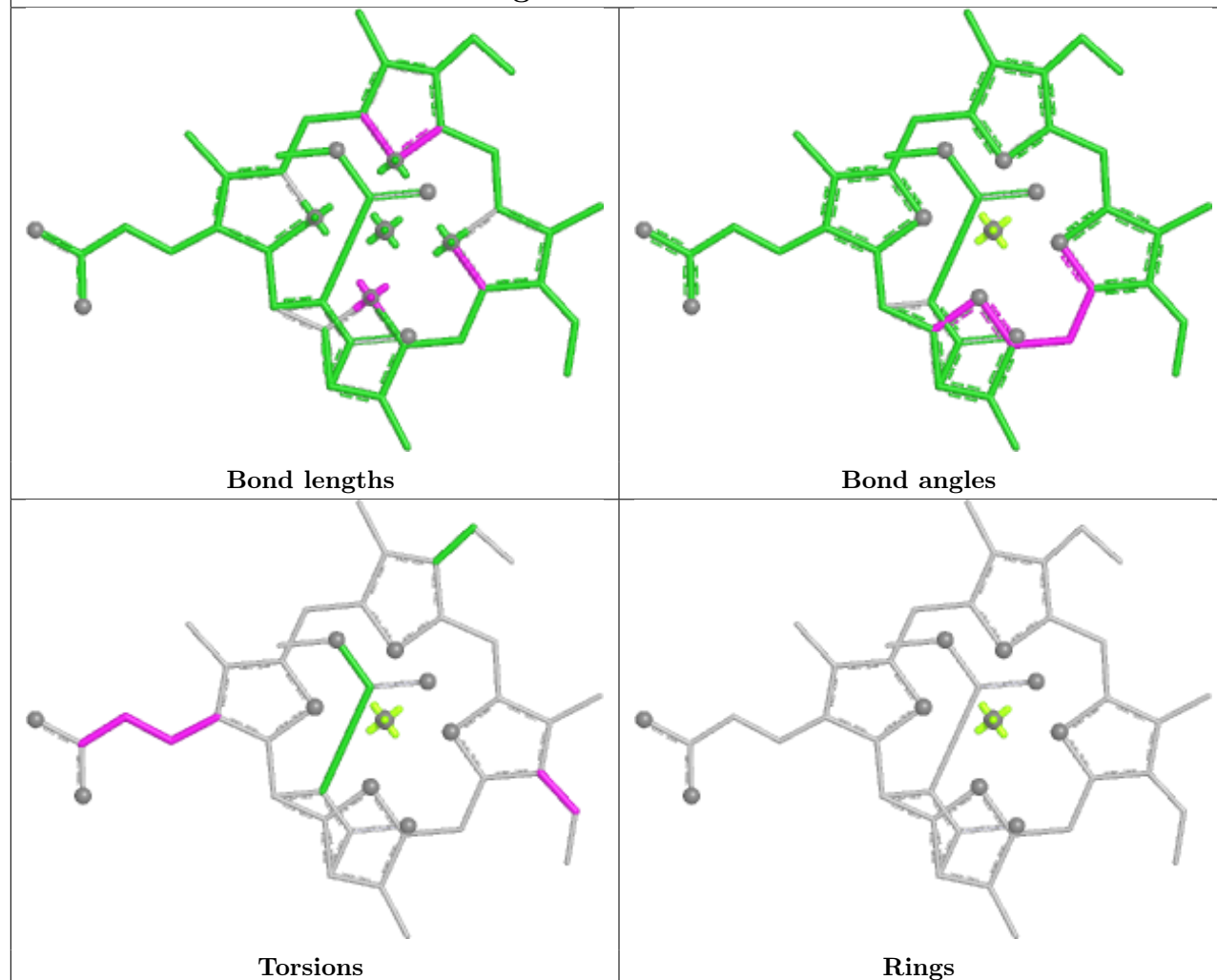


## Ligand CLA 8 601

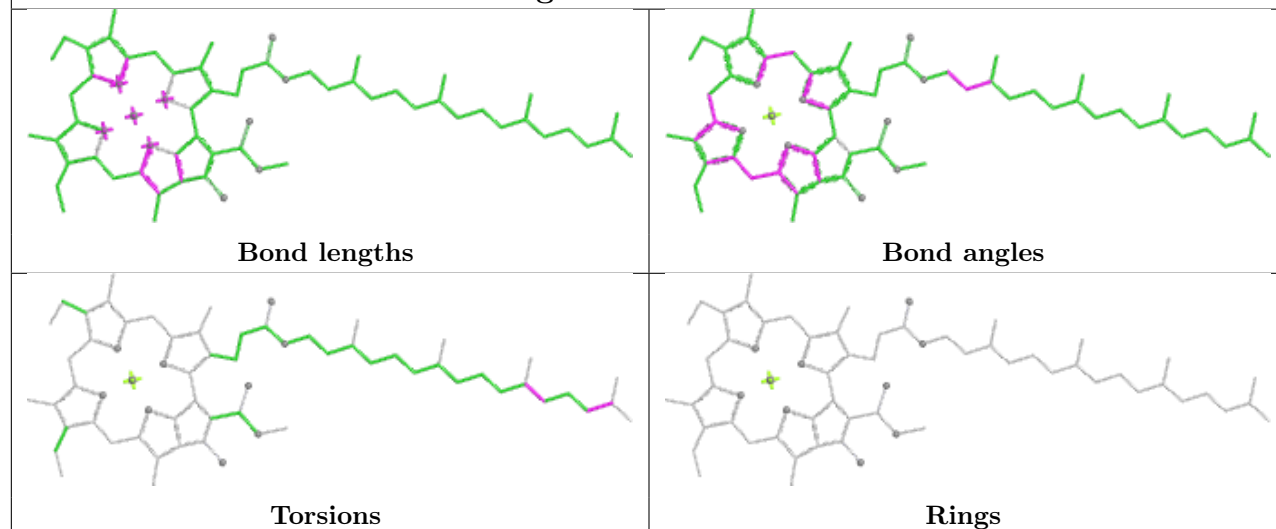




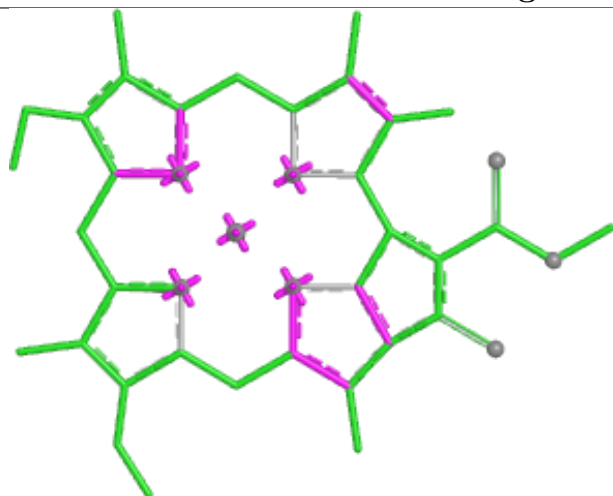
## Ligand KC2 6 610



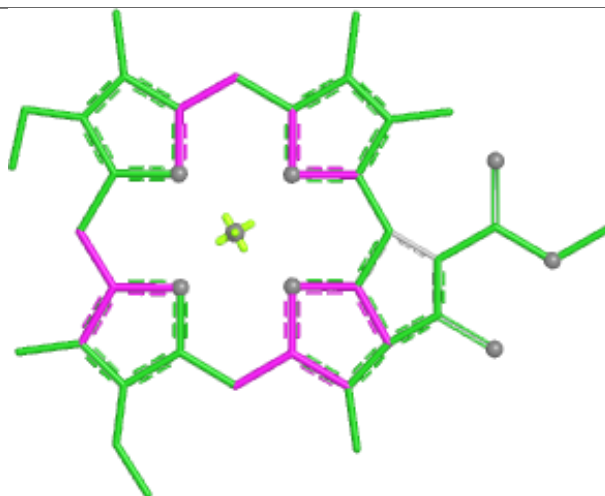
## Ligand CLA 7 303



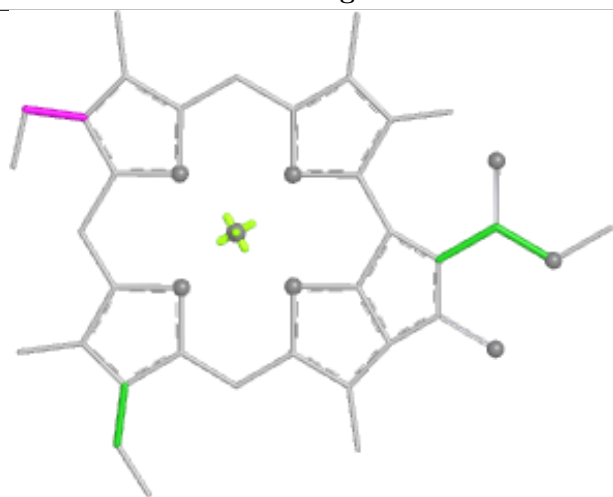
## Ligand CLA 2 609



Bond lengths



Bond angles

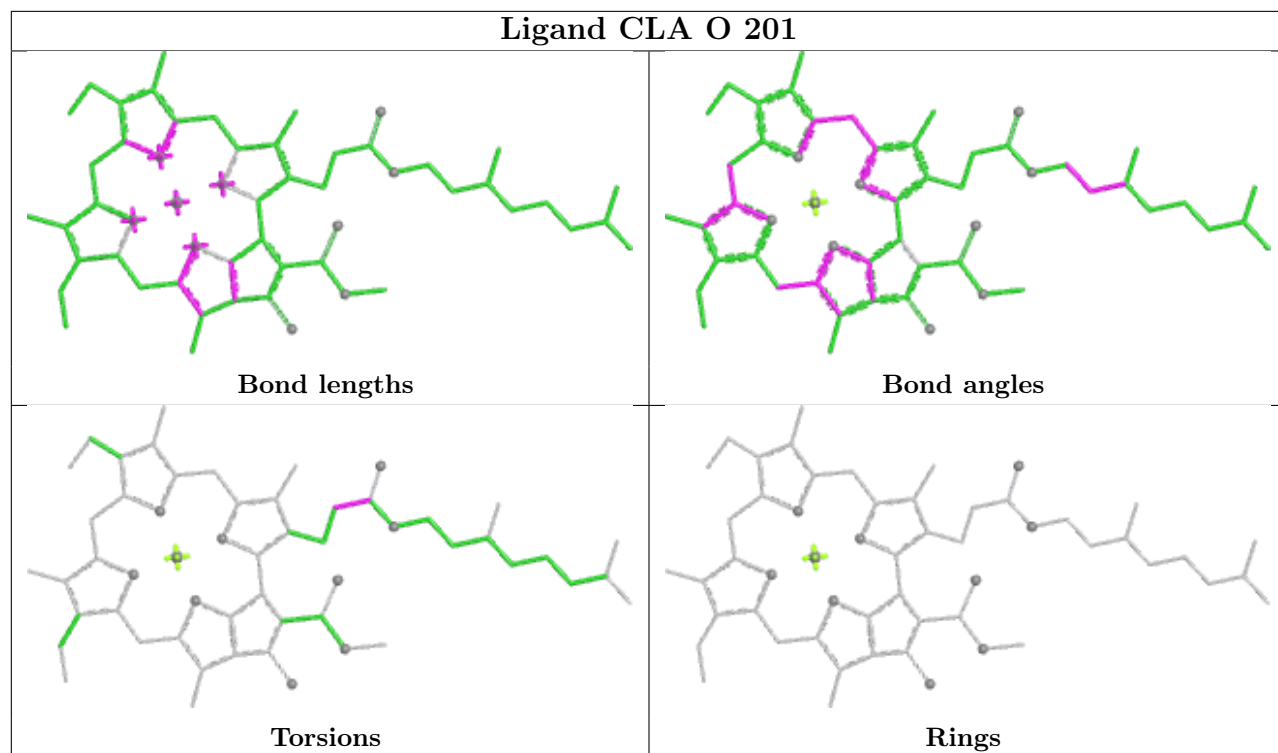


Torsions

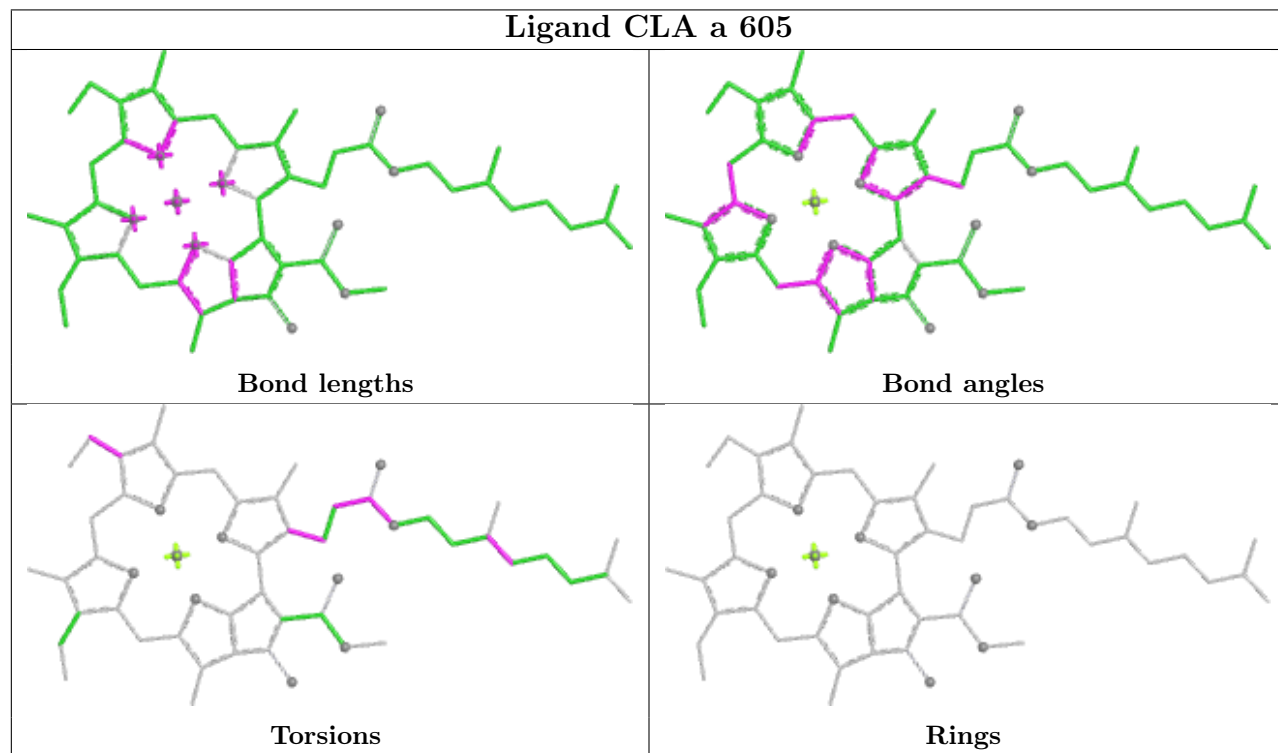


Rings

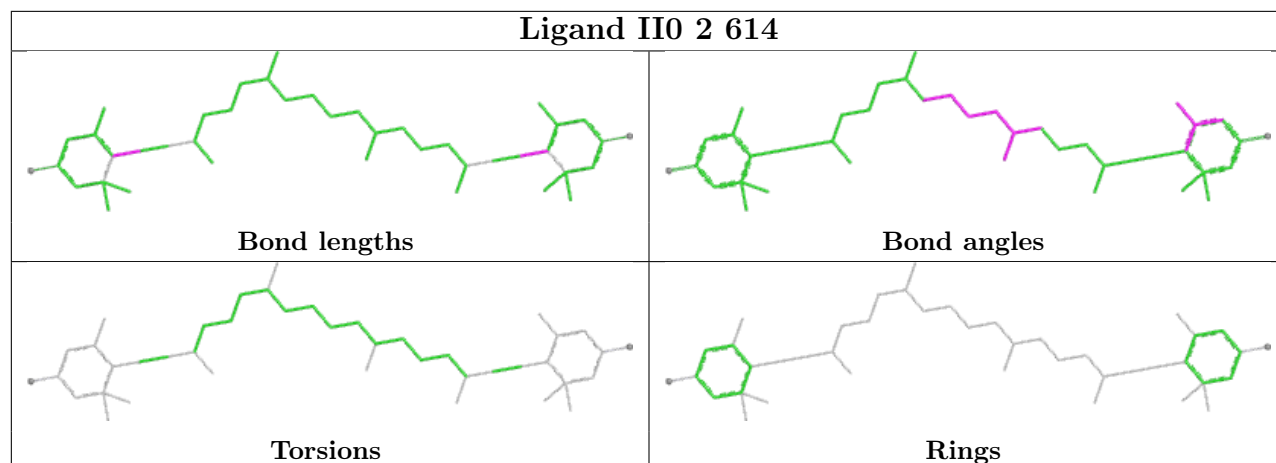
## Ligand CLA O 201



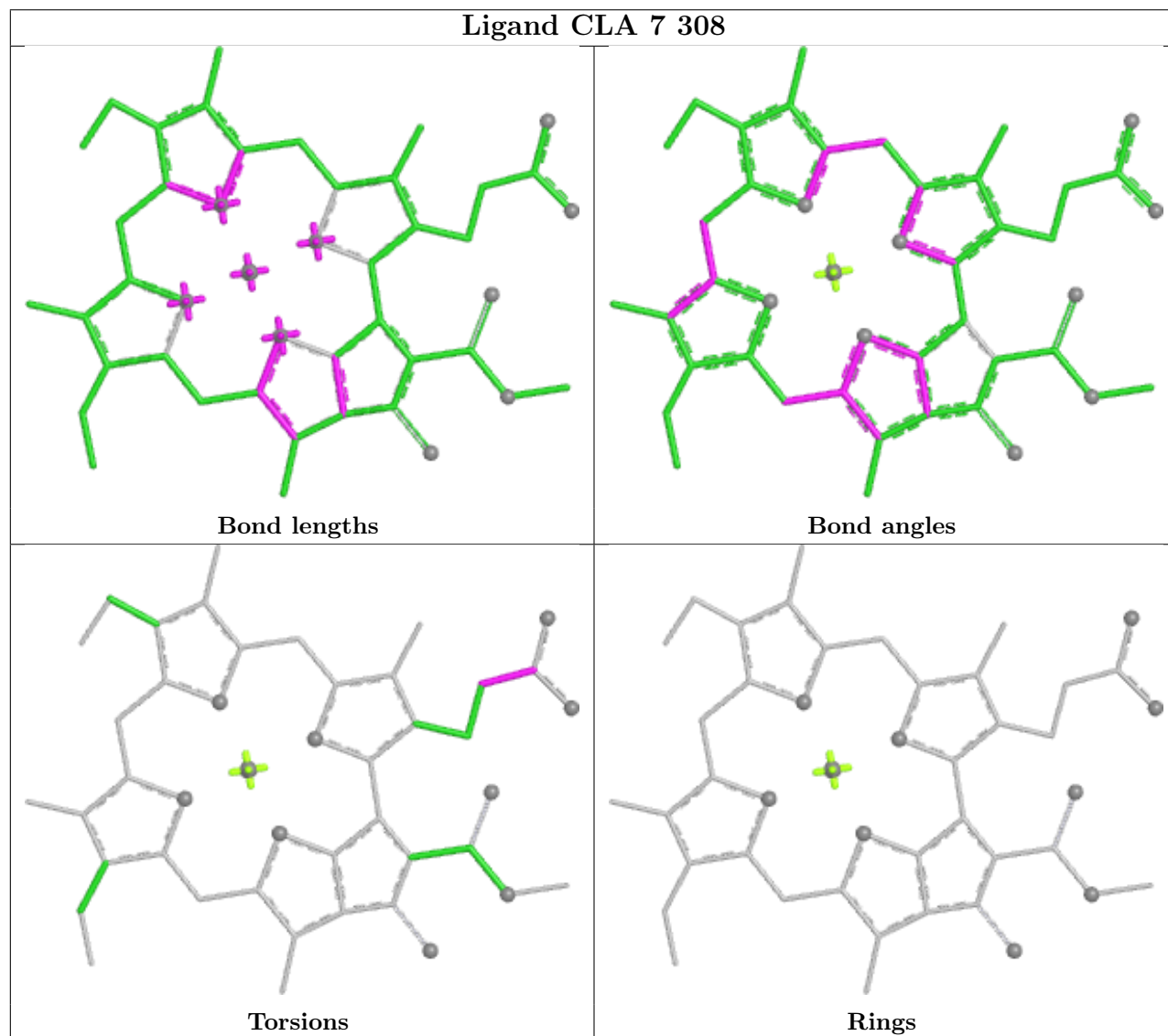
## Ligand CLA a 605



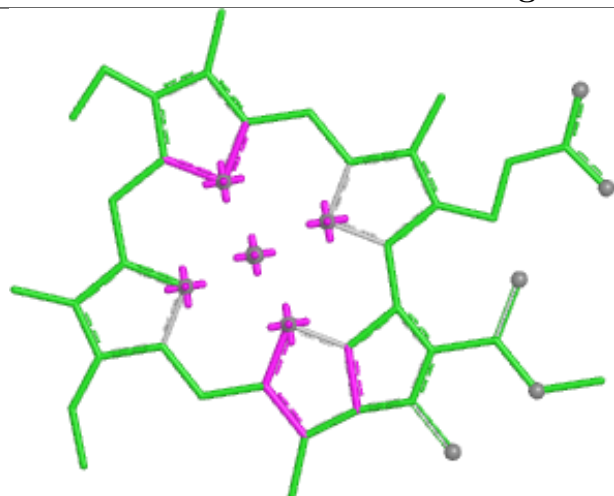
## Ligand II0 2 614



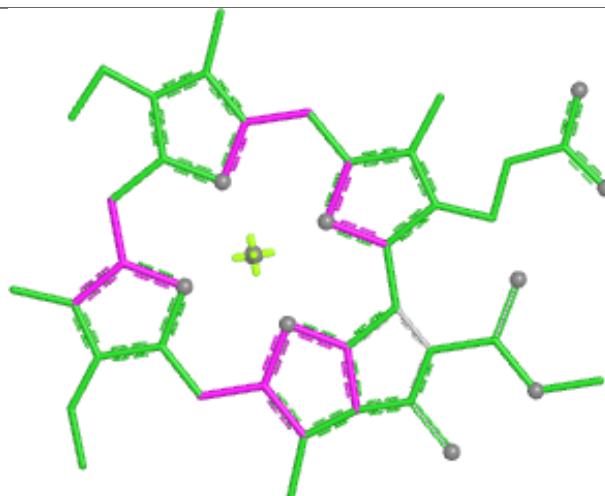
## Ligand CLA 7 308



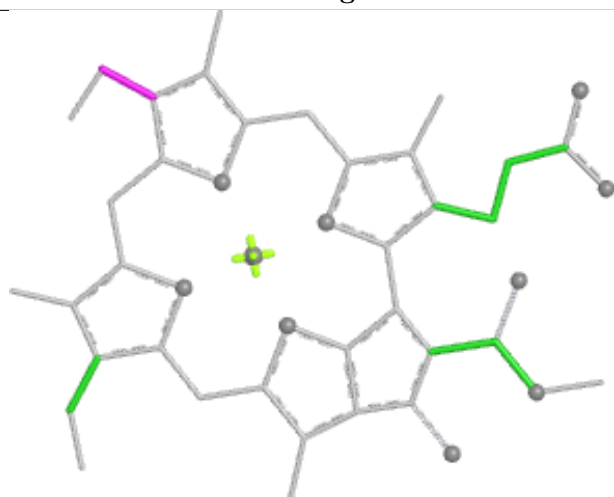
## Ligand CLA 2 607



Bond lengths



Bond angles

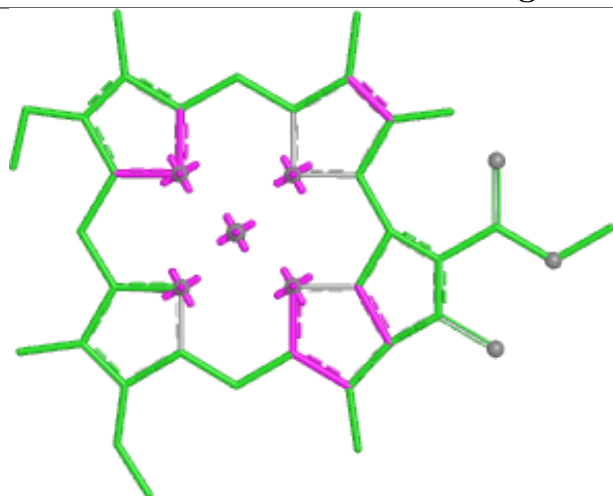


Torsions

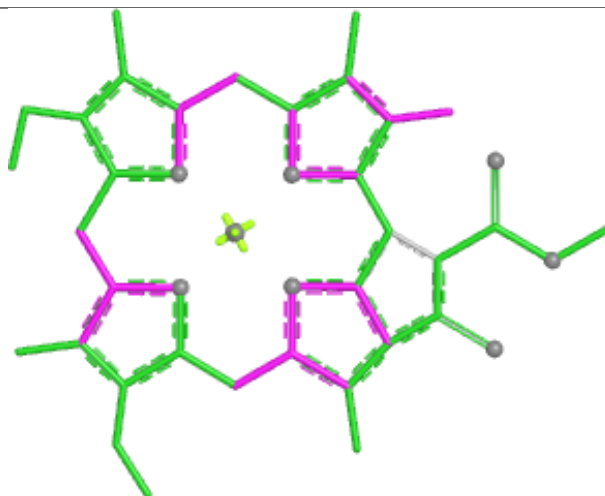


Rings

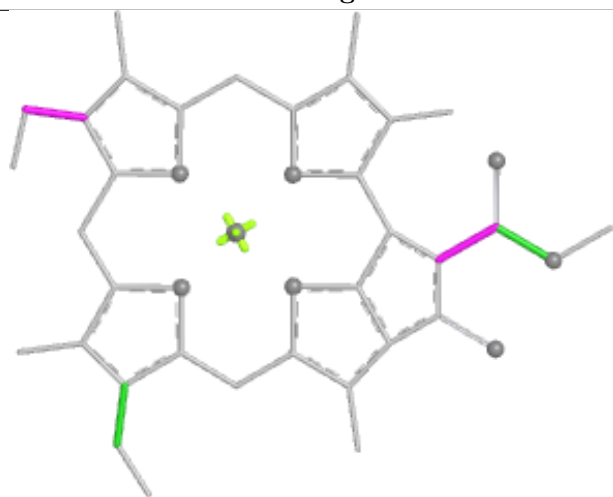
## Ligand CLA 5 613



Bond lengths



Bond angles

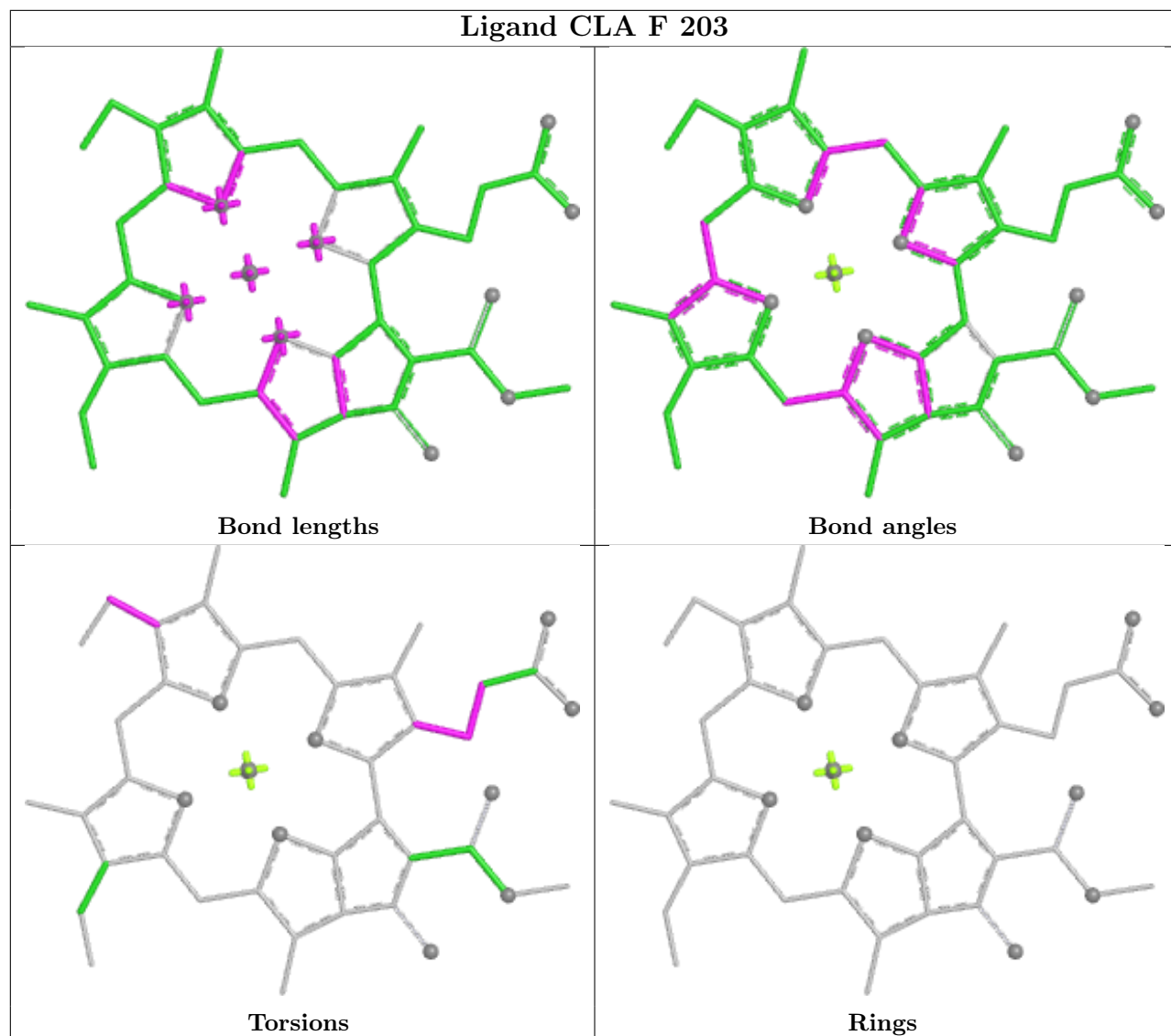


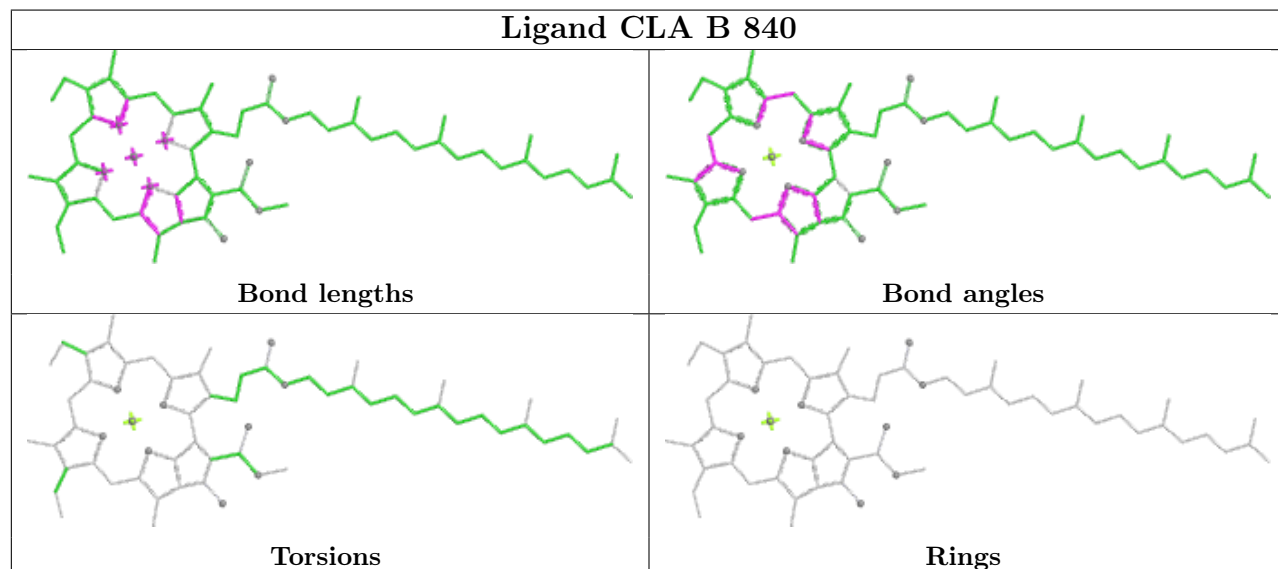
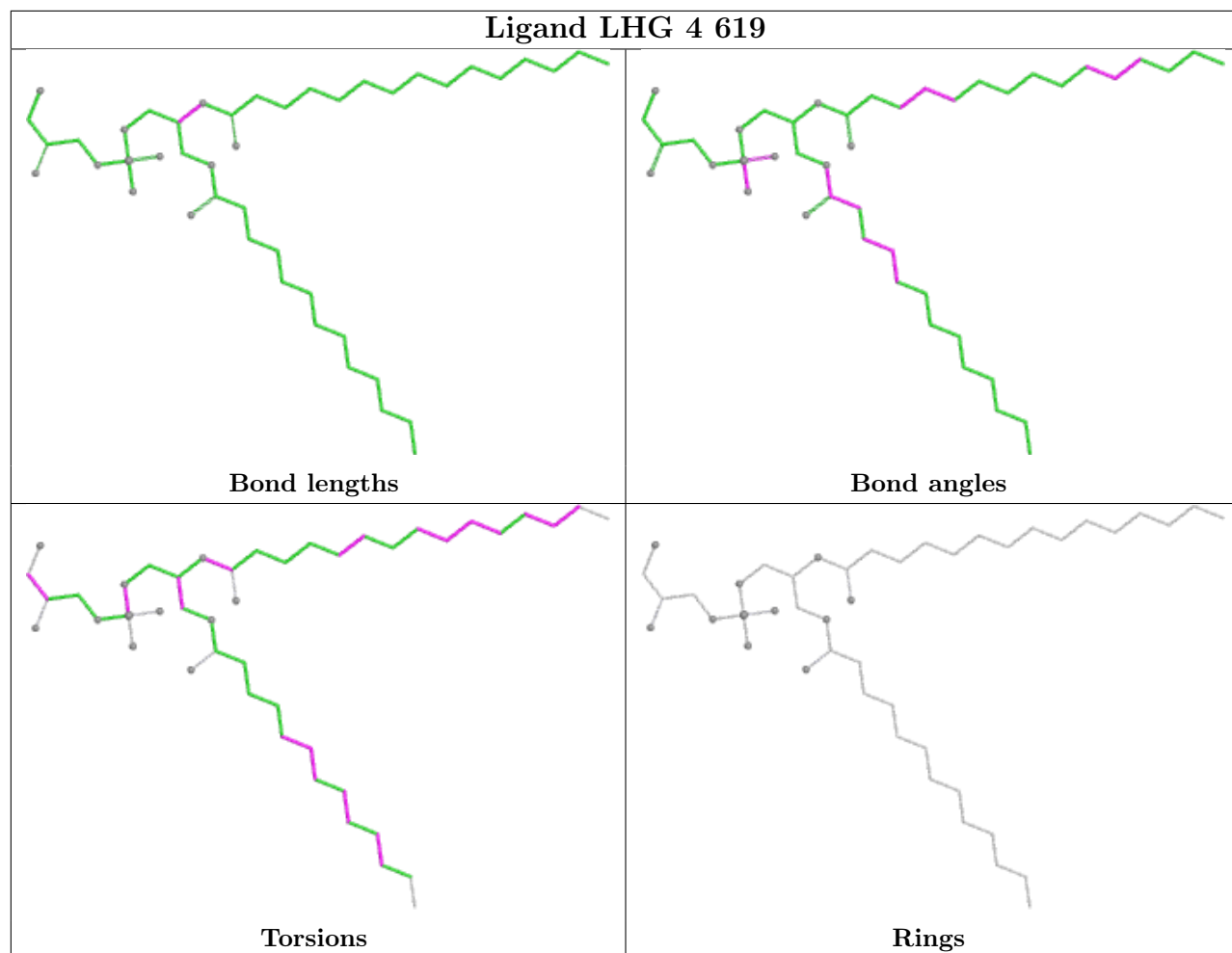
Torsions



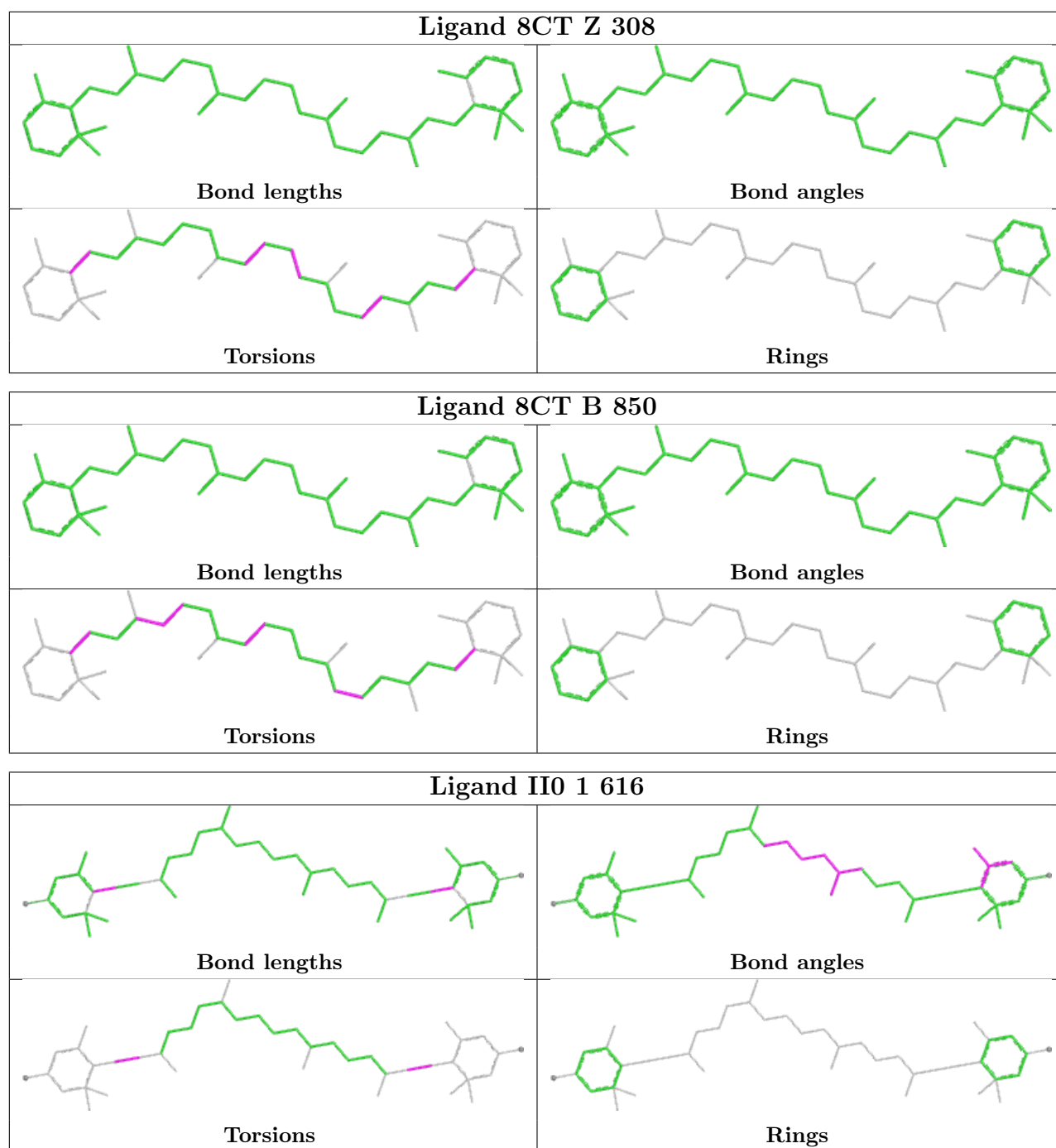
Rings

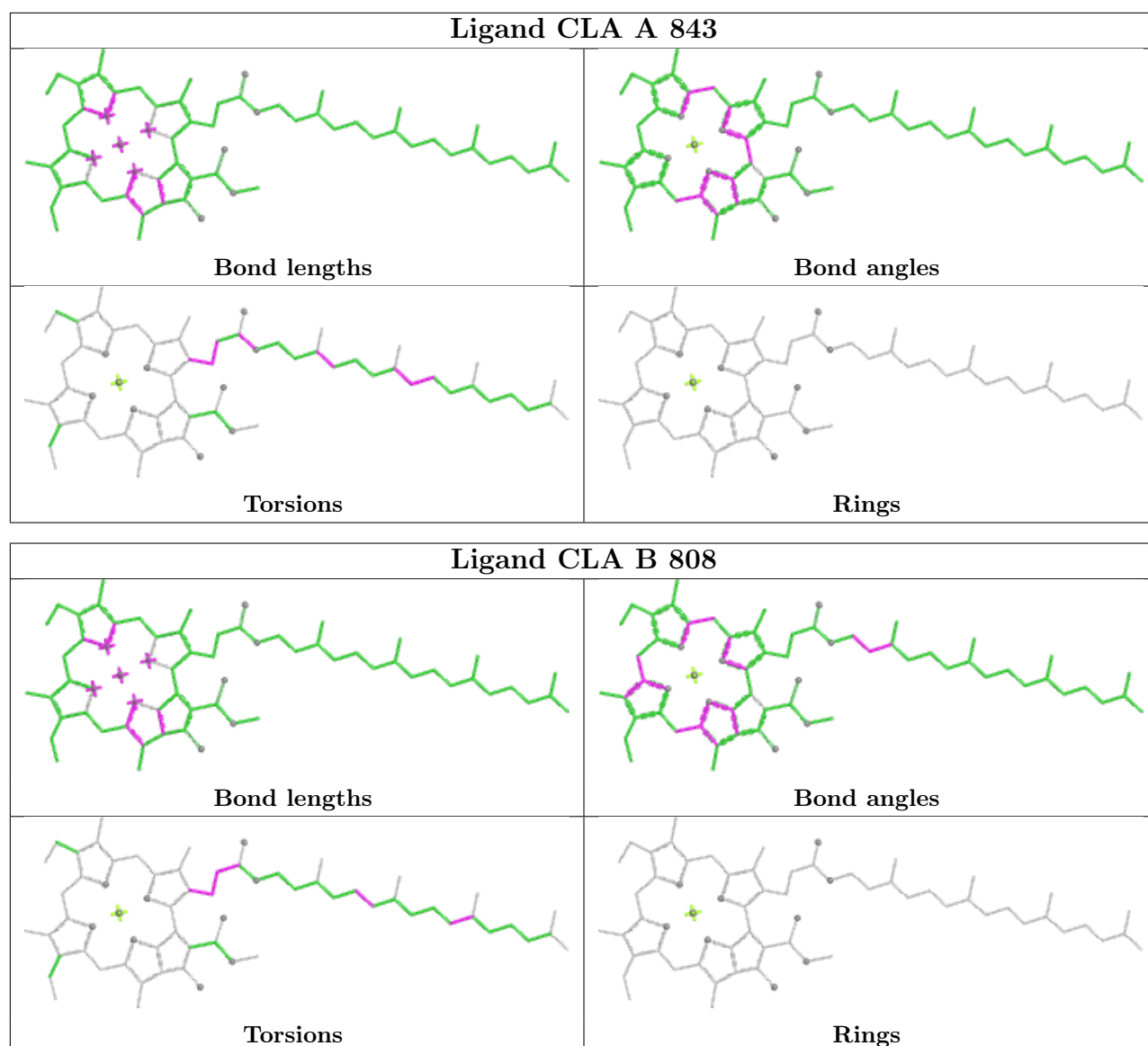
## Ligand CLA F 203



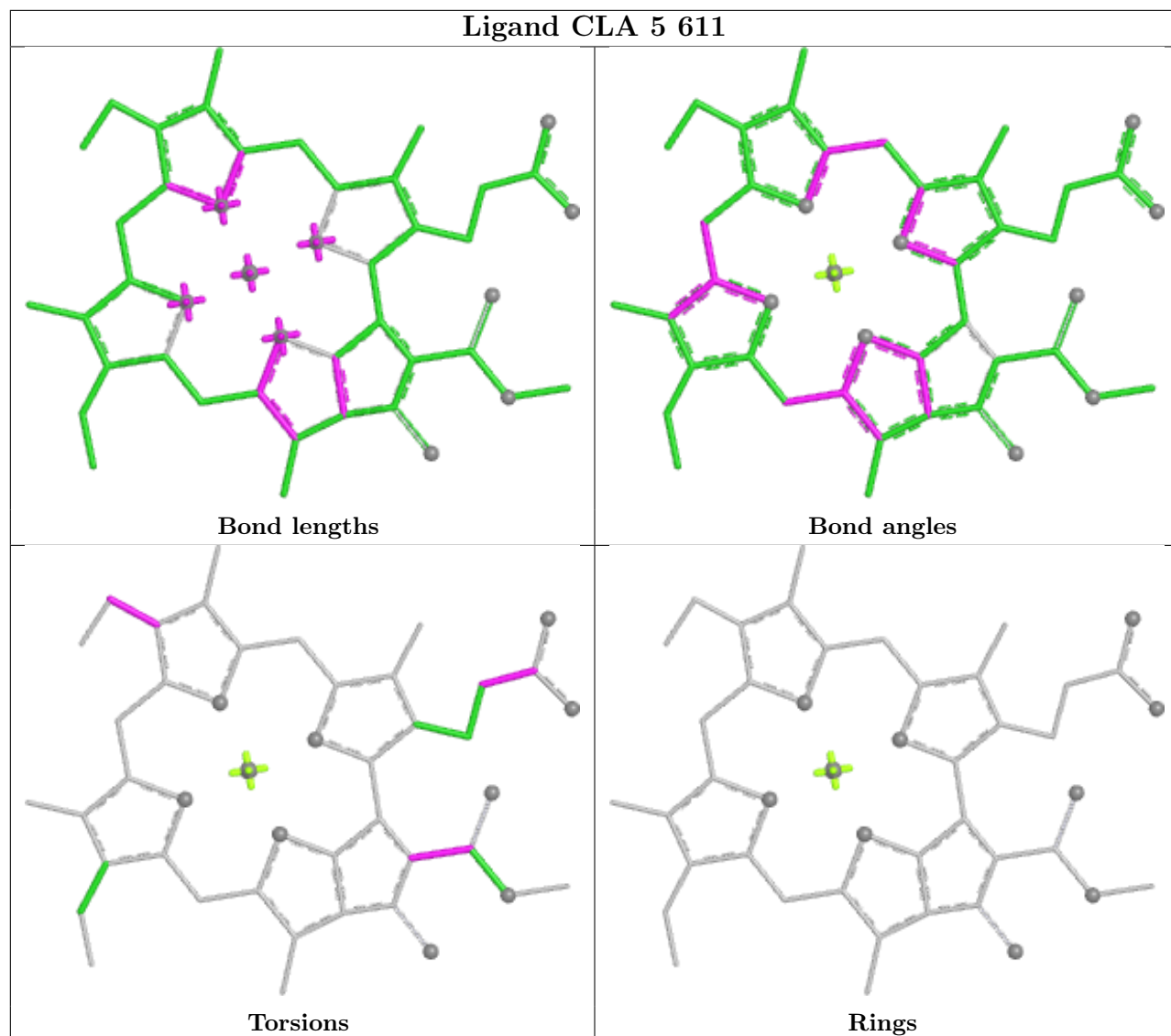


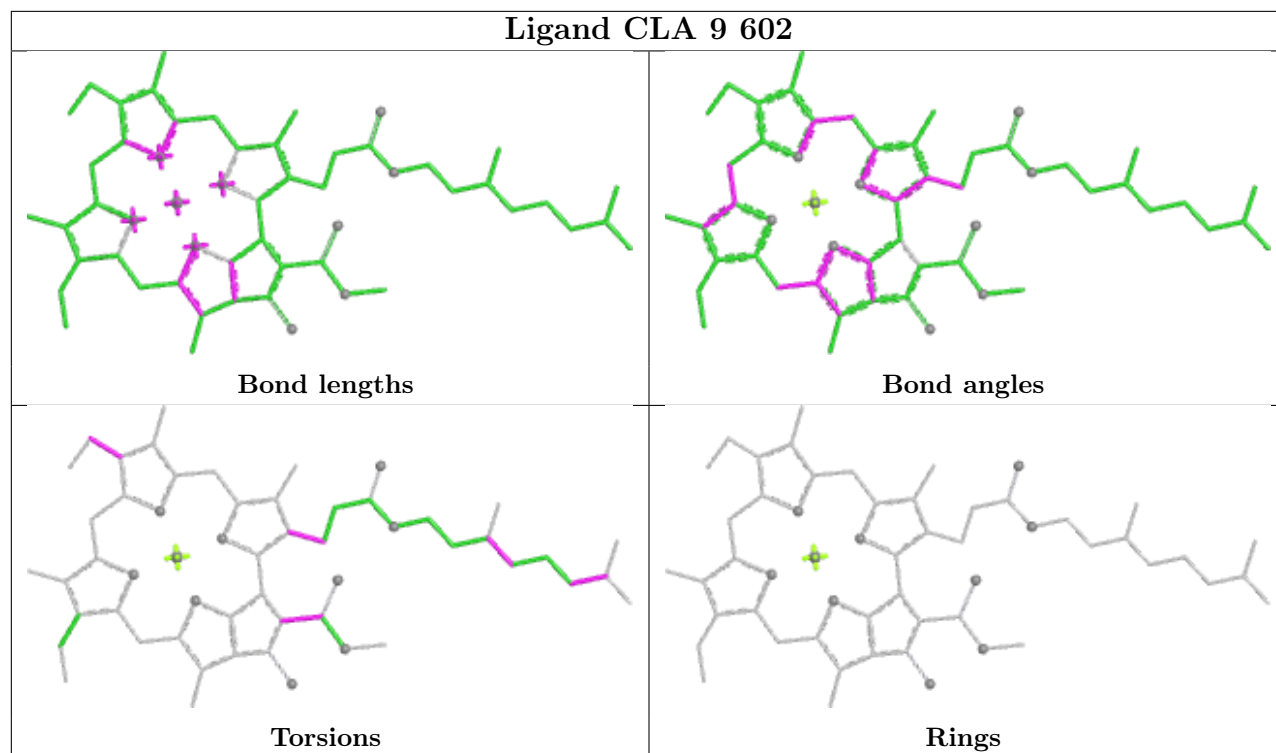
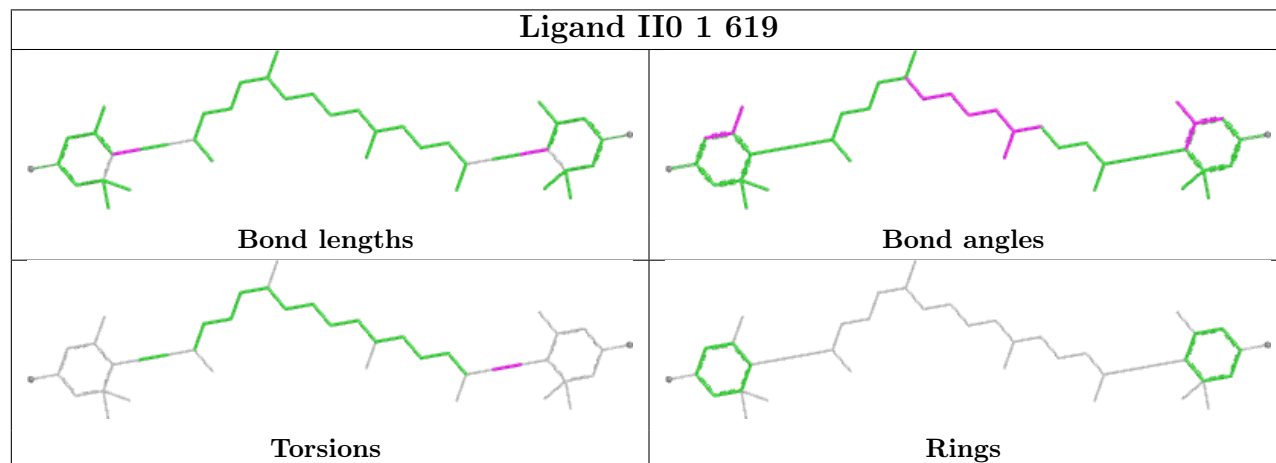


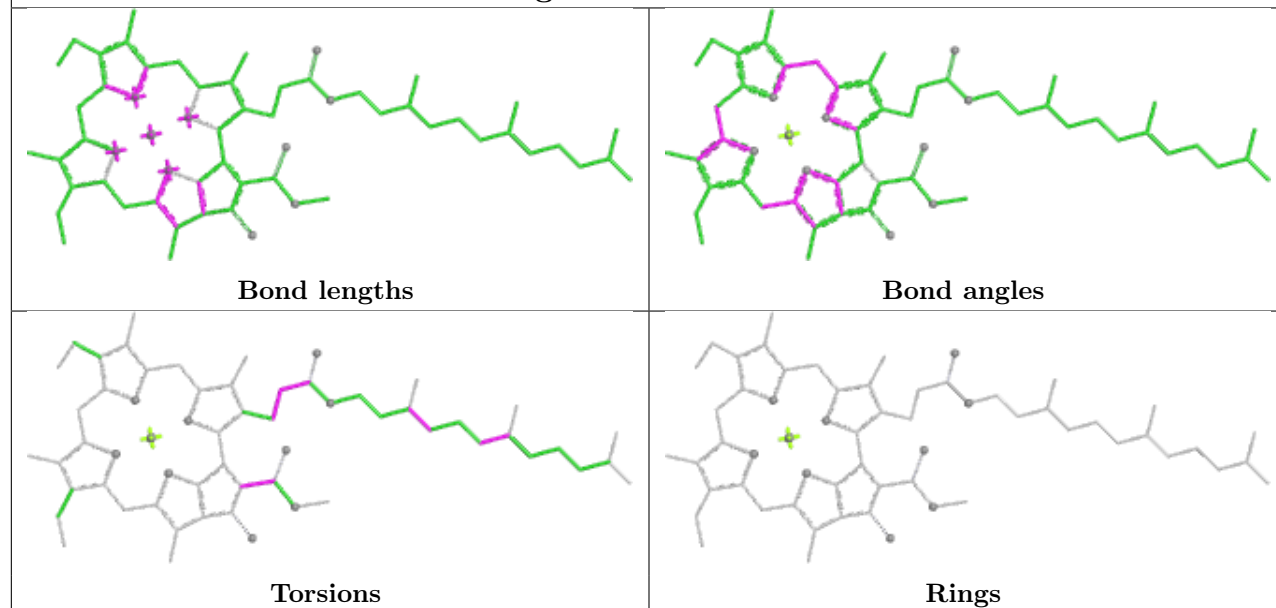
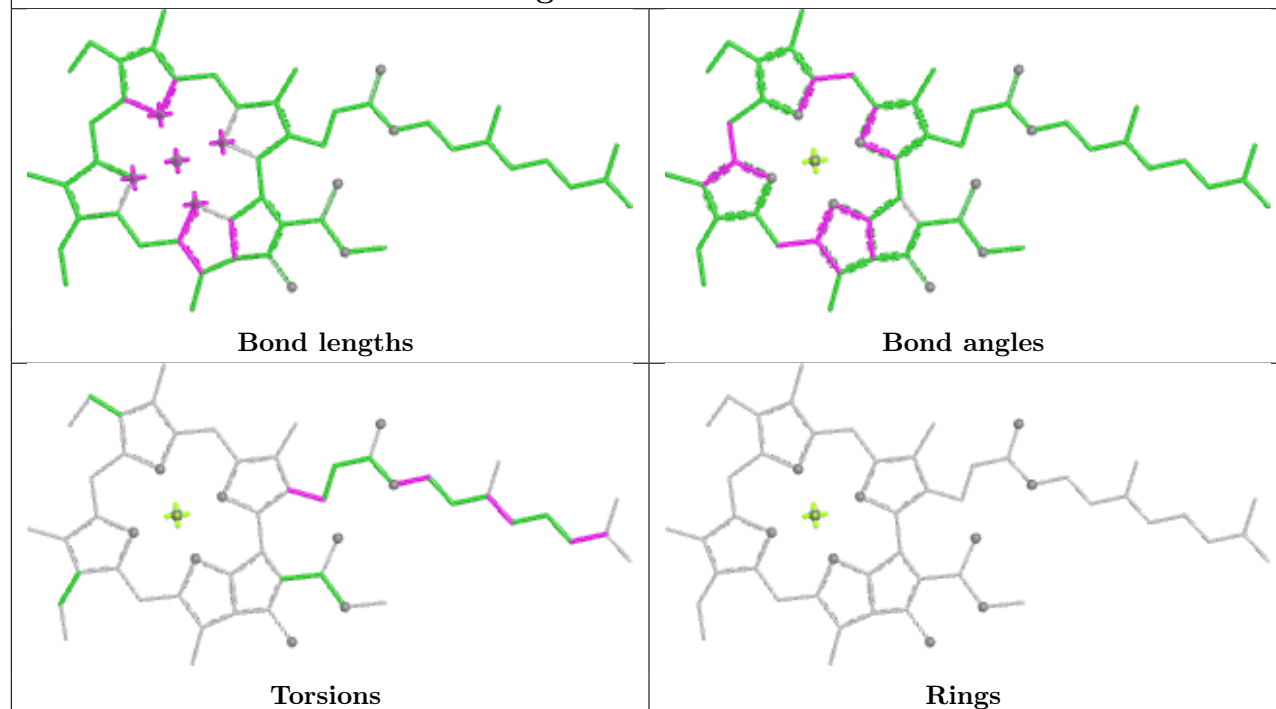


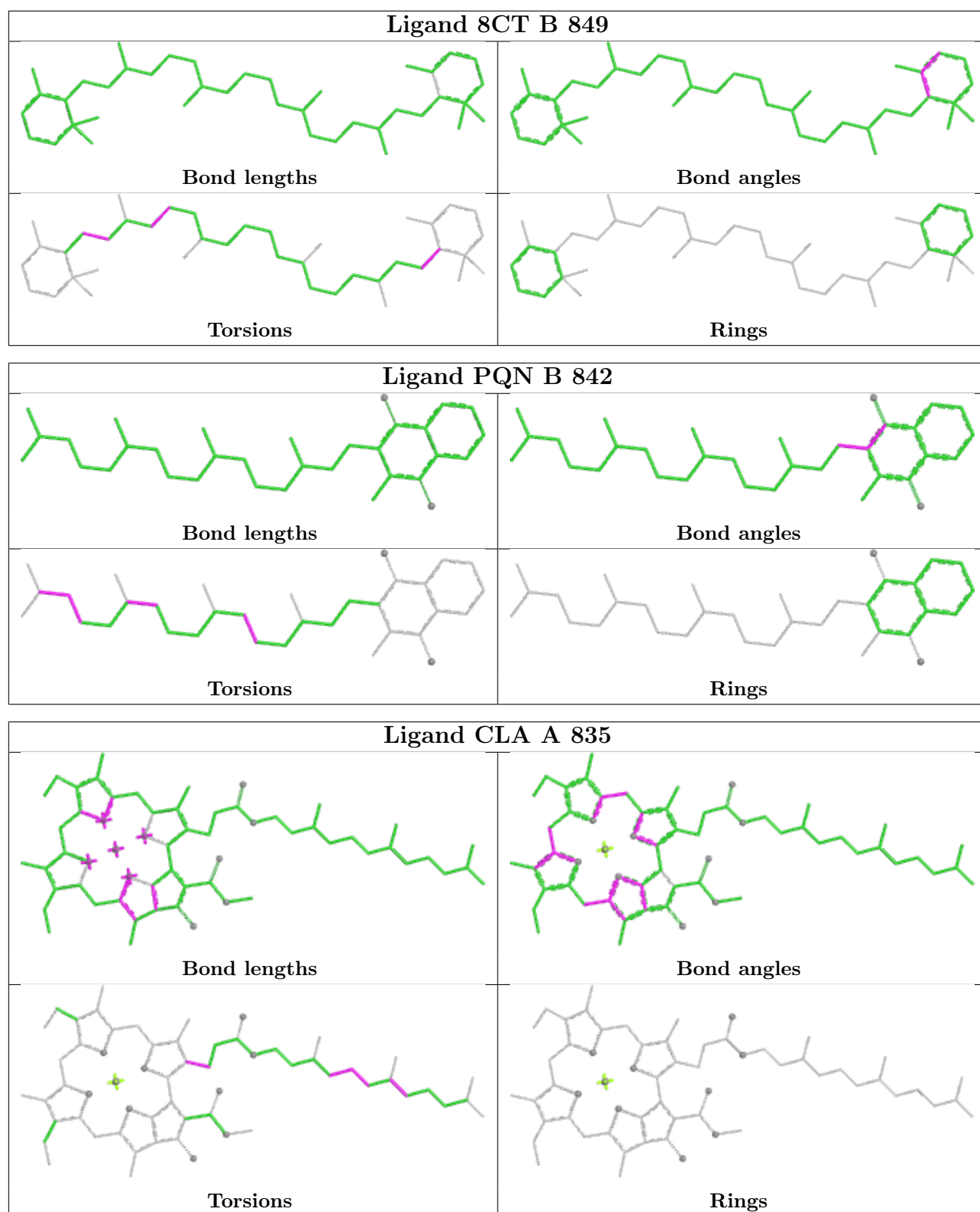


## Ligand CLA 5 611

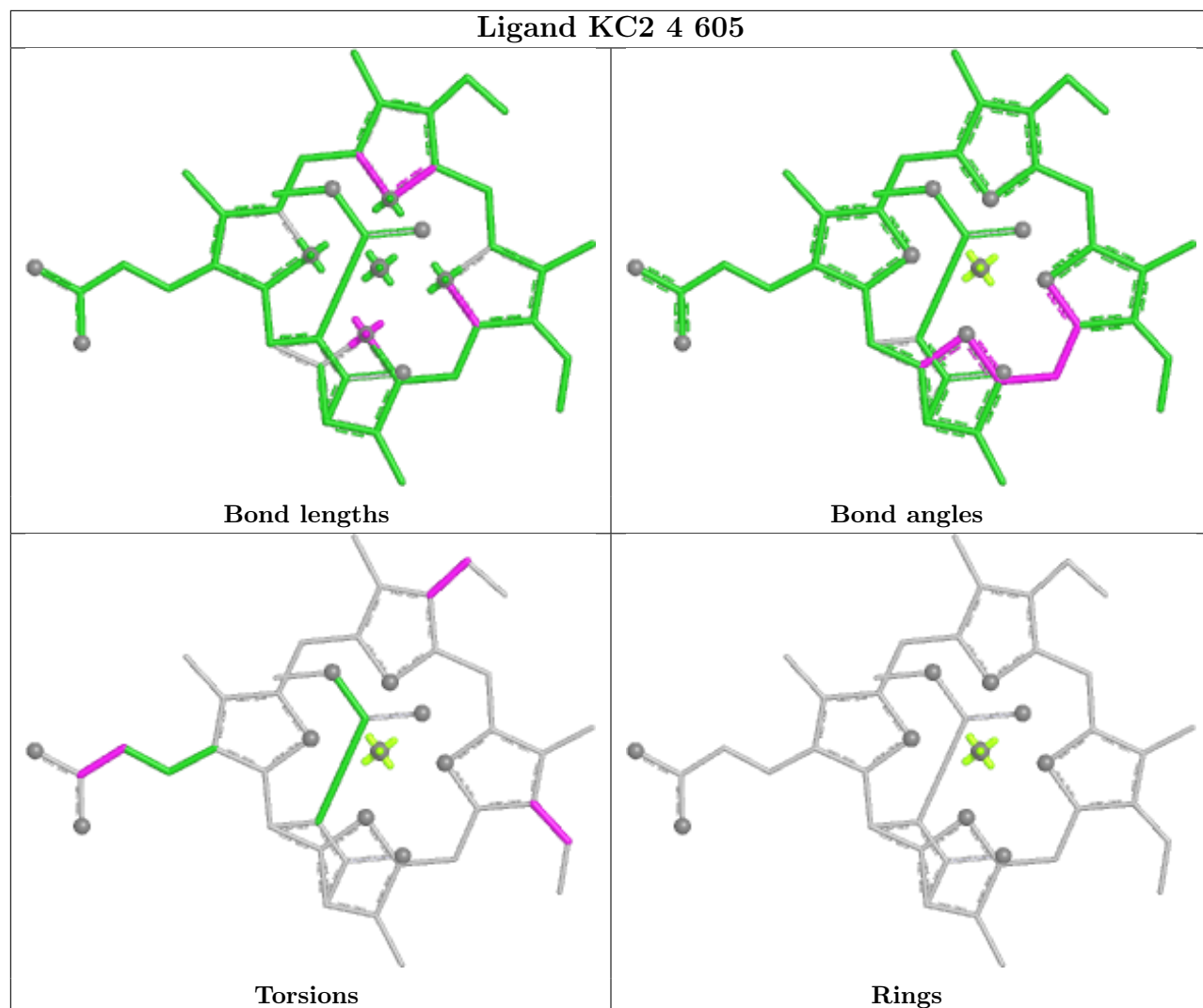


**Ligand CLA 9 602****Ligand II0 1 619**

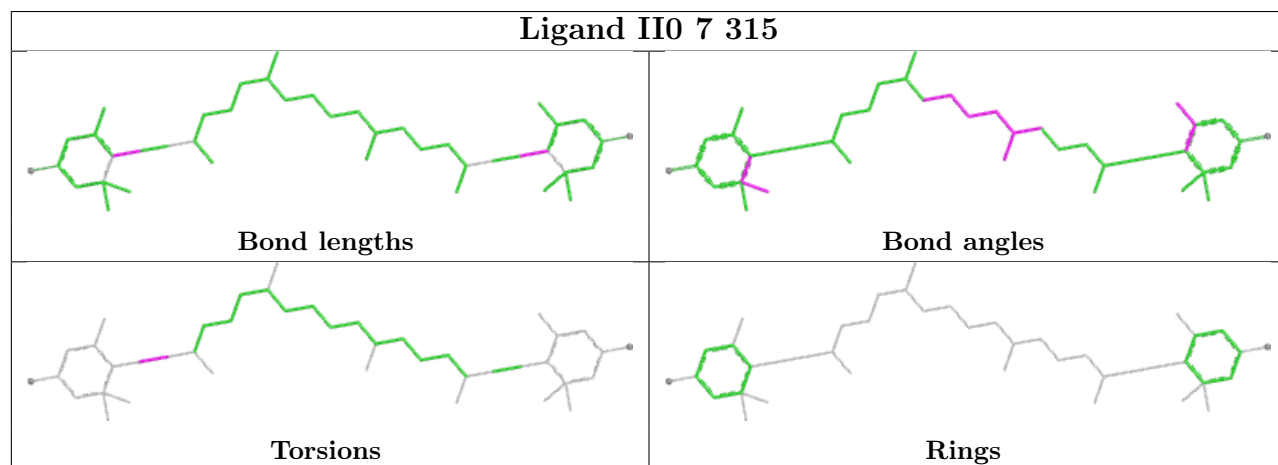
**Ligand CLA b 603****Ligand CLA a 610**

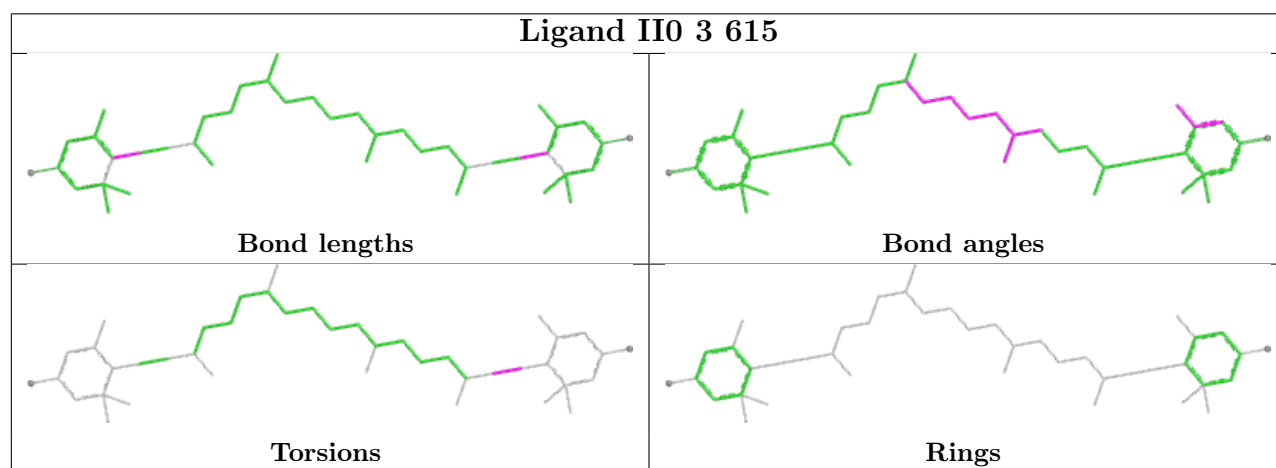
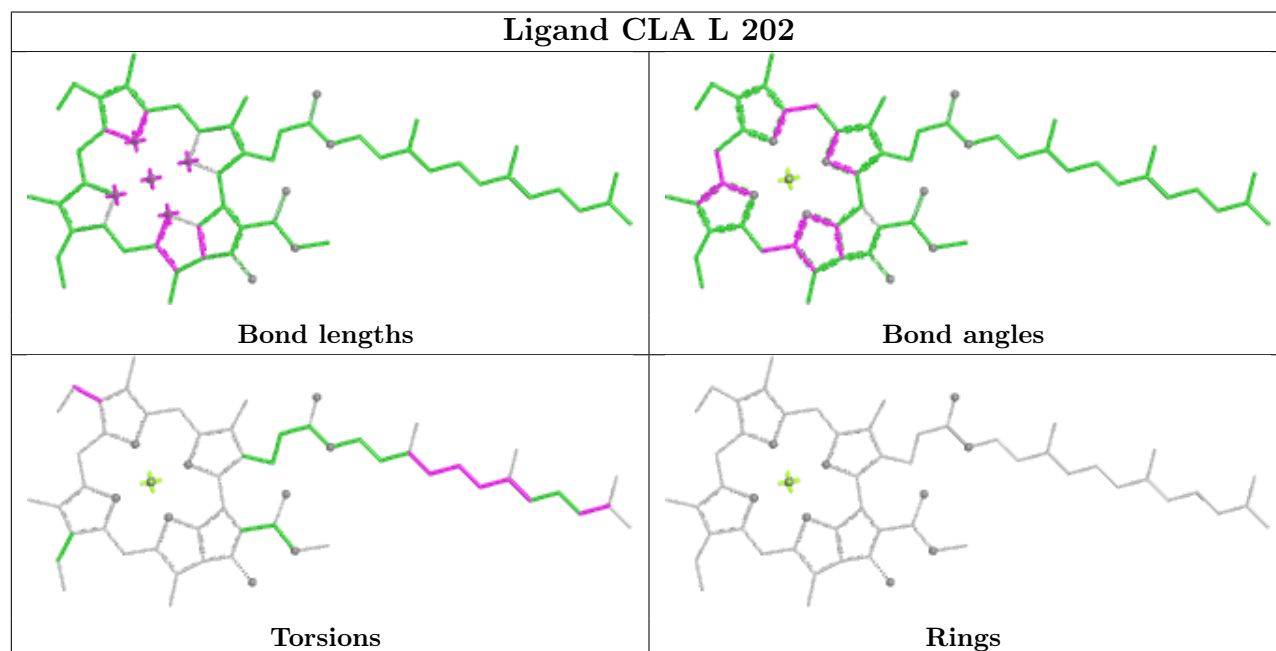
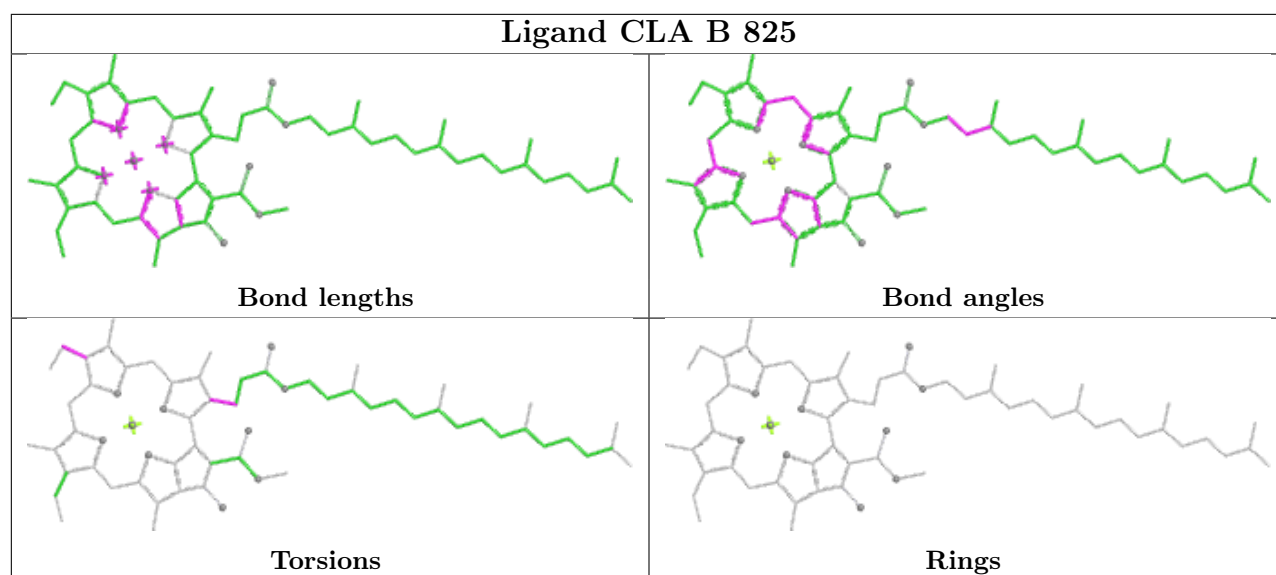


## Ligand KC2 4 605

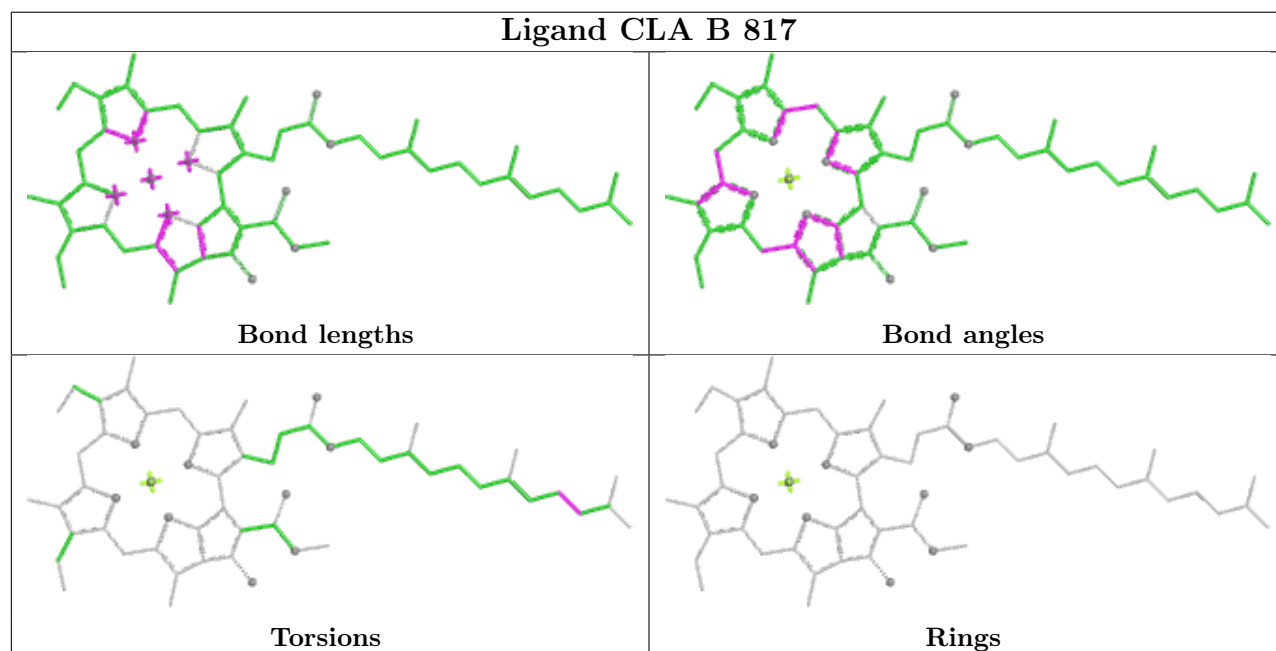
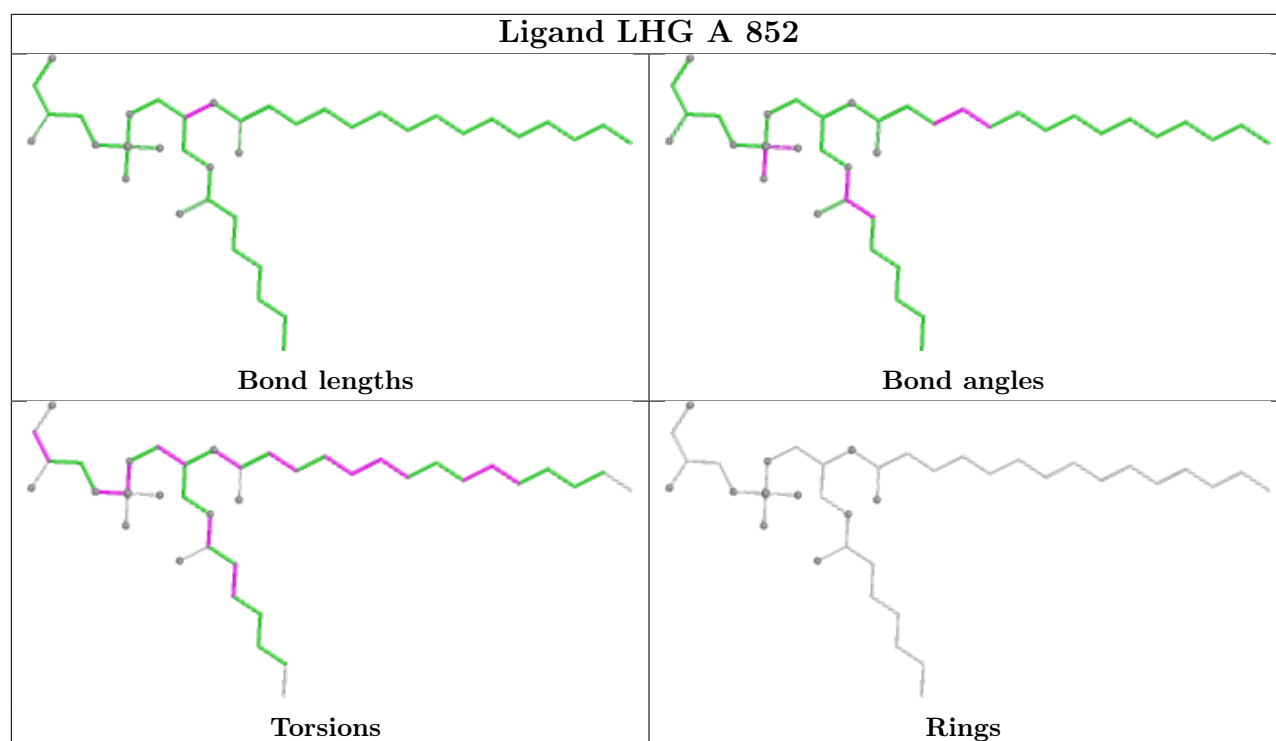


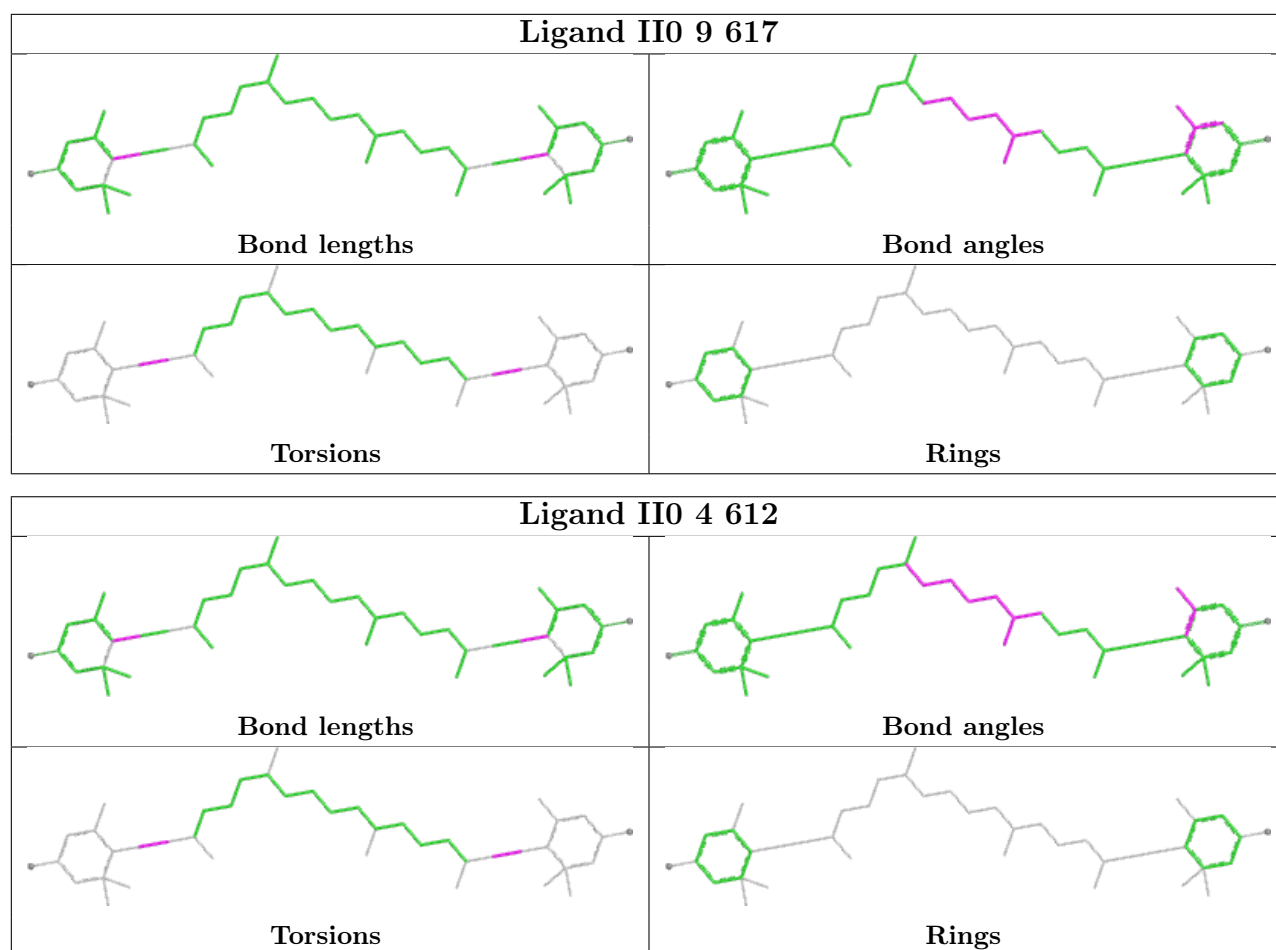
## Ligand II0 7 315



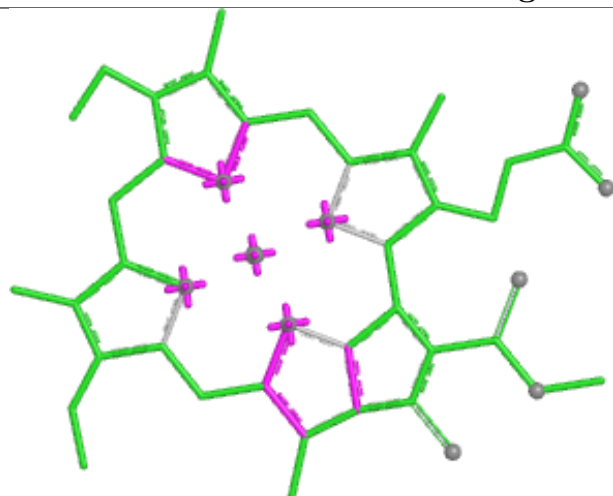




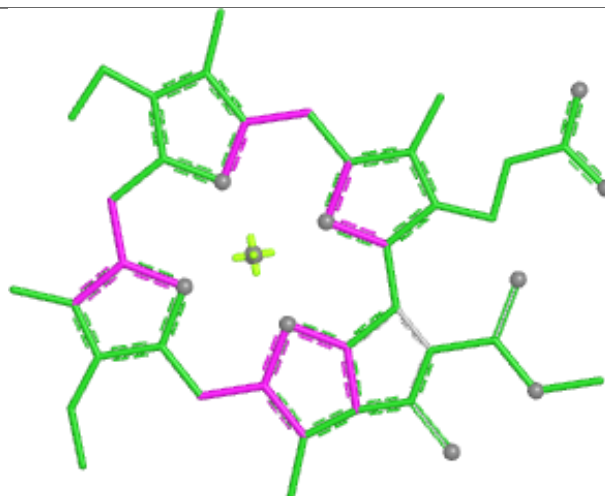




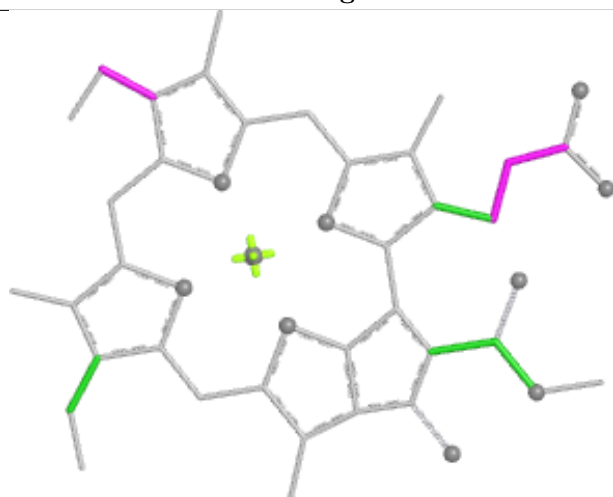
## Ligand CLA 9 603



Bond lengths



Bond angles

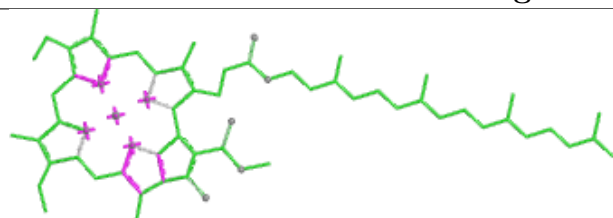


Torsions

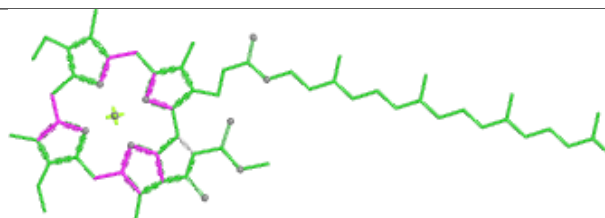


Rings

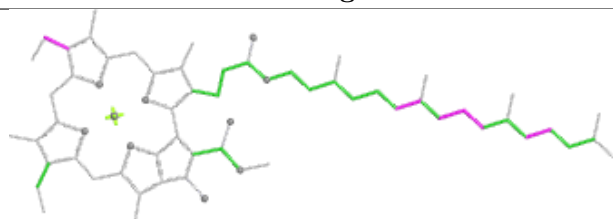
## Ligand CLA A 818



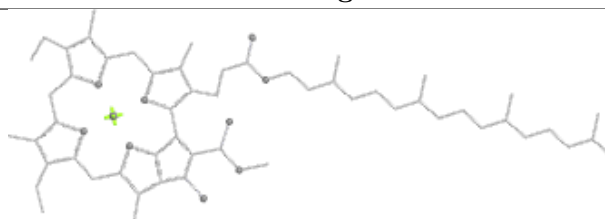
Bond lengths



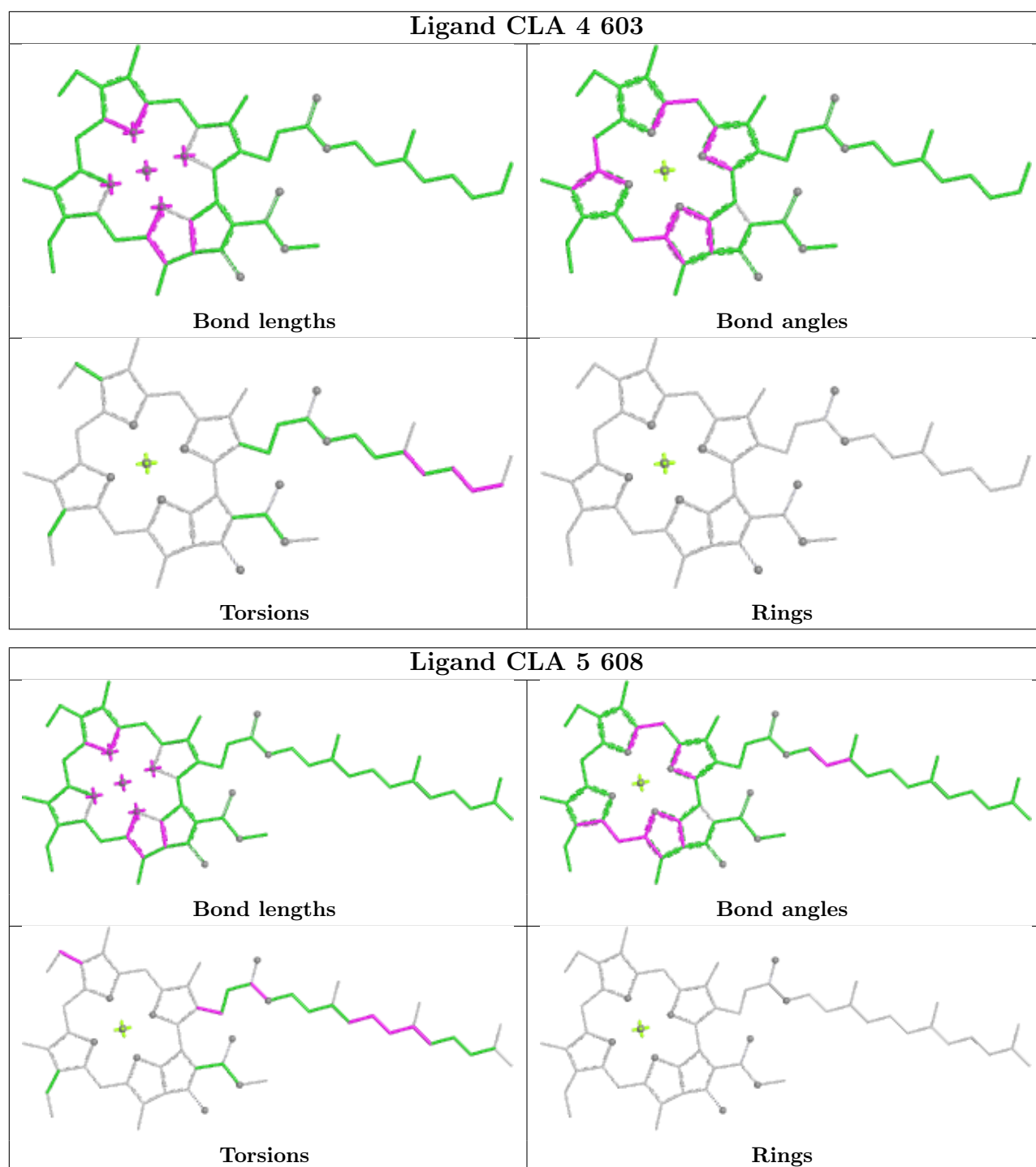
Bond angles

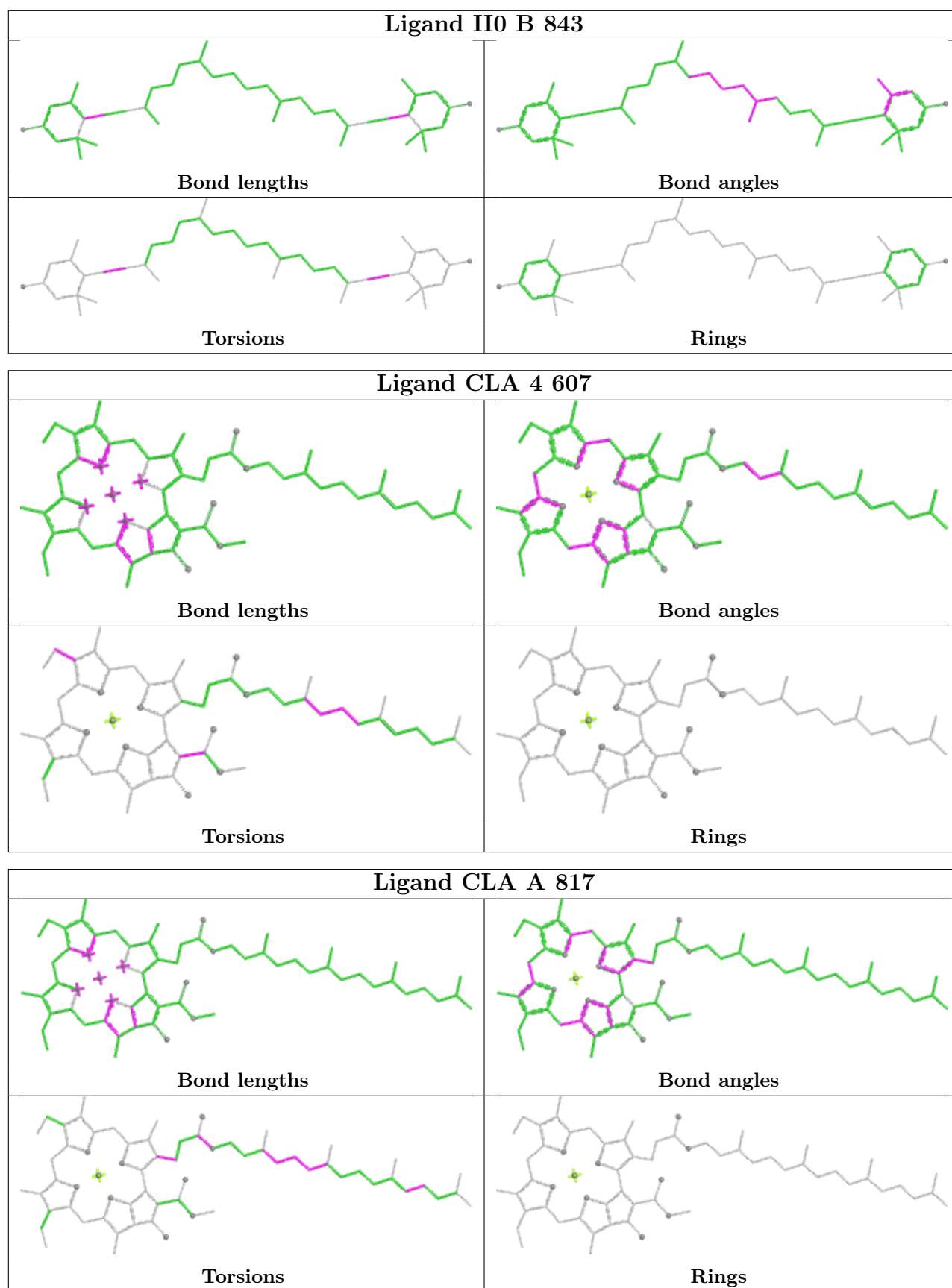


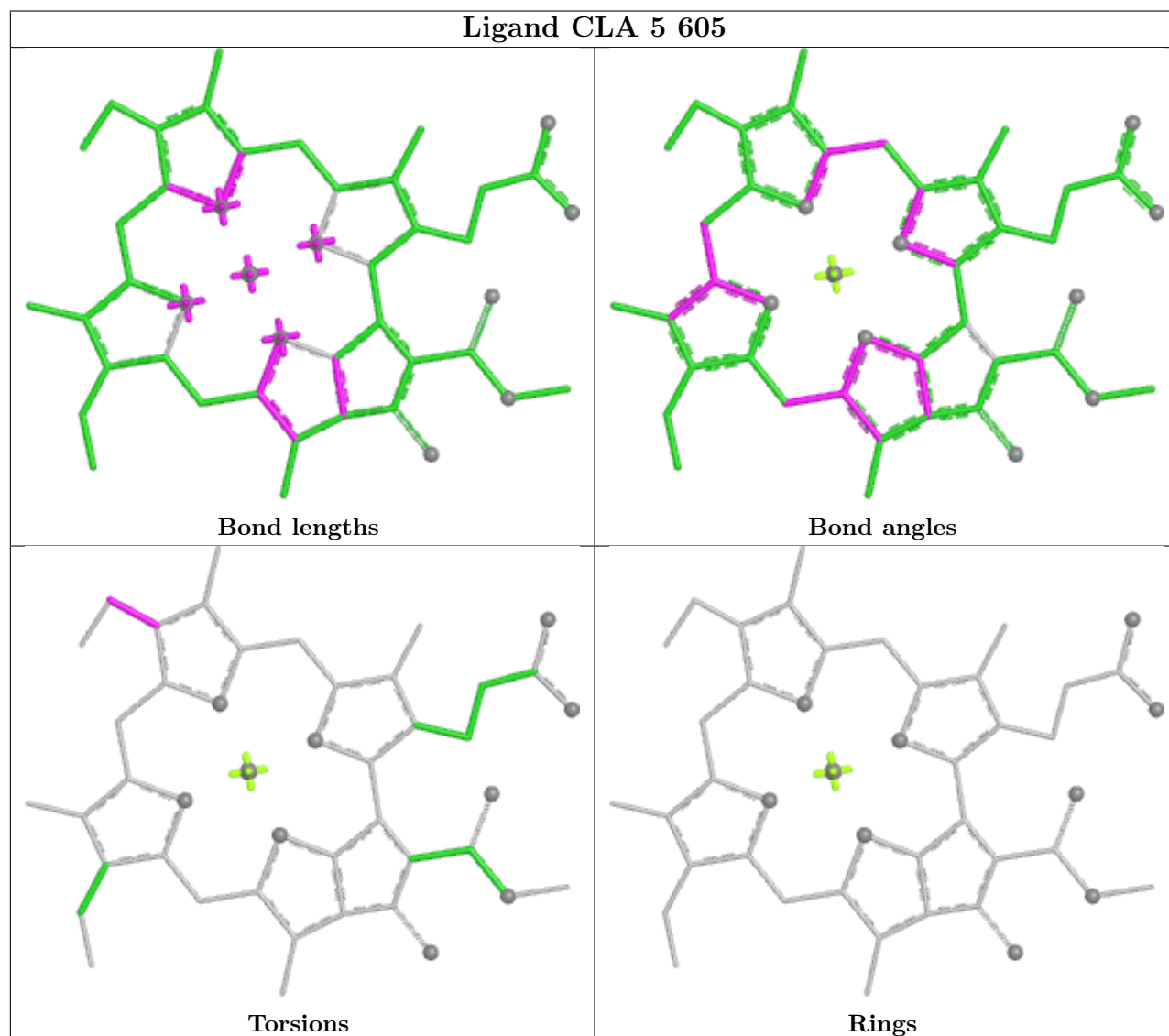
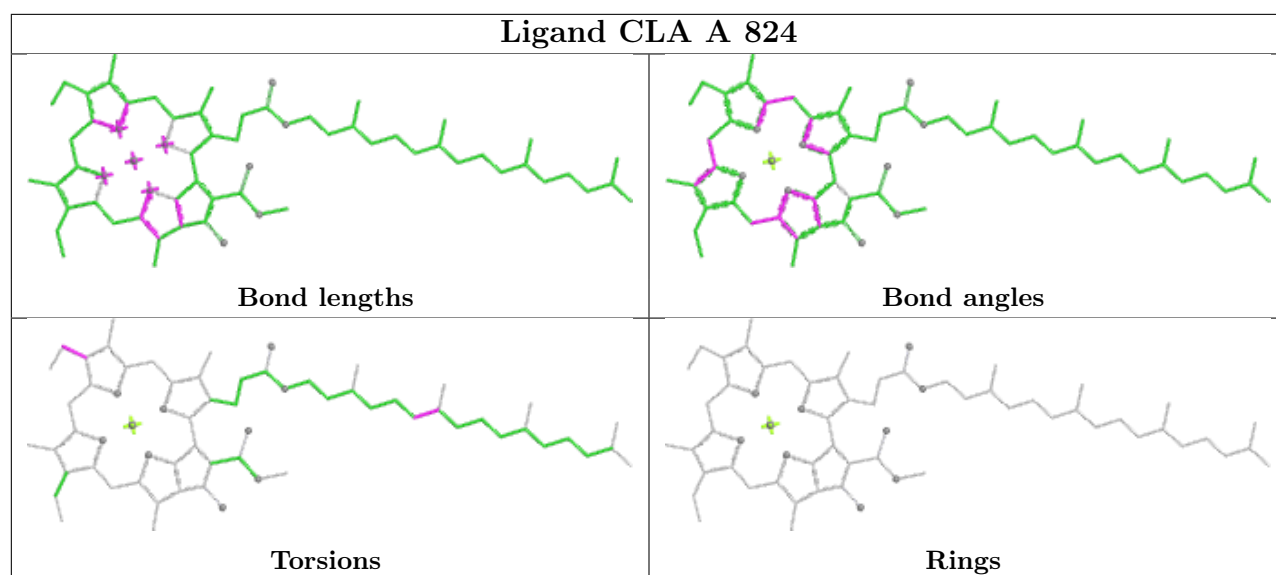
Torsions

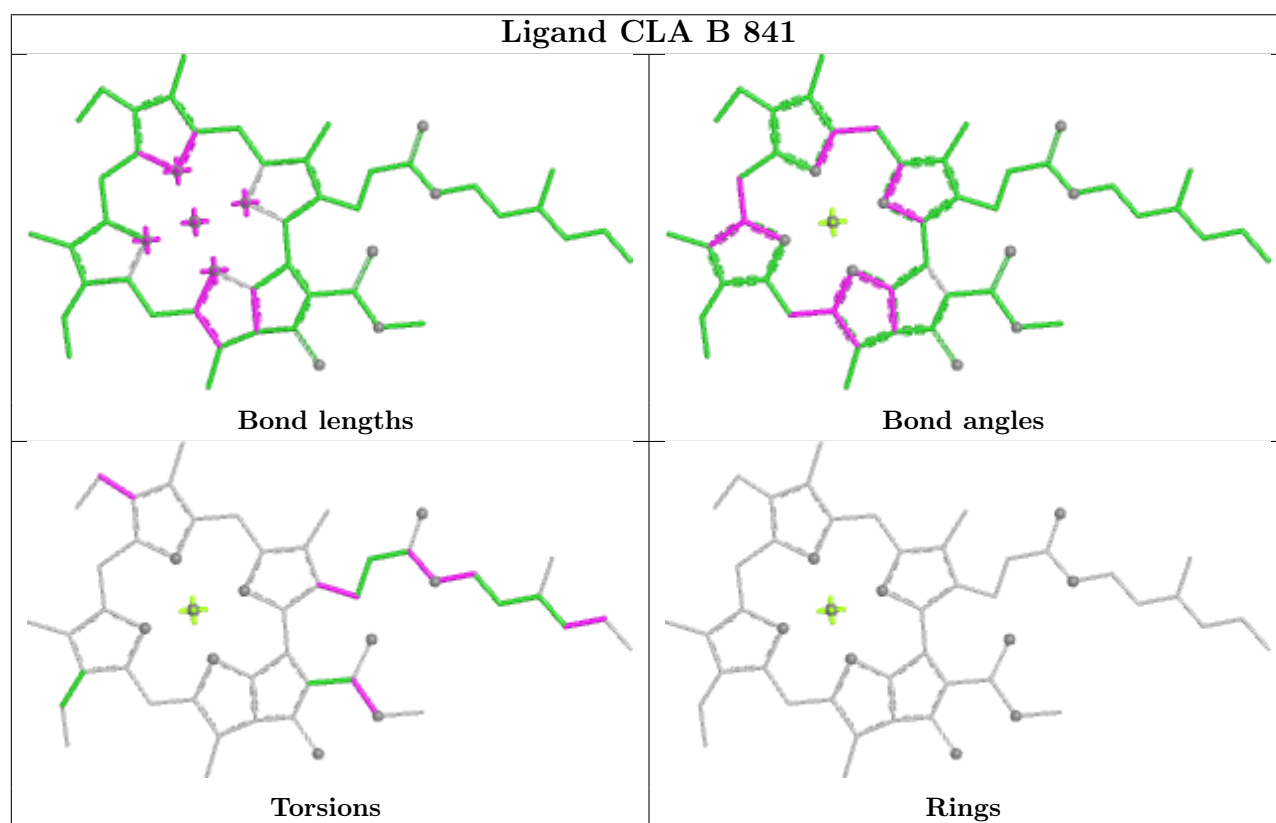
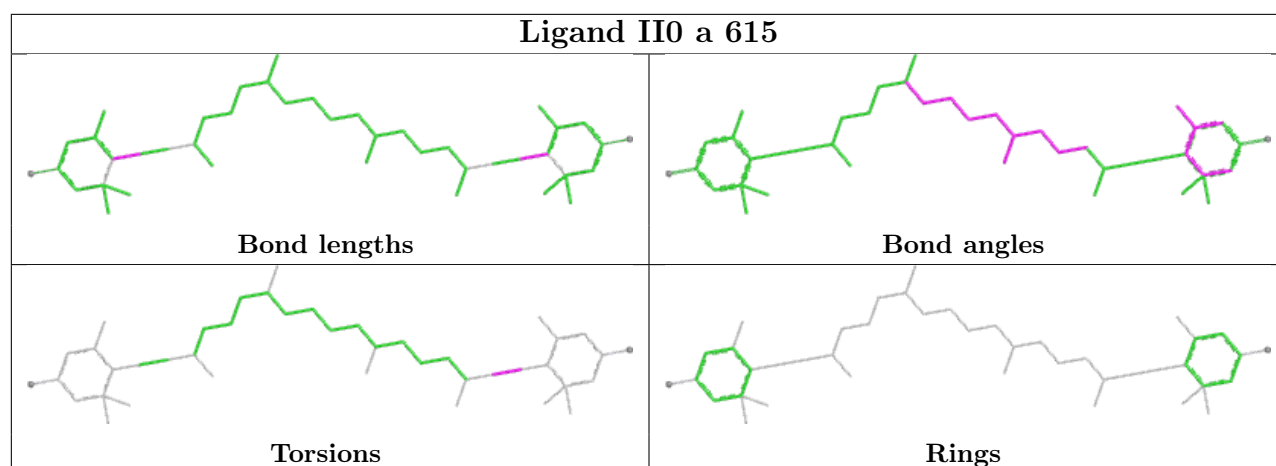


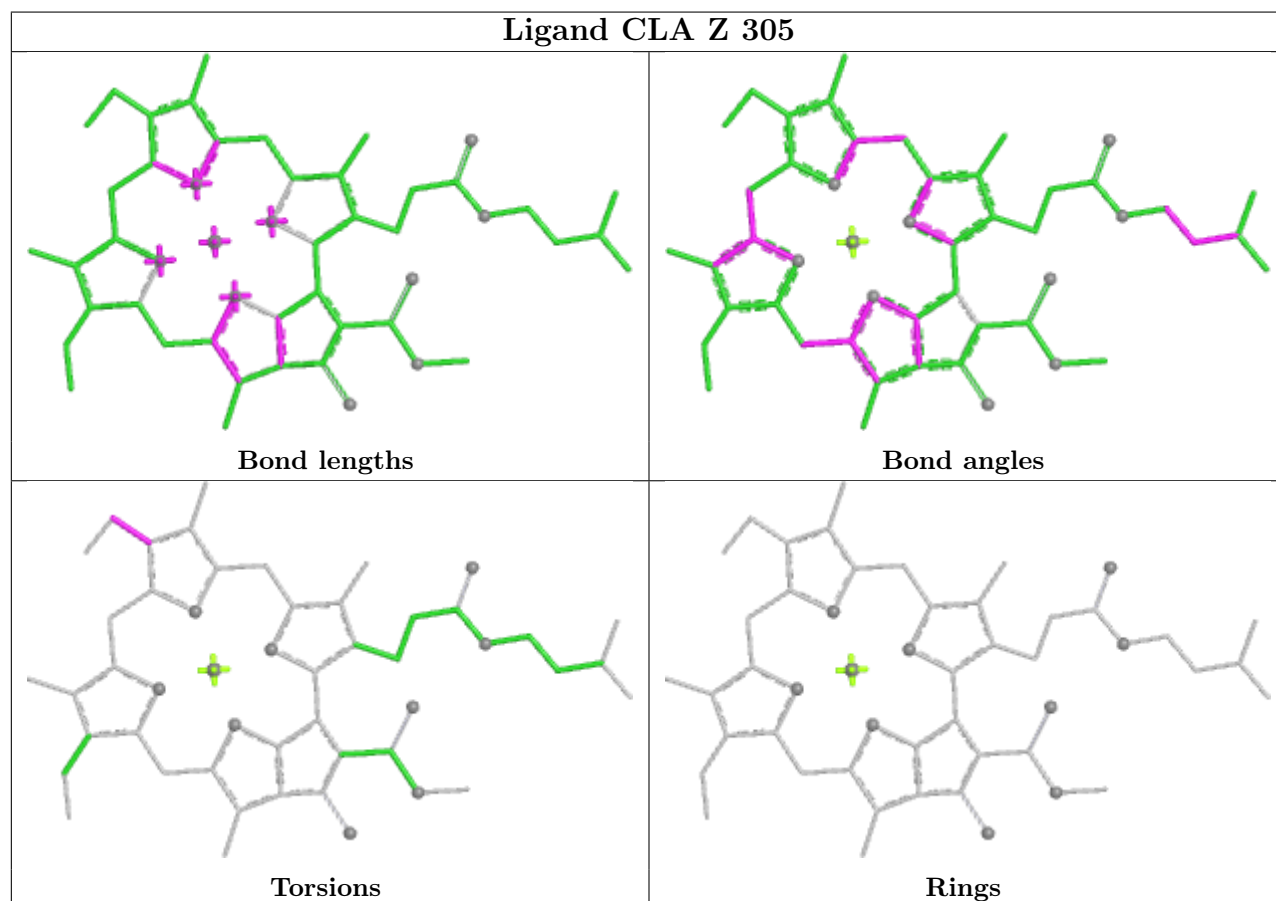
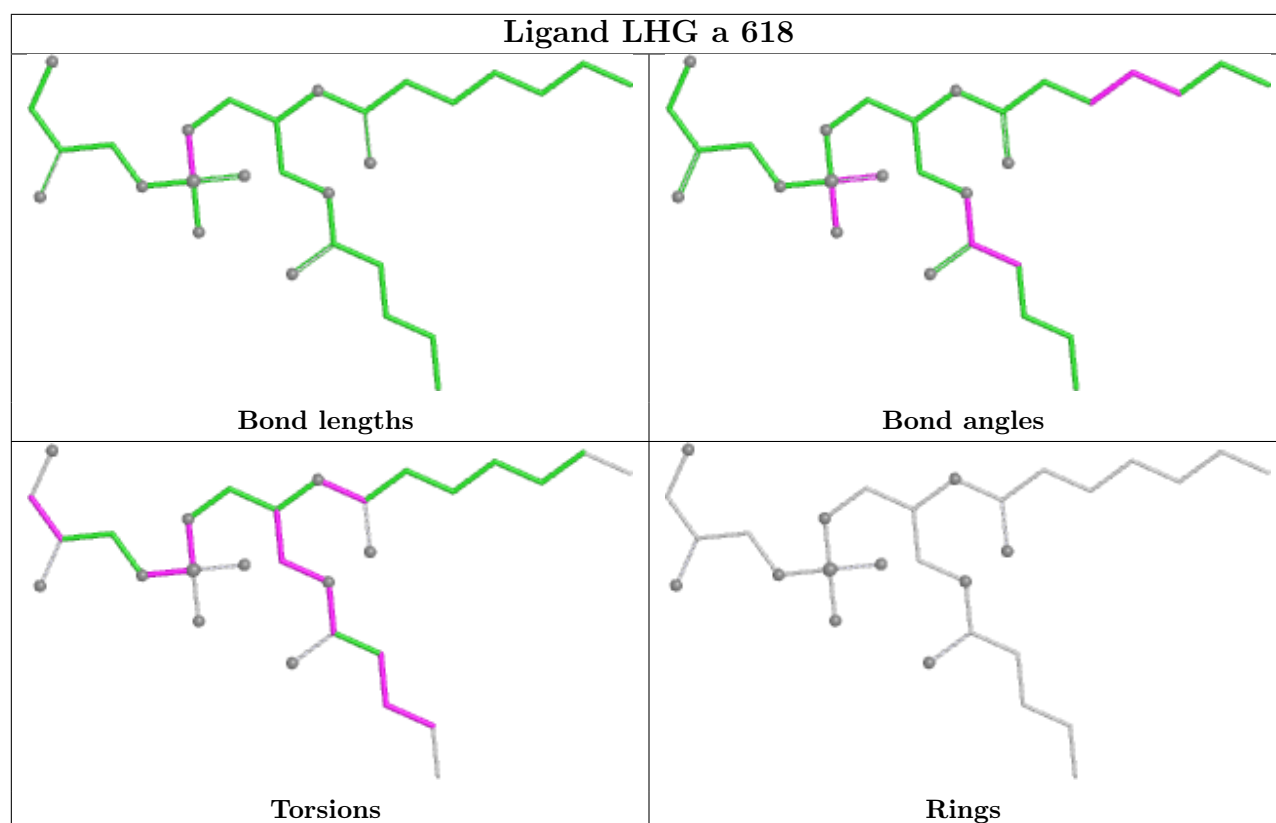
Rings





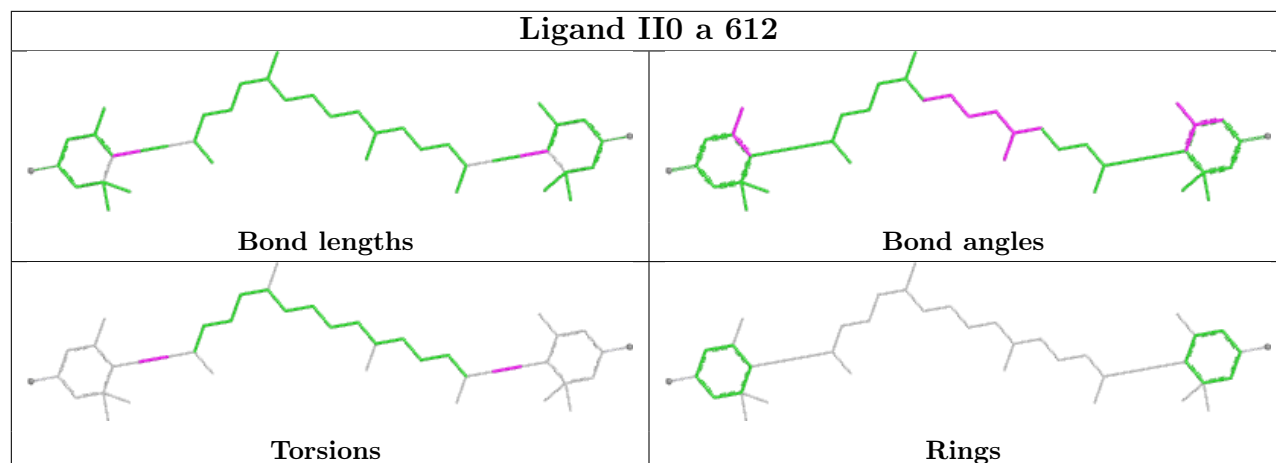




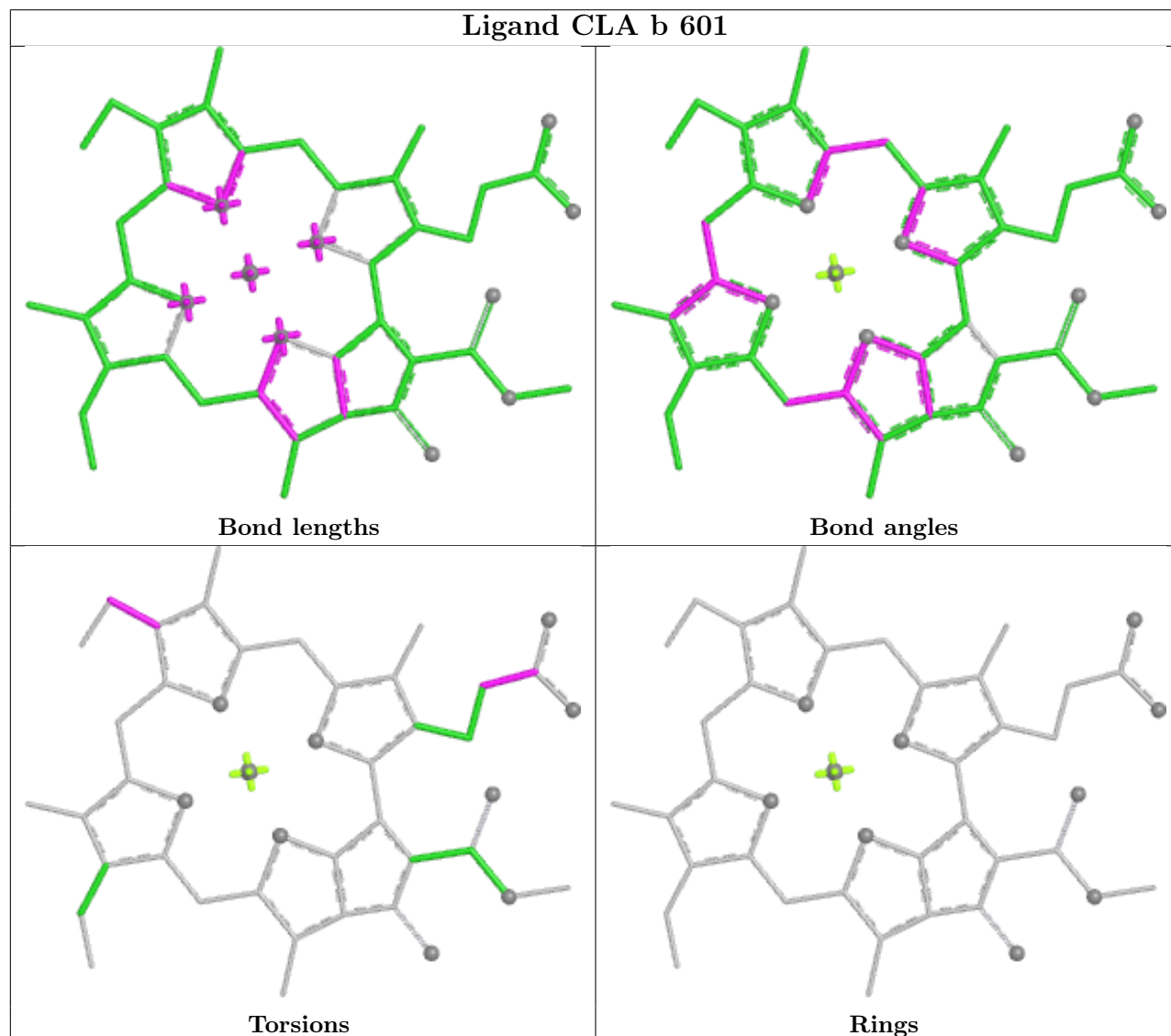




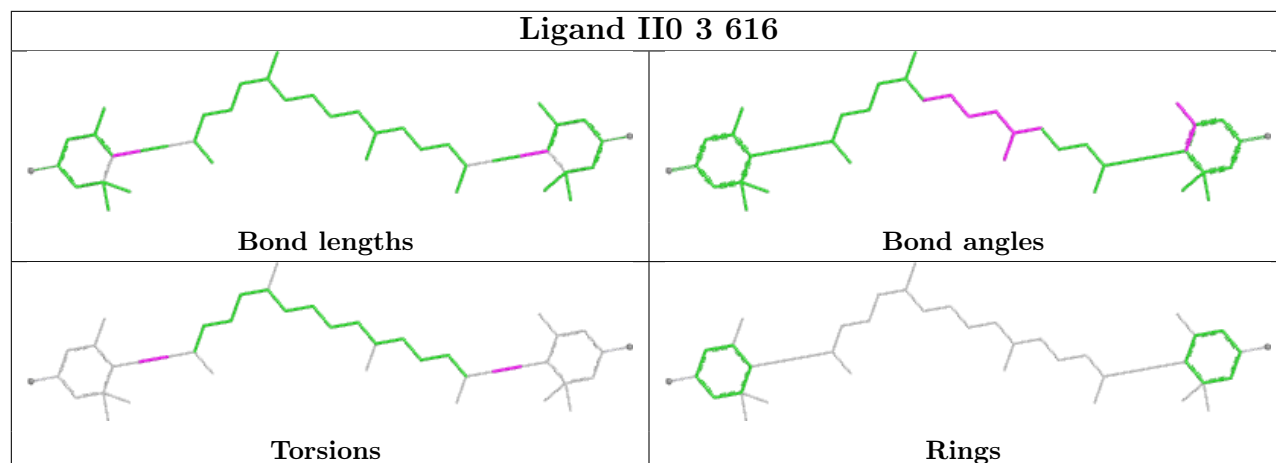
## Ligand II0 a 612



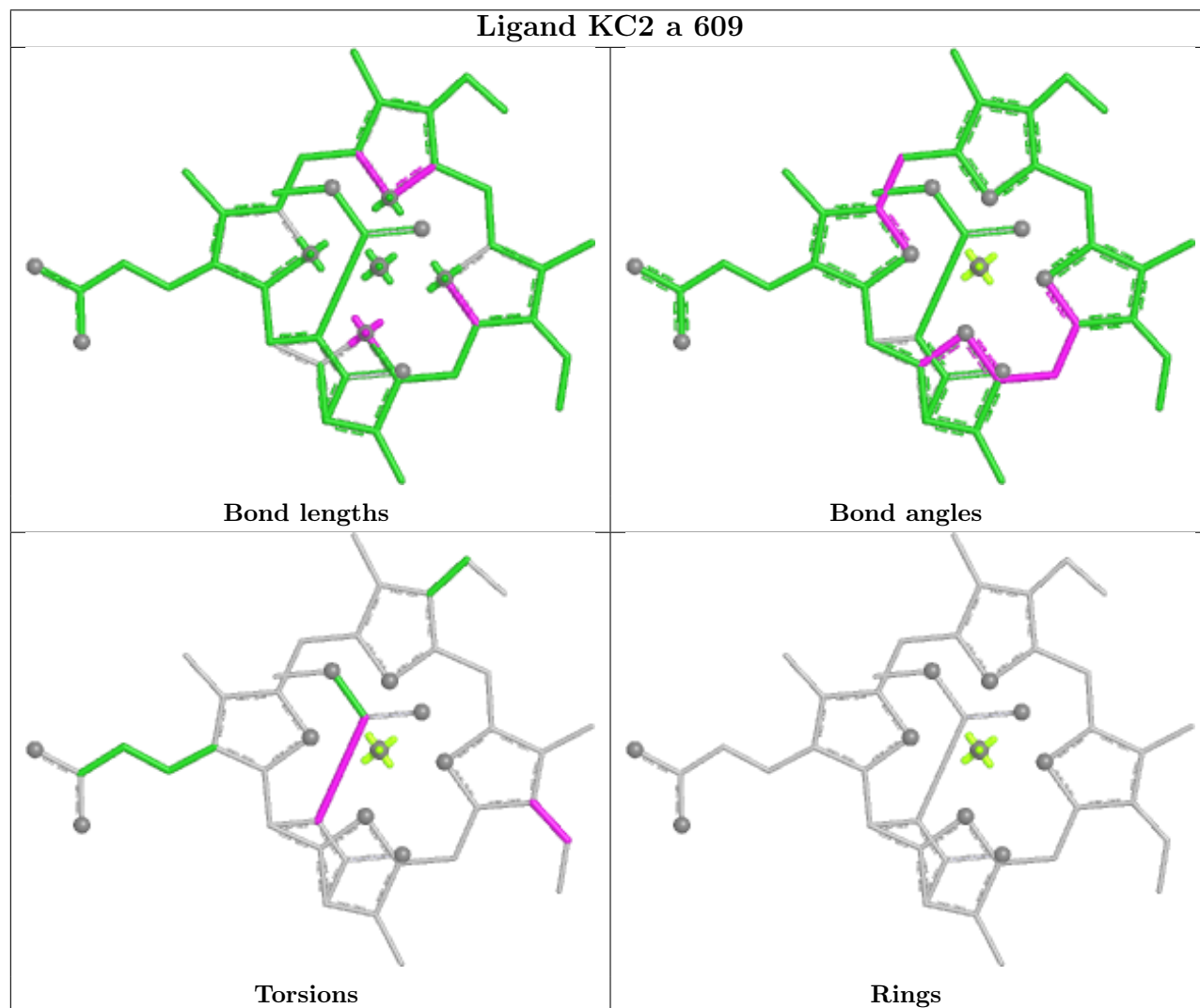
## Ligand CLA b 601

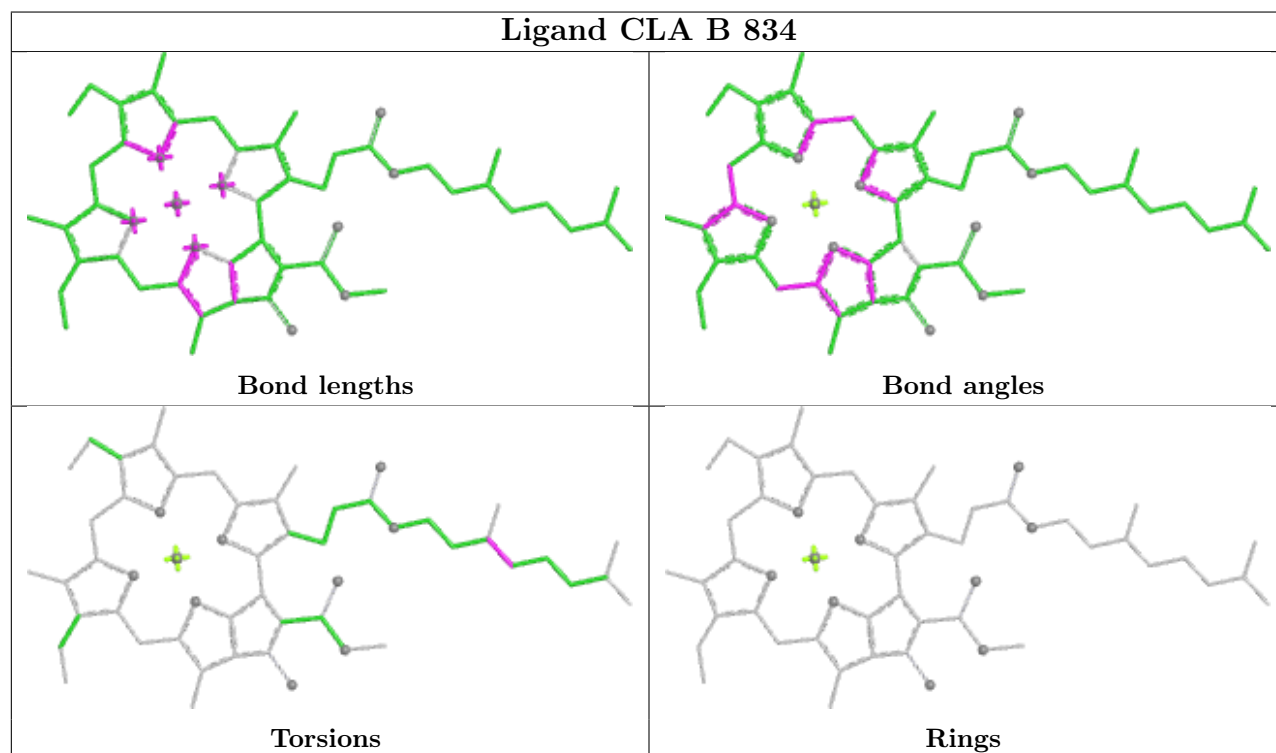
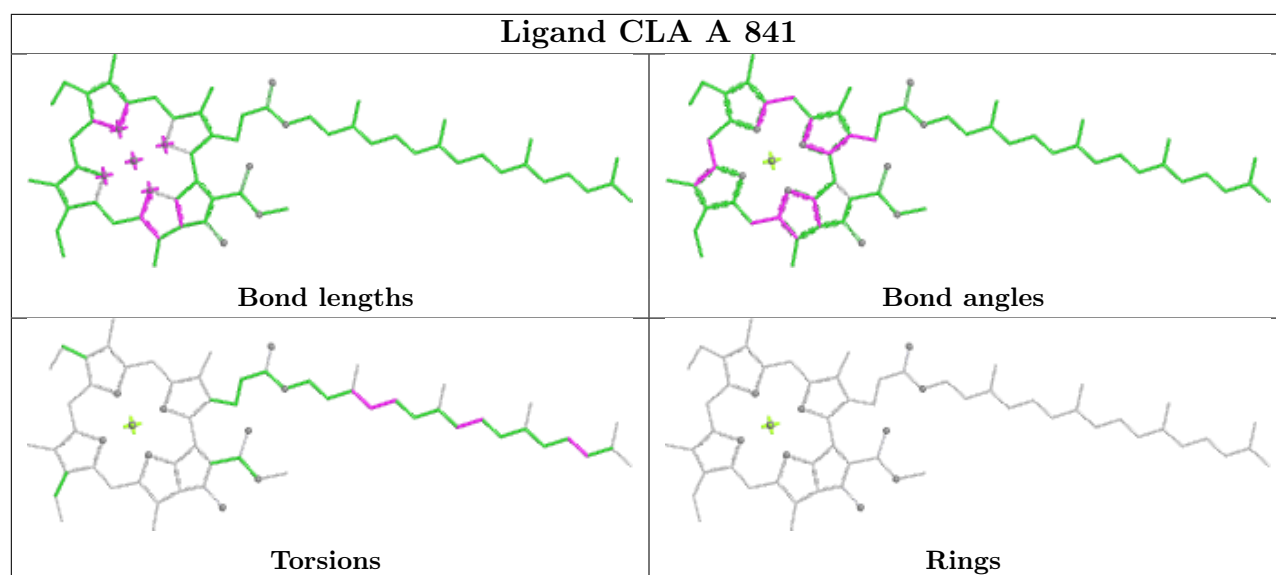


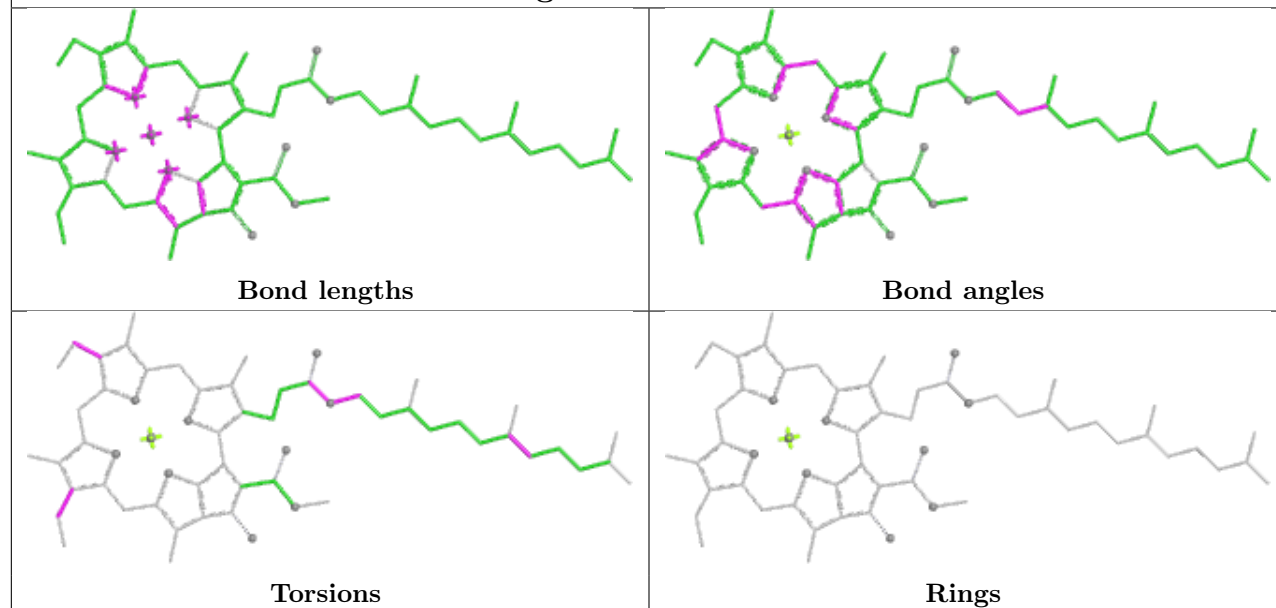
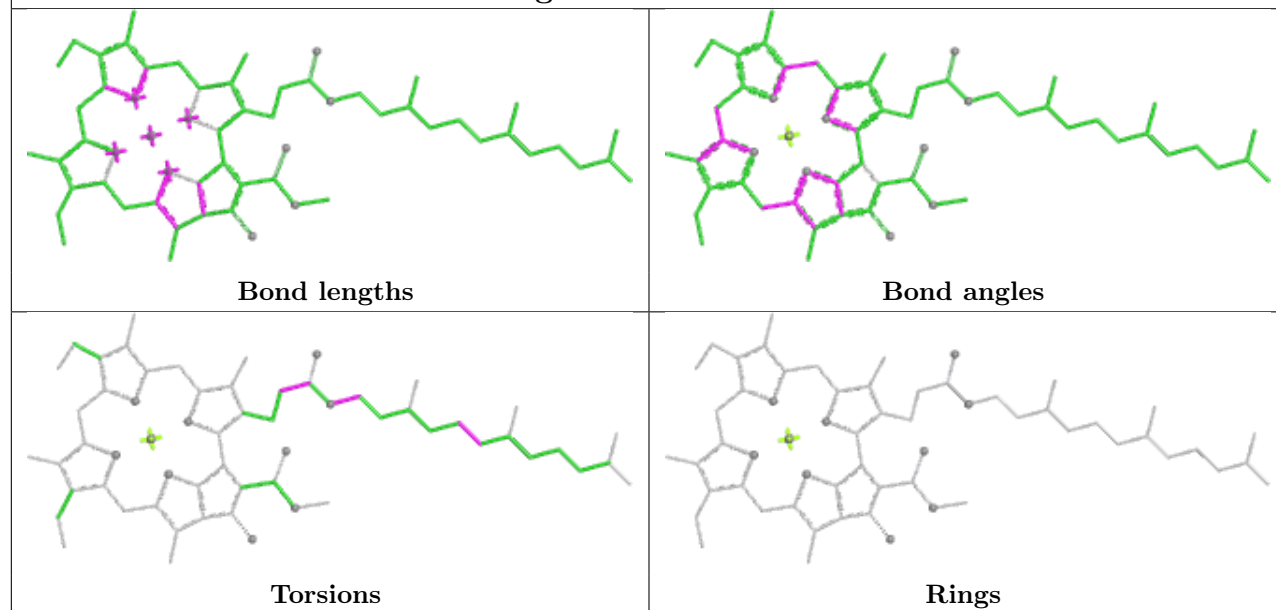
## Ligand II0 3 616

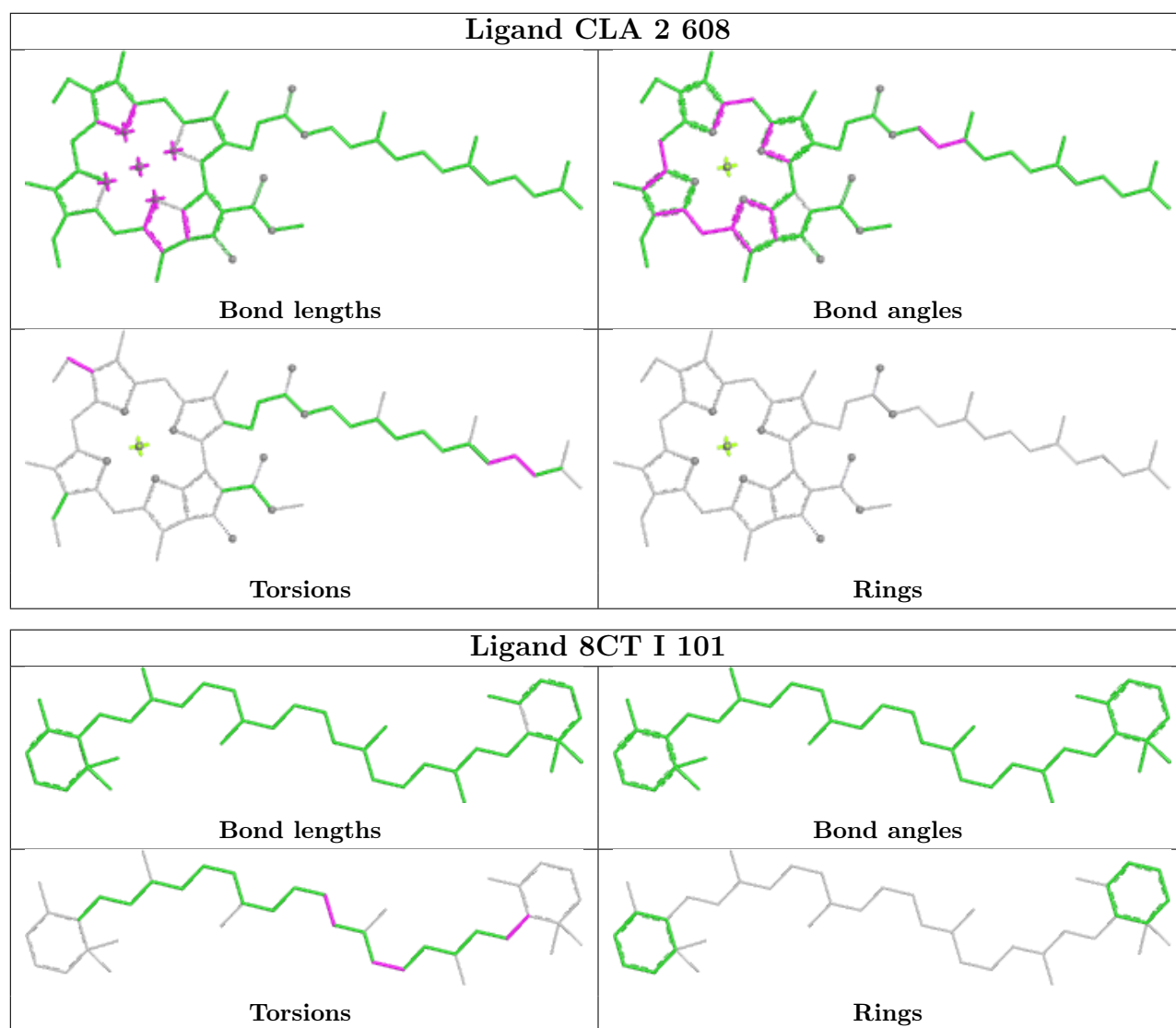


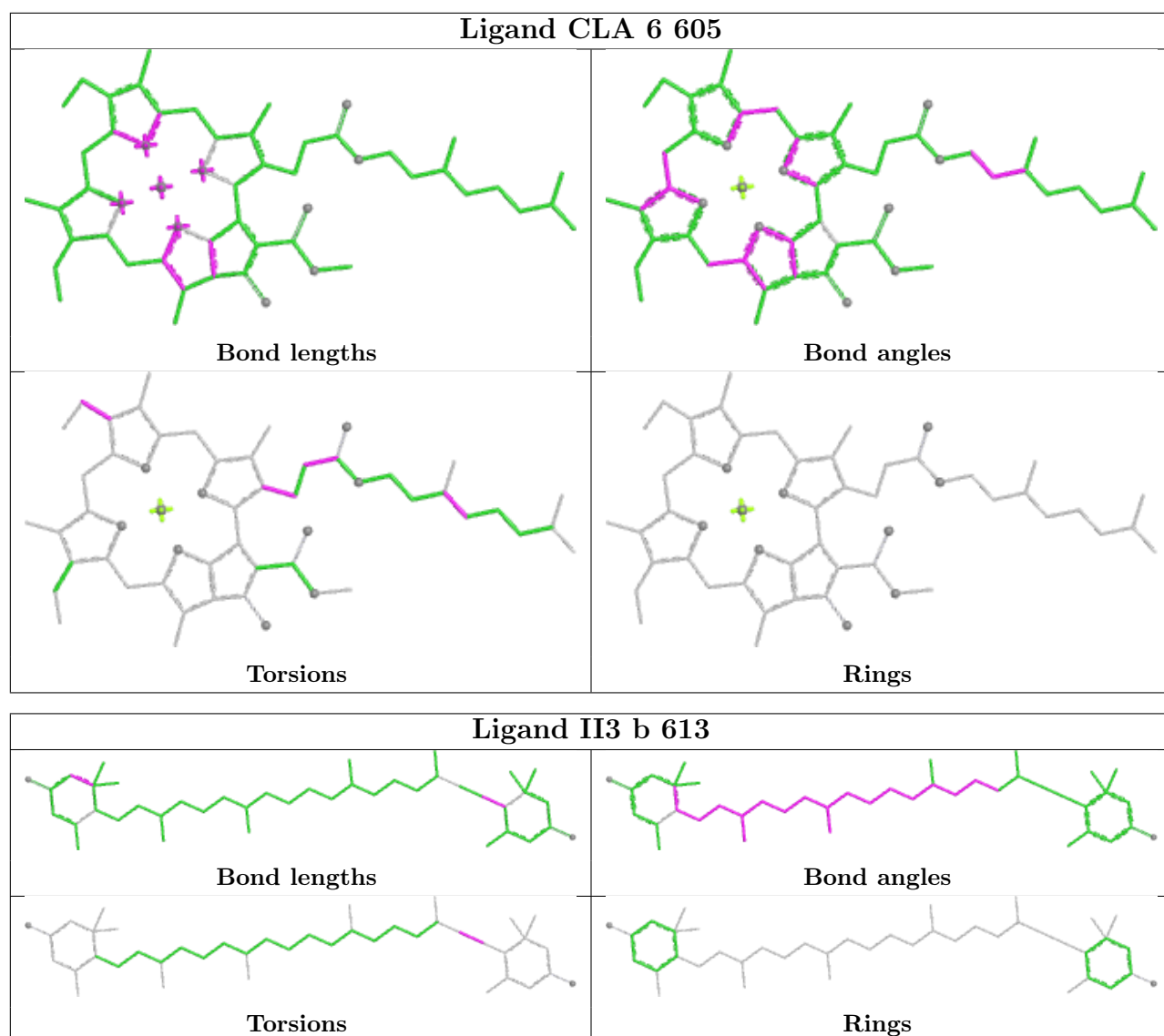
## Ligand KC2 a 609

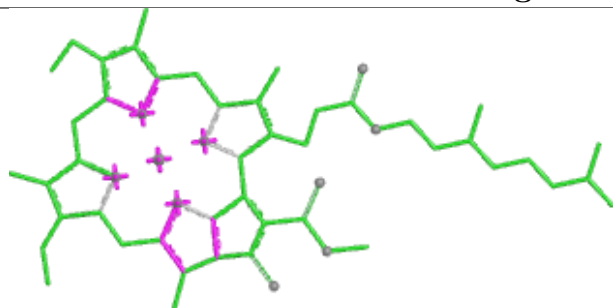
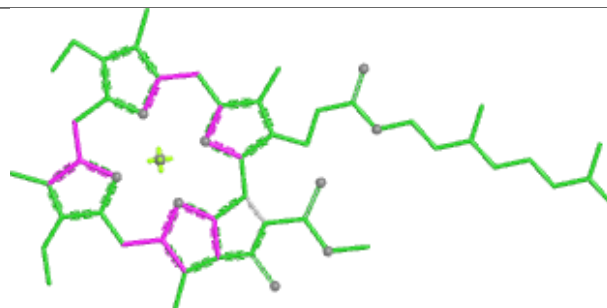
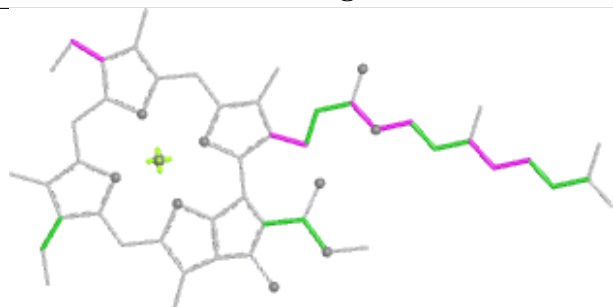
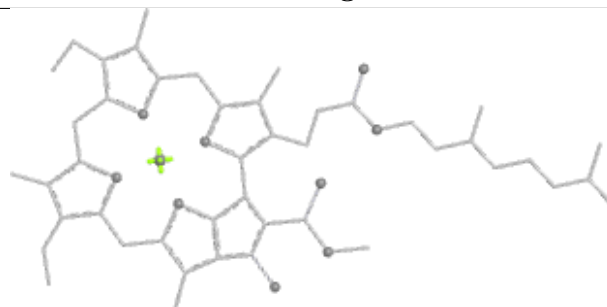
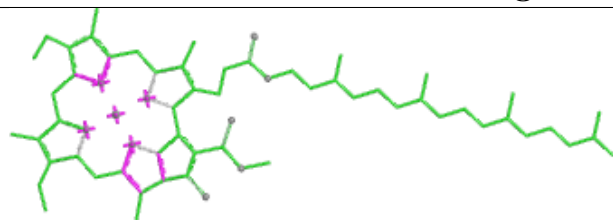
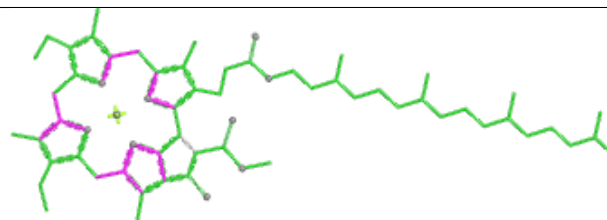
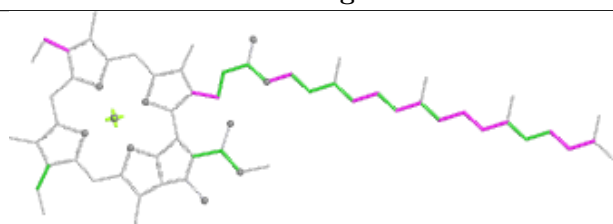
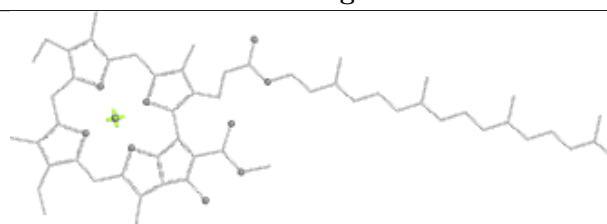




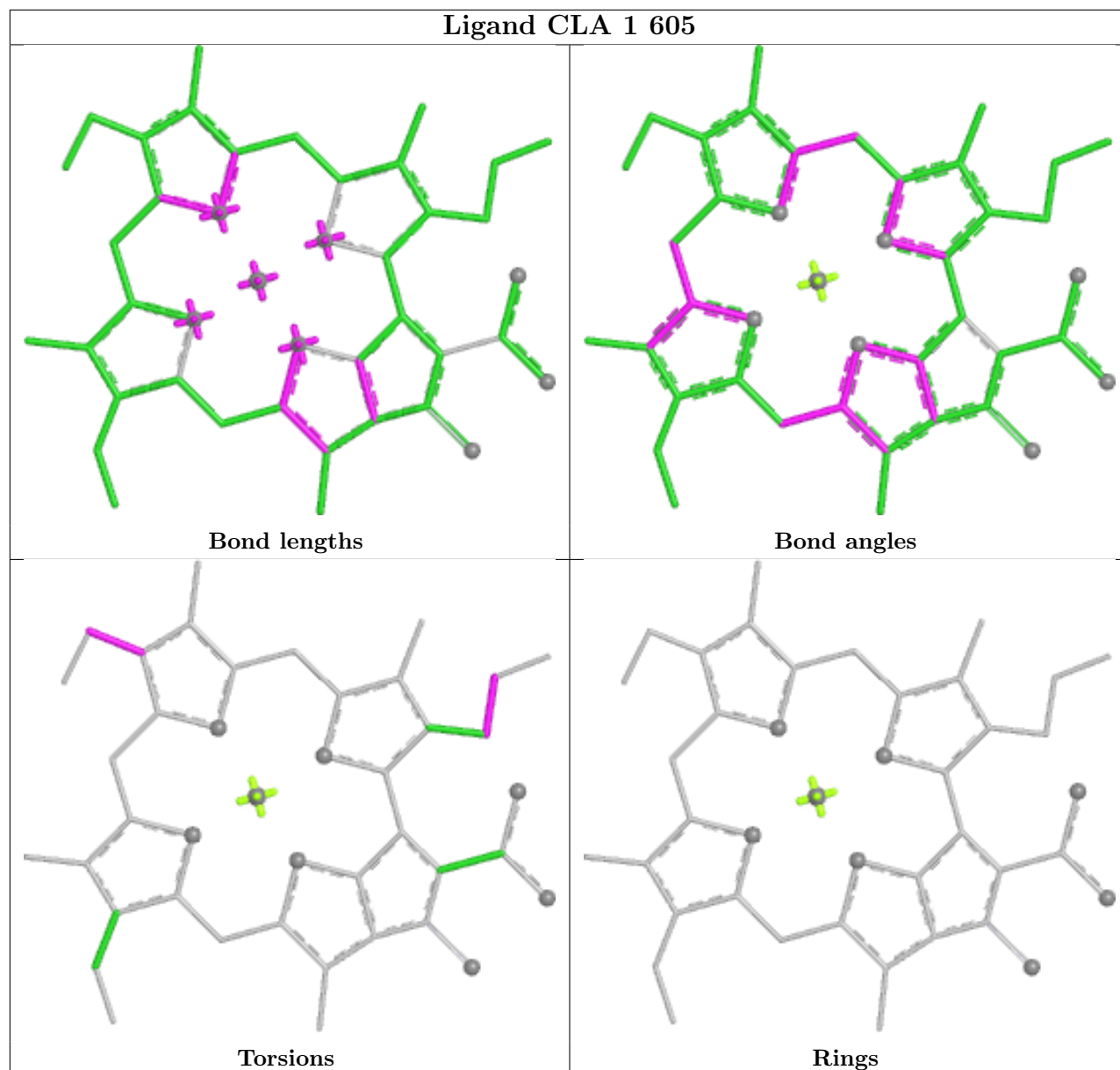
**Ligand CLA a 608****Ligand CLA b 607**



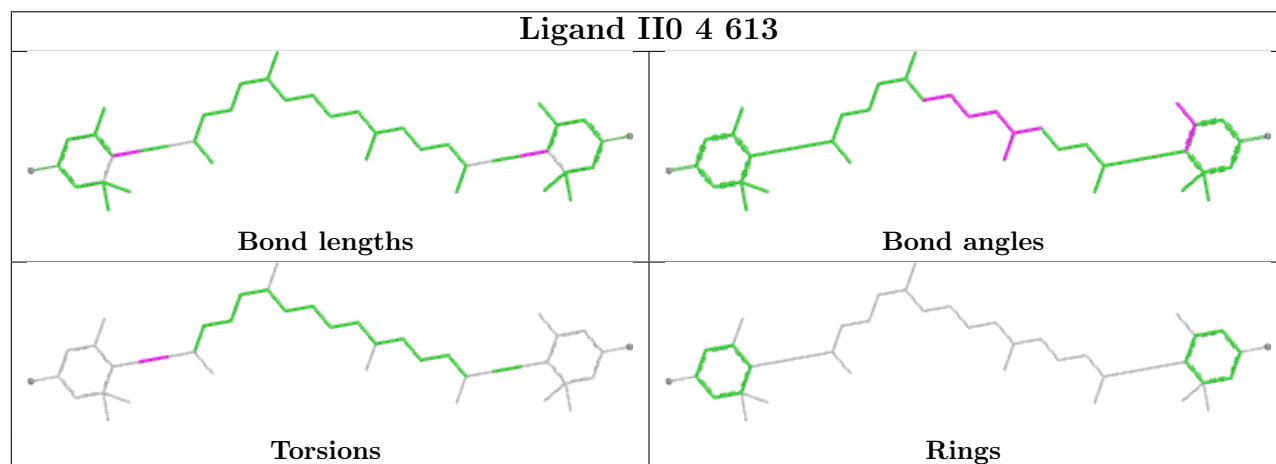


**Ligand CLA B 811****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 826****Bond lengths****Bond angles****Torsions****Rings**

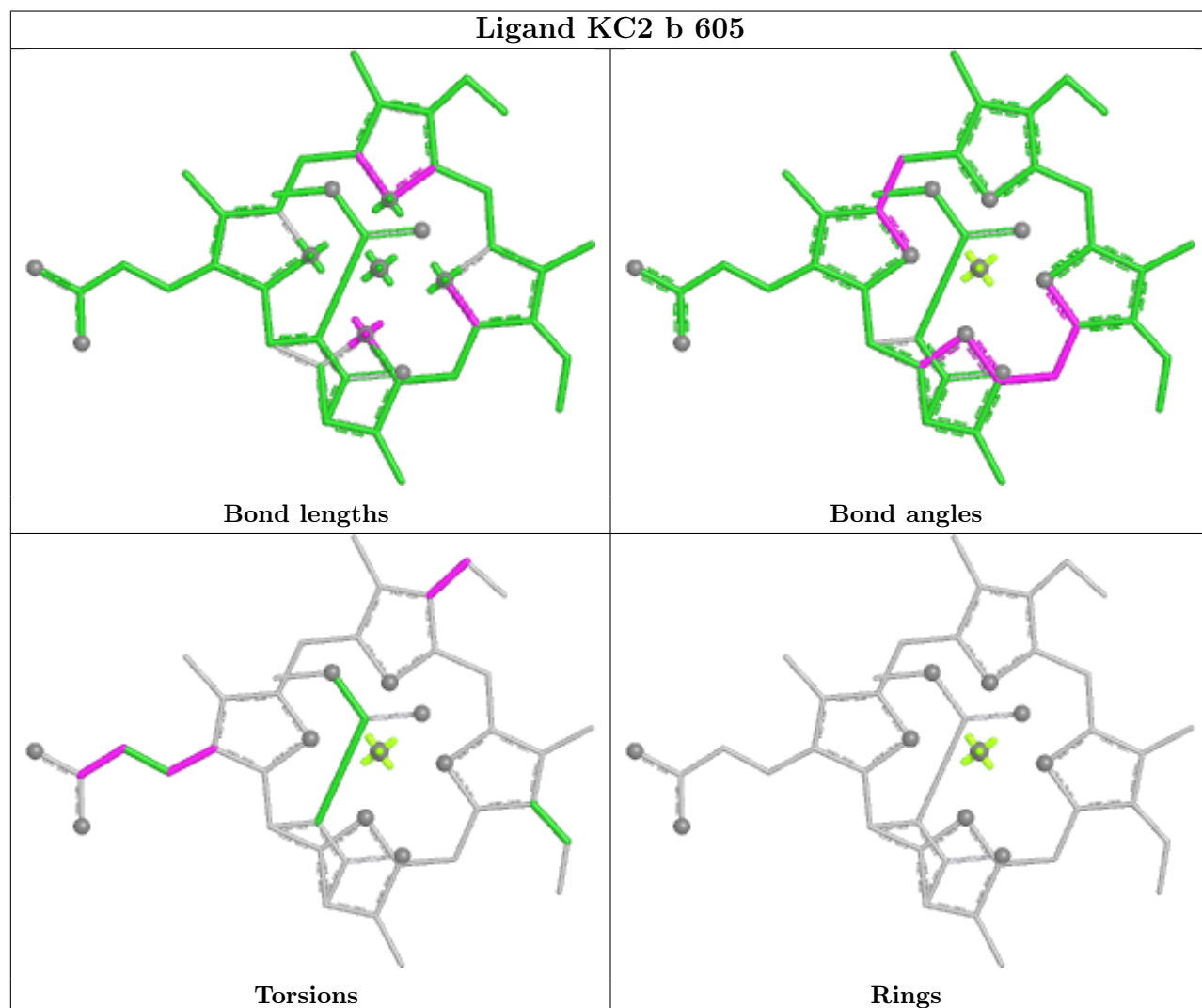
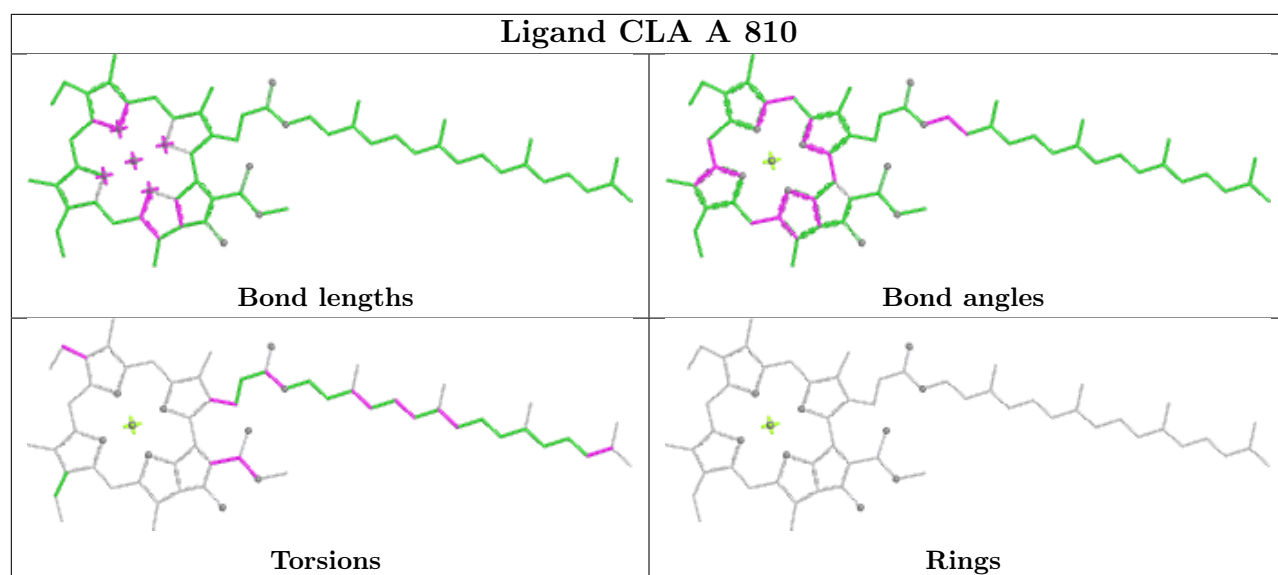
## Ligand CLA 1 605

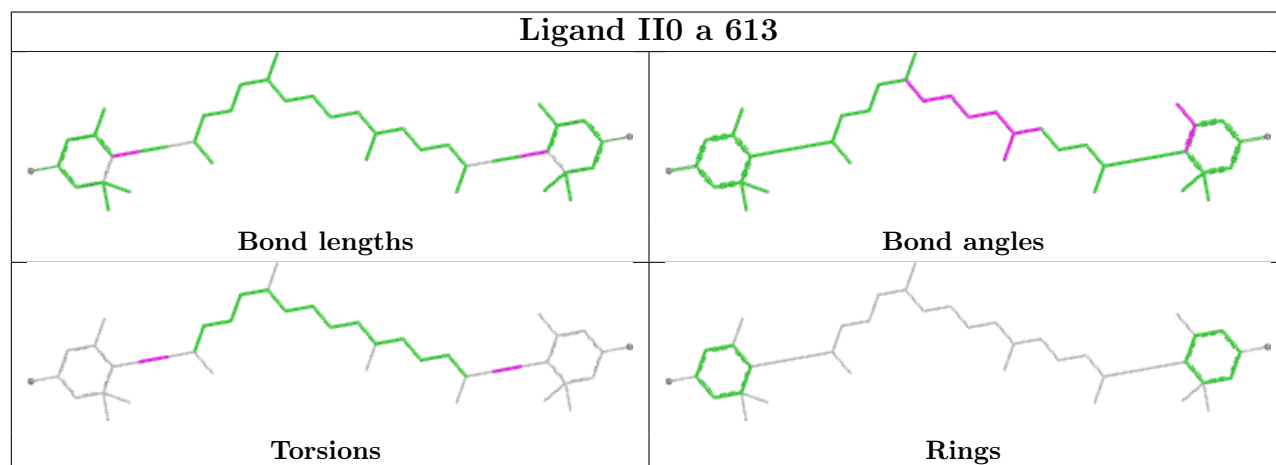
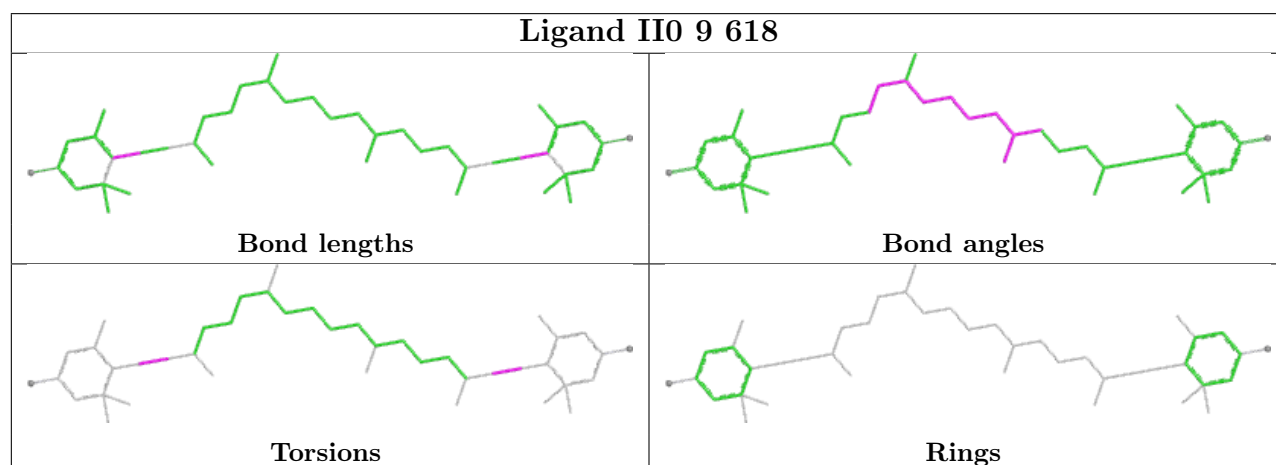
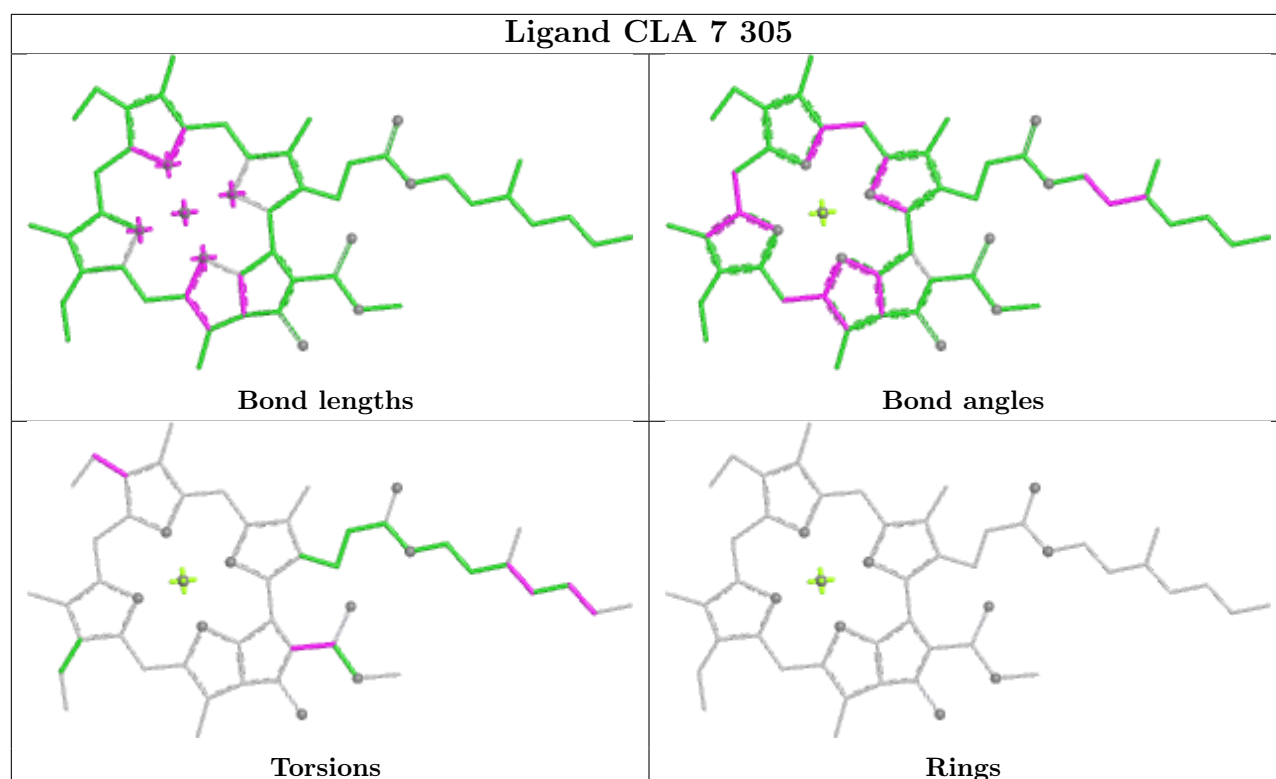


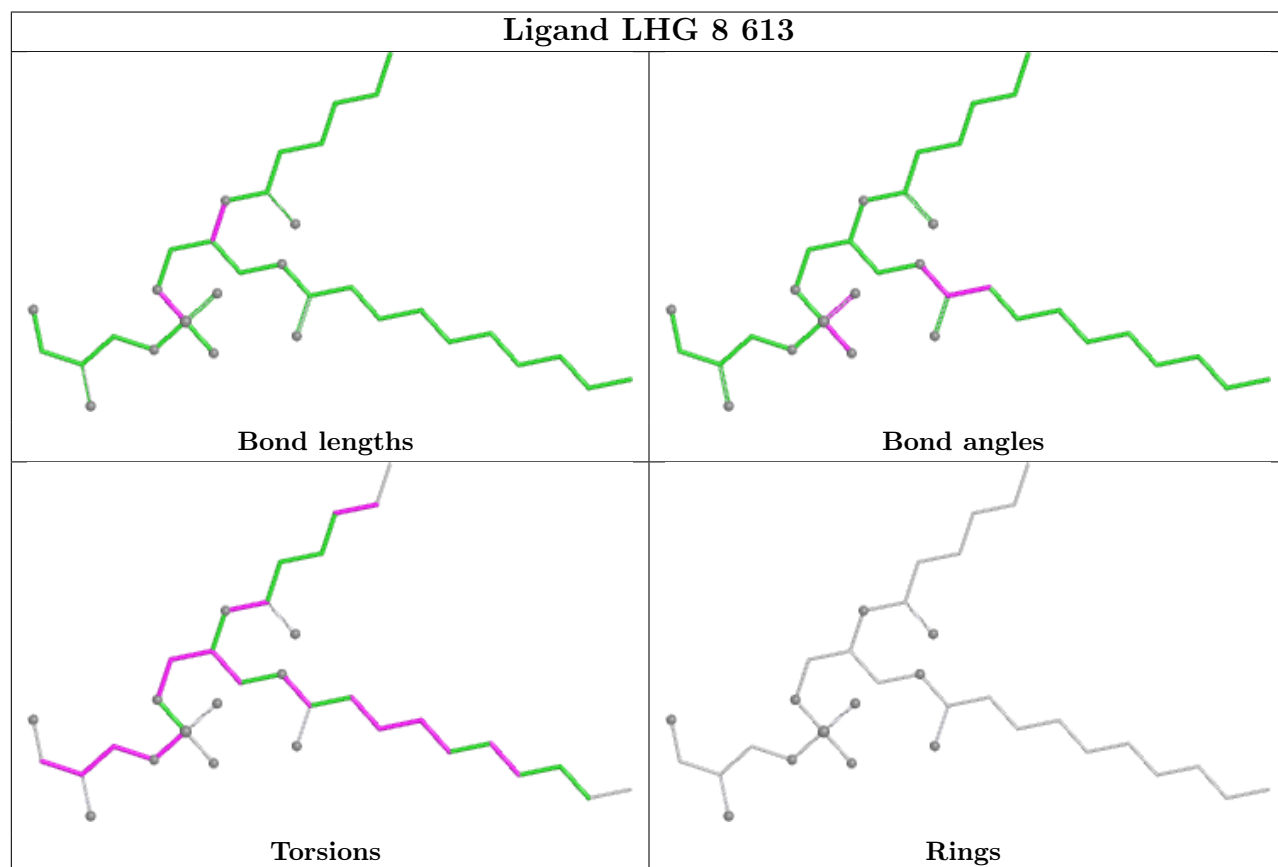
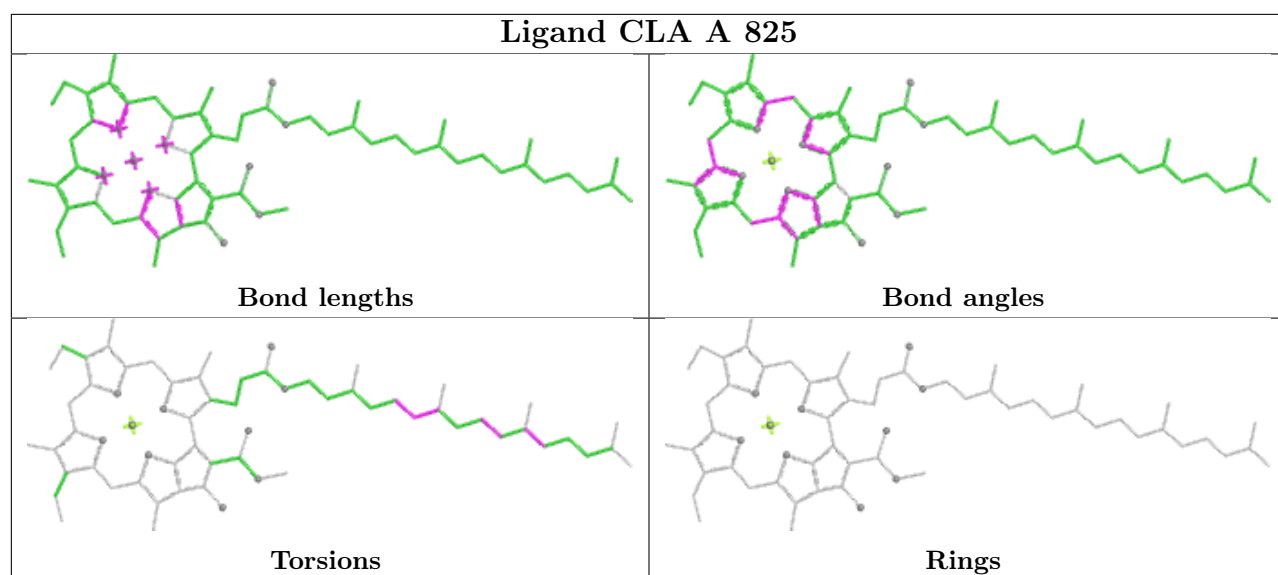
## Ligand II0 4 613

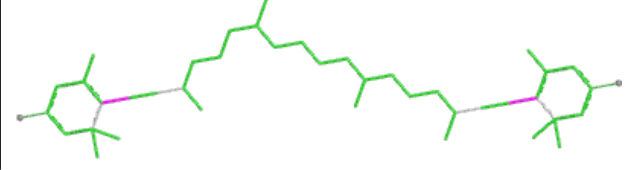
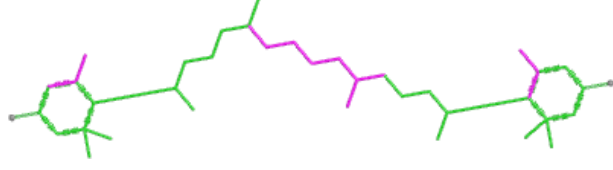
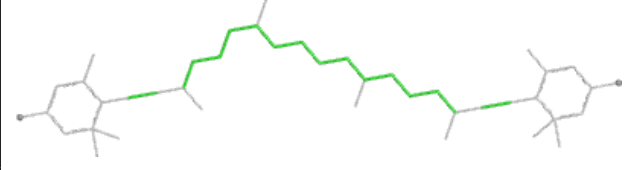
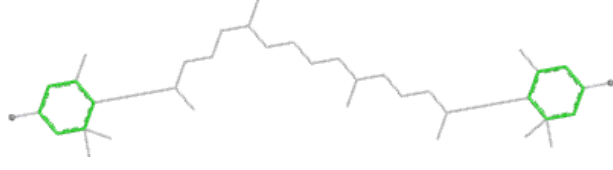
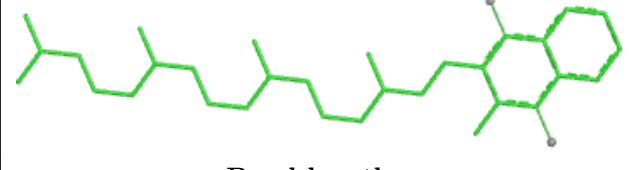
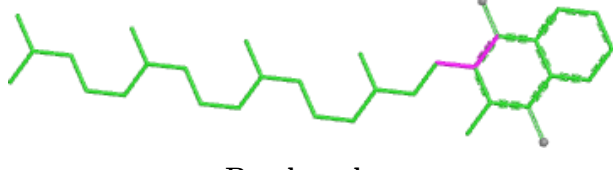
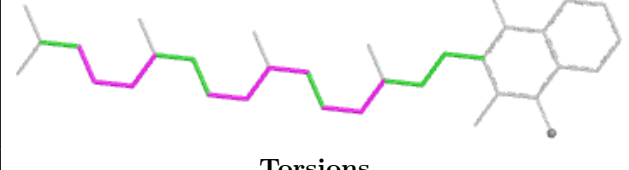
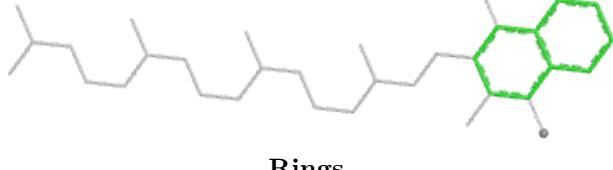
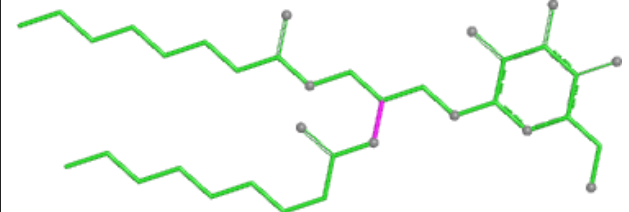
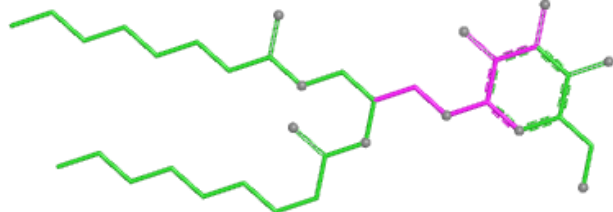
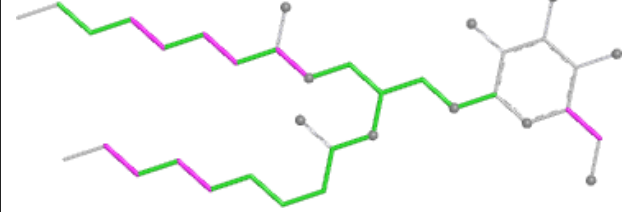
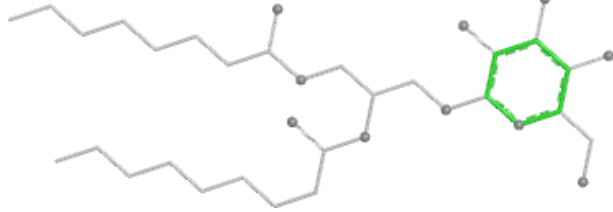


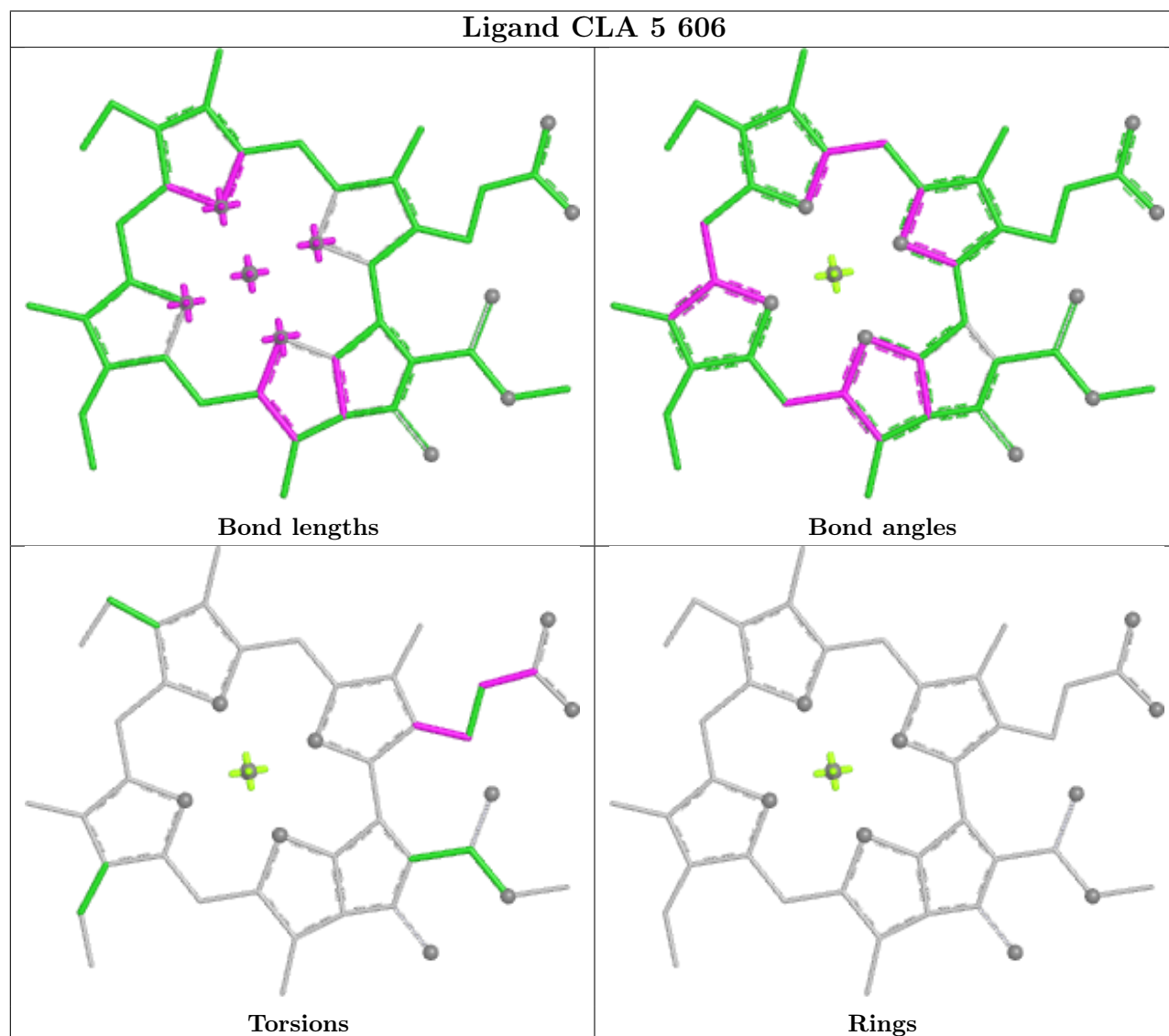
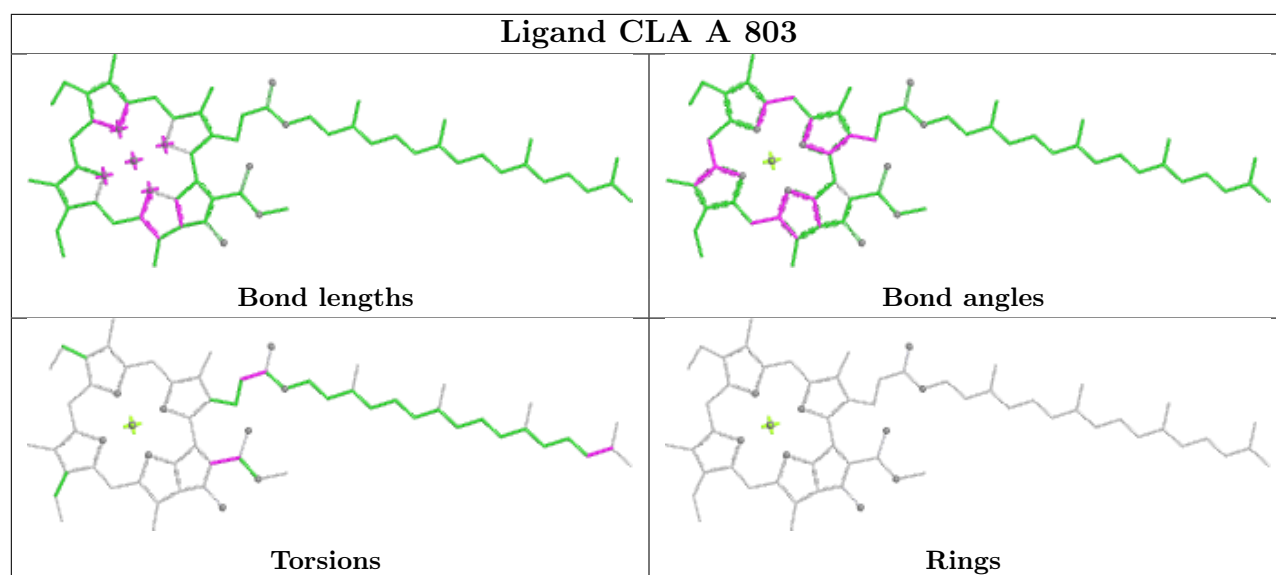


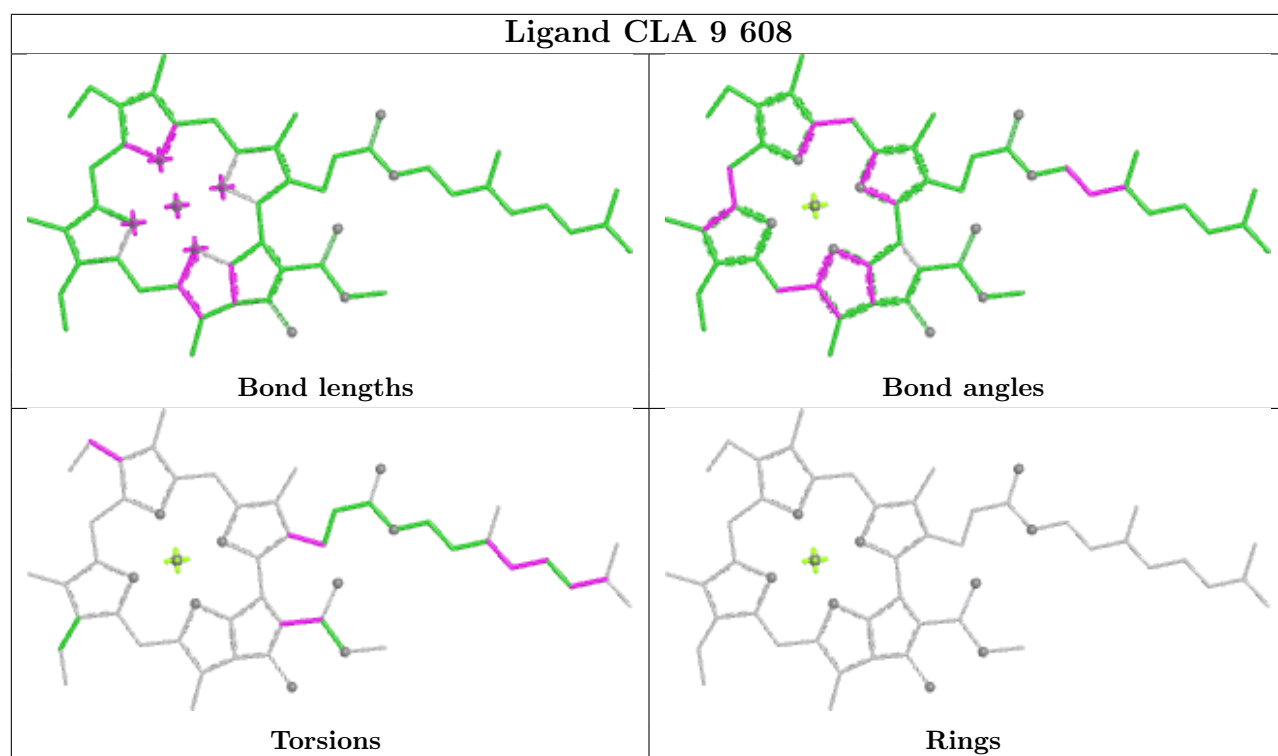




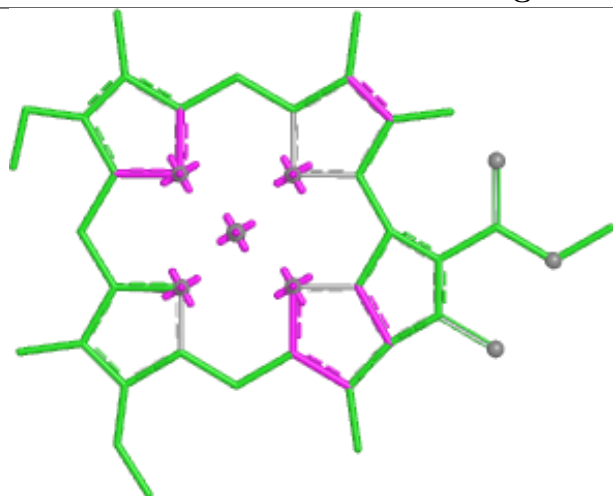


| Ligand II0 4 615                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand PQN A 850                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>      |  <p>Rings</p>        |
| Ligand LMG 2 617                                                                                        |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

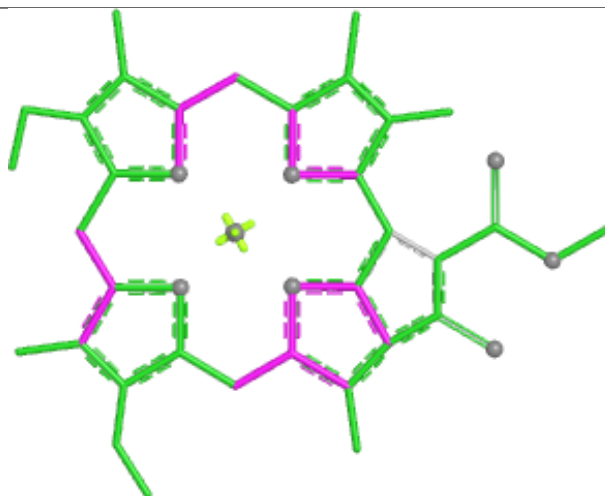




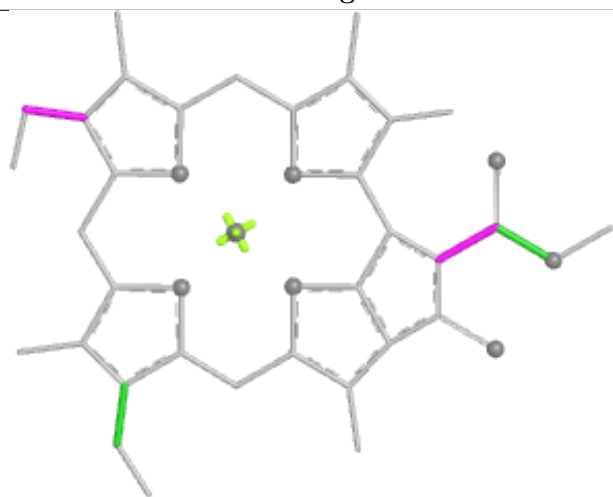
## Ligand CLA O 202



Bond lengths



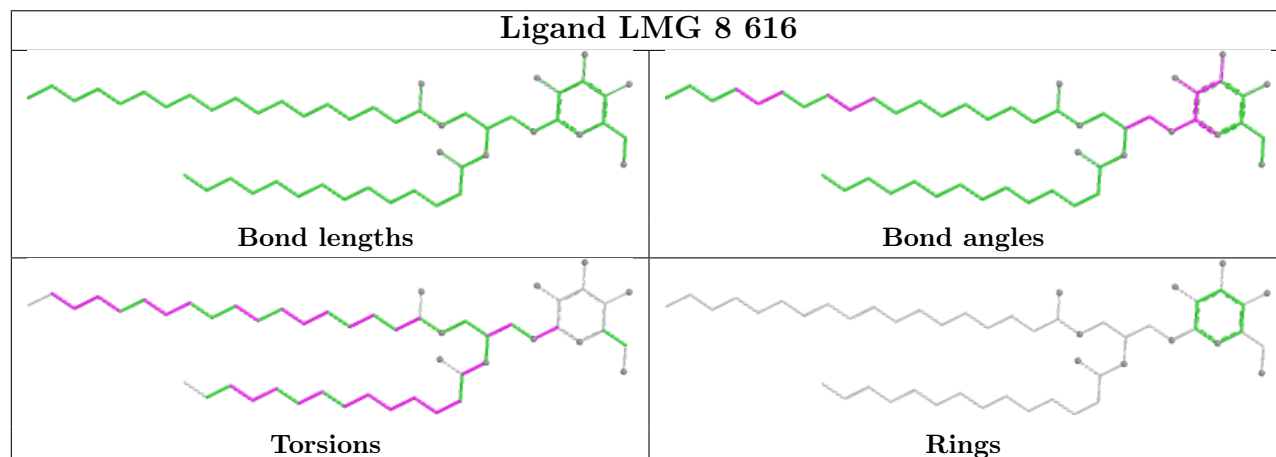
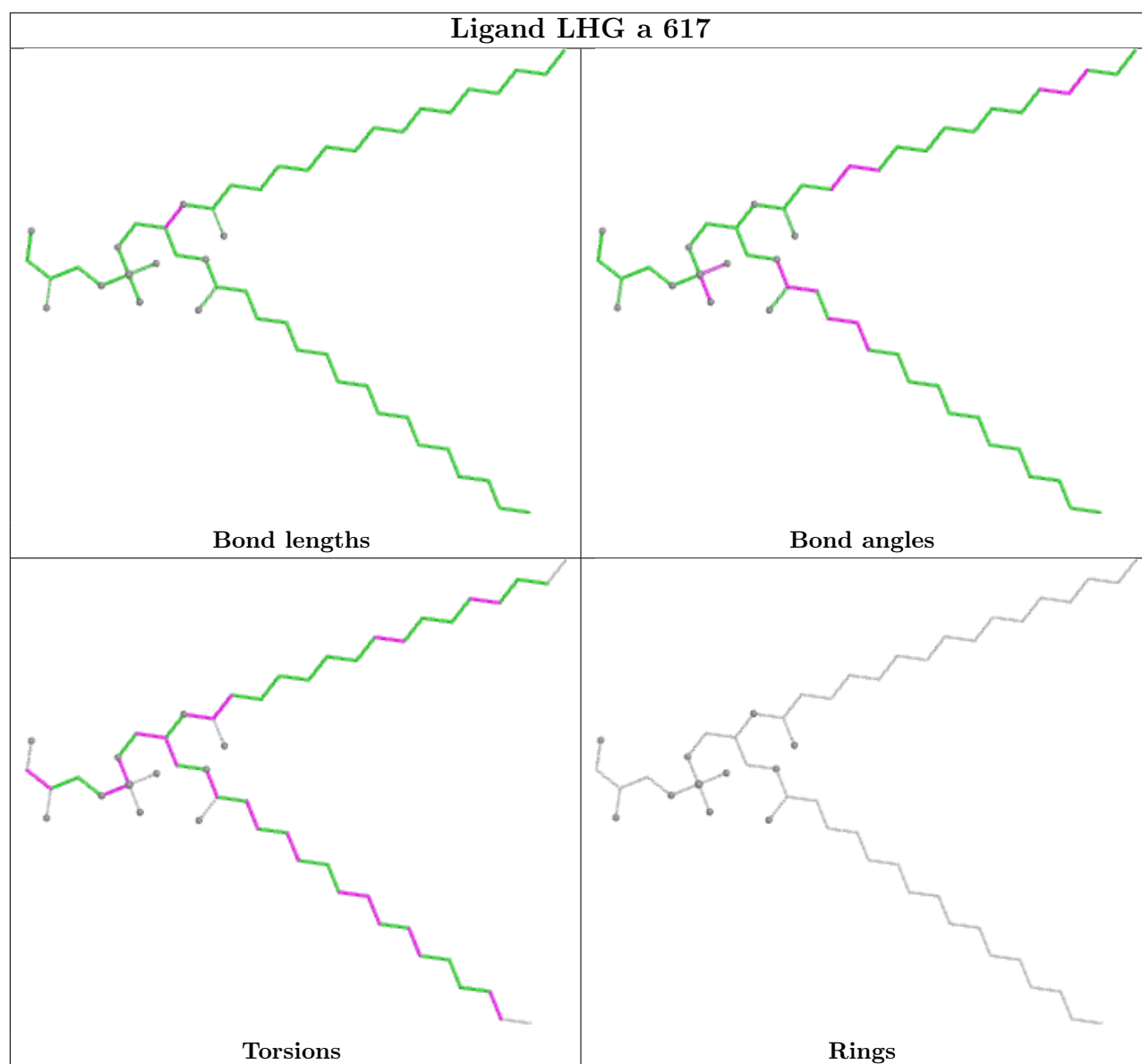
Bond angles



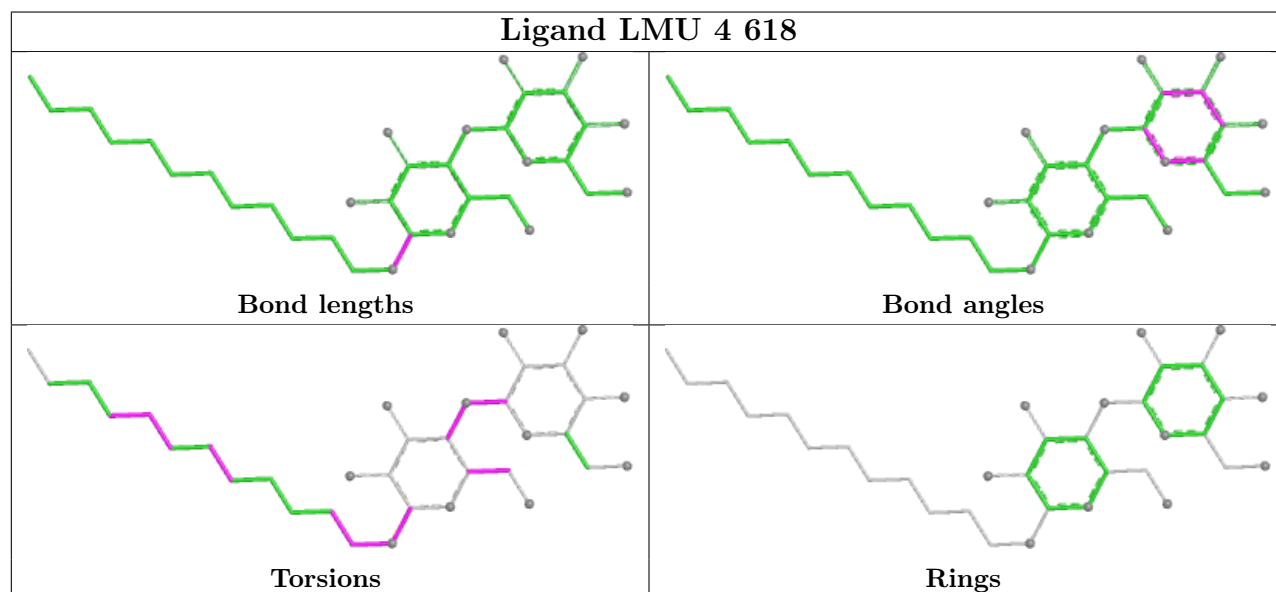
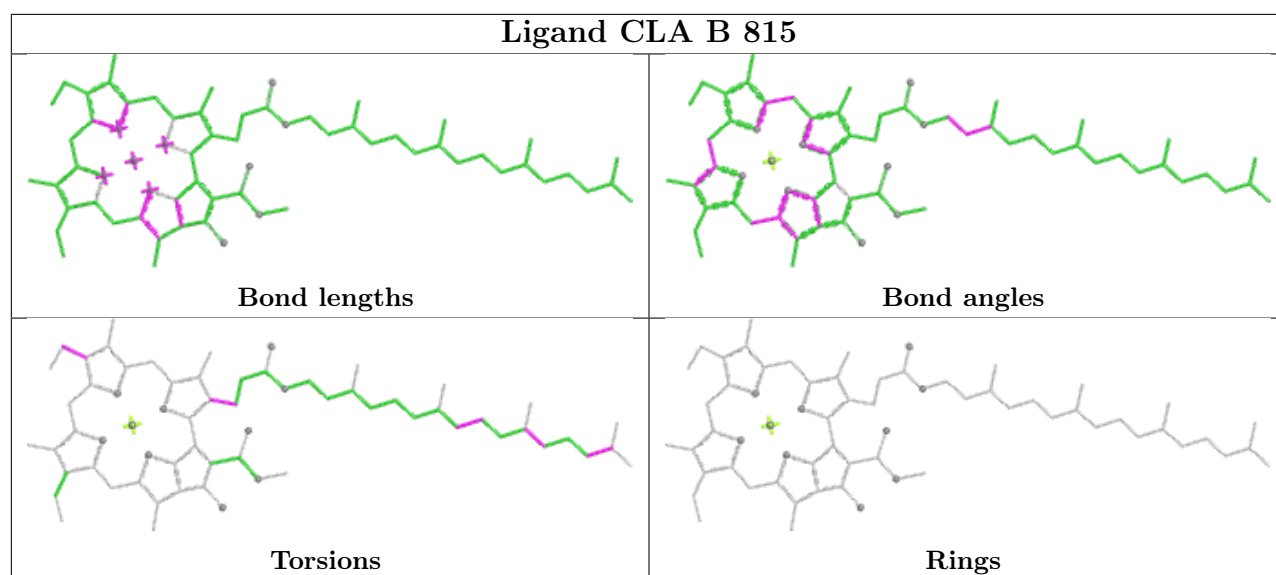
Torsions

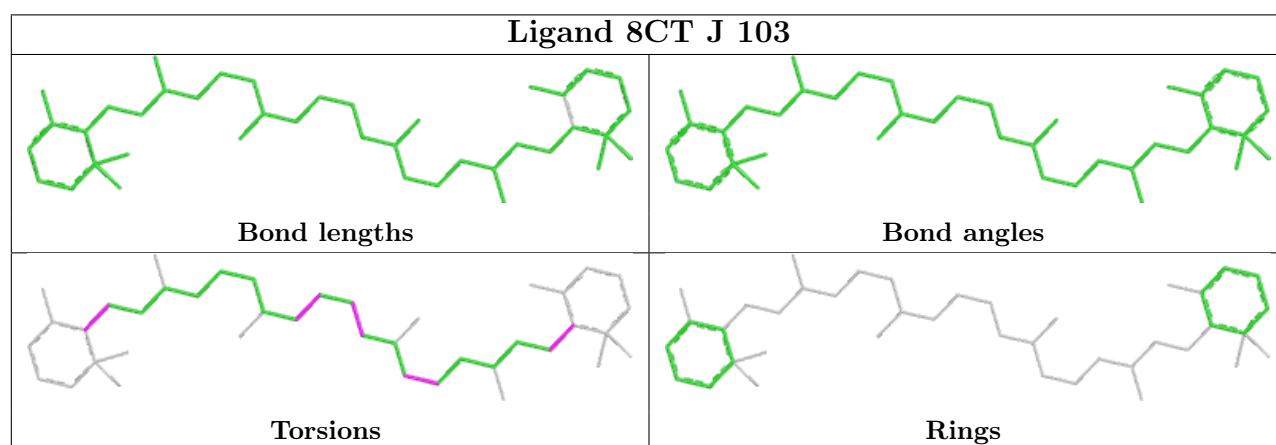
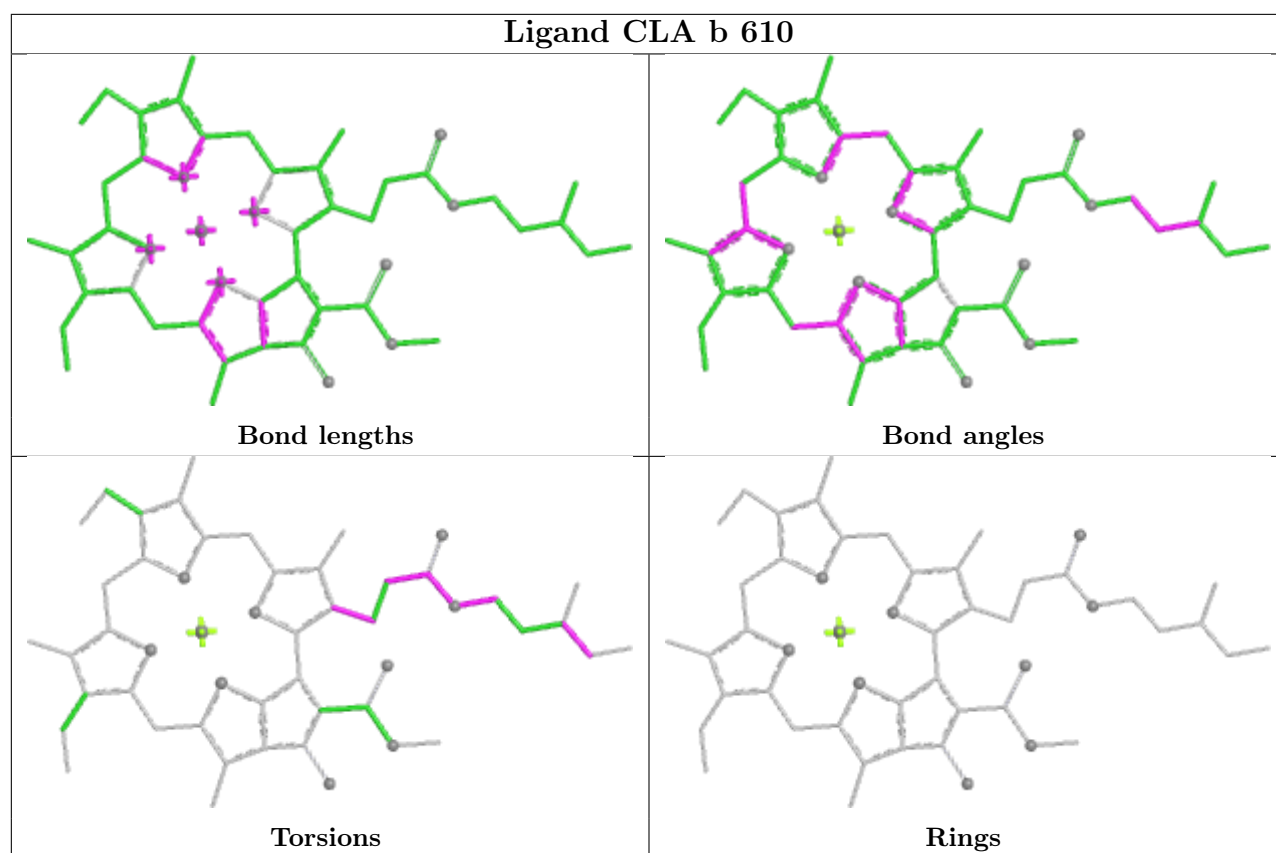


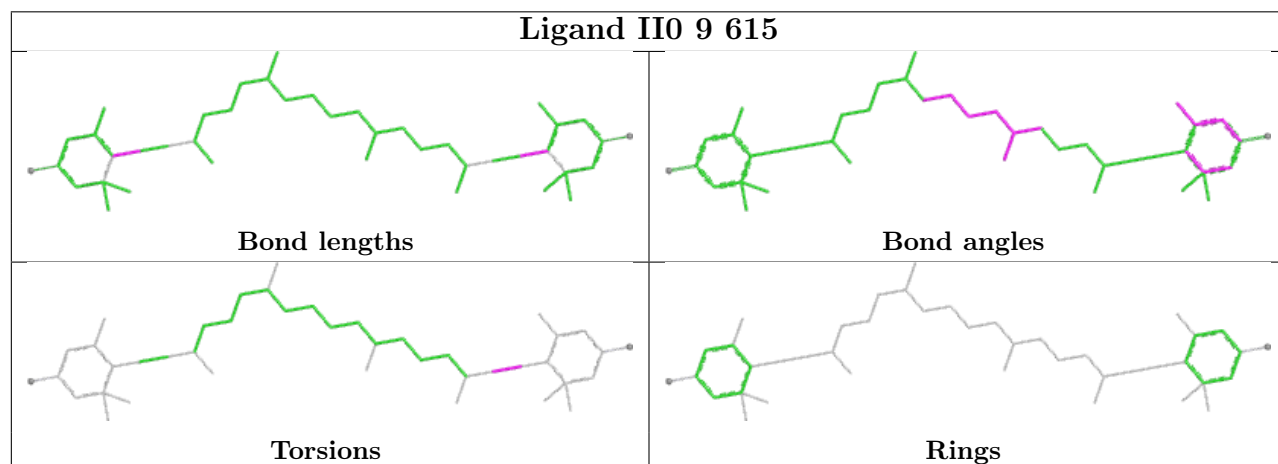
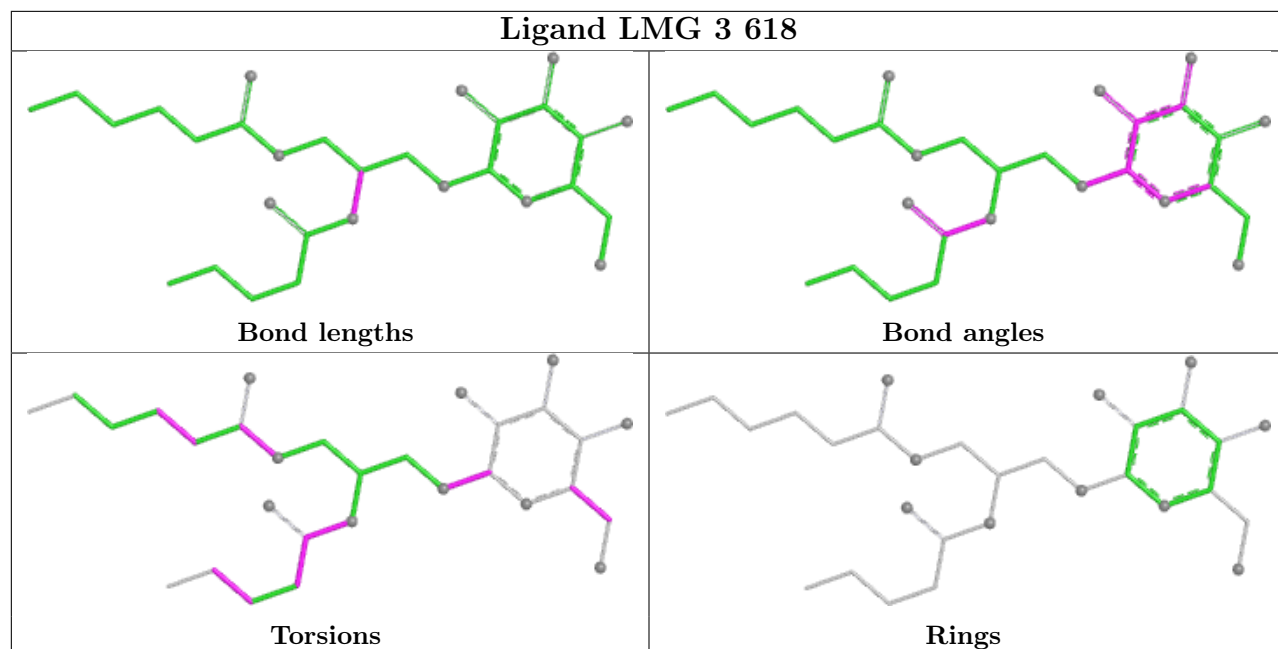
Rings



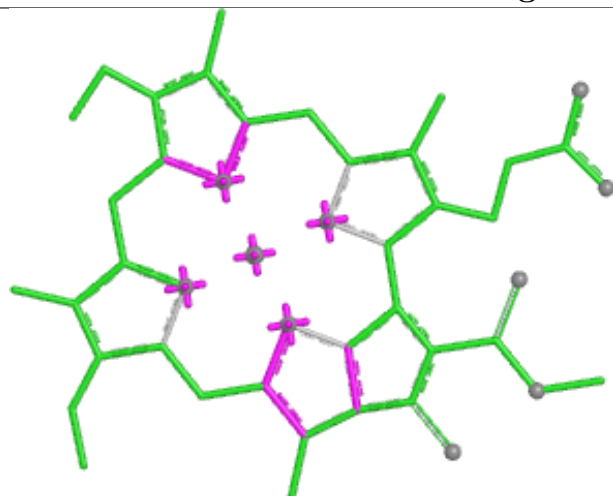




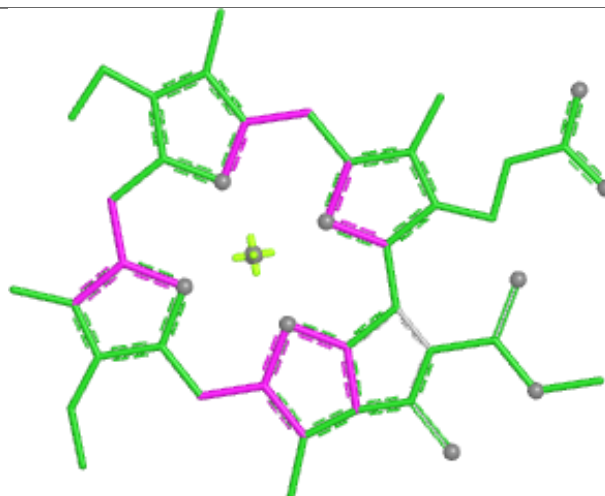




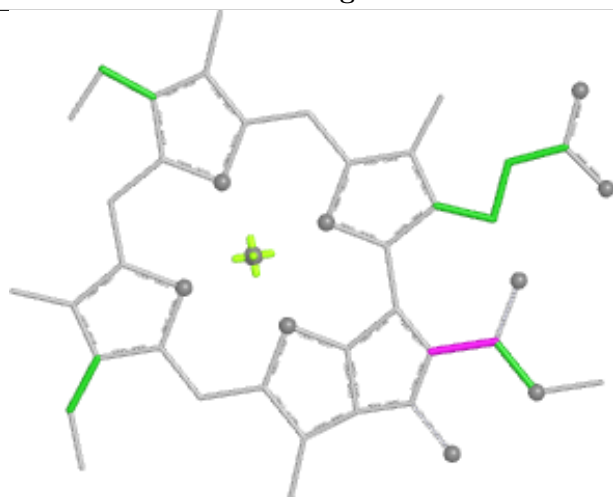
## Ligand CLA 2 606



Bond lengths



Bond angles

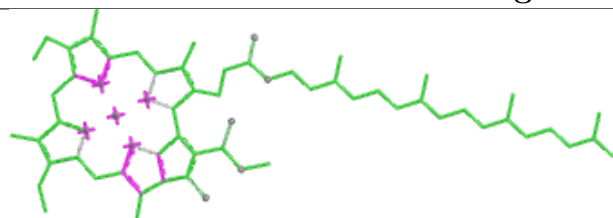


Torsions

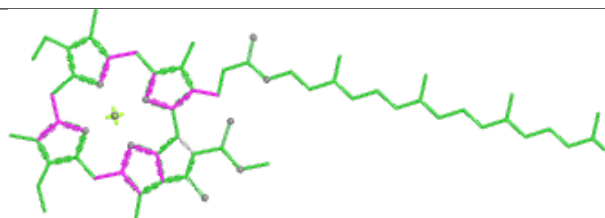


Rings

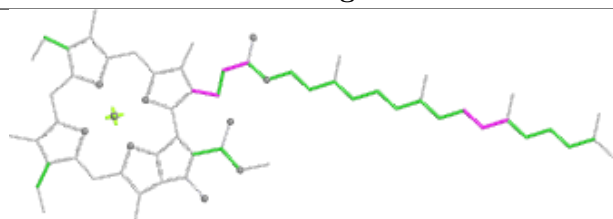
## Ligand CLA B 804



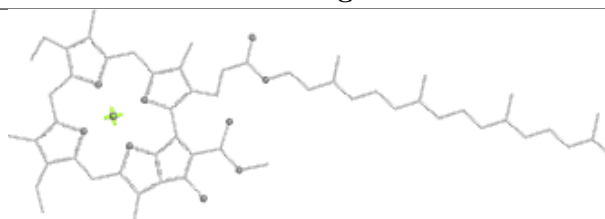
Bond lengths



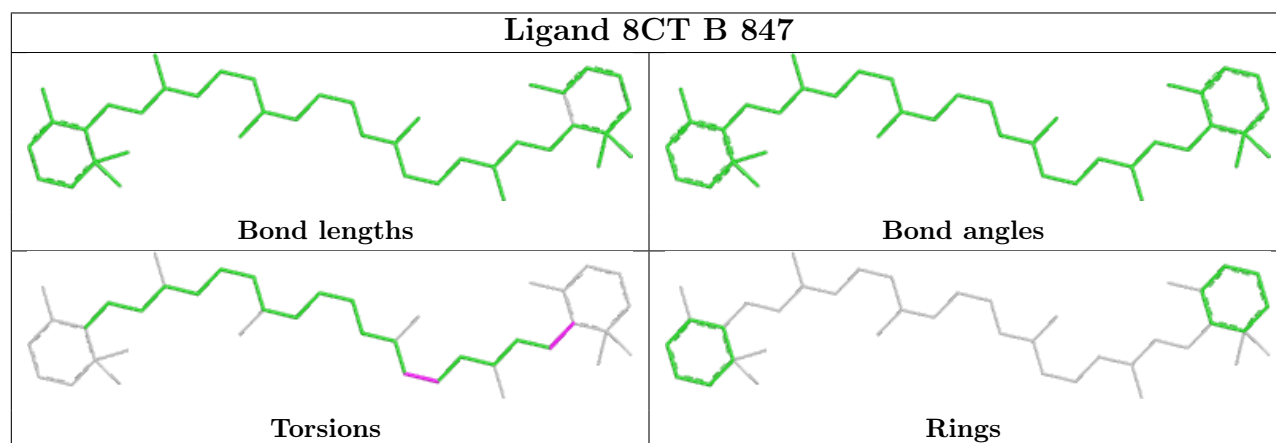
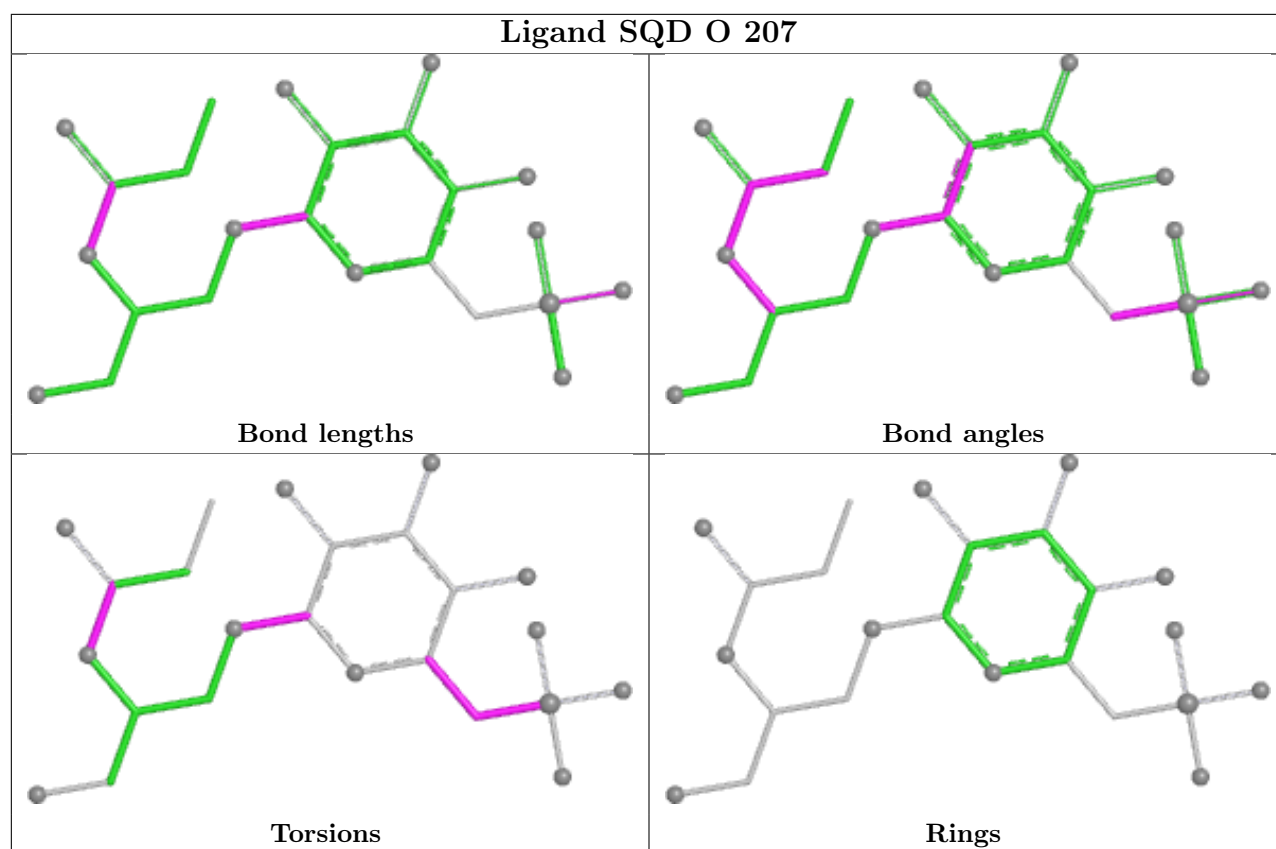
Bond angles



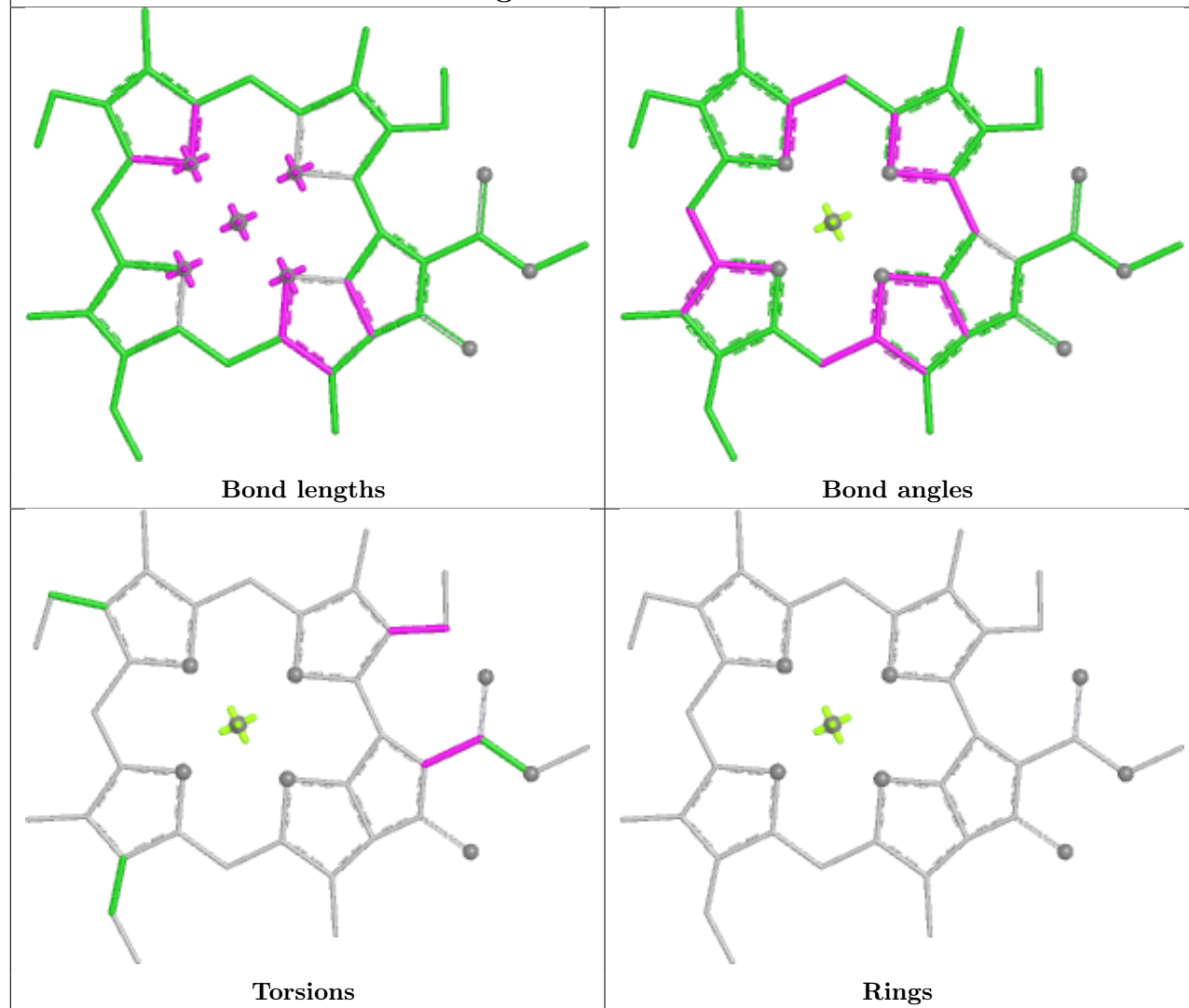
Torsions



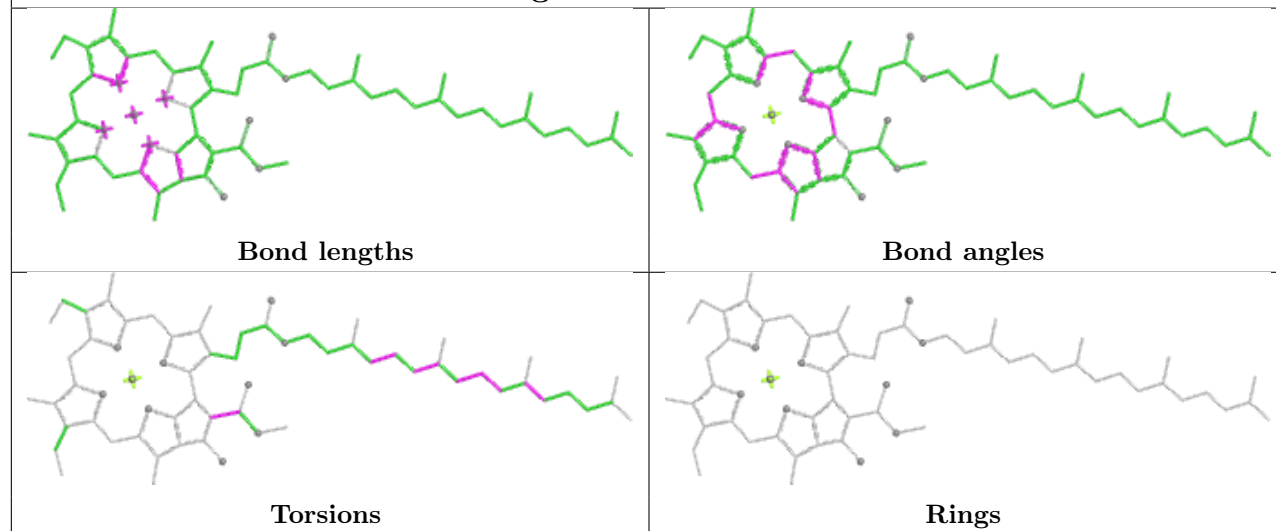
Rings

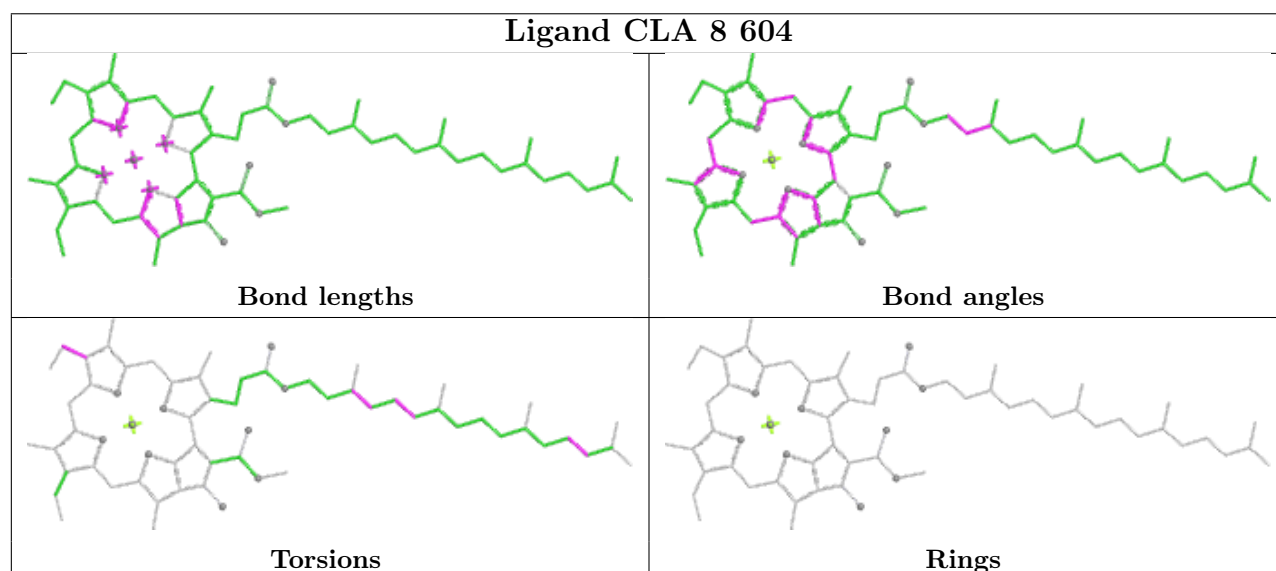
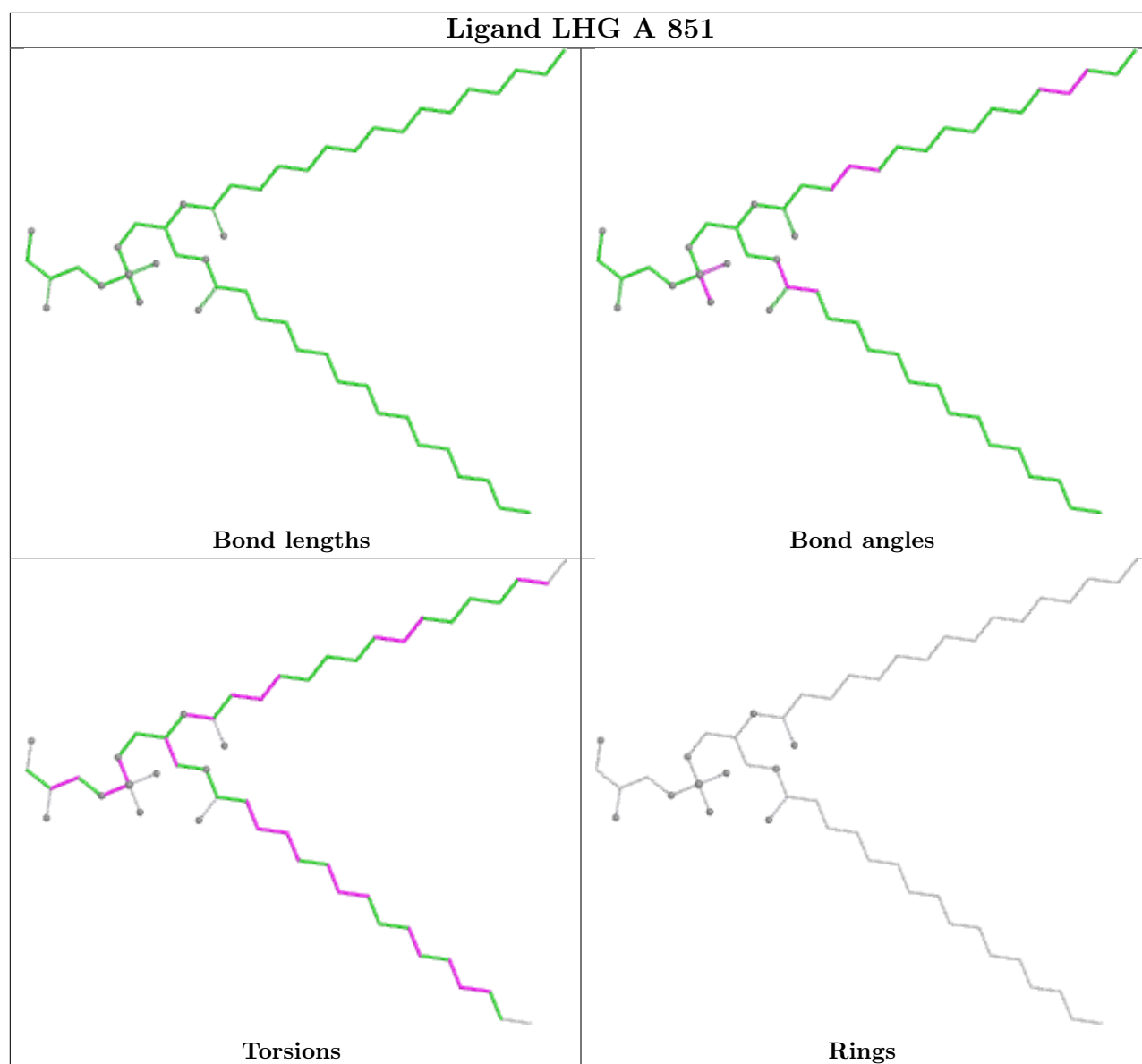


## Ligand CLA B 814

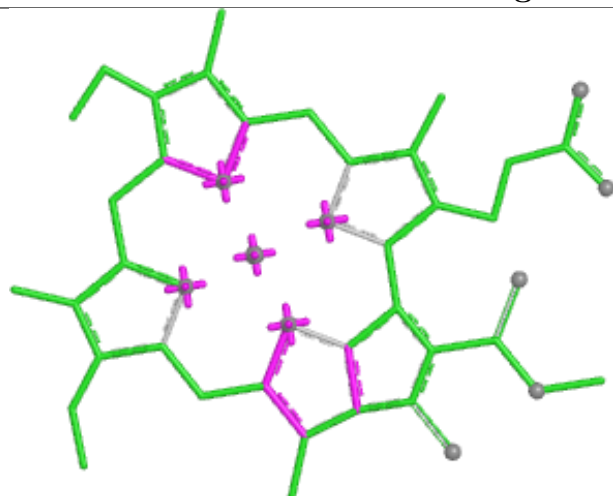


## Ligand CLA A 806

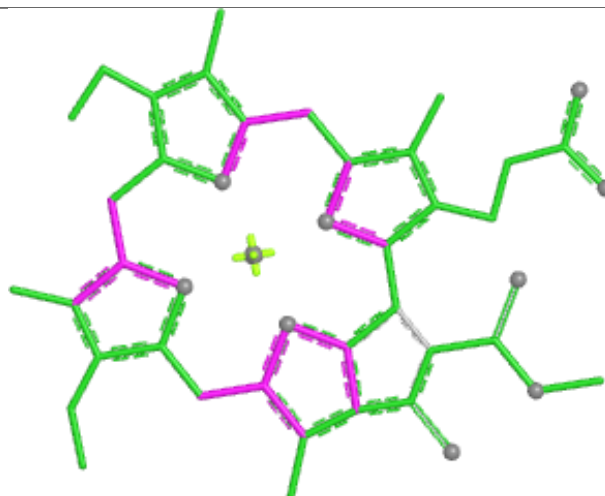




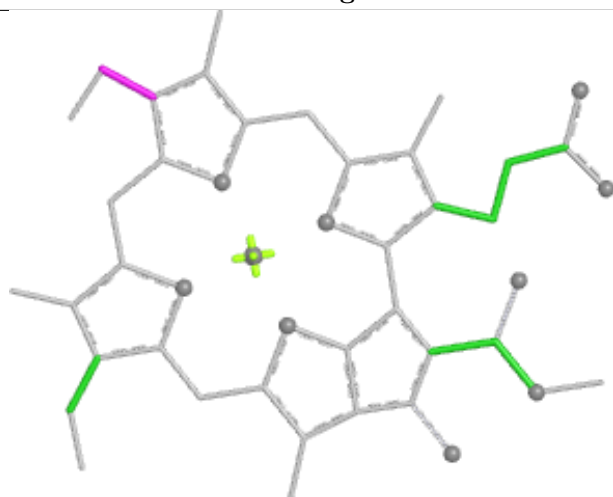
## Ligand CLA B 833



Bond lengths



Bond angles

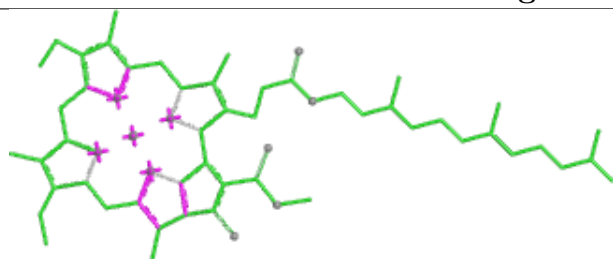


Torsions

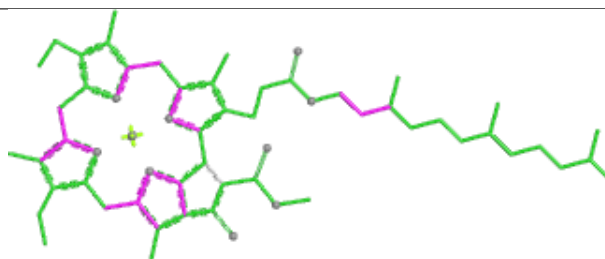


Rings

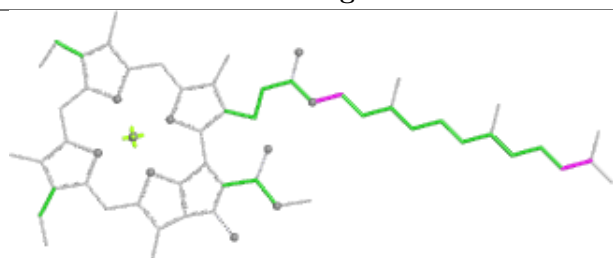
## Ligand CLA 4 606



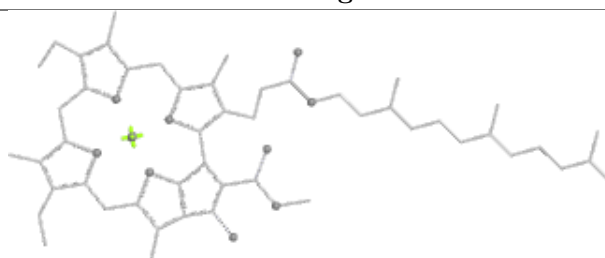
Bond lengths



Bond angles

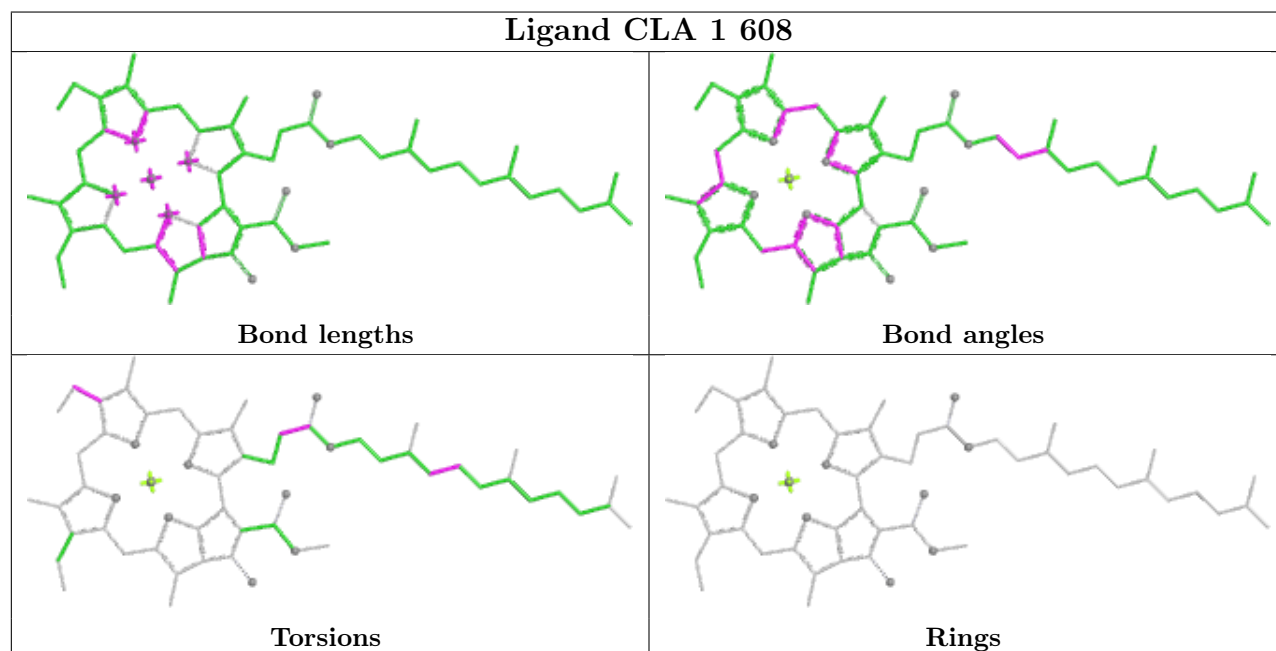
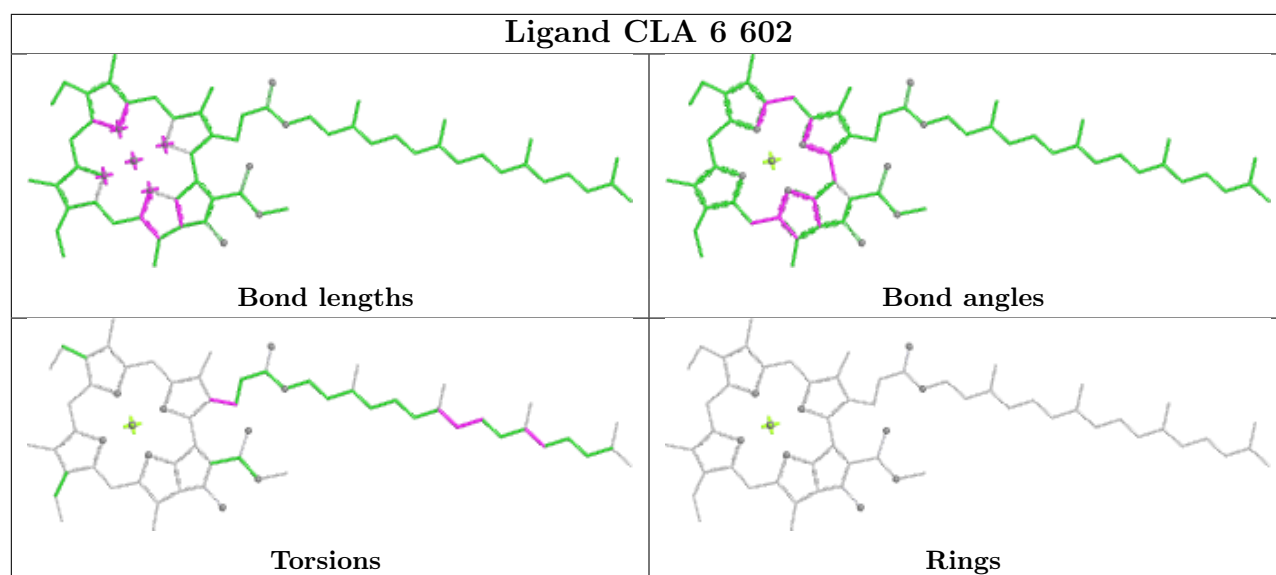


Torsions

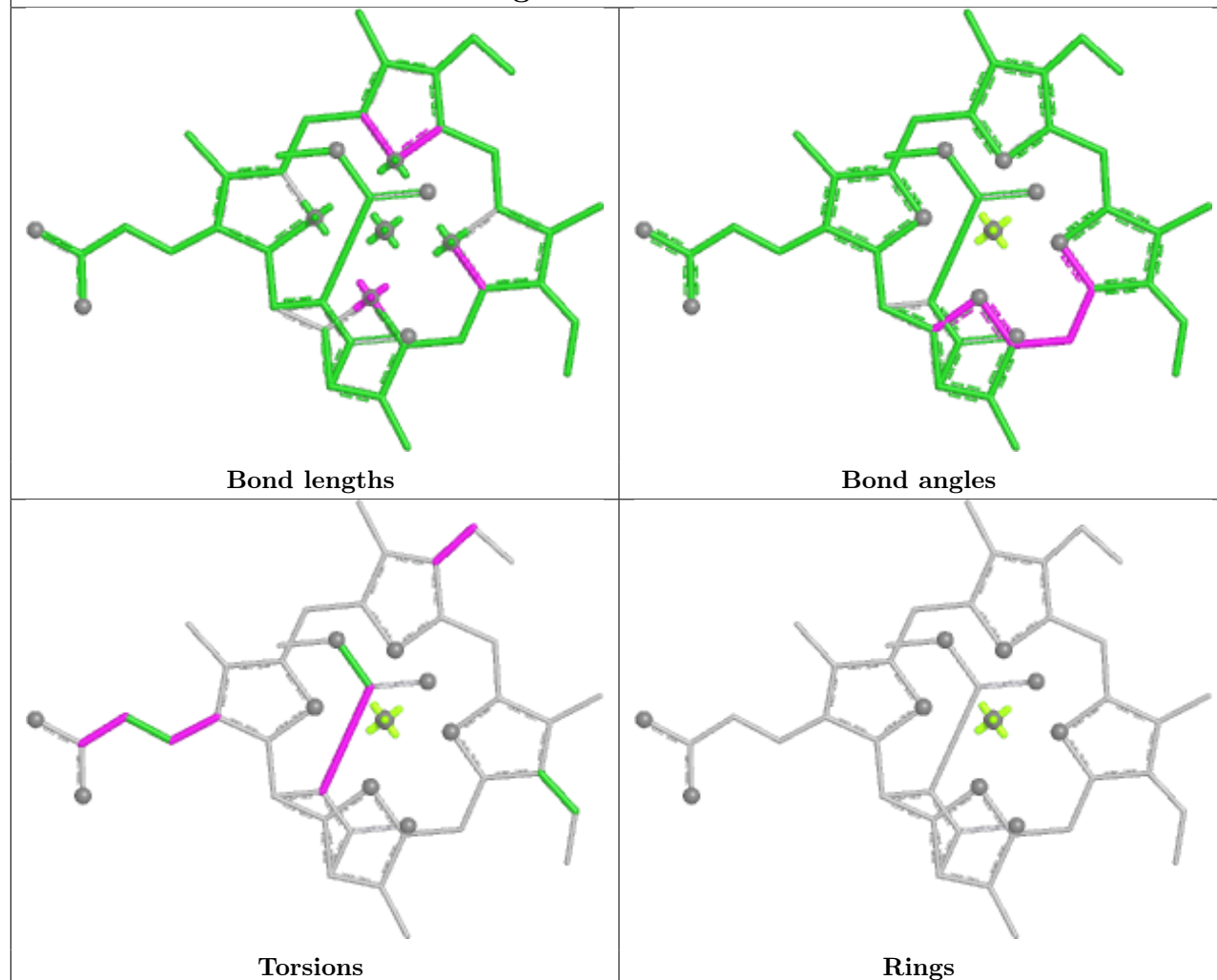


Rings

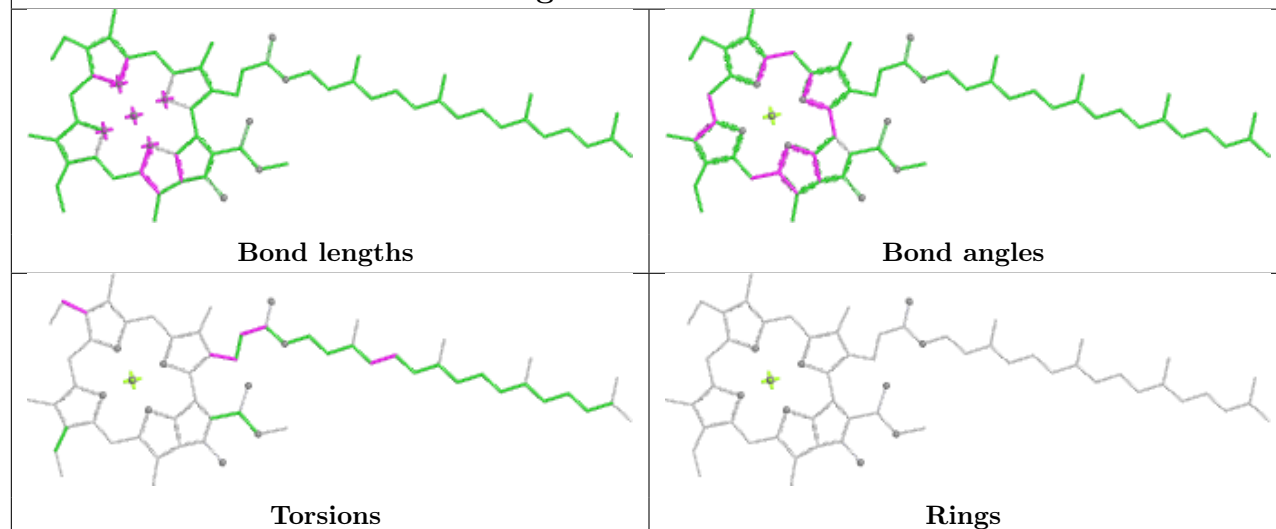


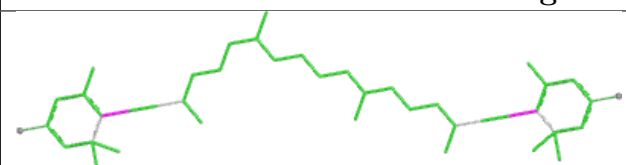
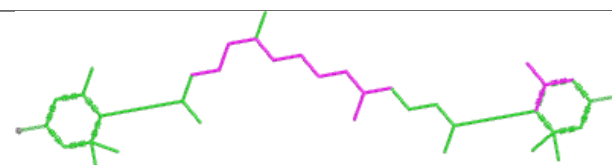
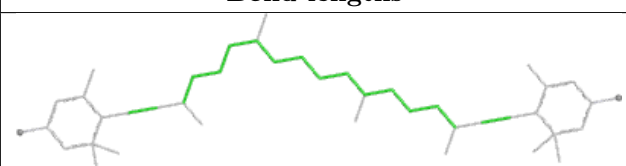
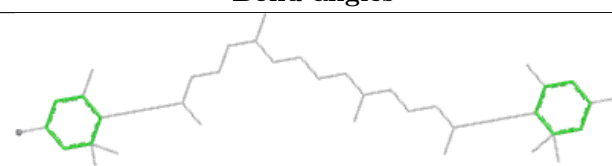


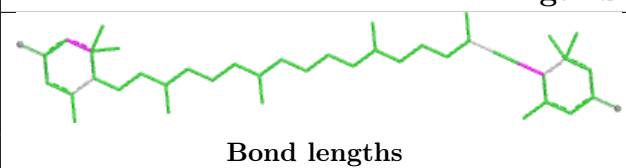
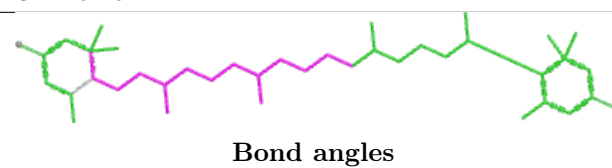
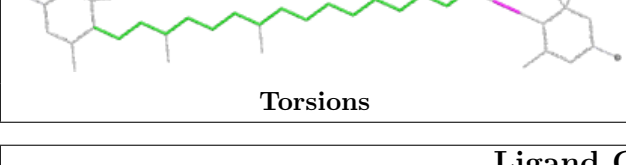
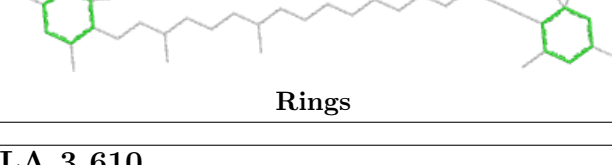
## Ligand KC2 1 610

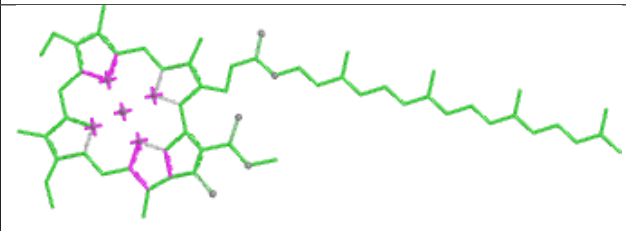
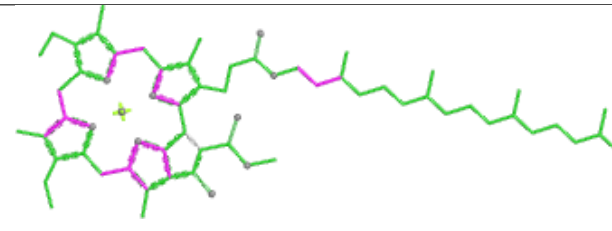
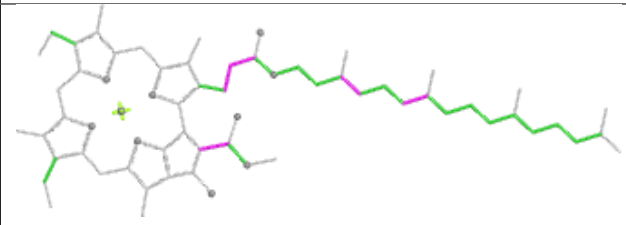
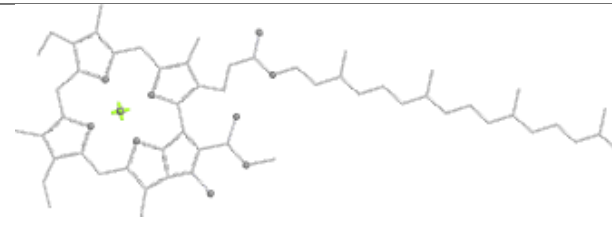


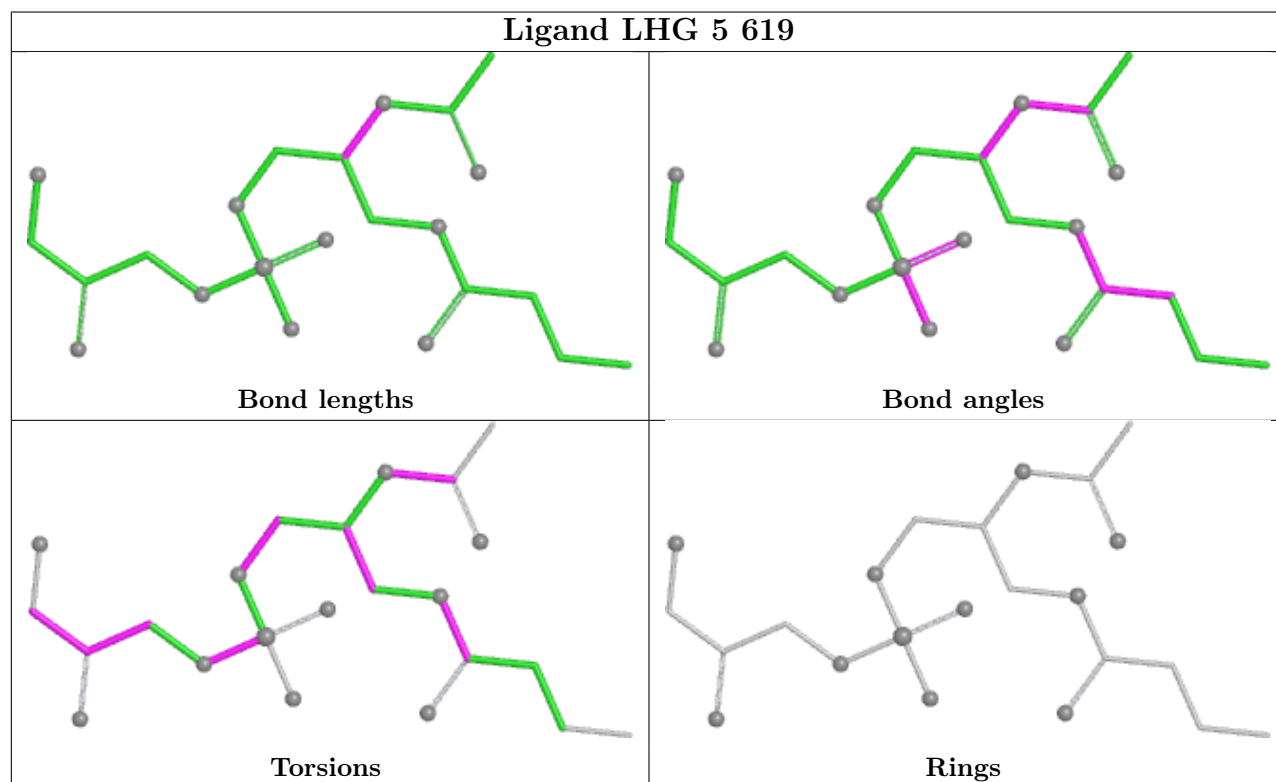
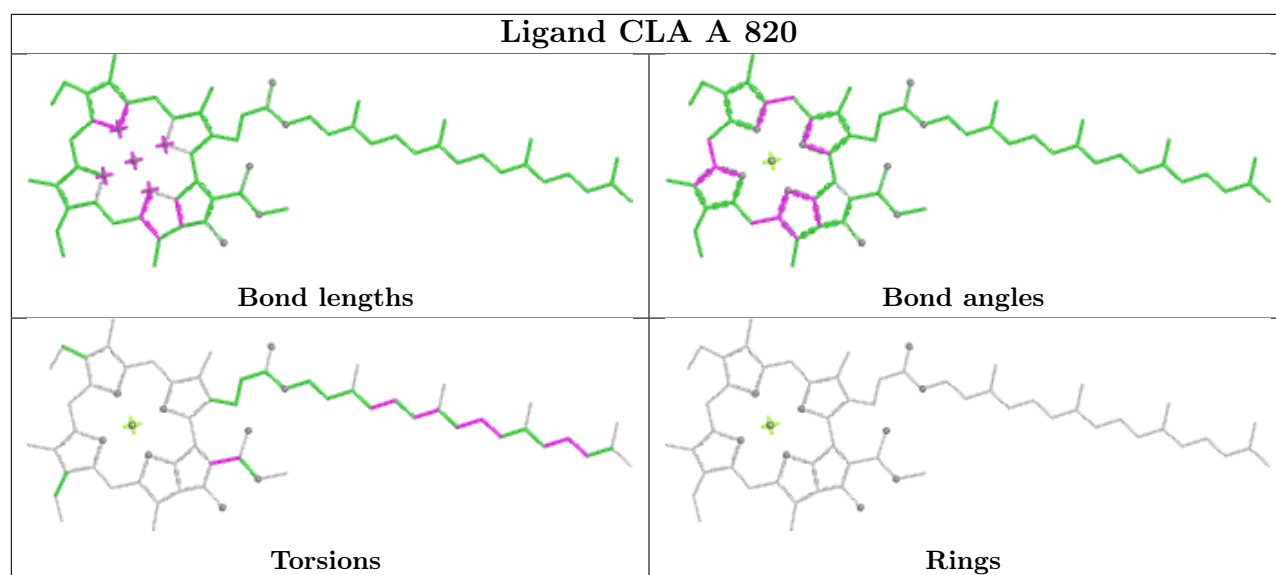
## Ligand CLA a 611



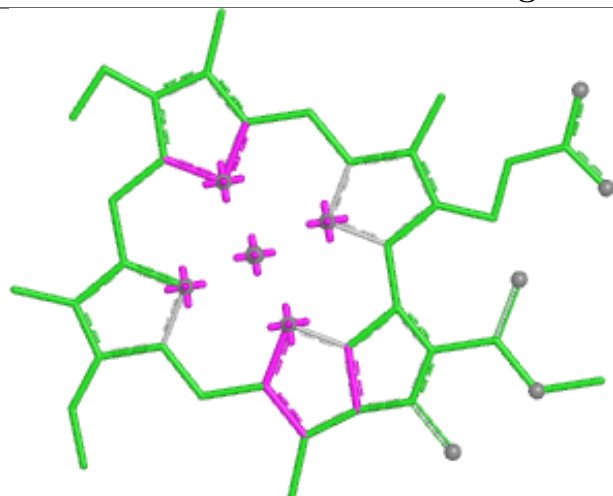
| Ligand II0 7 317                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand II3 1 615                                                                   |                                                                                     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                       | Bond angles                                                                         |
|  |  |
| Torsions                                                                           | Rings                                                                               |

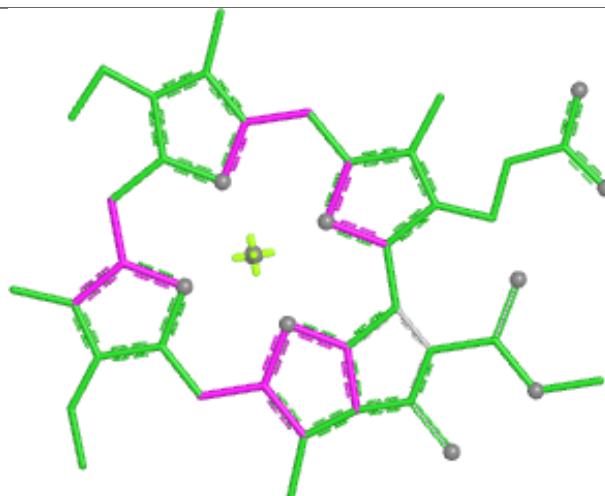
| Ligand CLA 3 610                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |



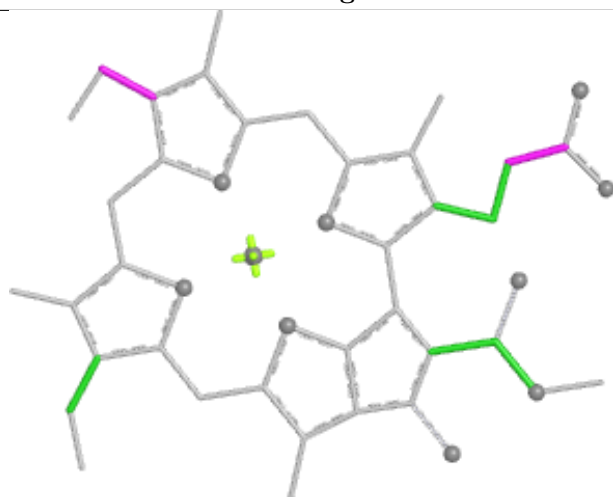
## Ligand CLA 9 605



Bond lengths



Bond angles

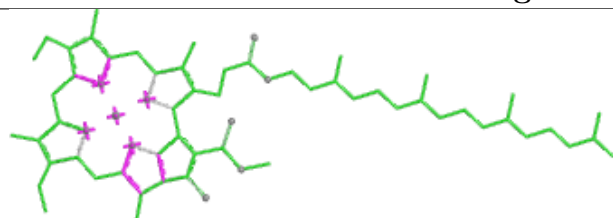


Torsions

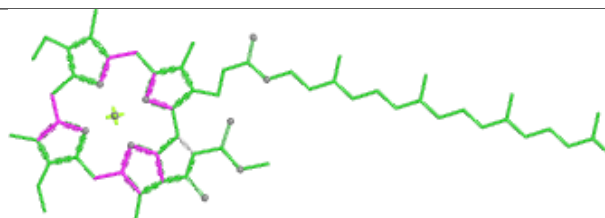


Rings

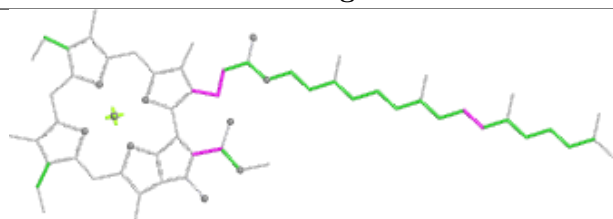
## Ligand CLA A 842



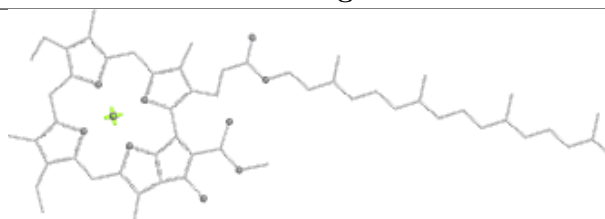
Bond lengths



Bond angles

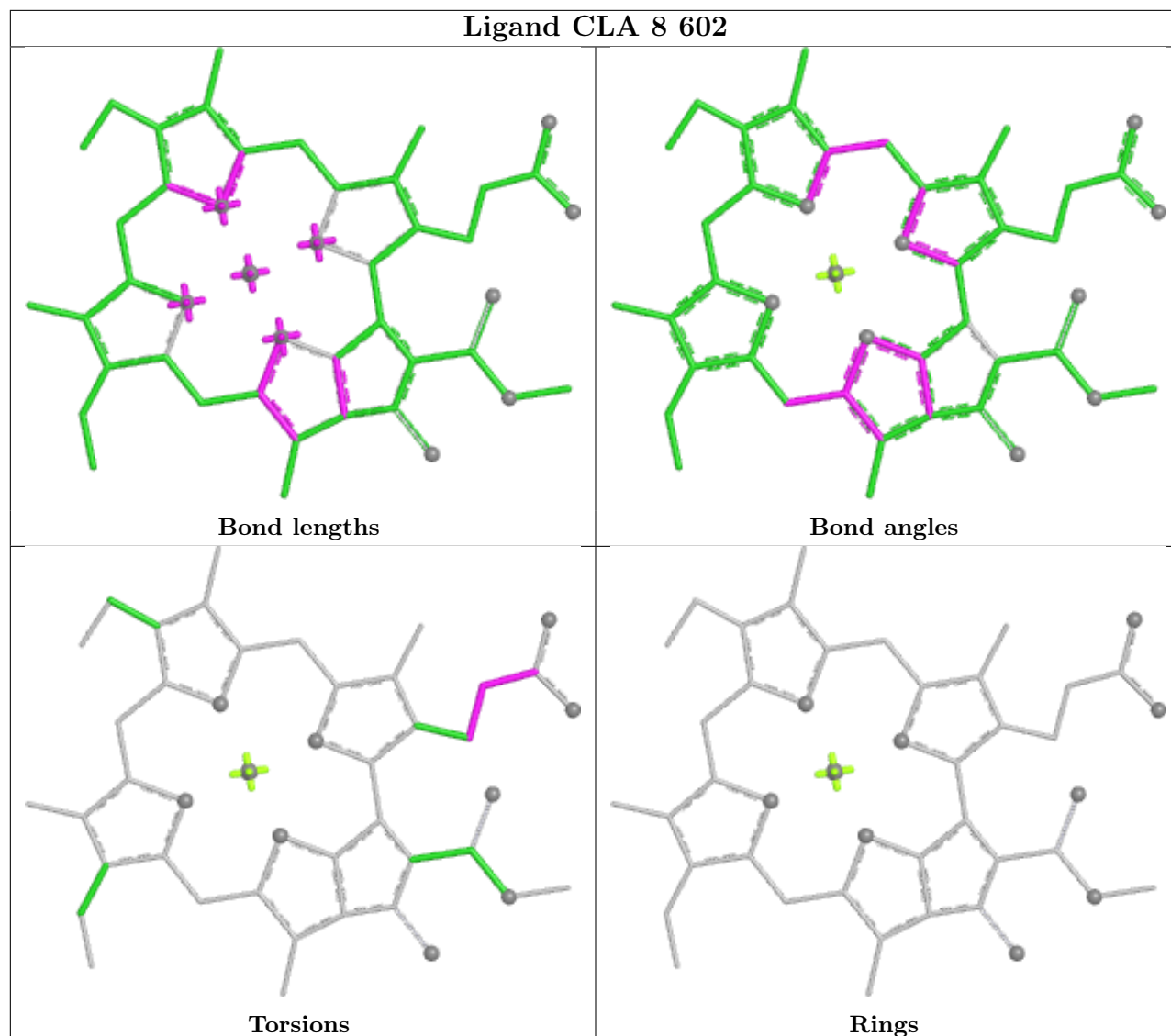


Torsions

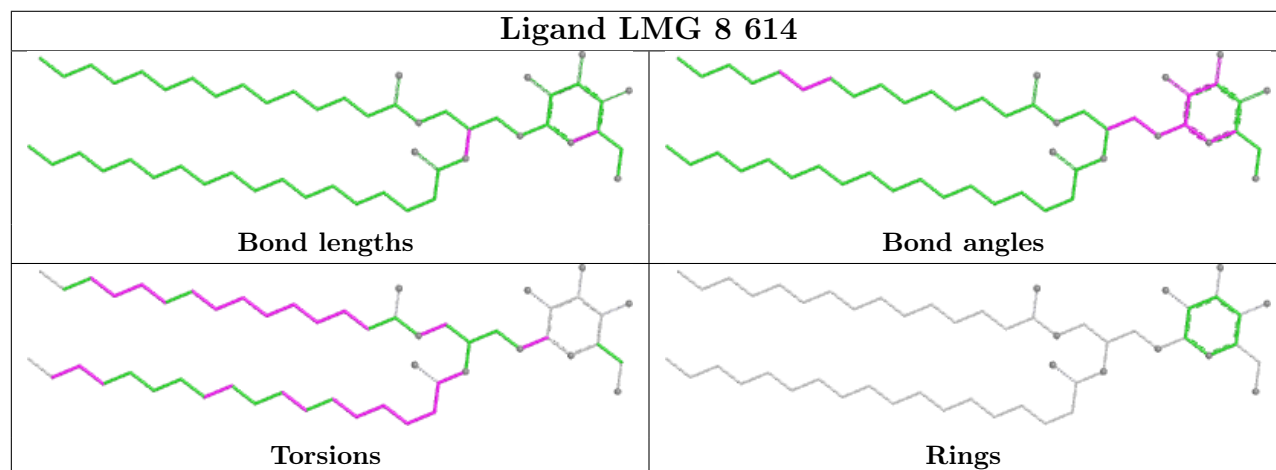


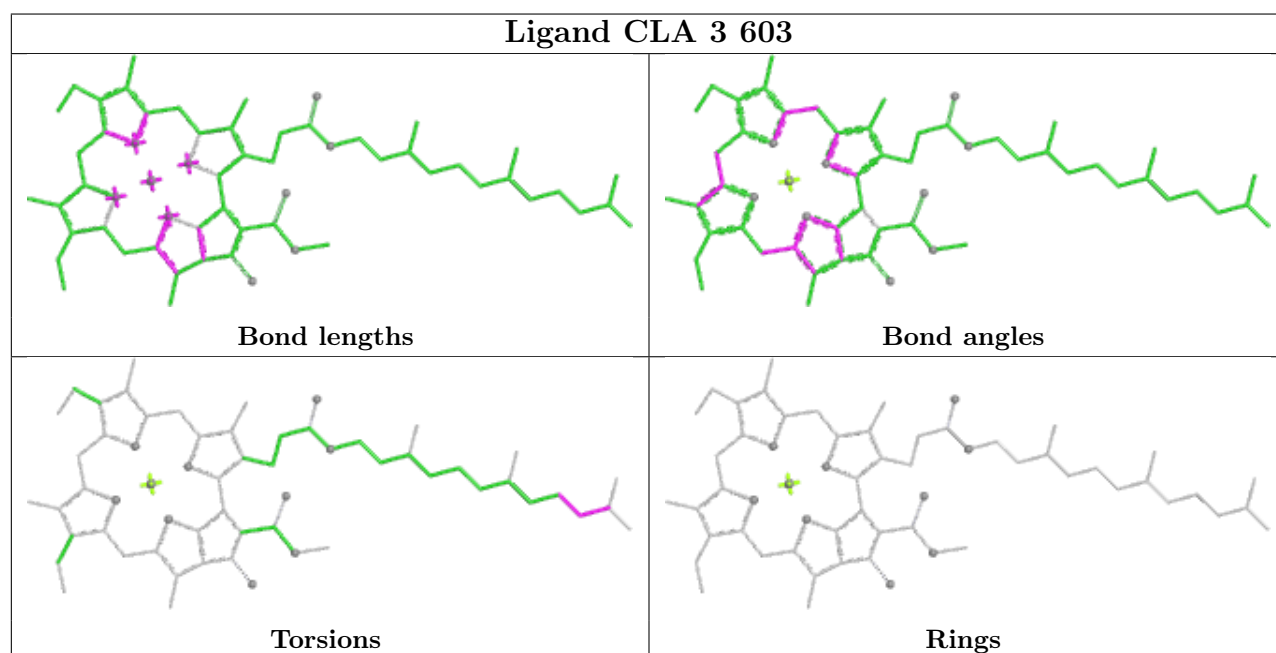
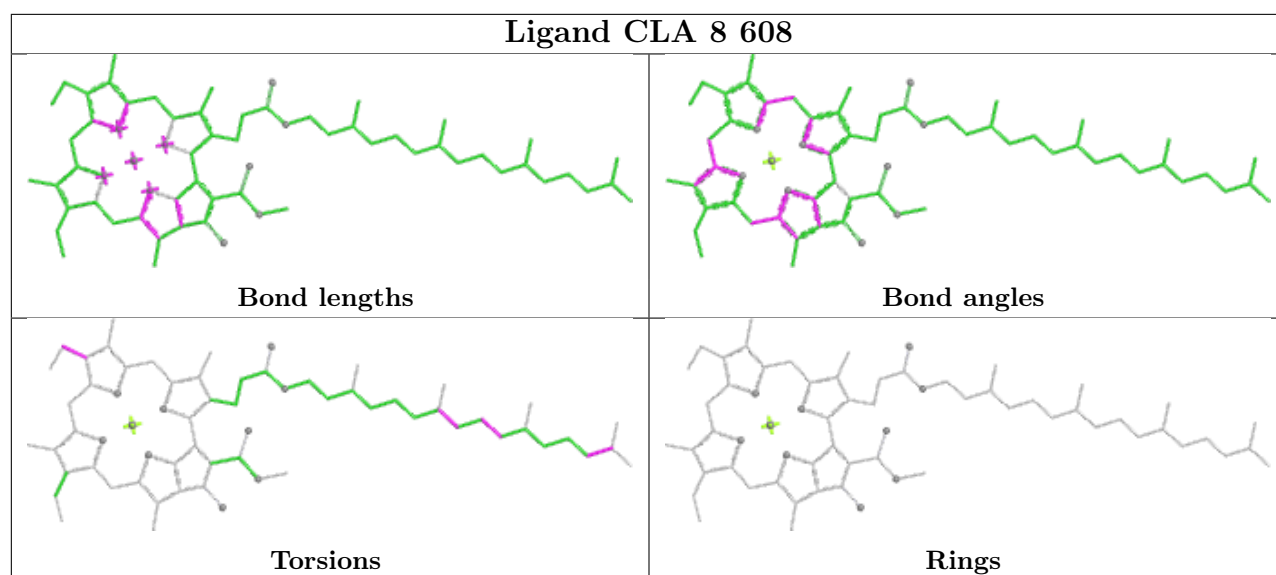
Rings

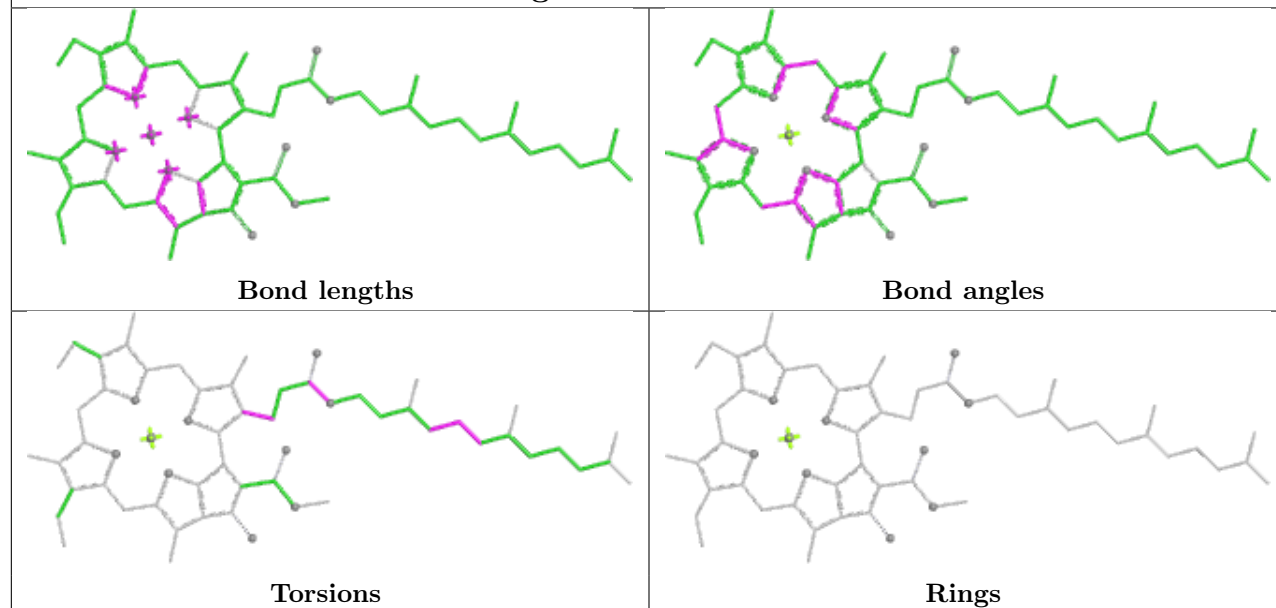
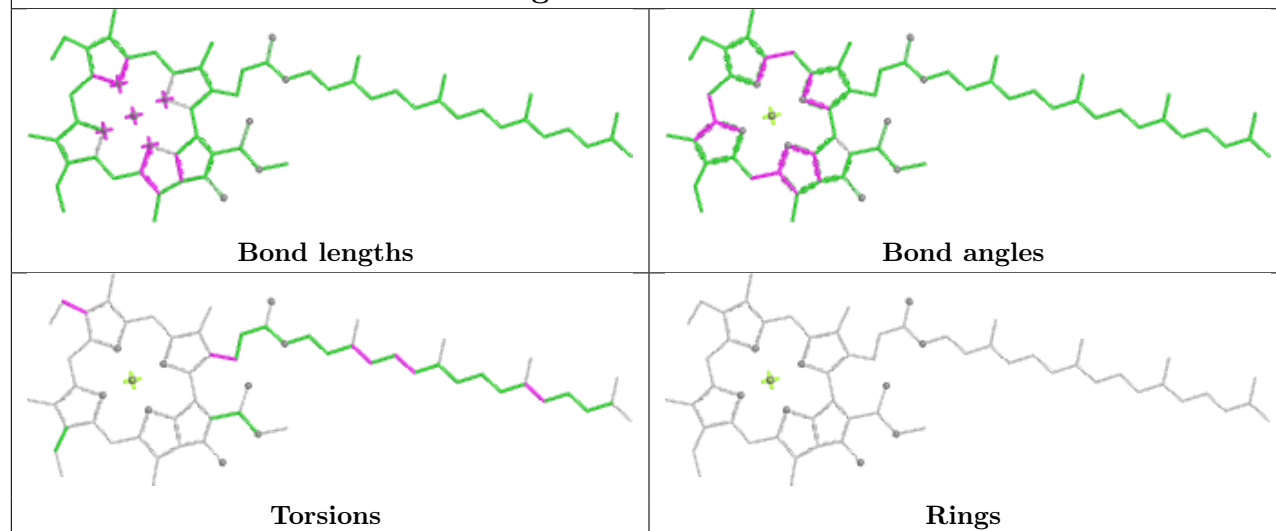
## Ligand CLA 8 602



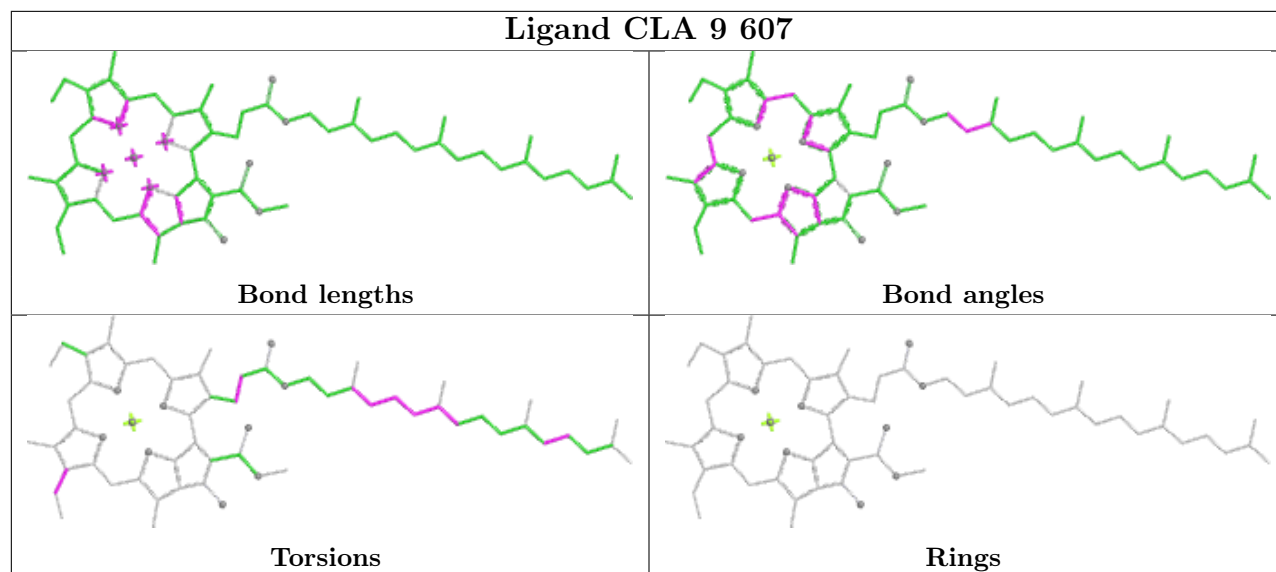
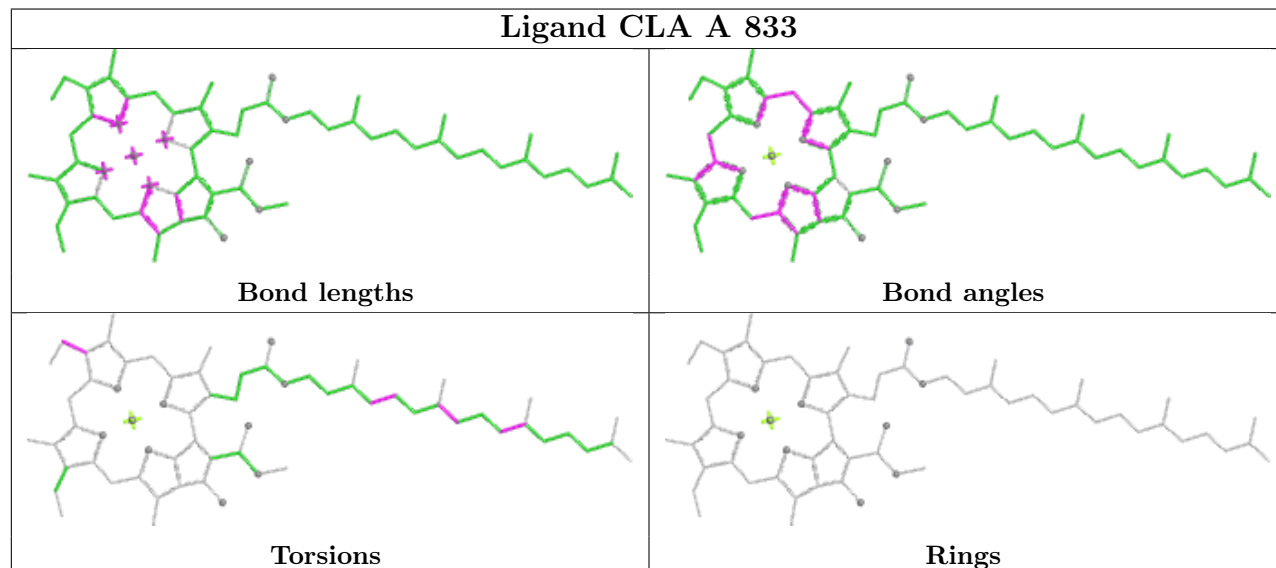
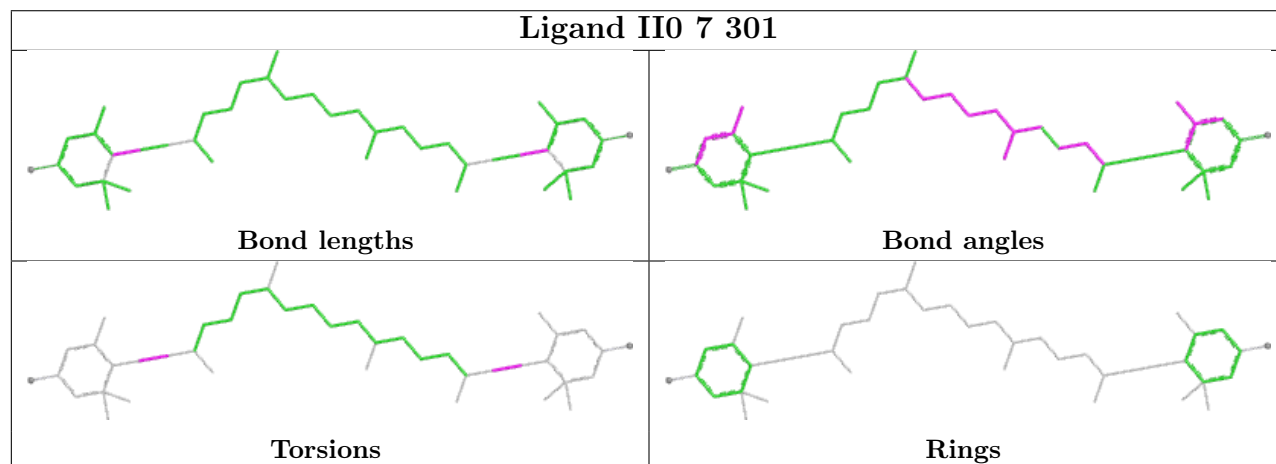
## Ligand LMG 8 614

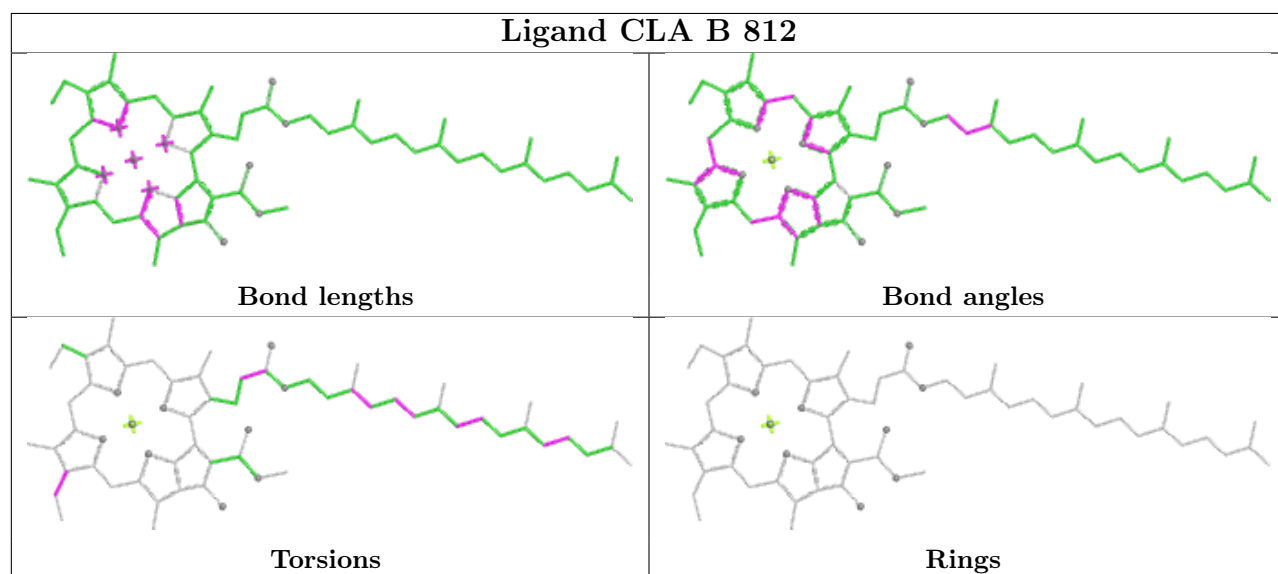
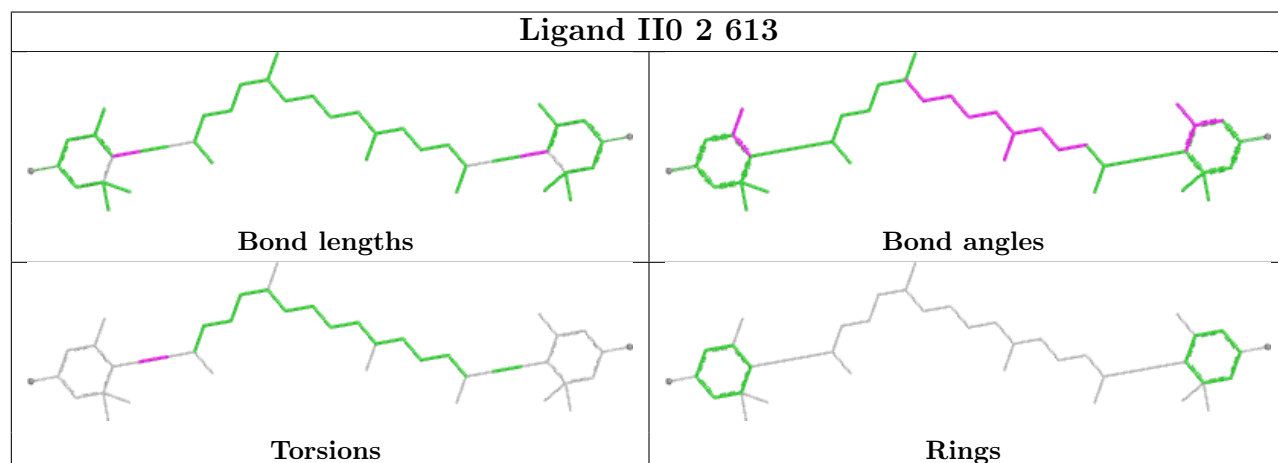
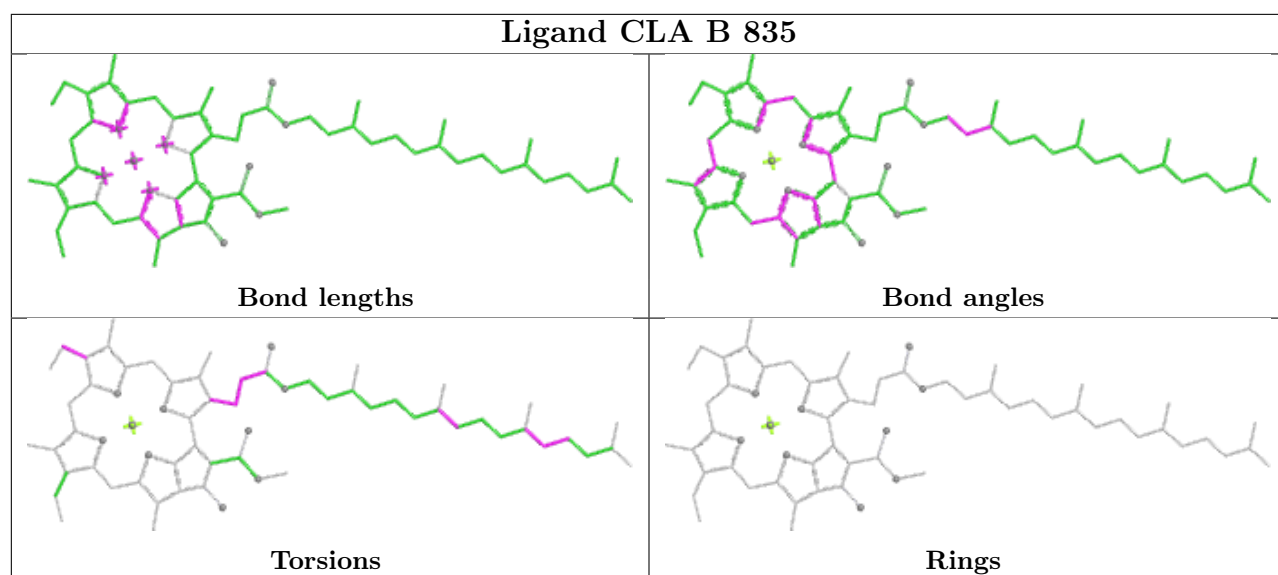




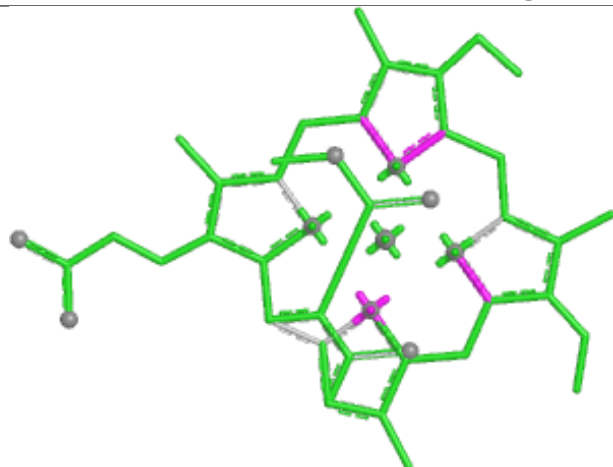
**Ligand CLA A 830****Ligand CLA A 822**



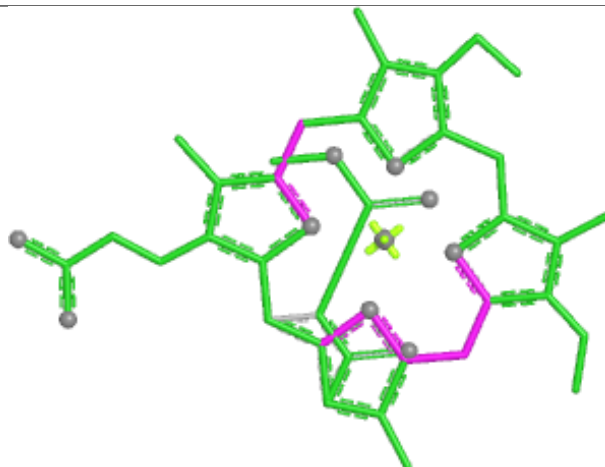
**Ligand CLA 9 607****Ligand CLA A 833****Ligand II0 7 301**



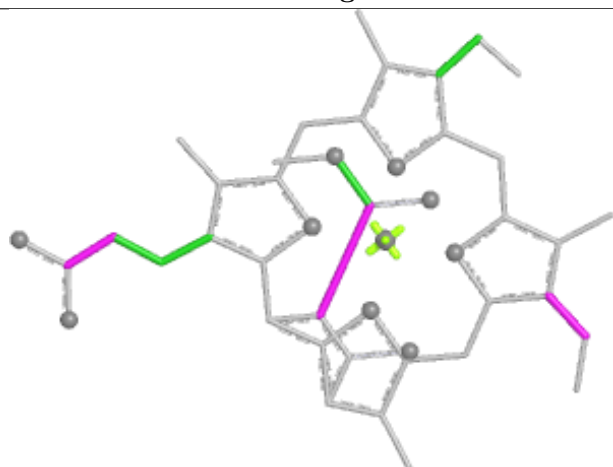
## Ligand KC2 9 610



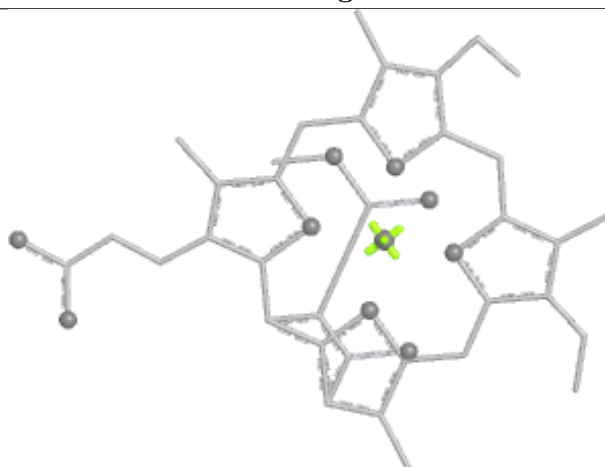
Bond lengths



Bond angles

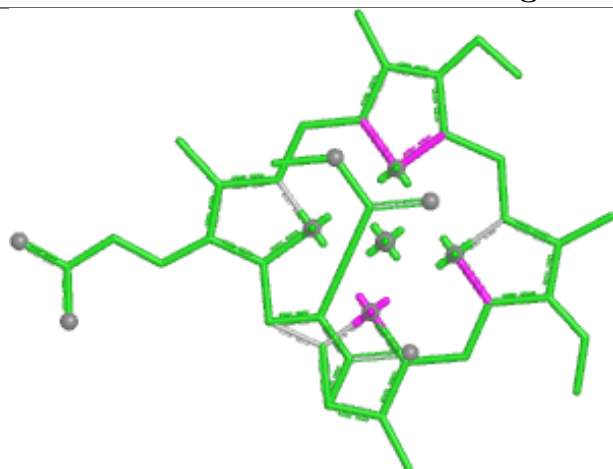


Torsions

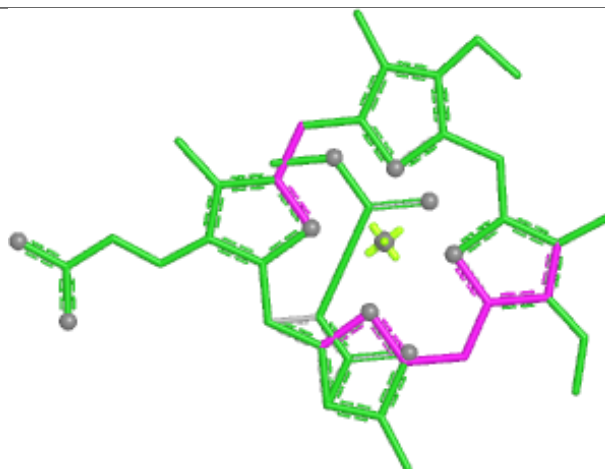


Rings

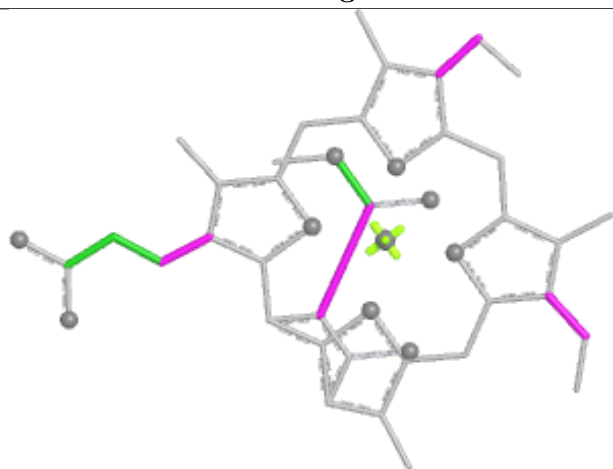
## Ligand KC2 3 606



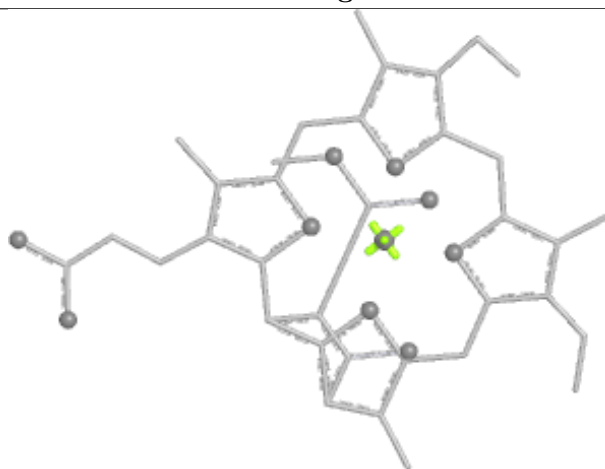
Bond lengths



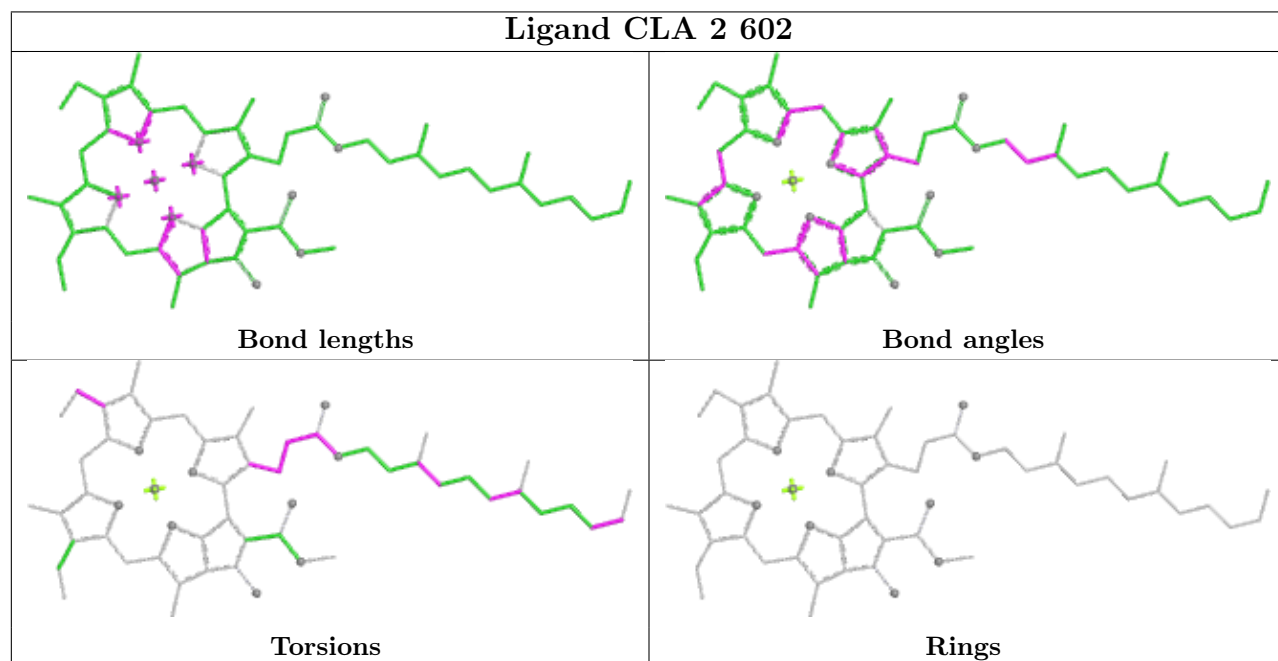
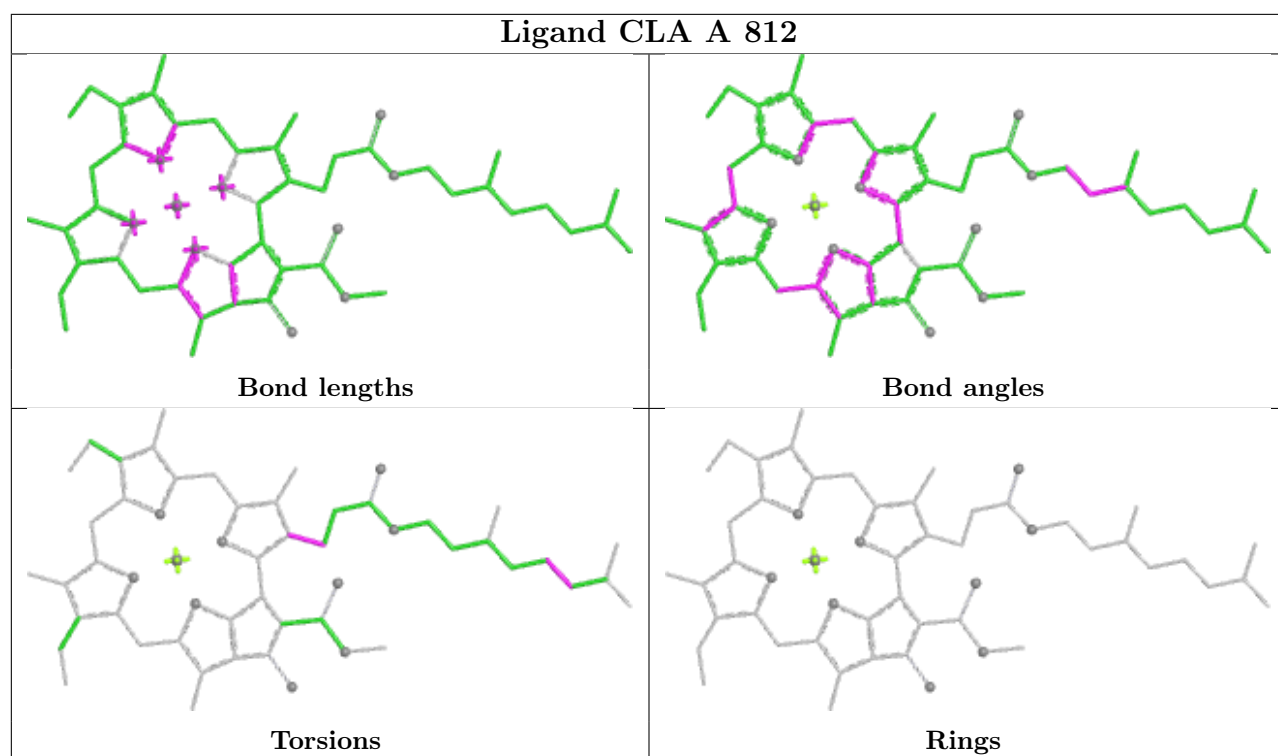
Bond angles

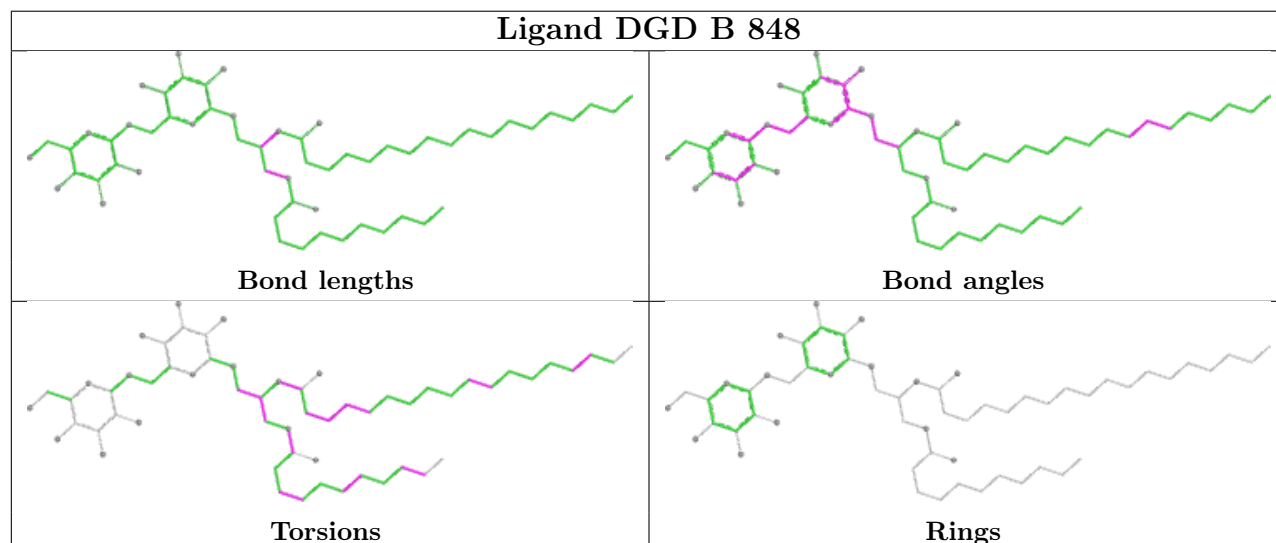
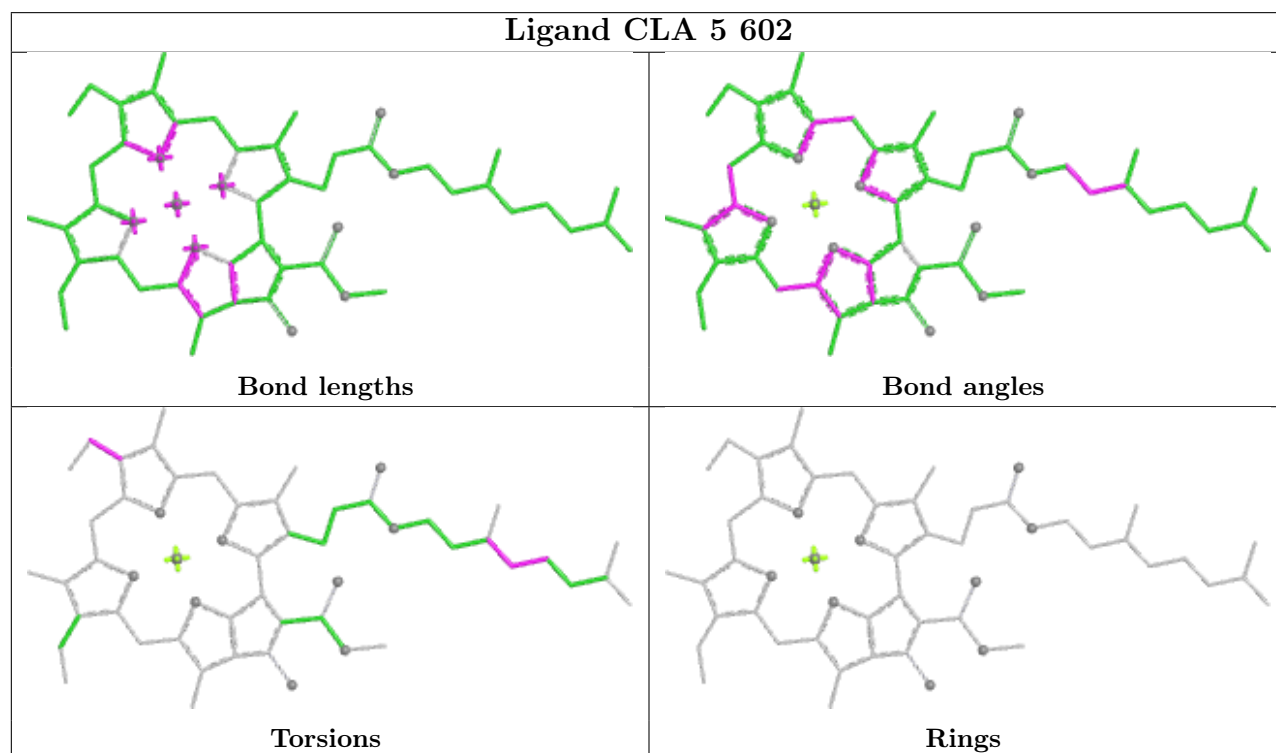
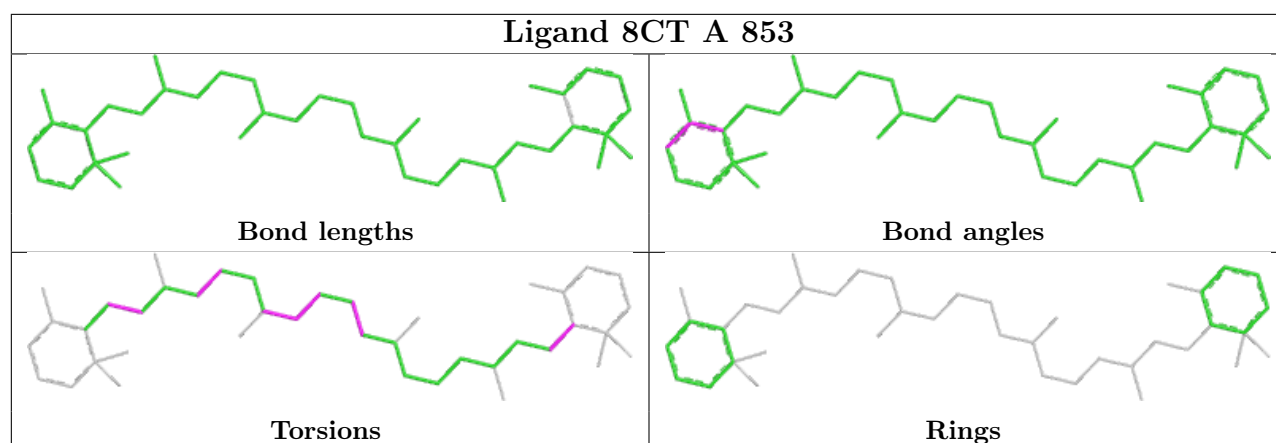


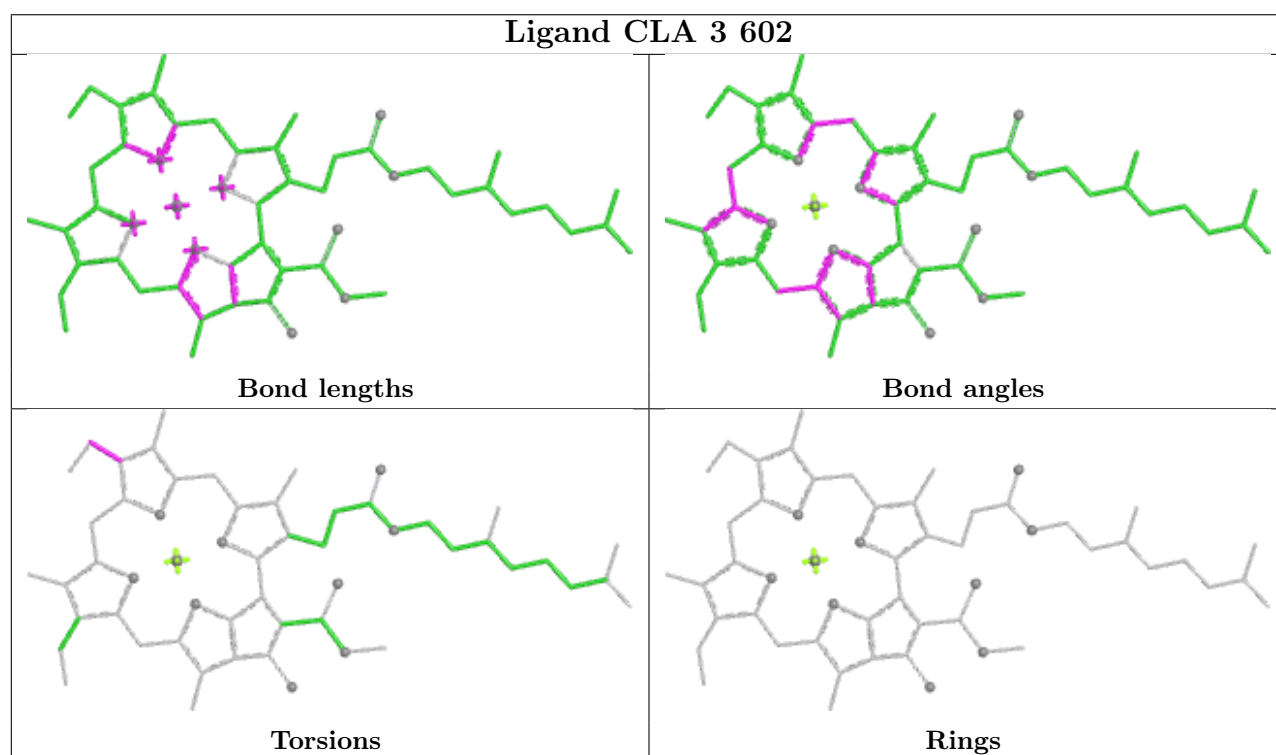
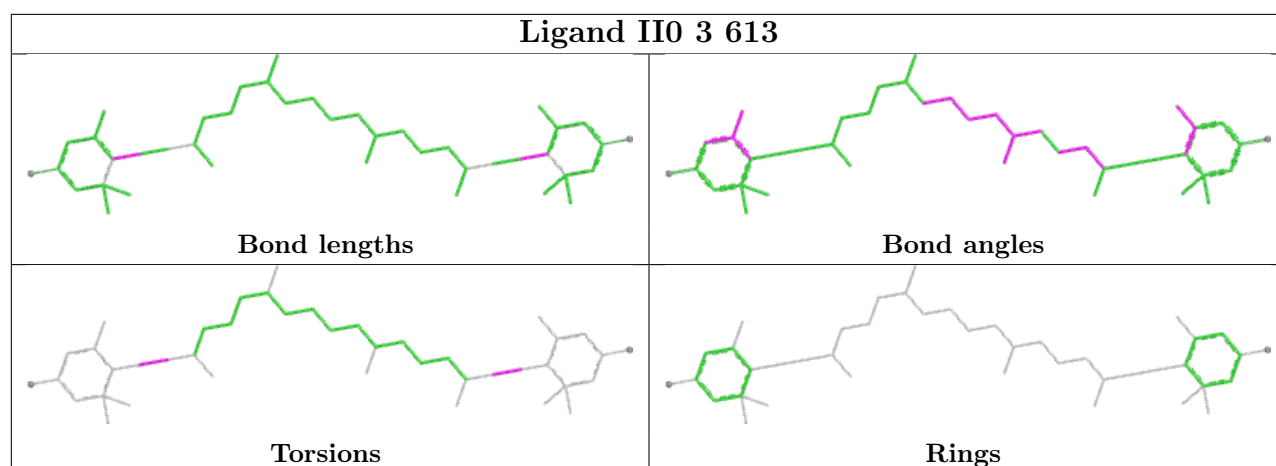
Torsions



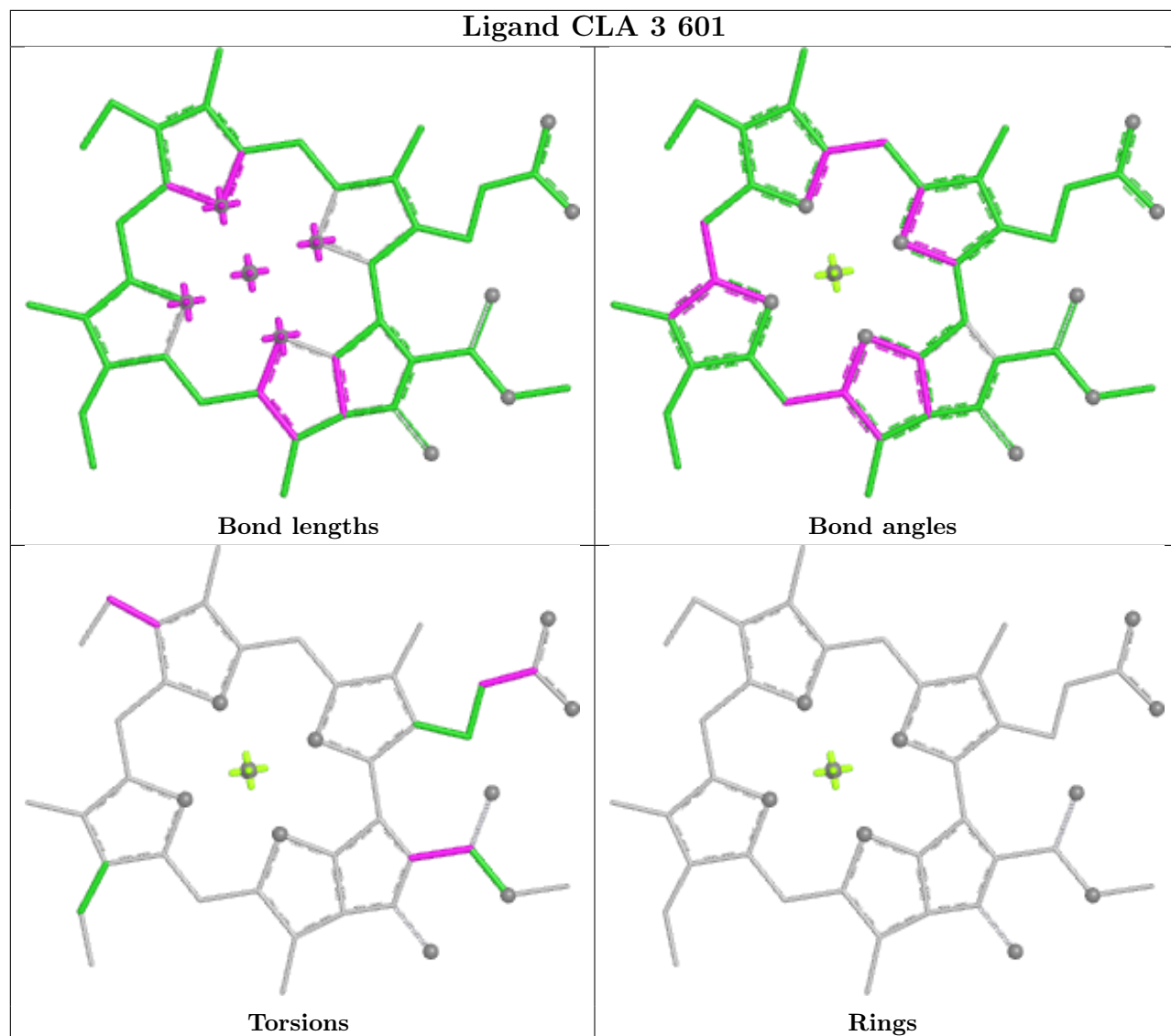
Rings



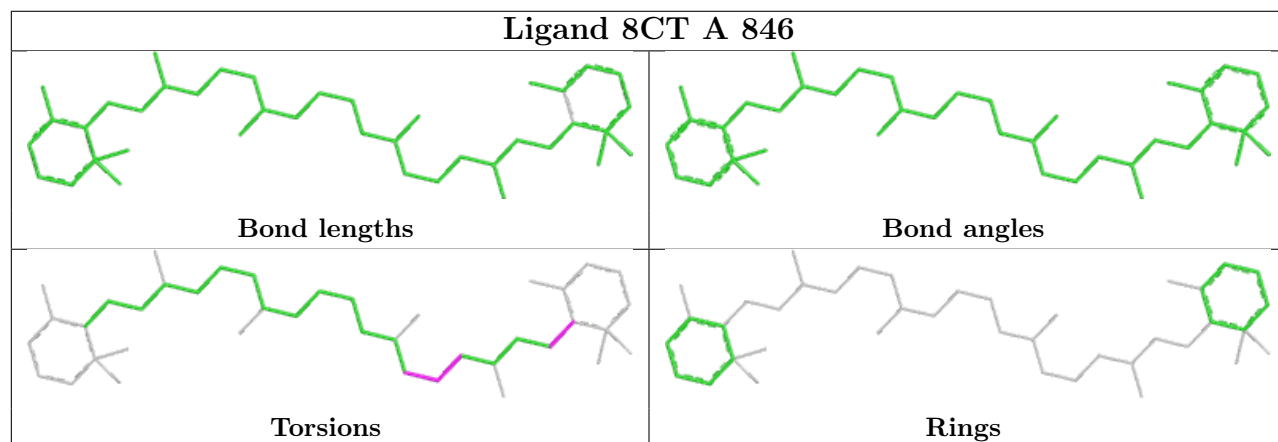




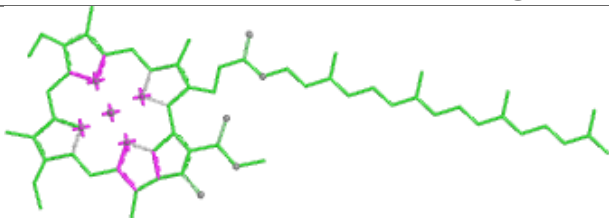
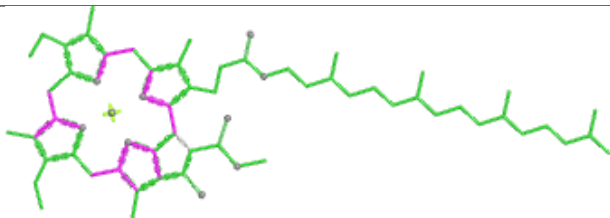
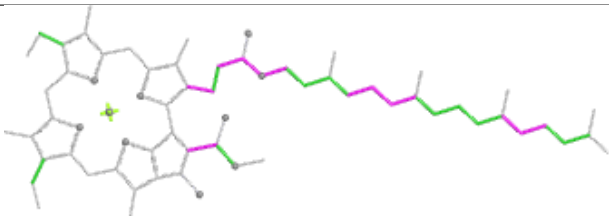
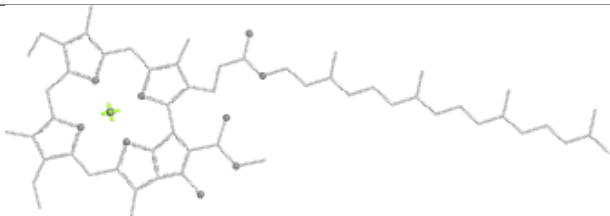
## Ligand CLA 3 601

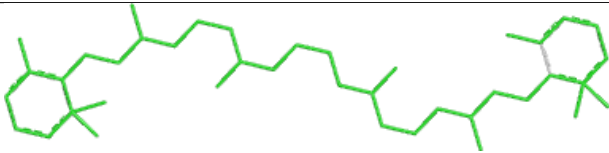
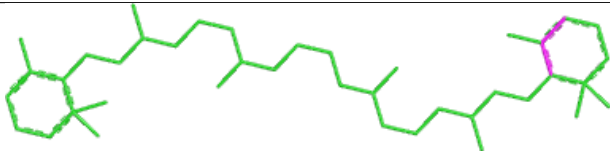
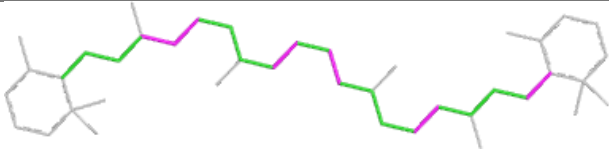
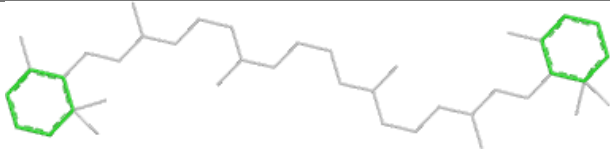


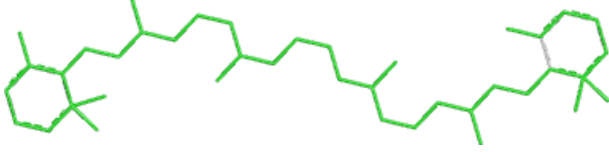
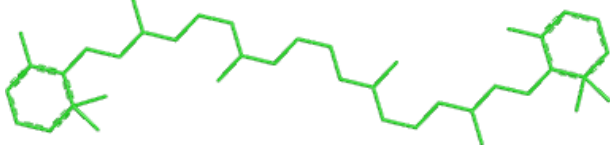
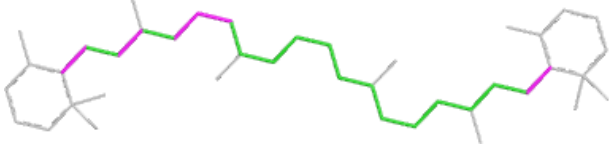
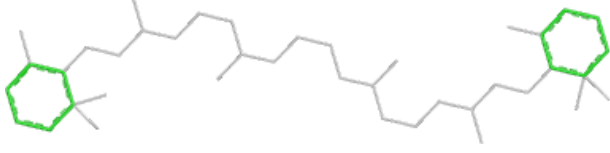
## Ligand 8CT A 846

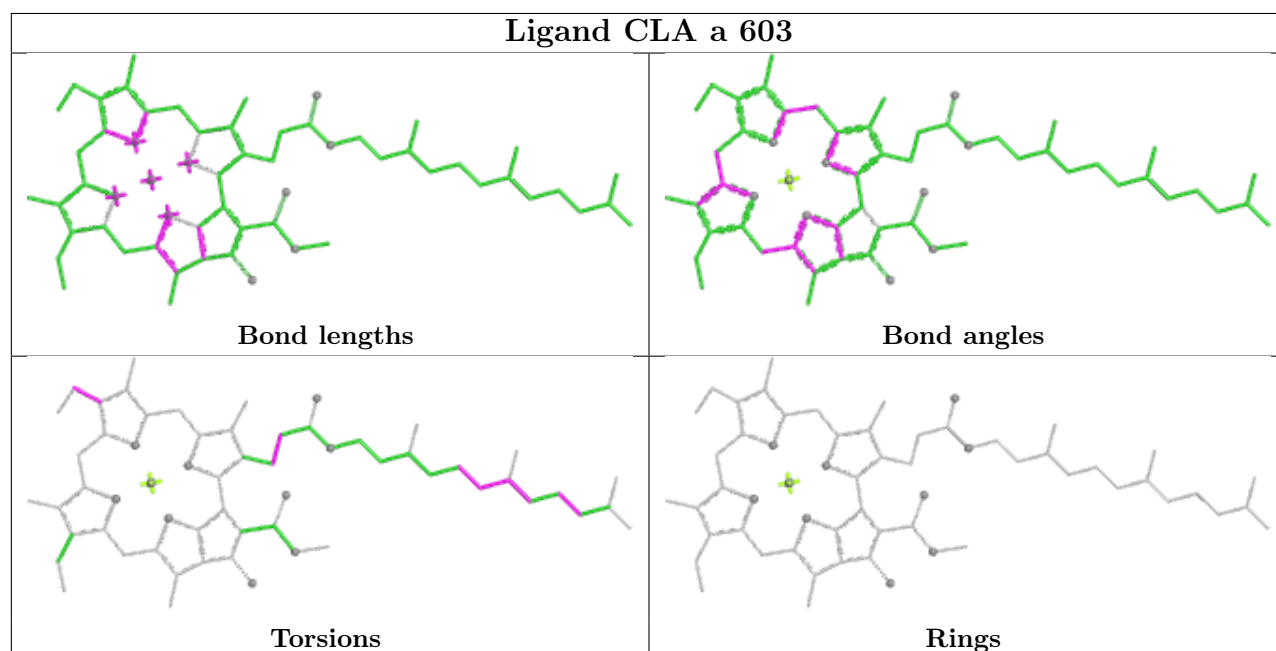
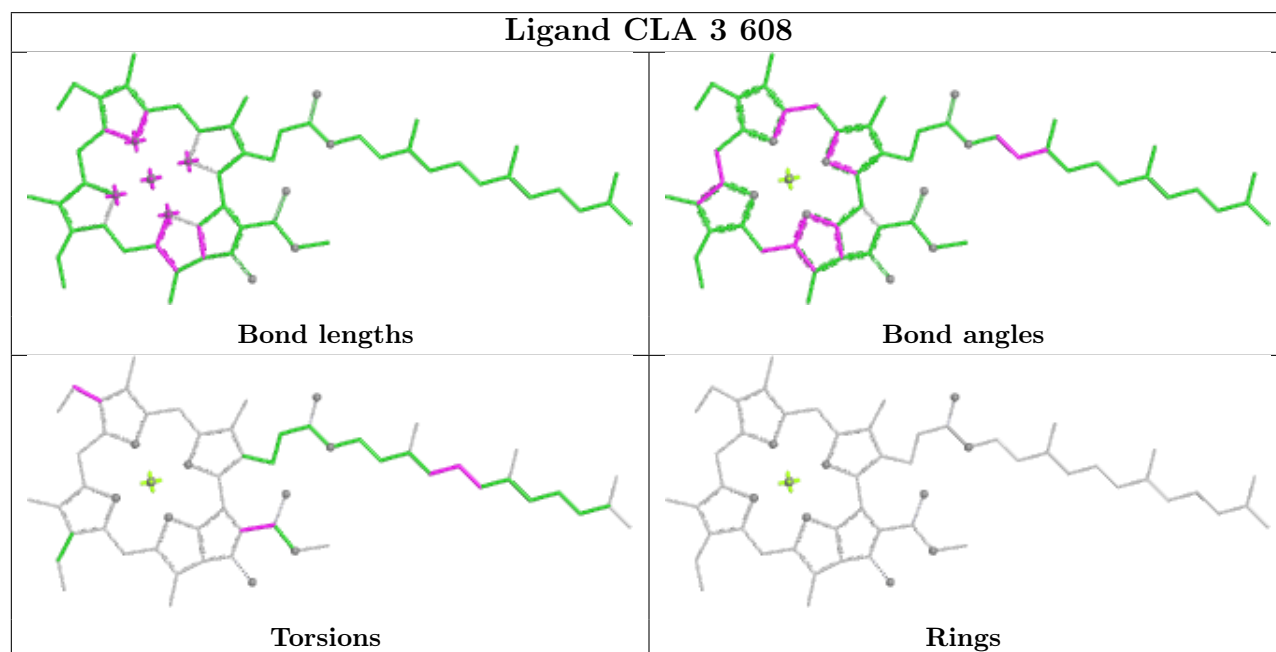
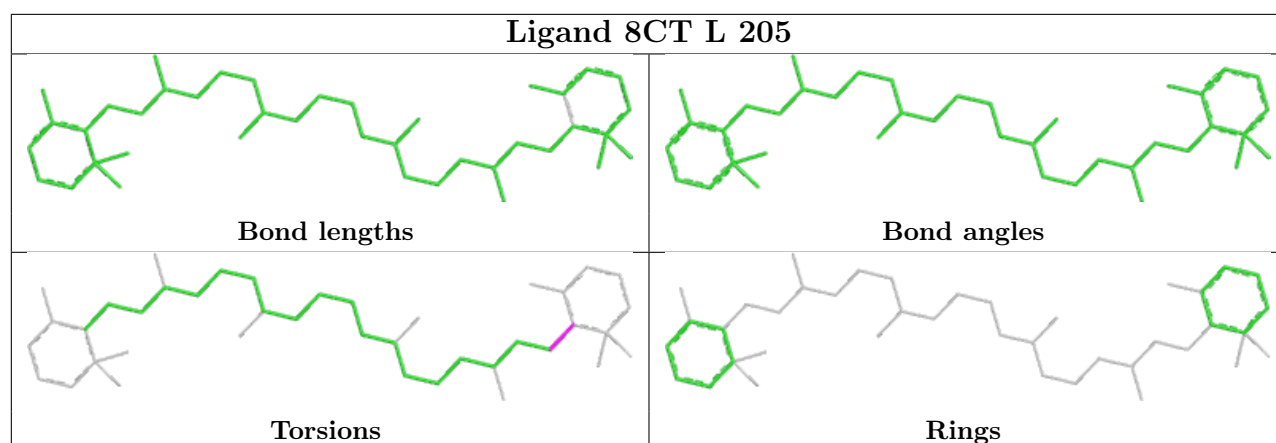




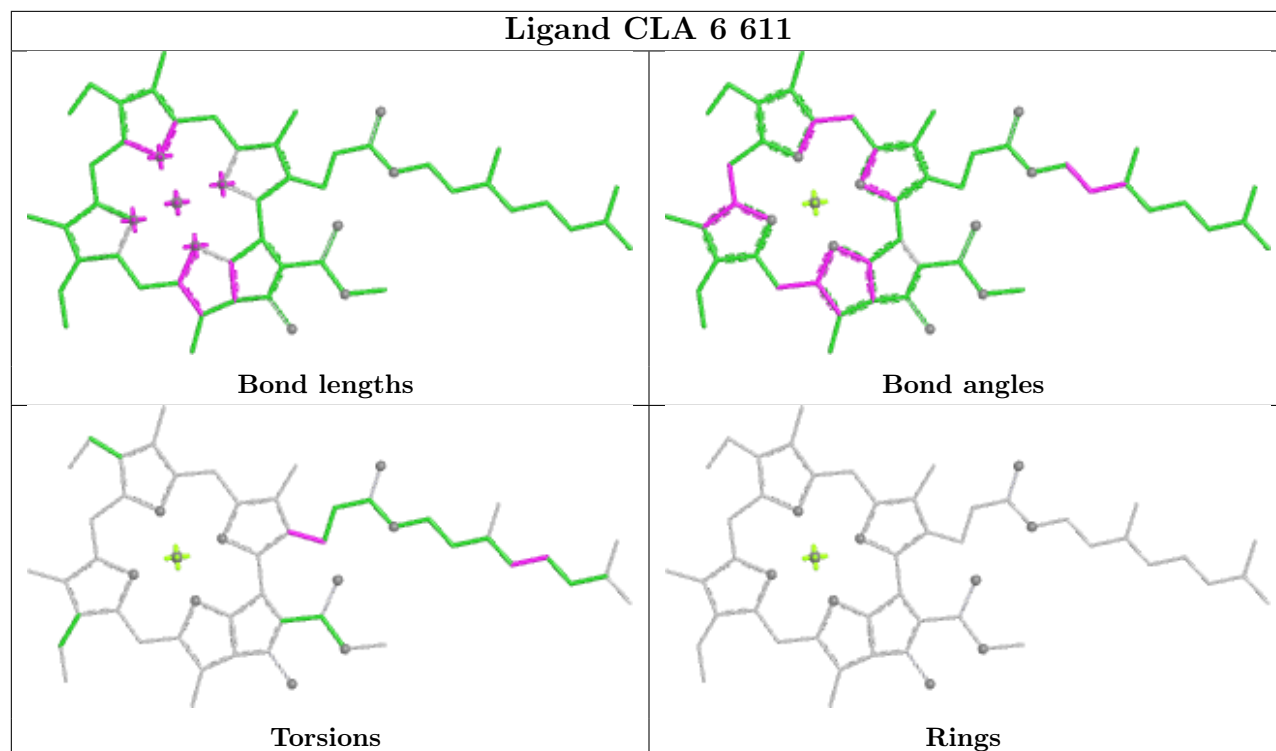
| Ligand CLA B 832                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand 8CT B 845                                                                   |                                                                                     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                       | Bond angles                                                                         |
|  |  |
| Torsions                                                                           | Rings                                                                               |

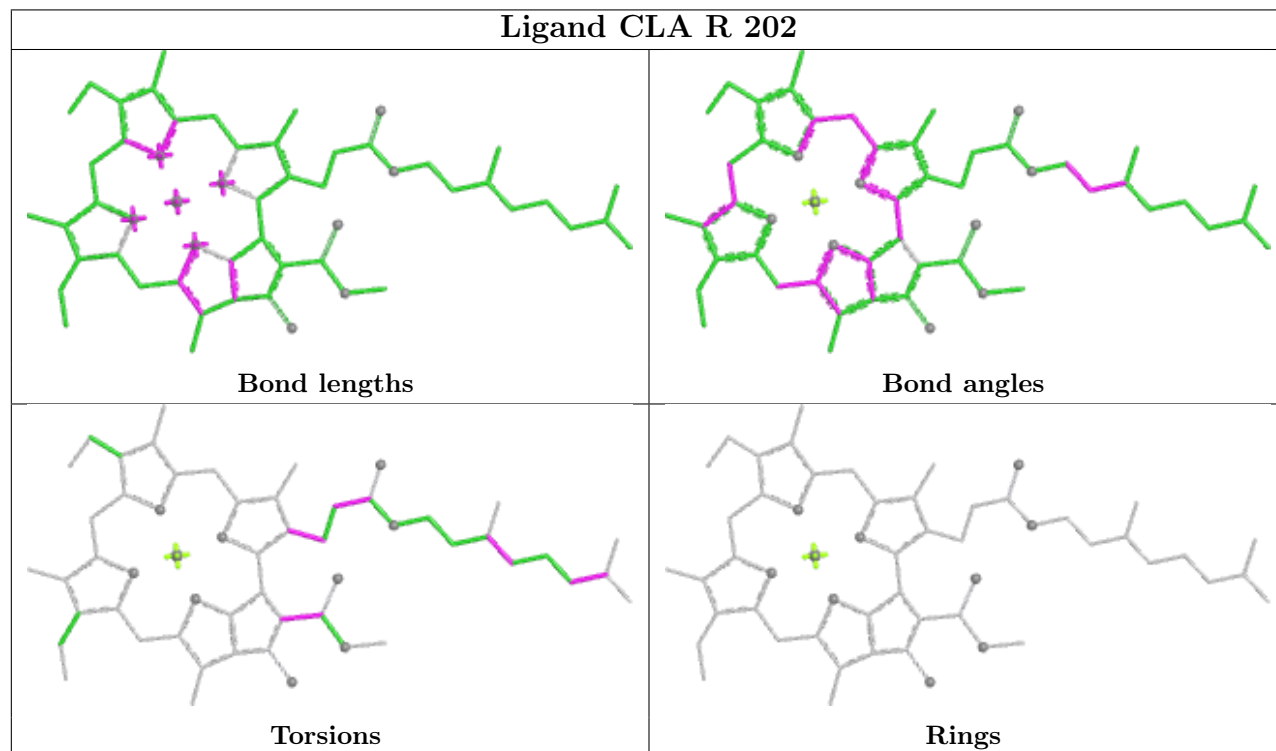
| Ligand 8CT R 201                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |



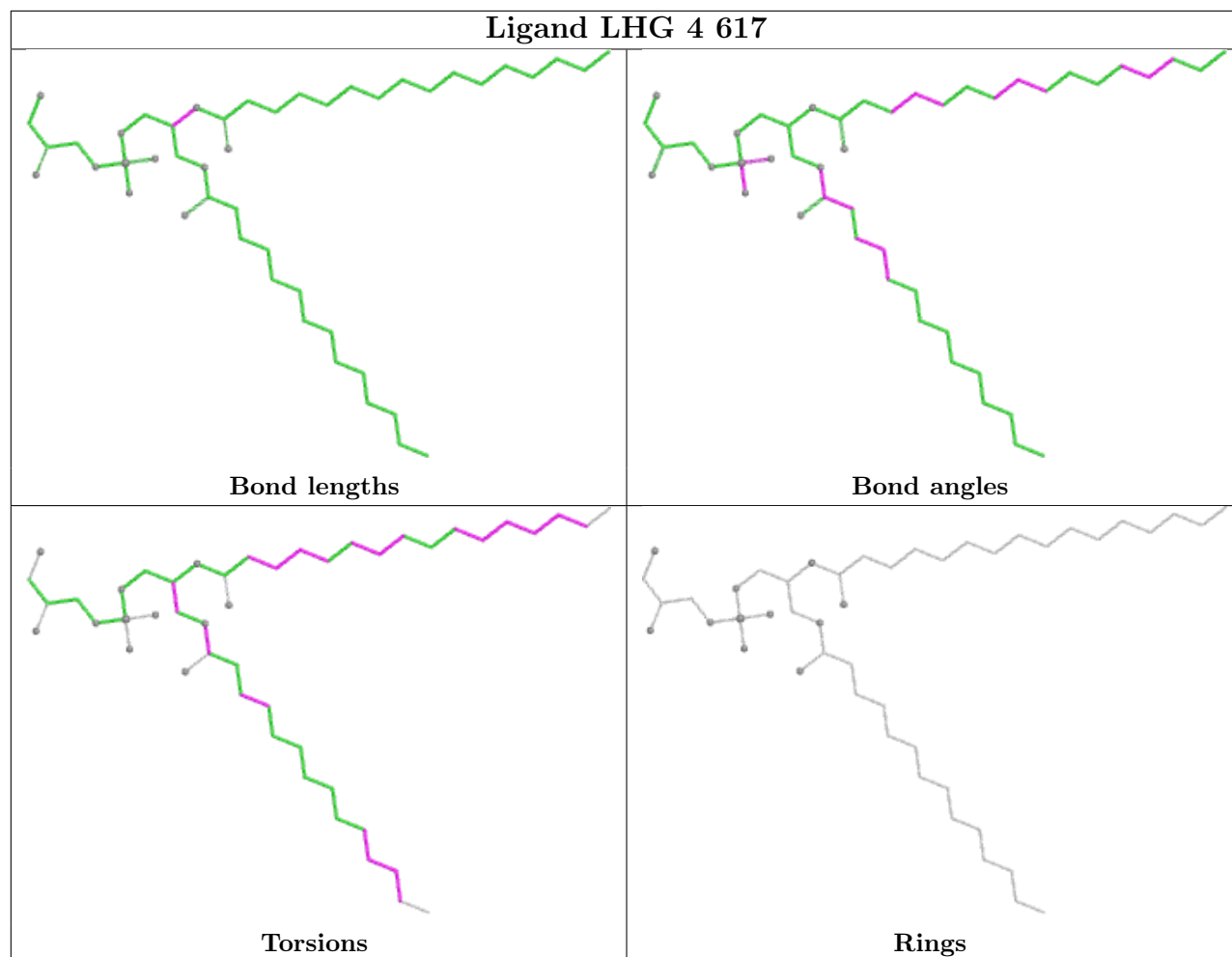
## Ligand CLA 6 611



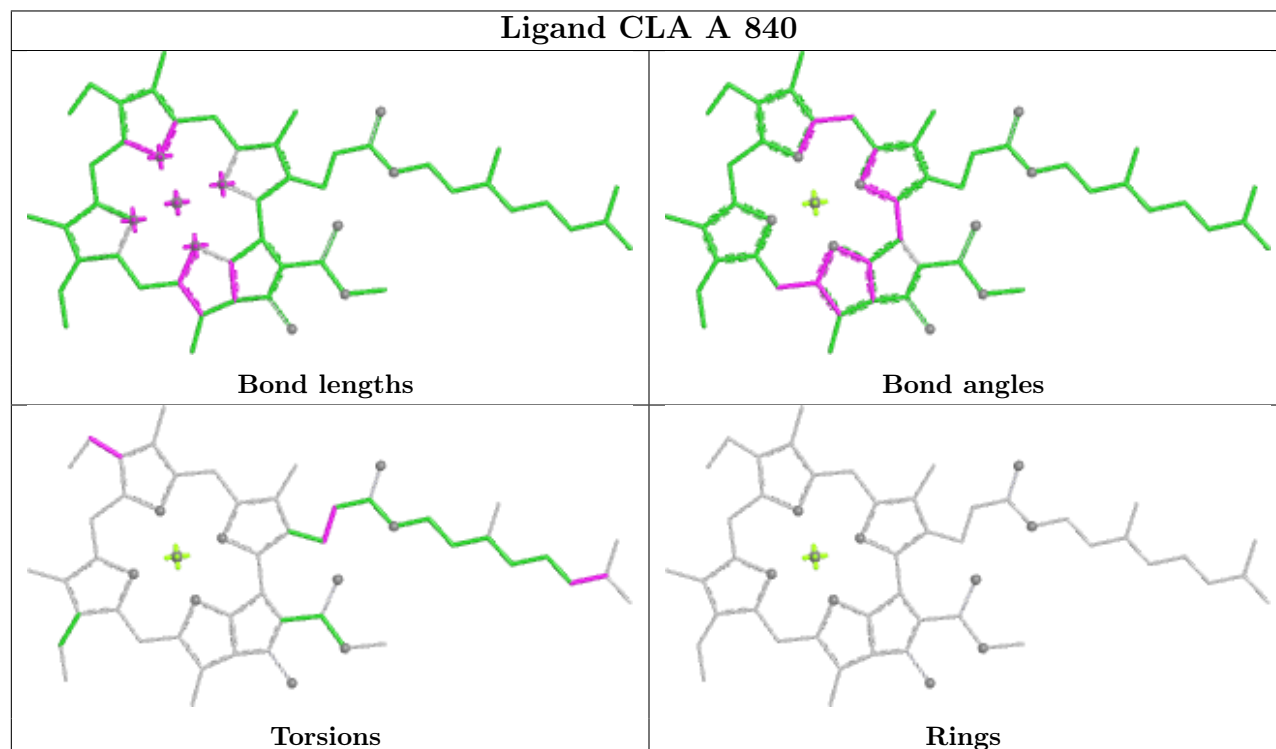
## Ligand CLA R 202

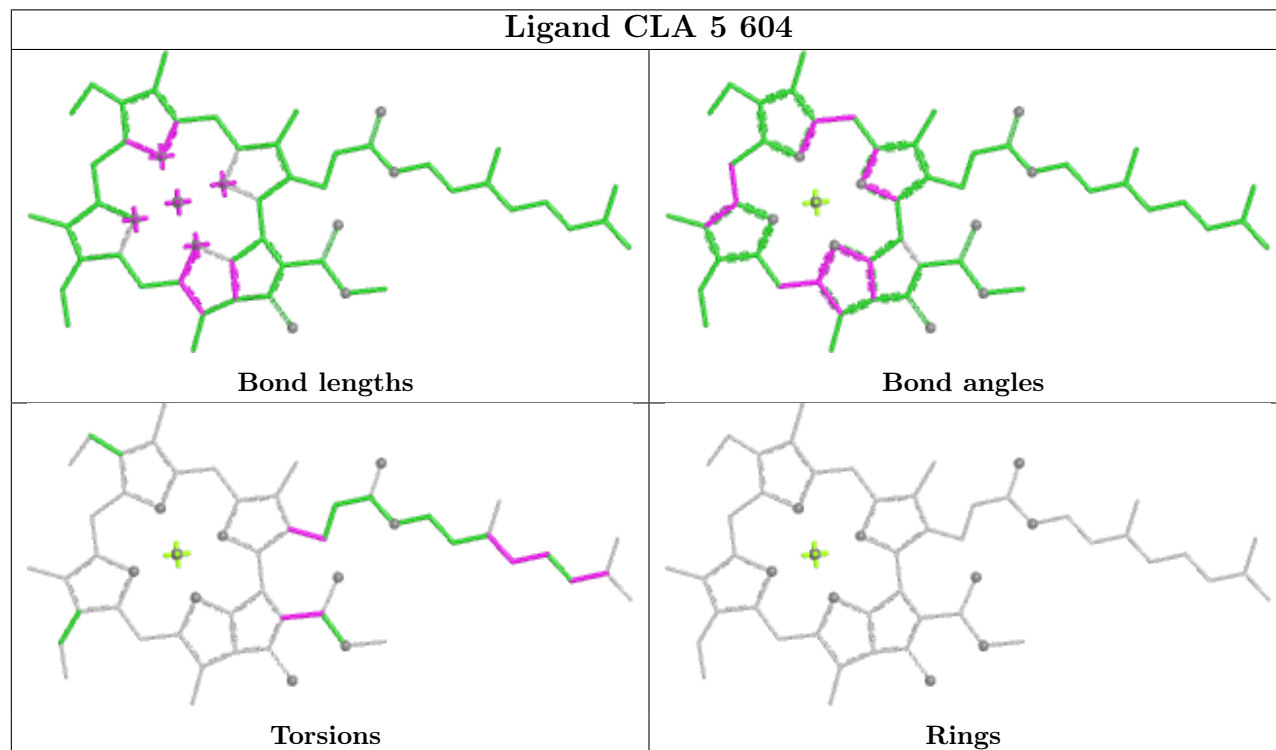
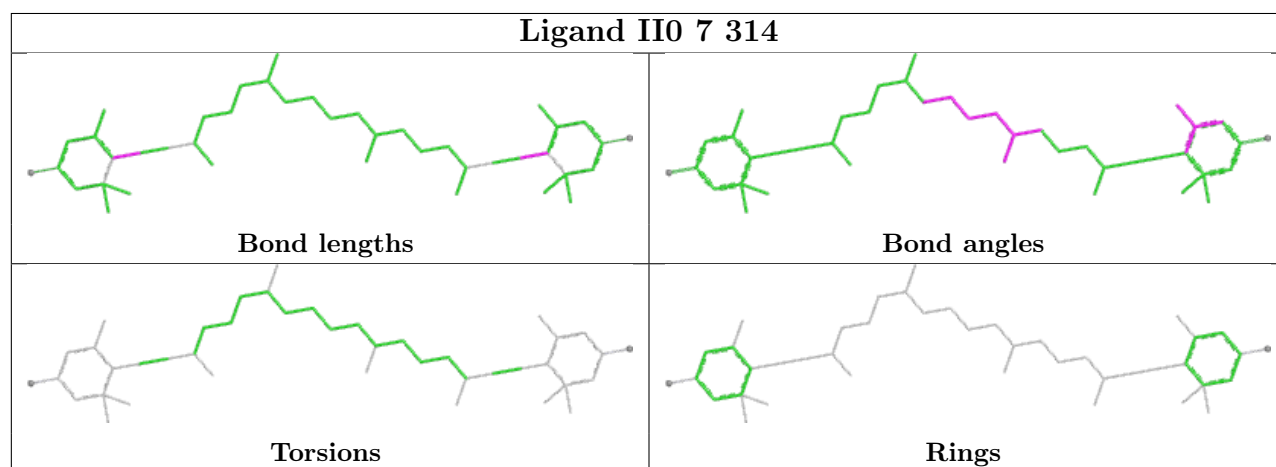
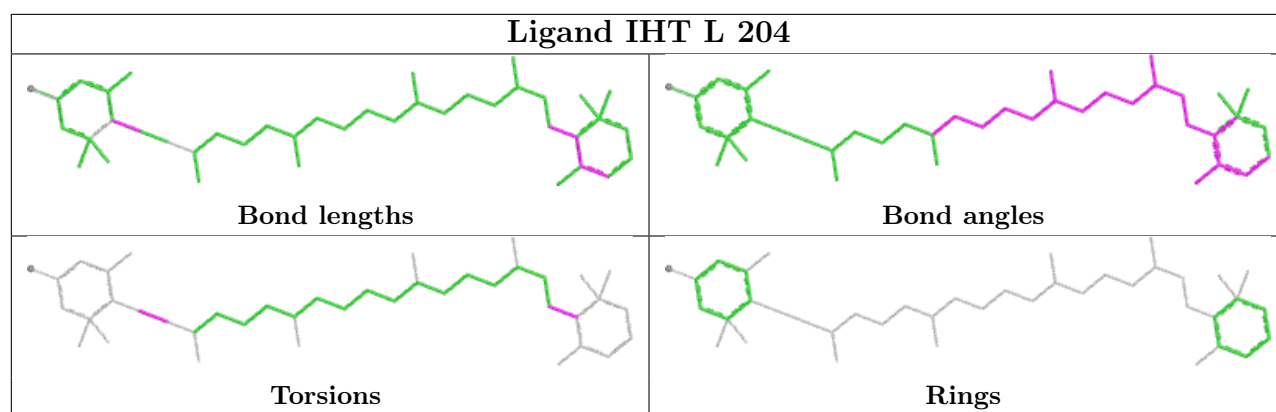


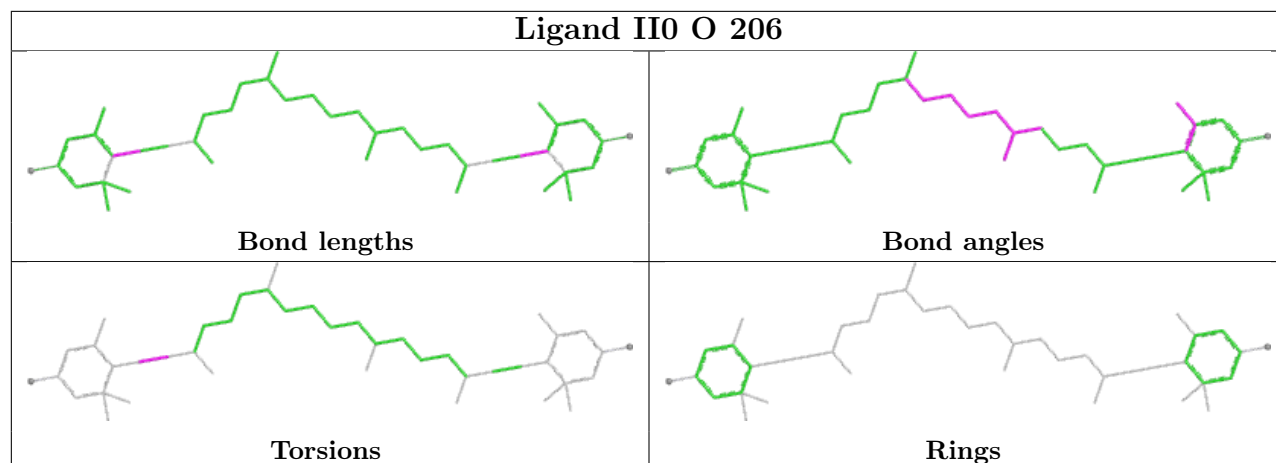
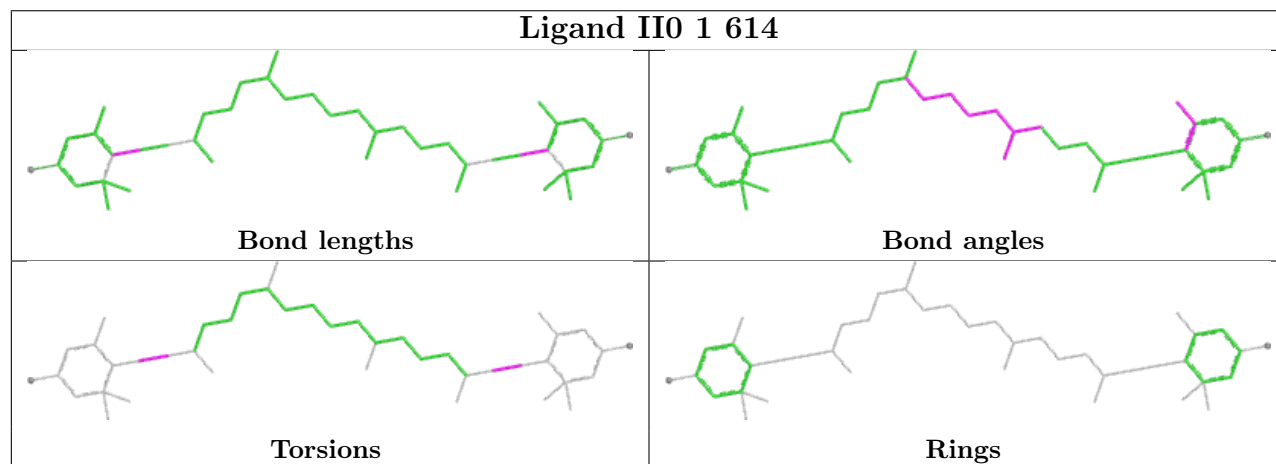
## Ligand LHG 4 617



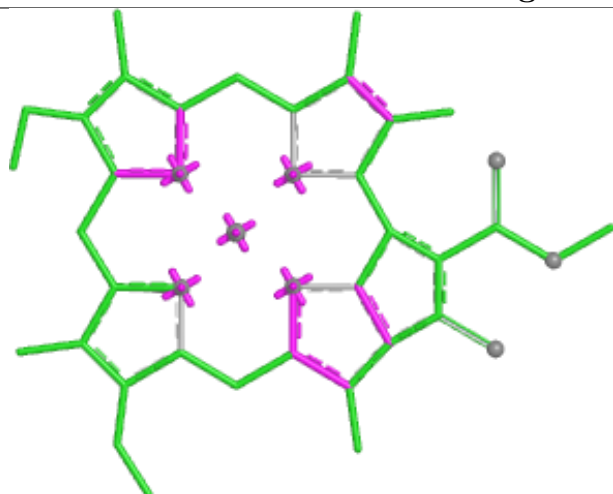
## Ligand CLA A 840



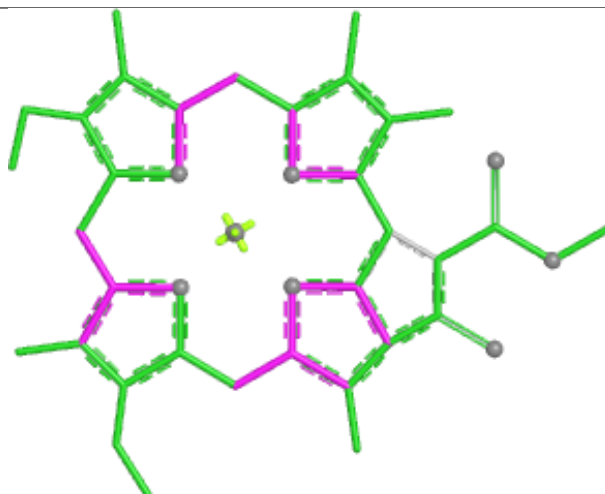


**Ligand II0 O 206****Ligand II0 1 614**

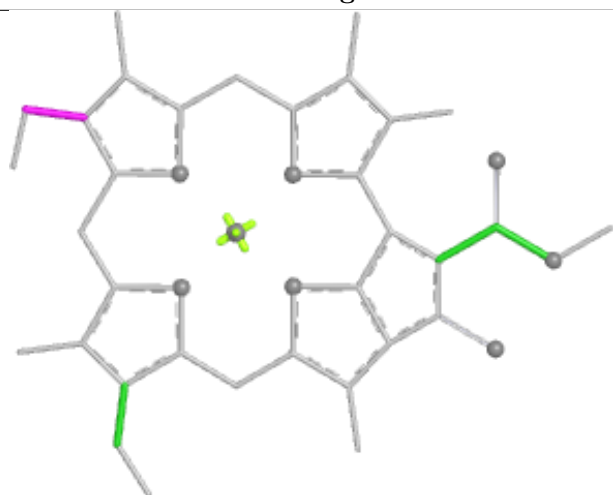
## Ligand CLA 5 601



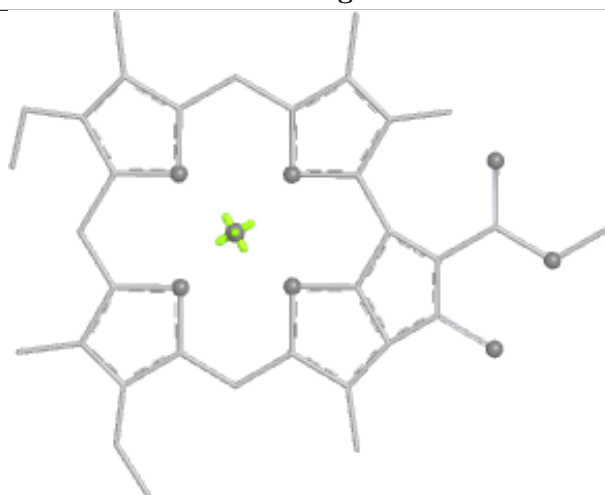
Bond lengths



Bond angles

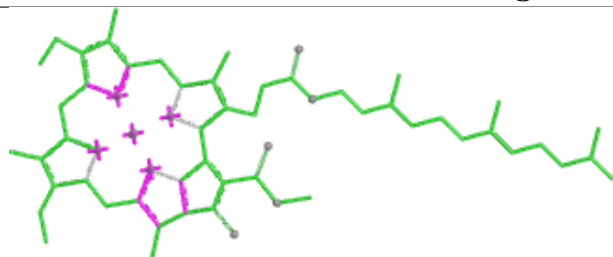


Torsions

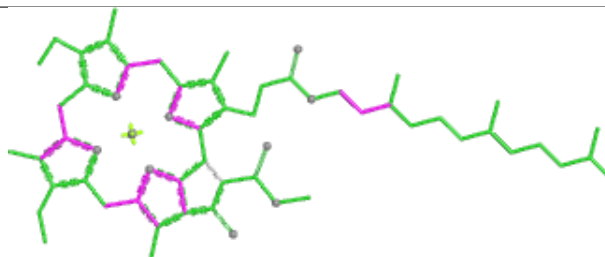


Rings

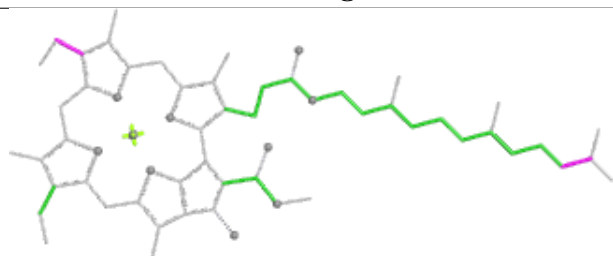
## Ligand CLA B 818



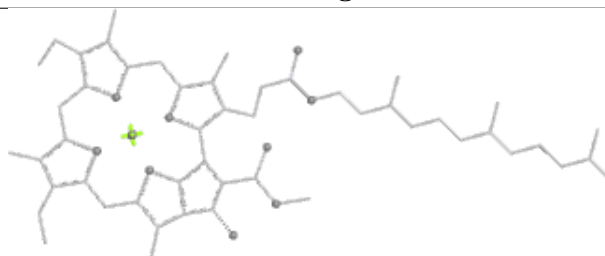
Bond lengths



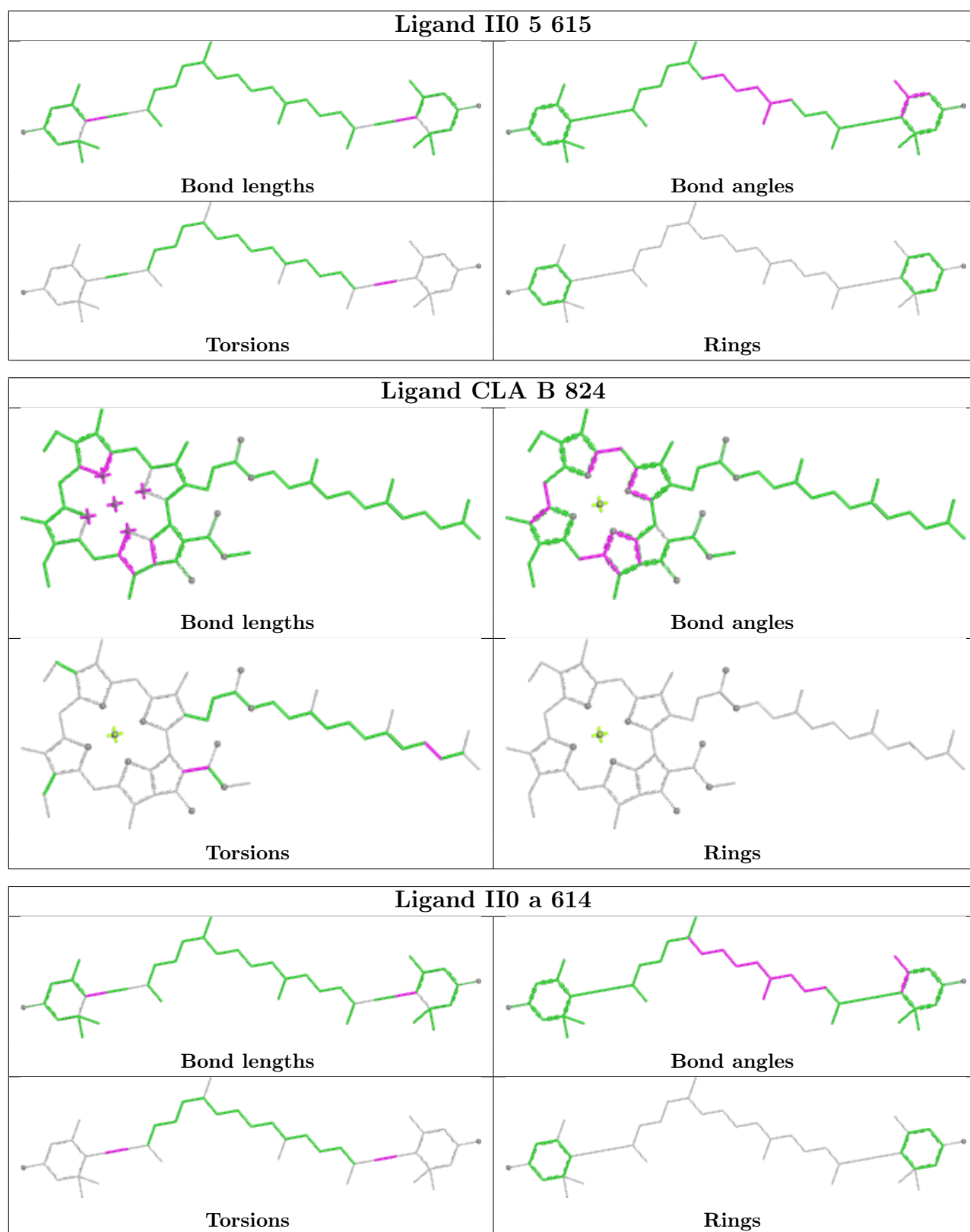
Bond angles



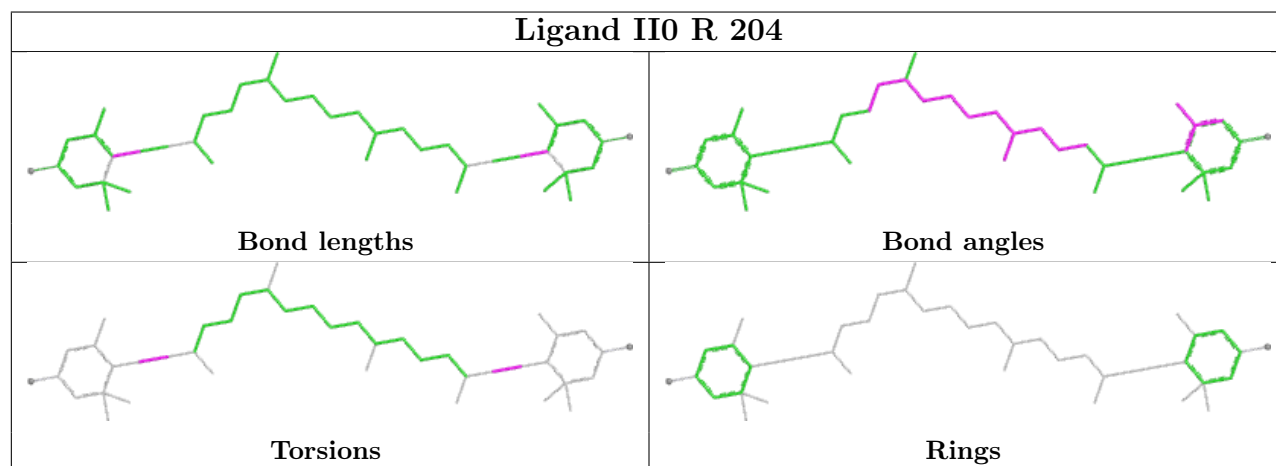
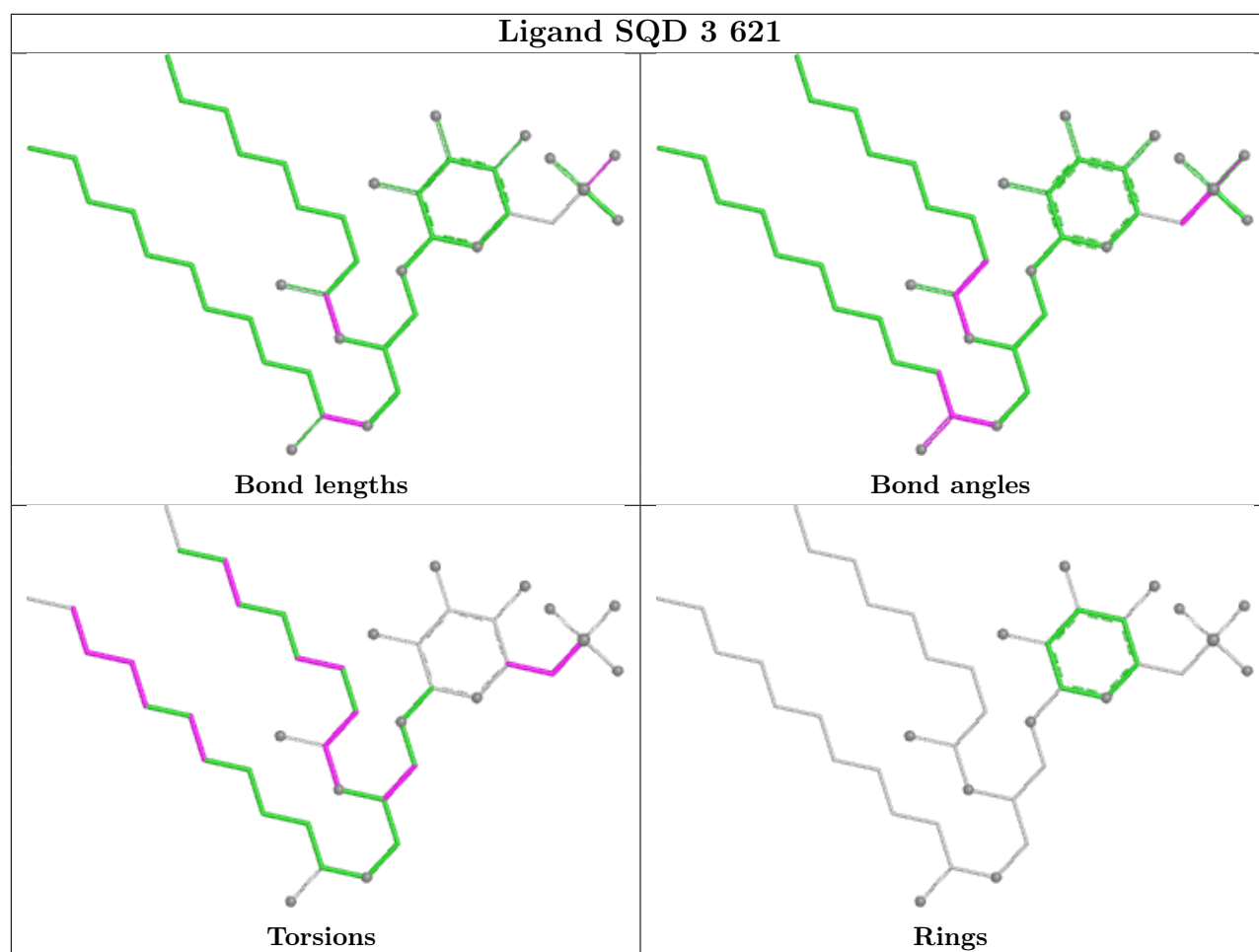
Torsions



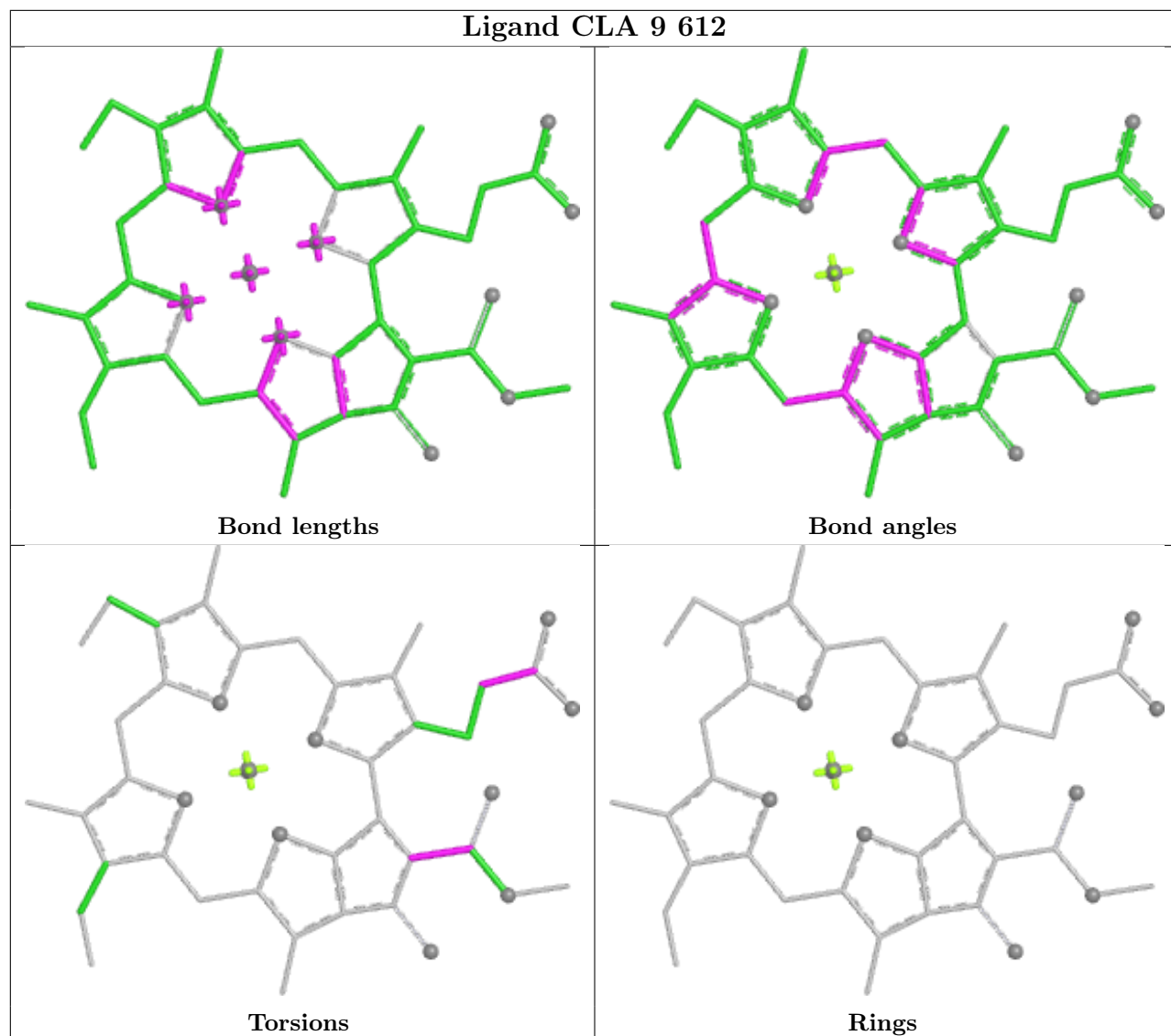
Rings



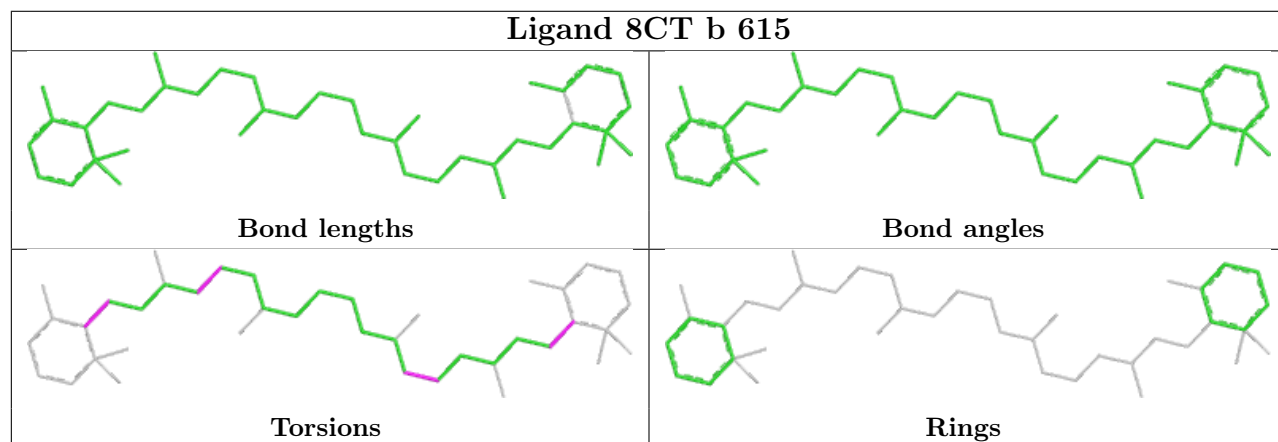


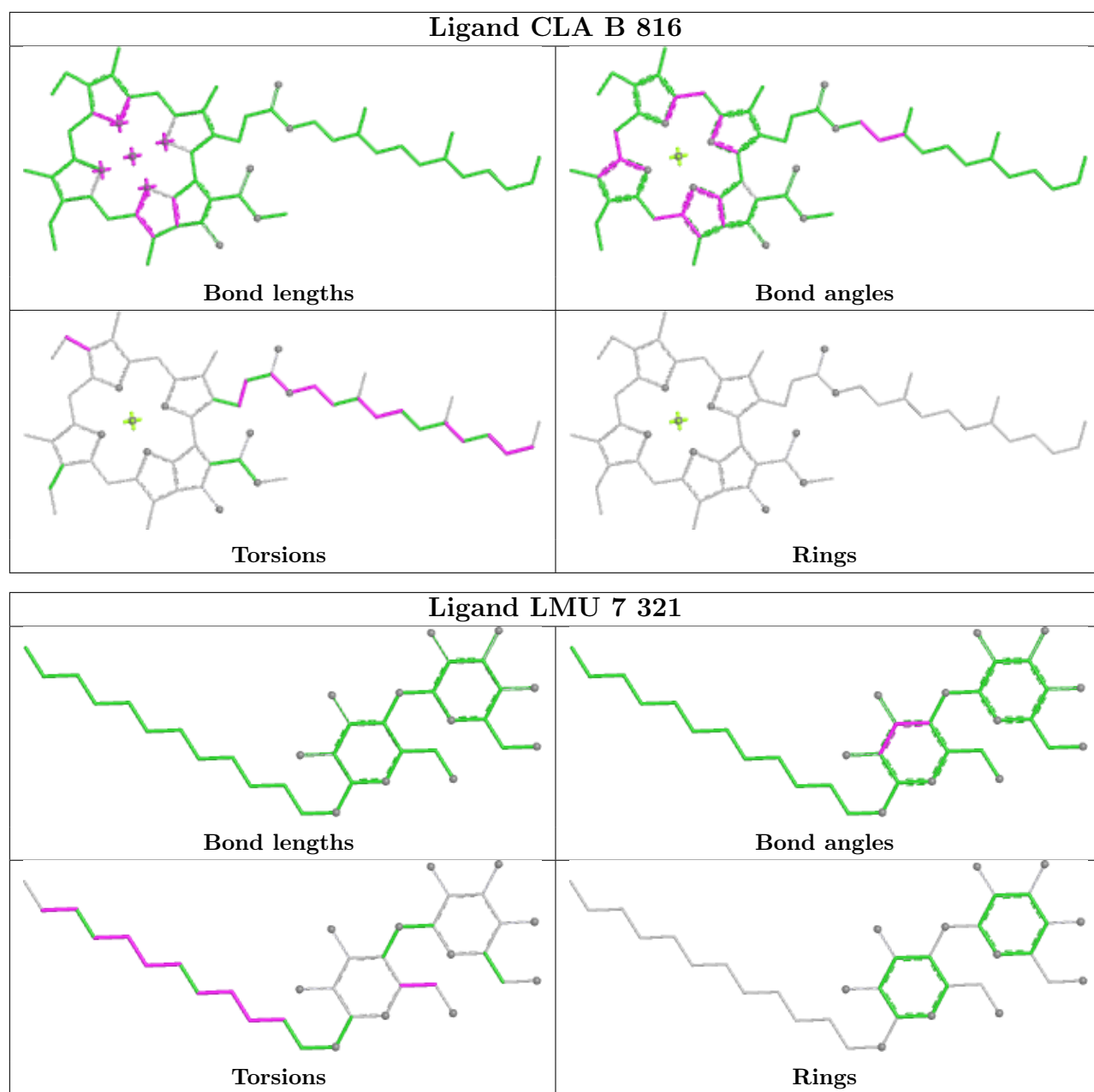


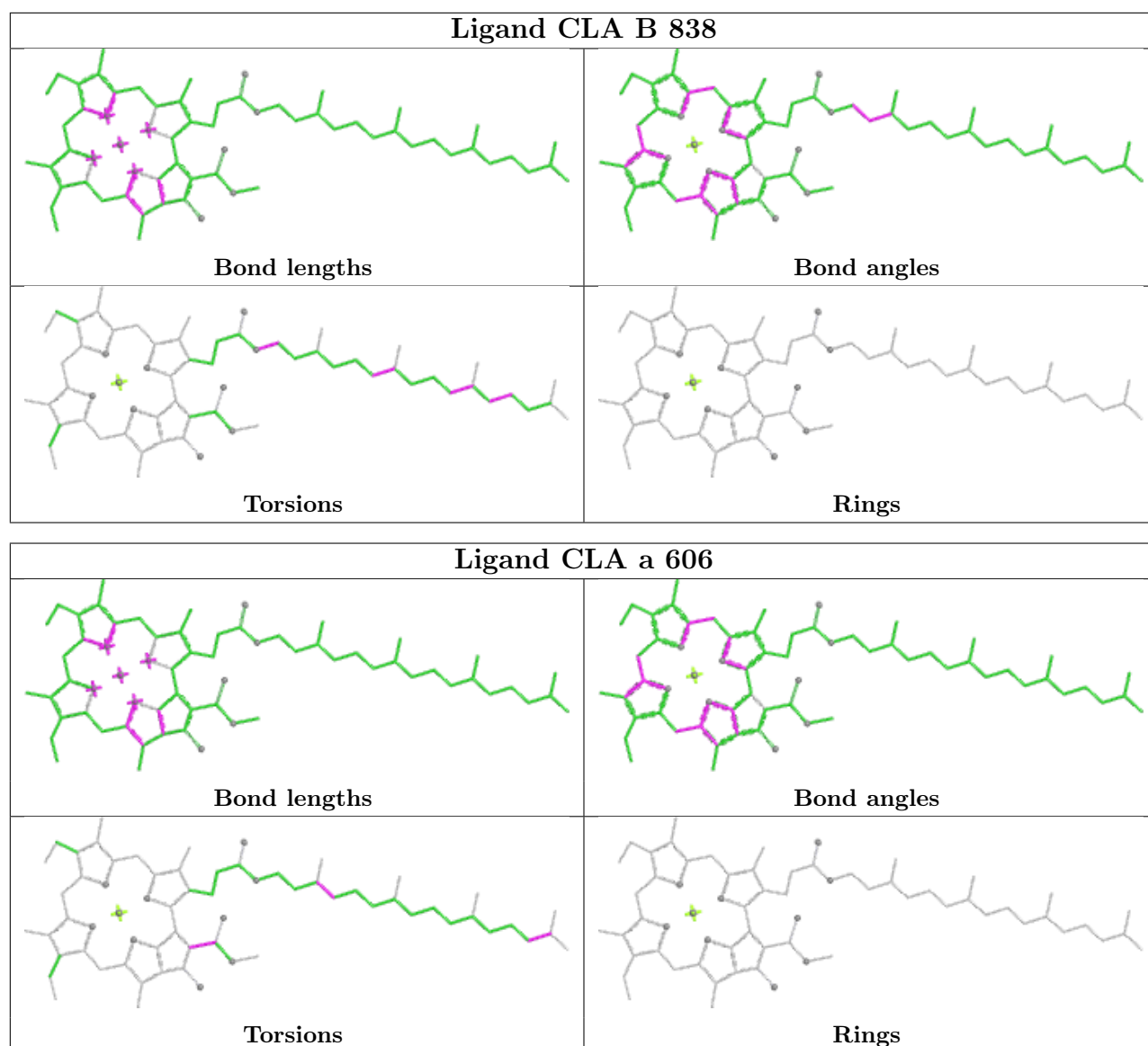
## Ligand CLA 9 612

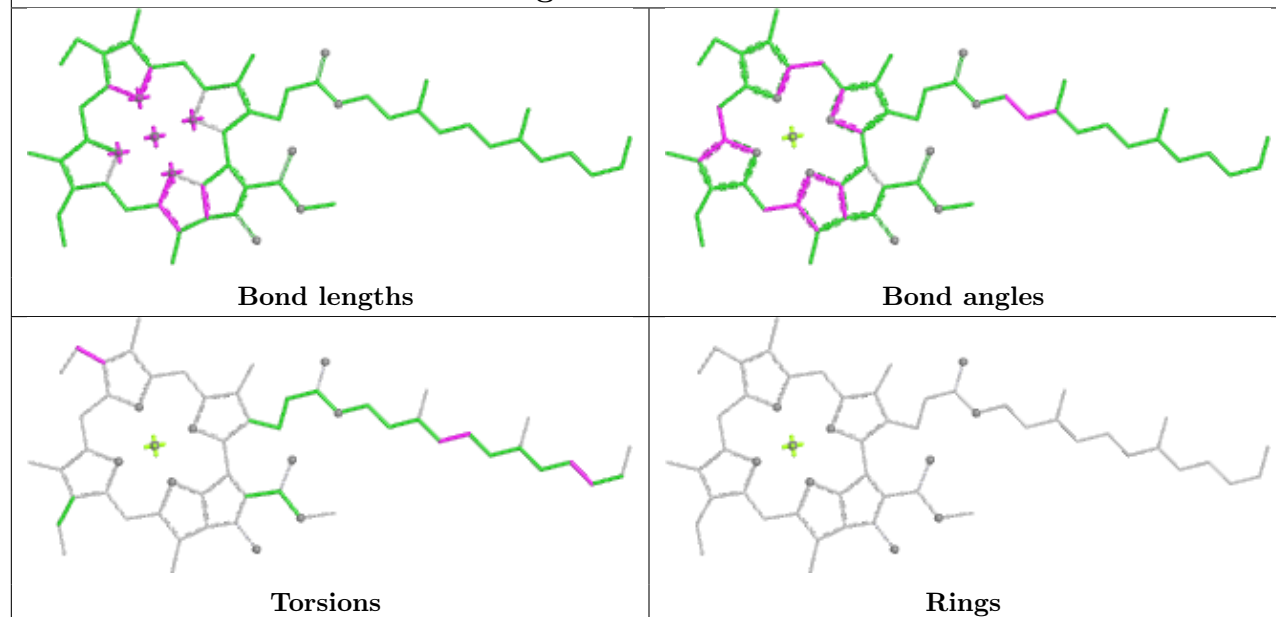
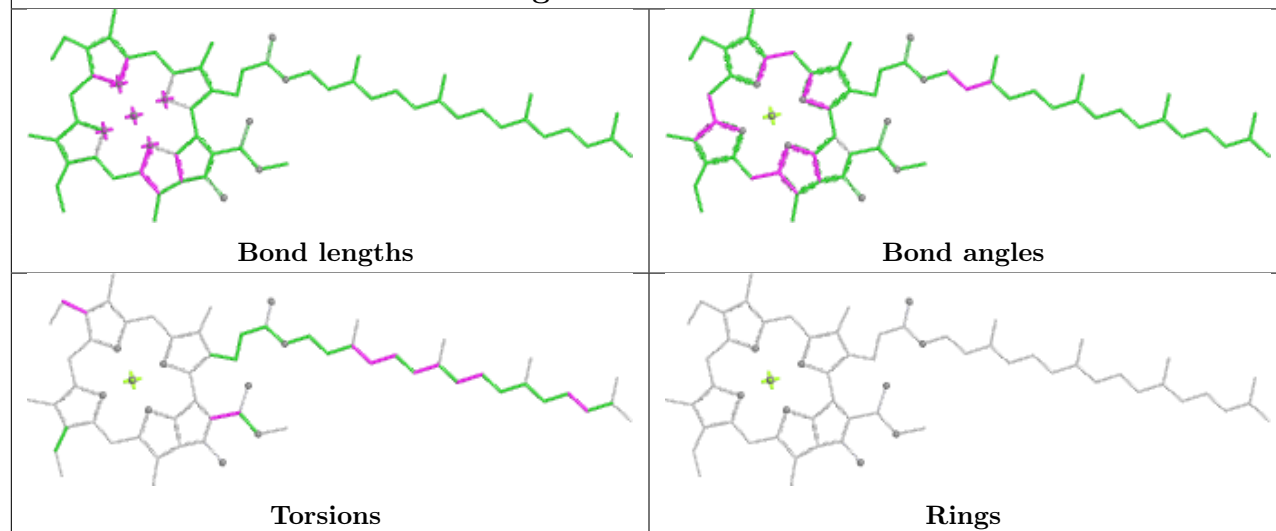


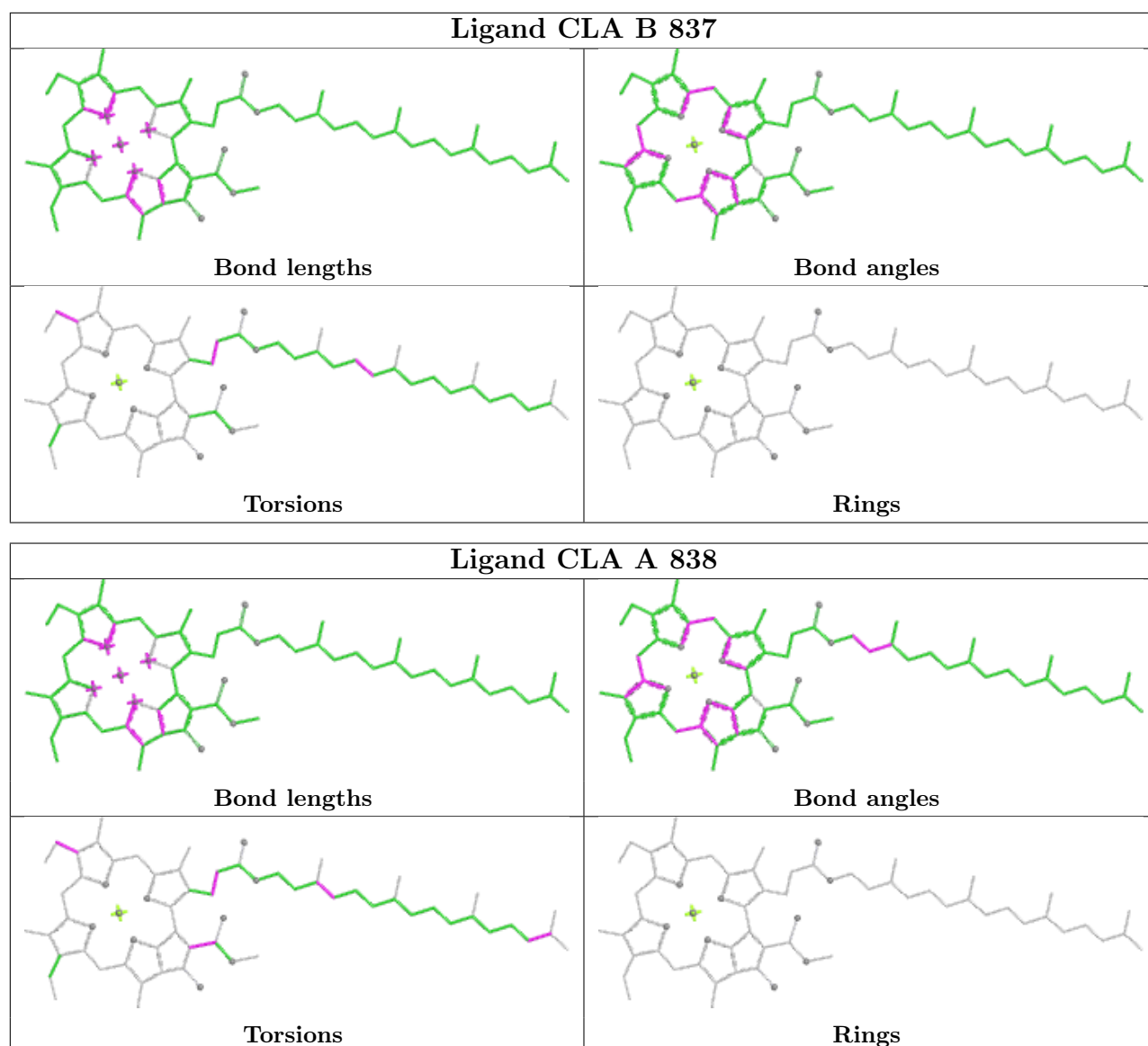
## Ligand 8CT b 615

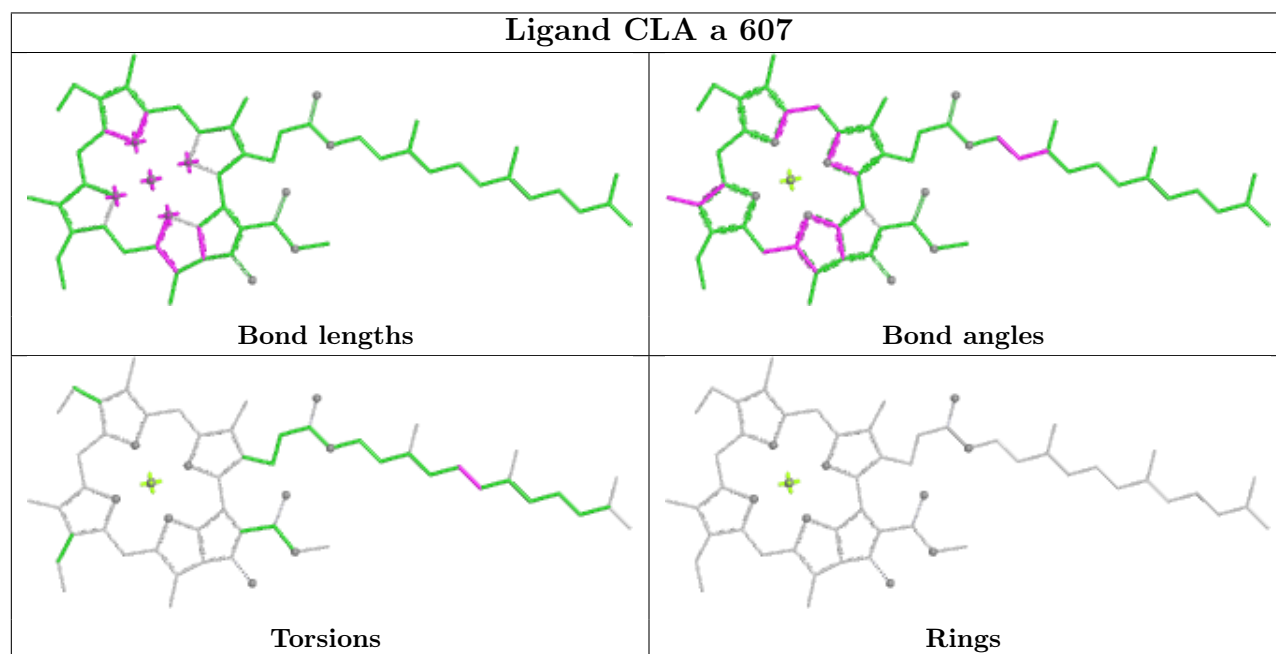
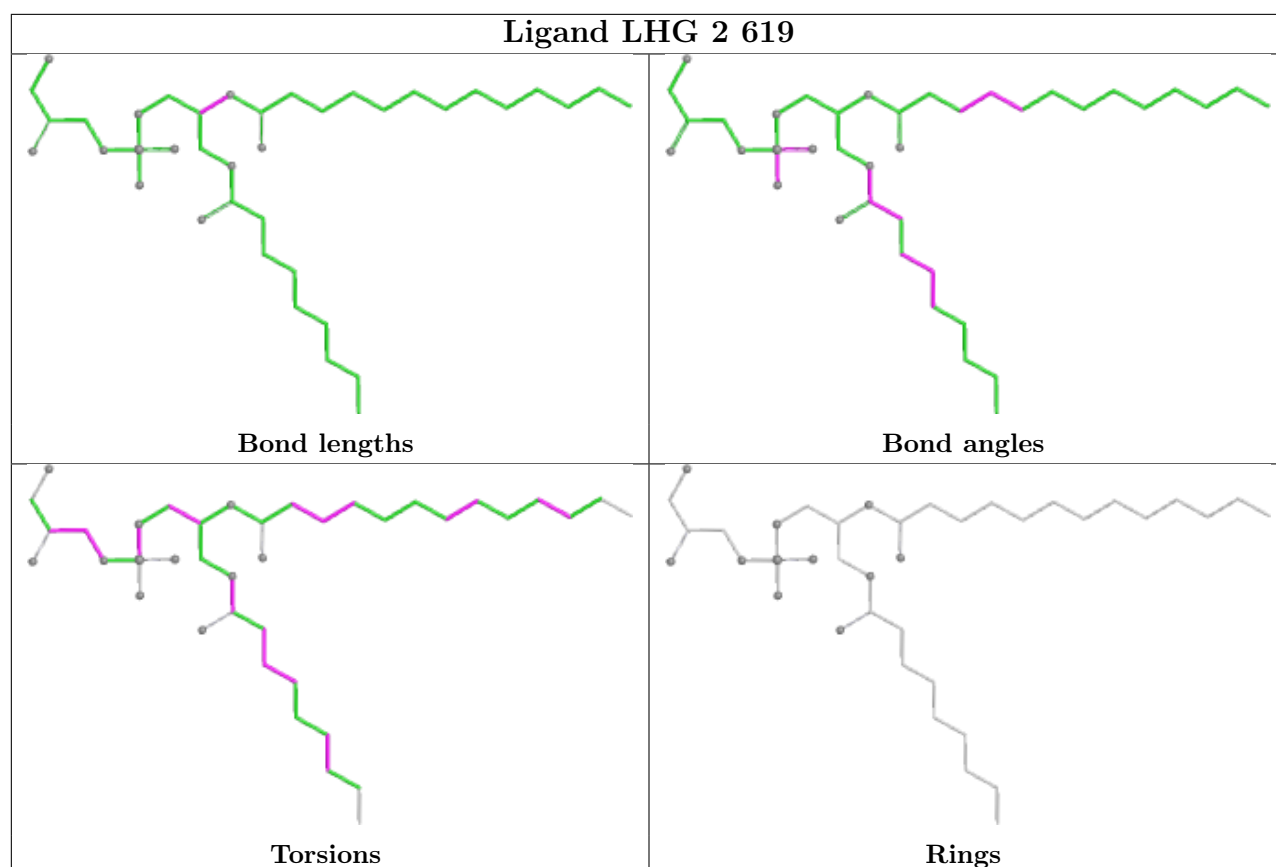


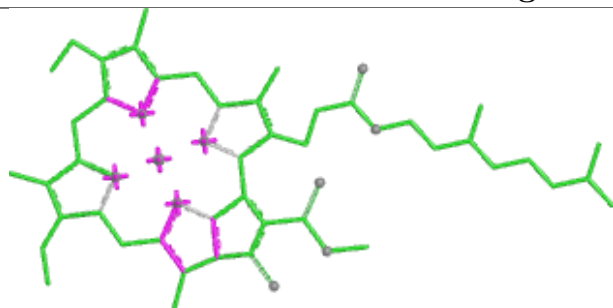




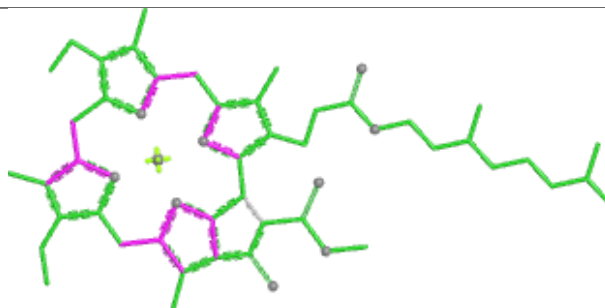
**Ligand CLA 1 602****Ligand CLA B 807**



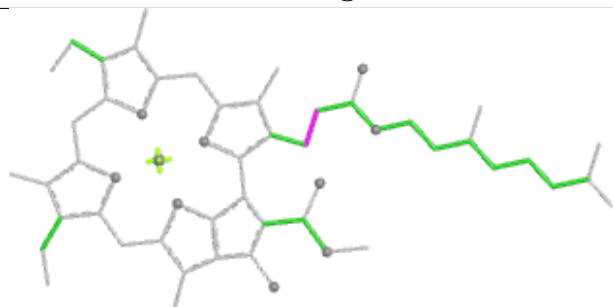


**Ligand CLA 9 604**

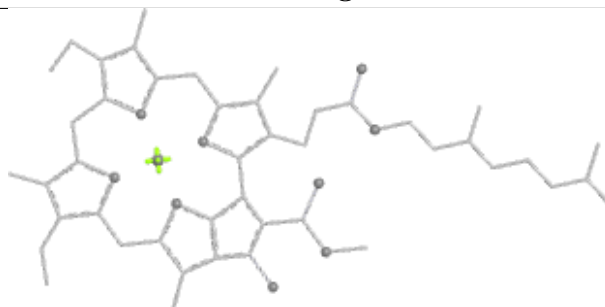
Bond lengths



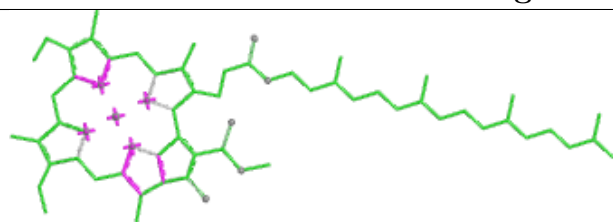
Bond angles



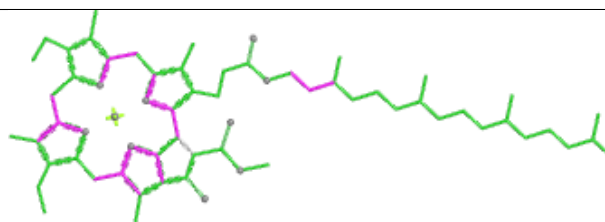
Torsions



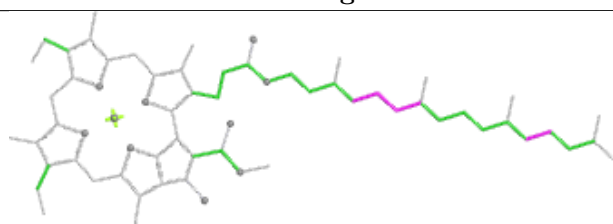
Rings

**Ligand CLA B 801**

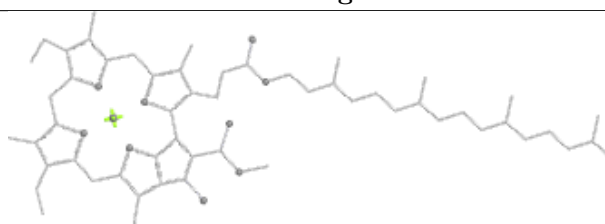
Bond lengths



Bond angles

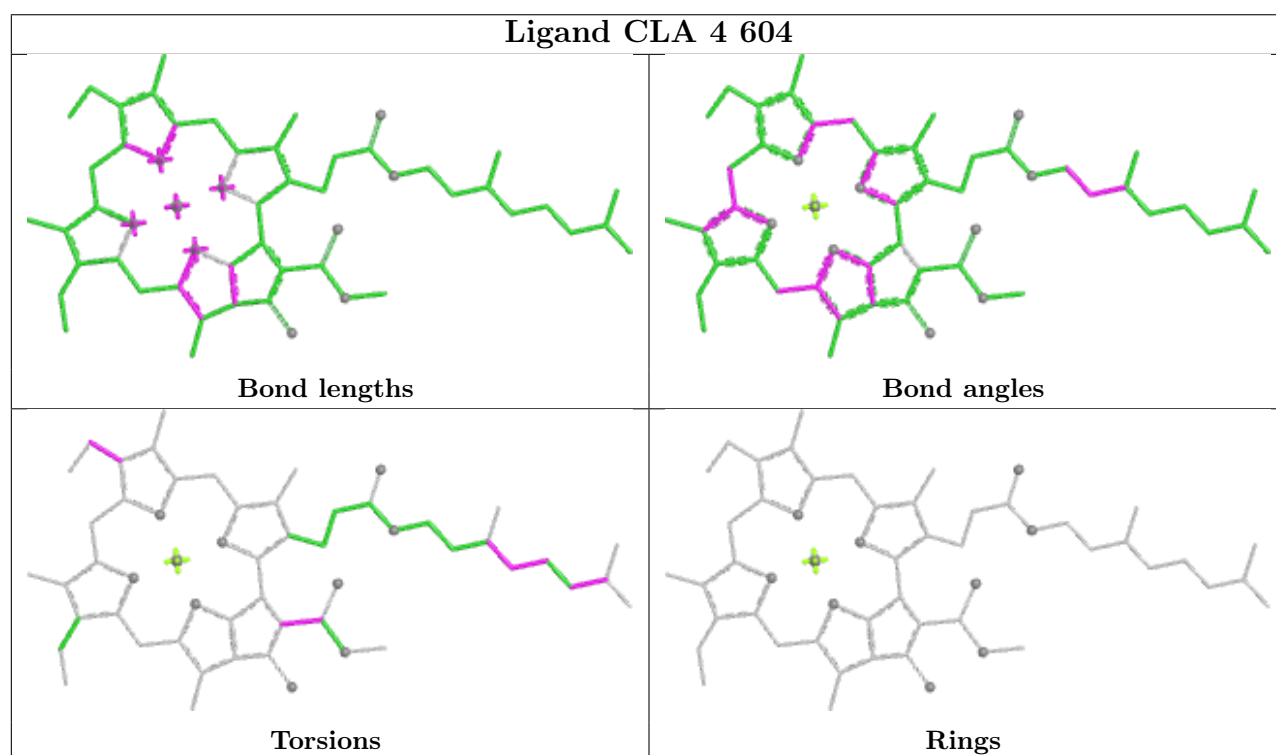
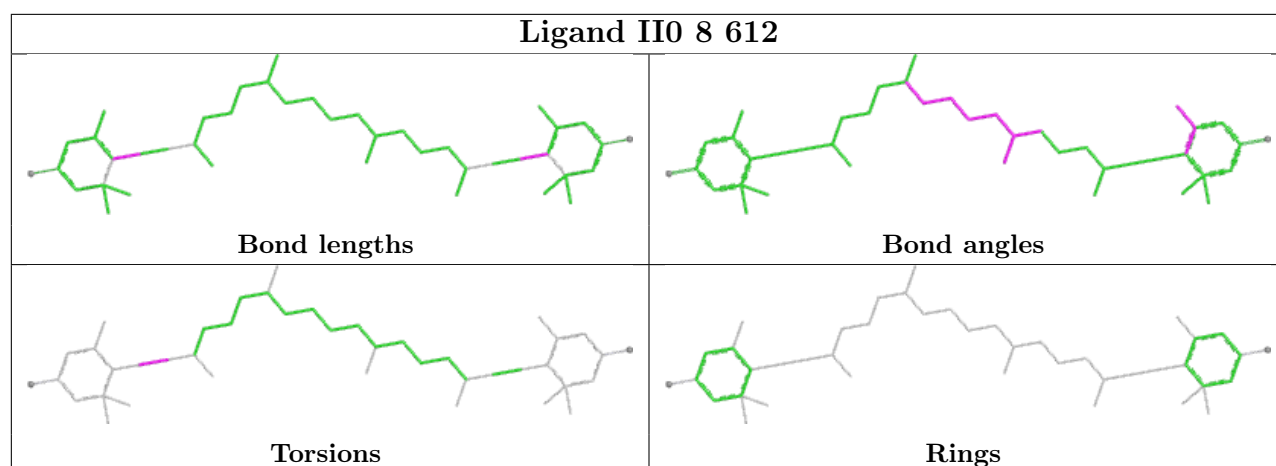


Torsions

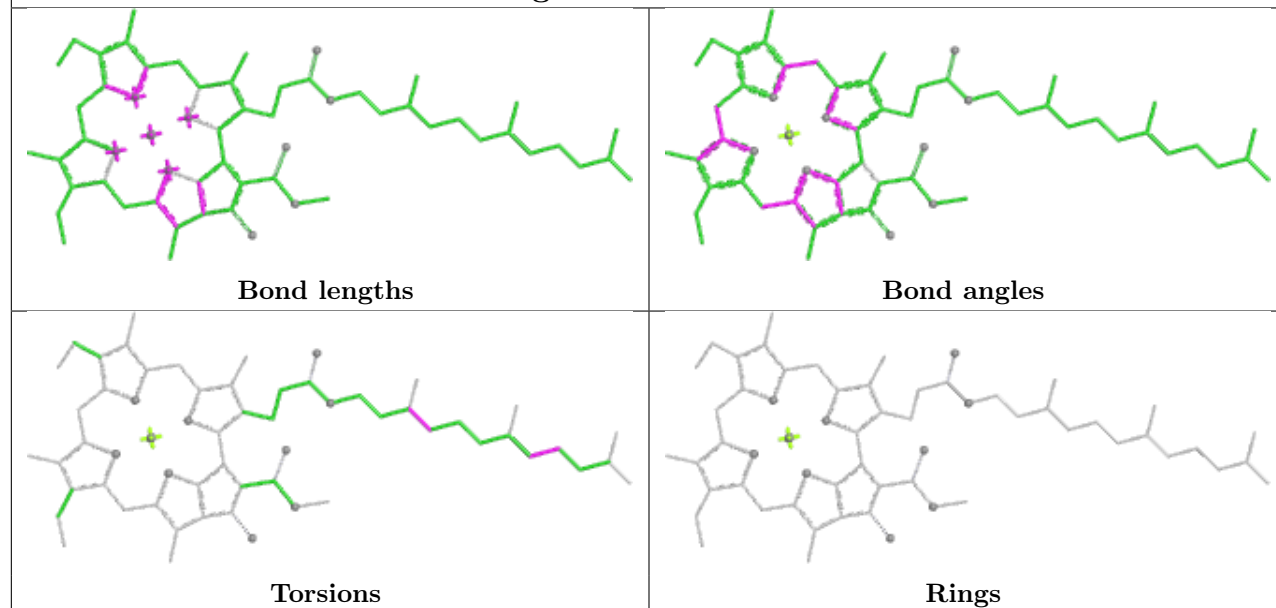


Rings

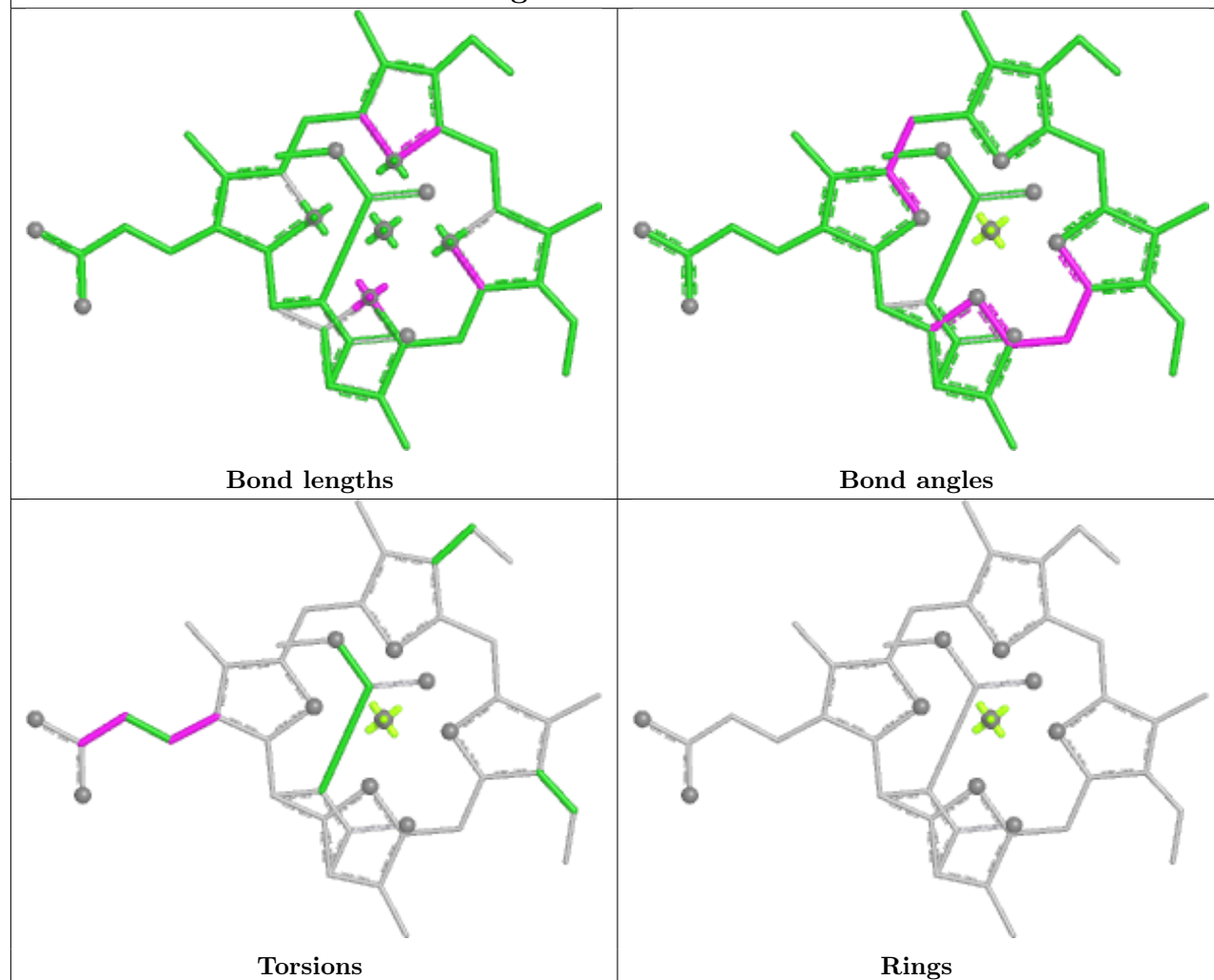


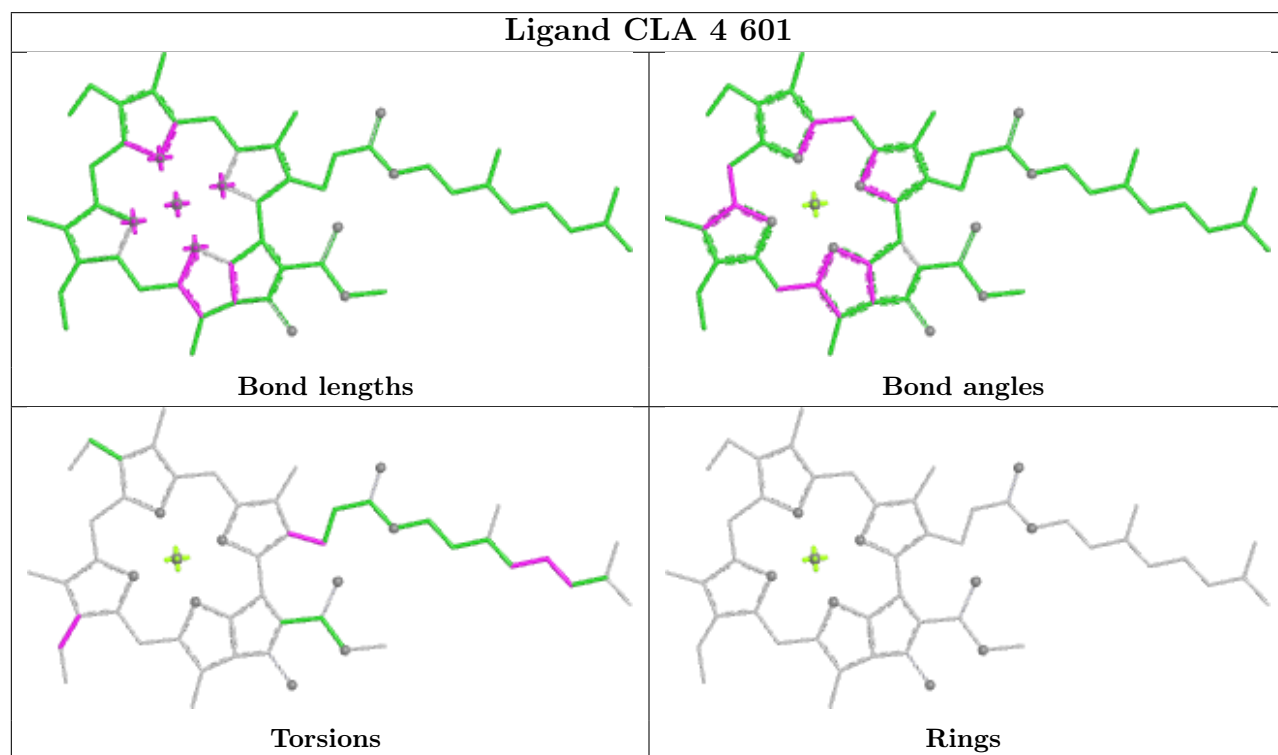
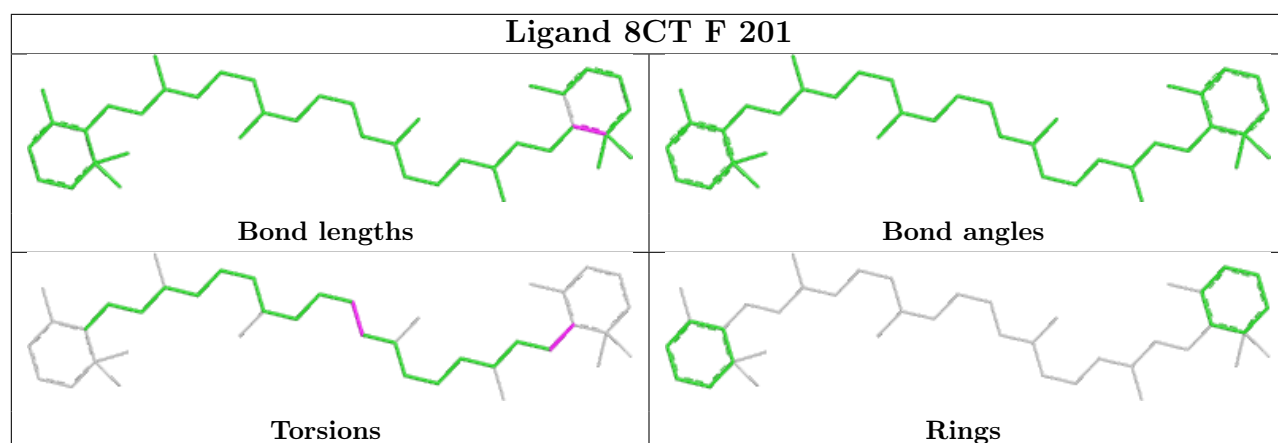


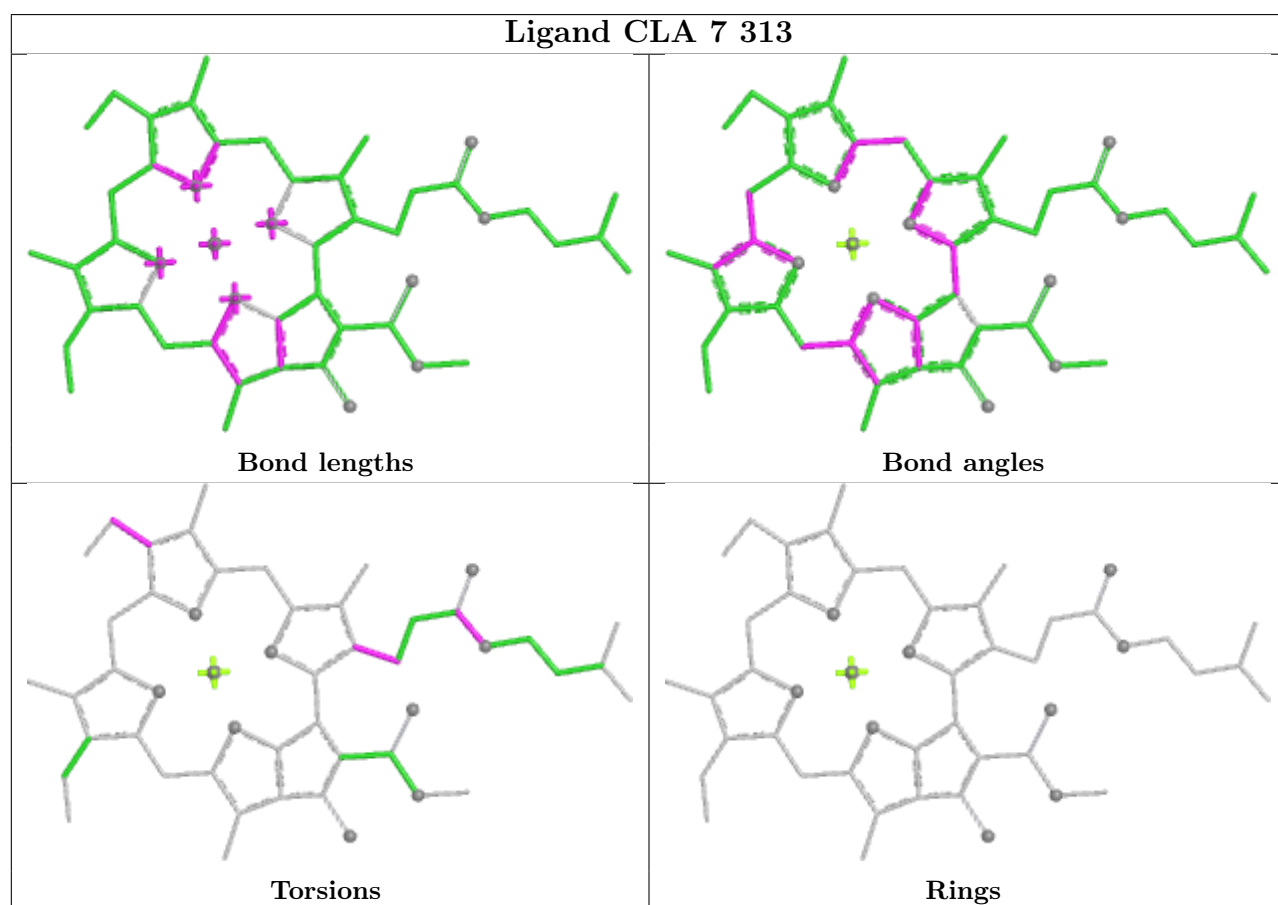
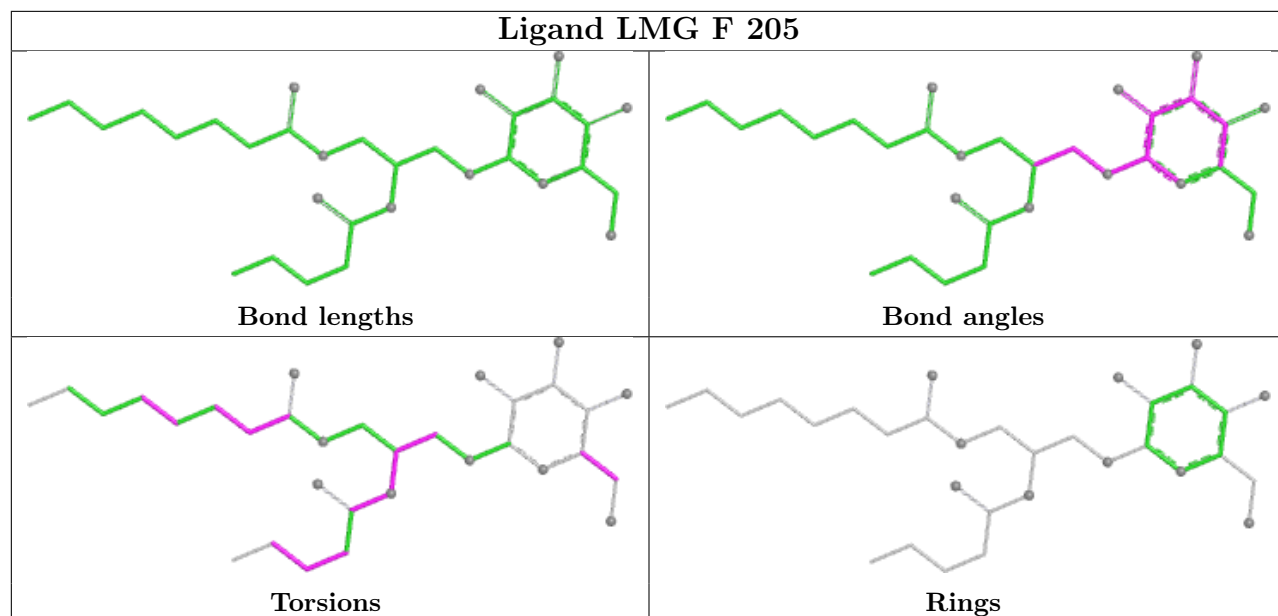
## Ligand CLA B 810

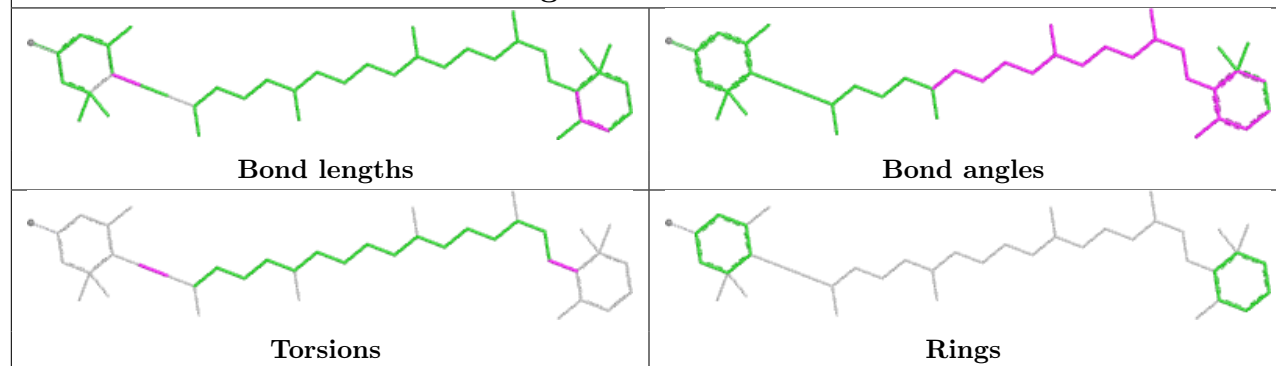
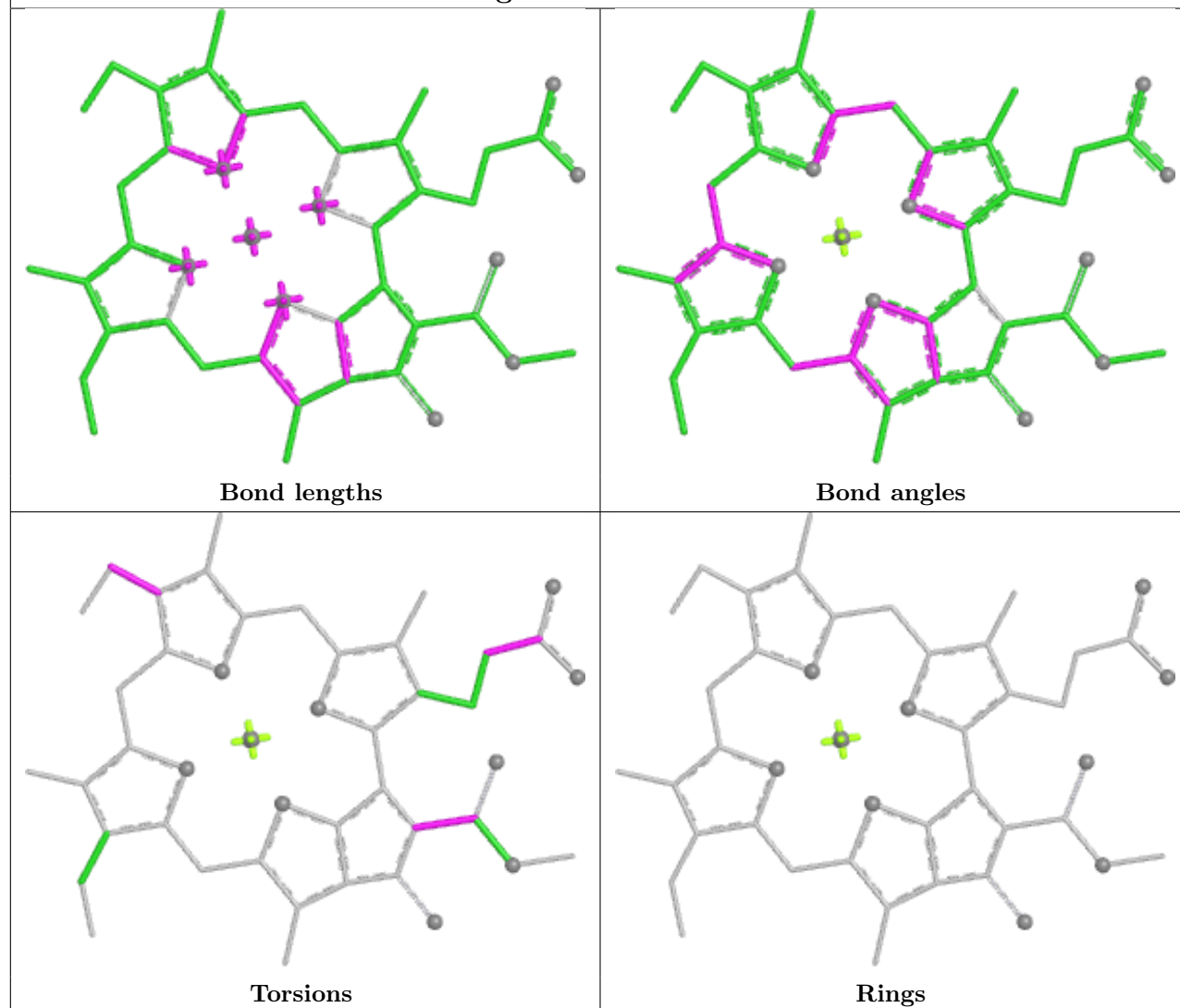


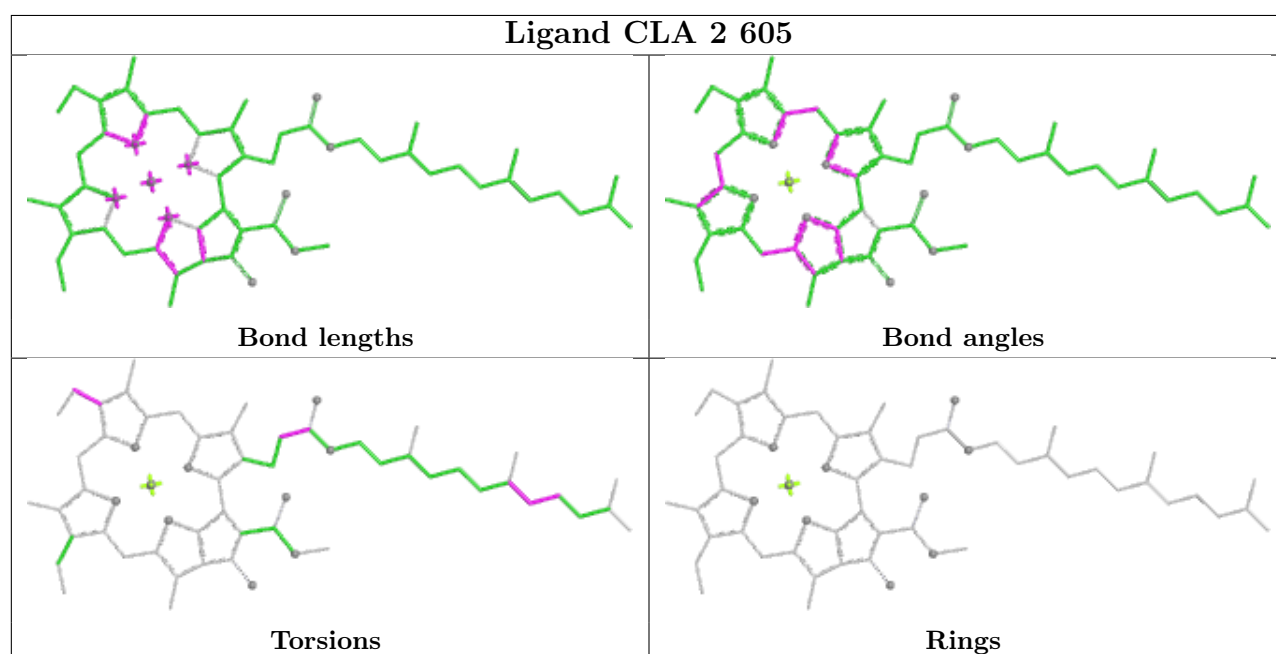
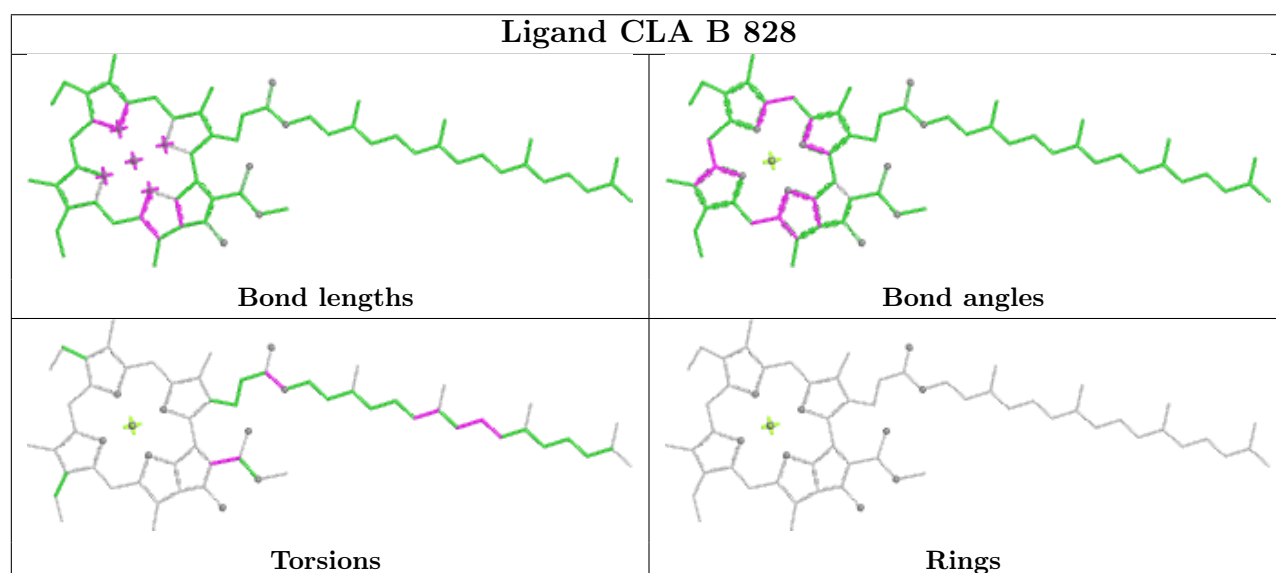
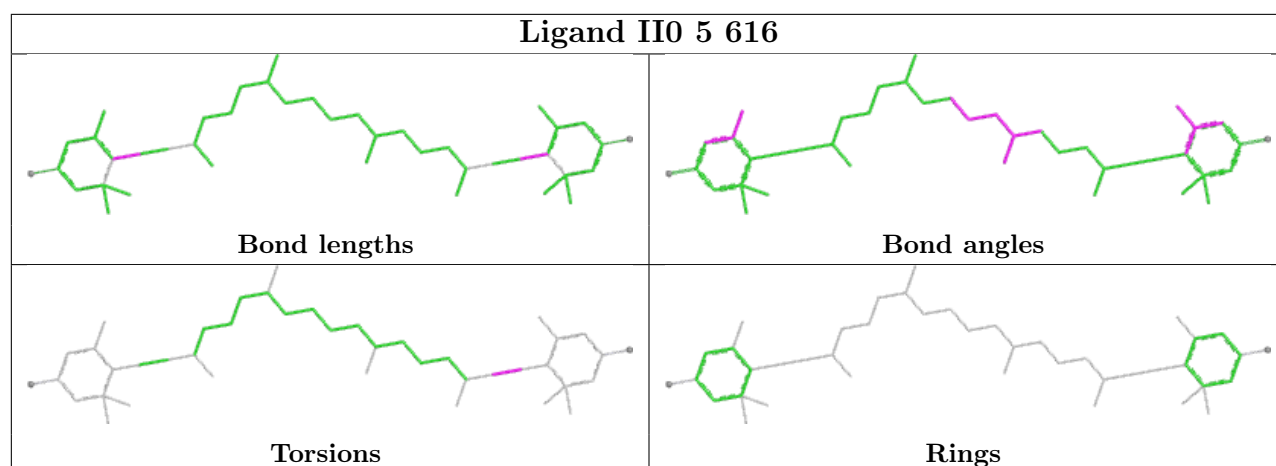
## Ligand KC2 b 609



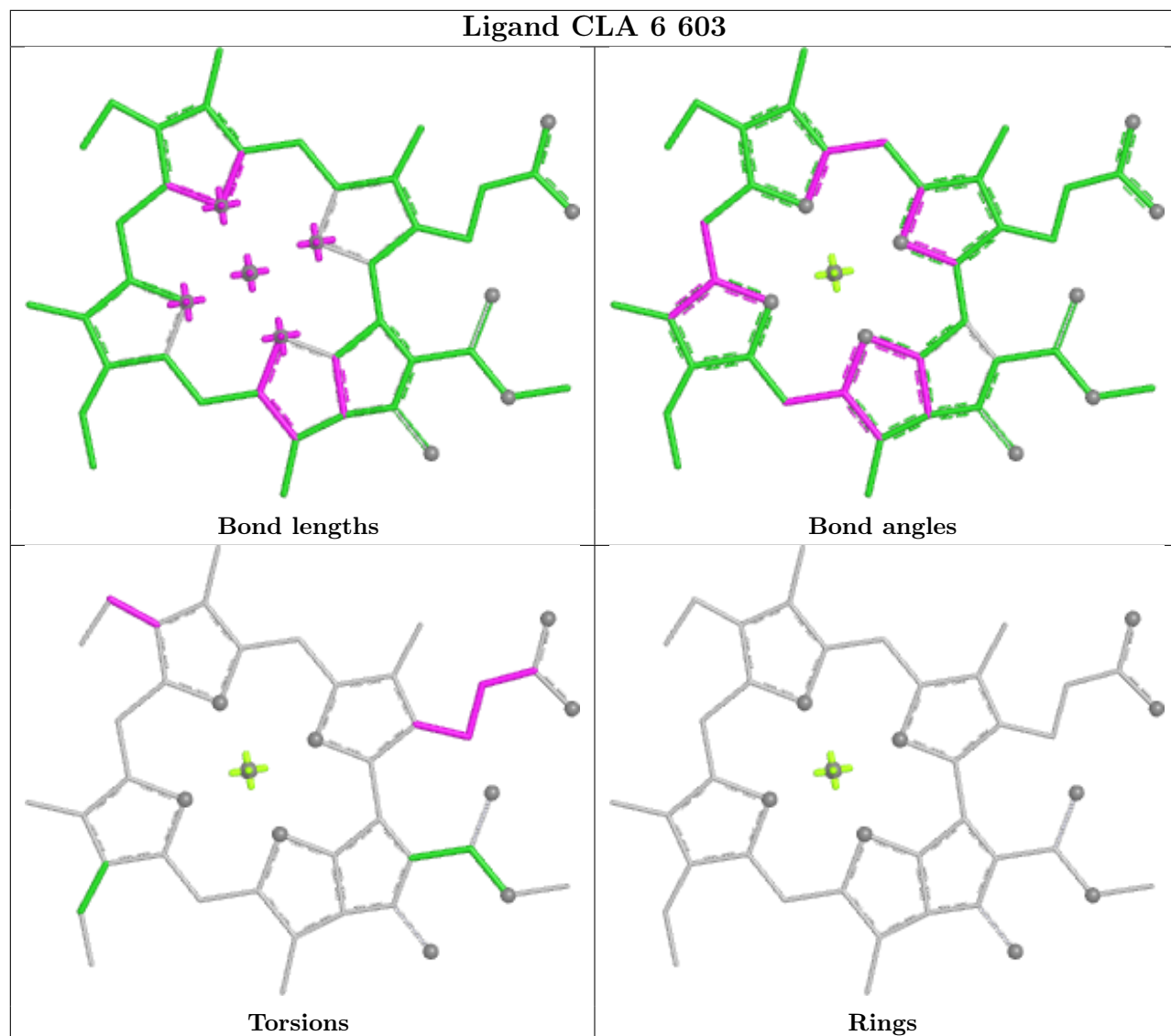




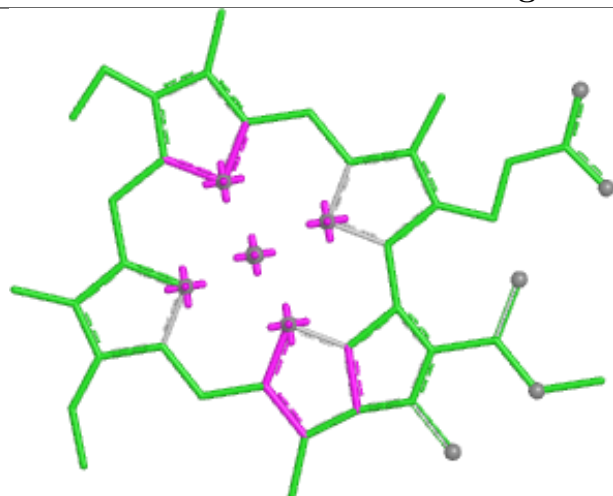
**Ligand IHT 6 616****Ligand CLA 7 306**



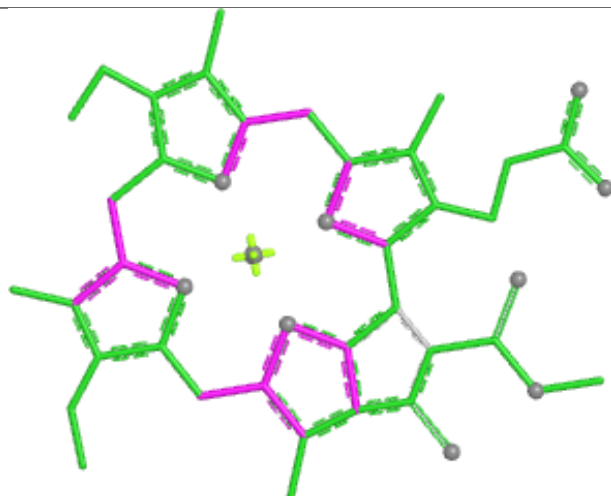
## Ligand CLA 6 603



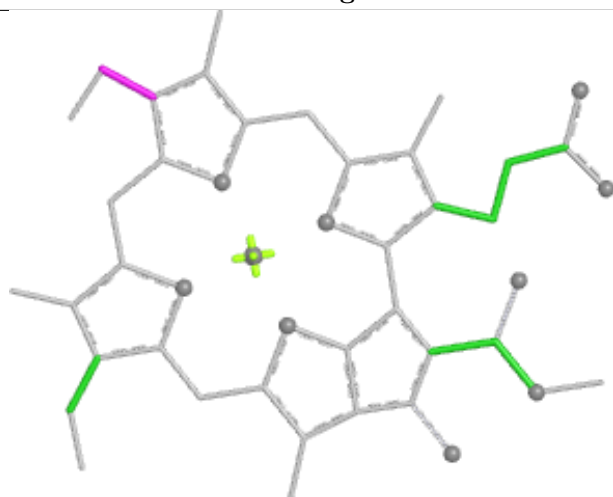
## Ligand CLA 3 612



Bond lengths



Bond angles

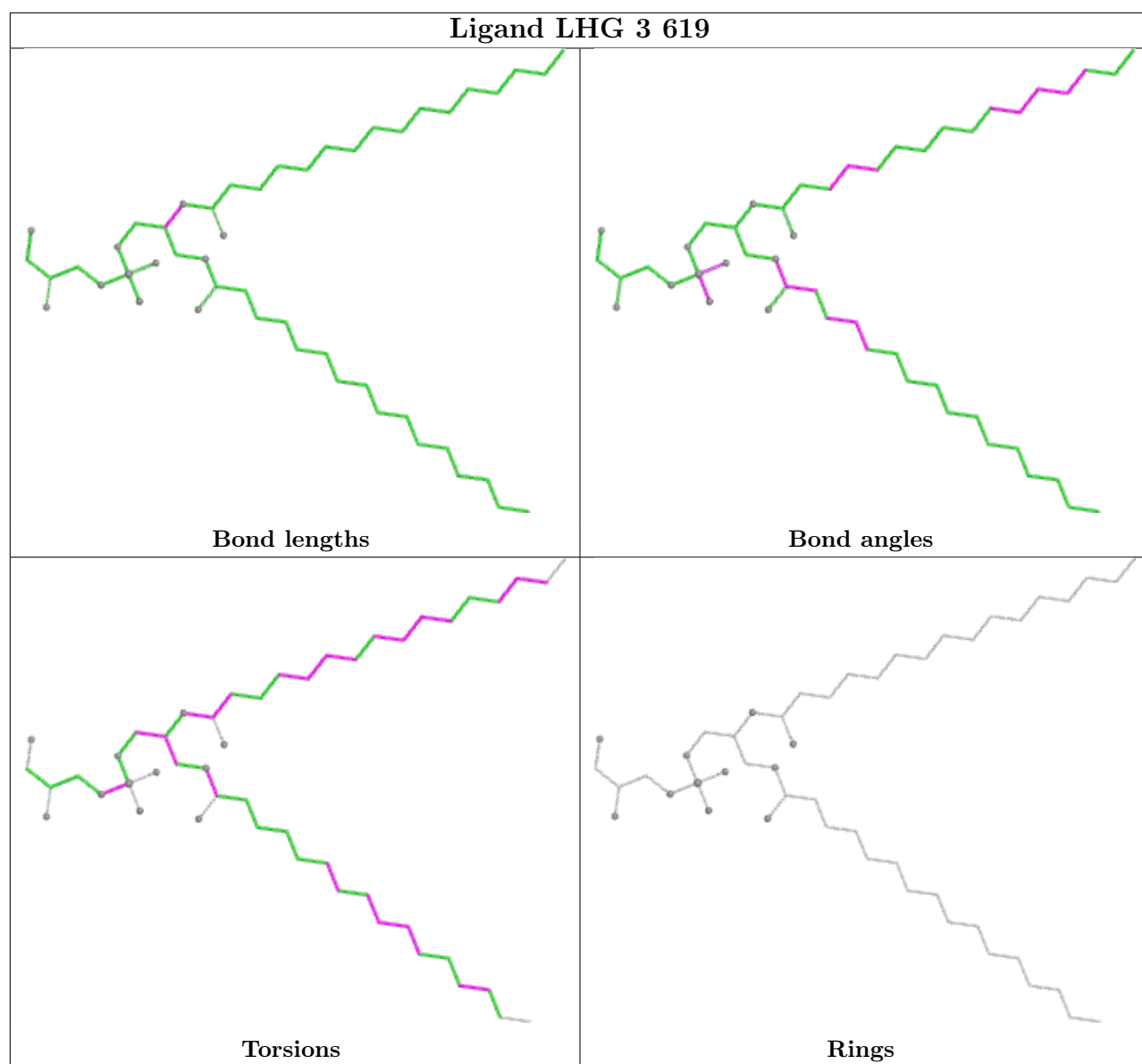


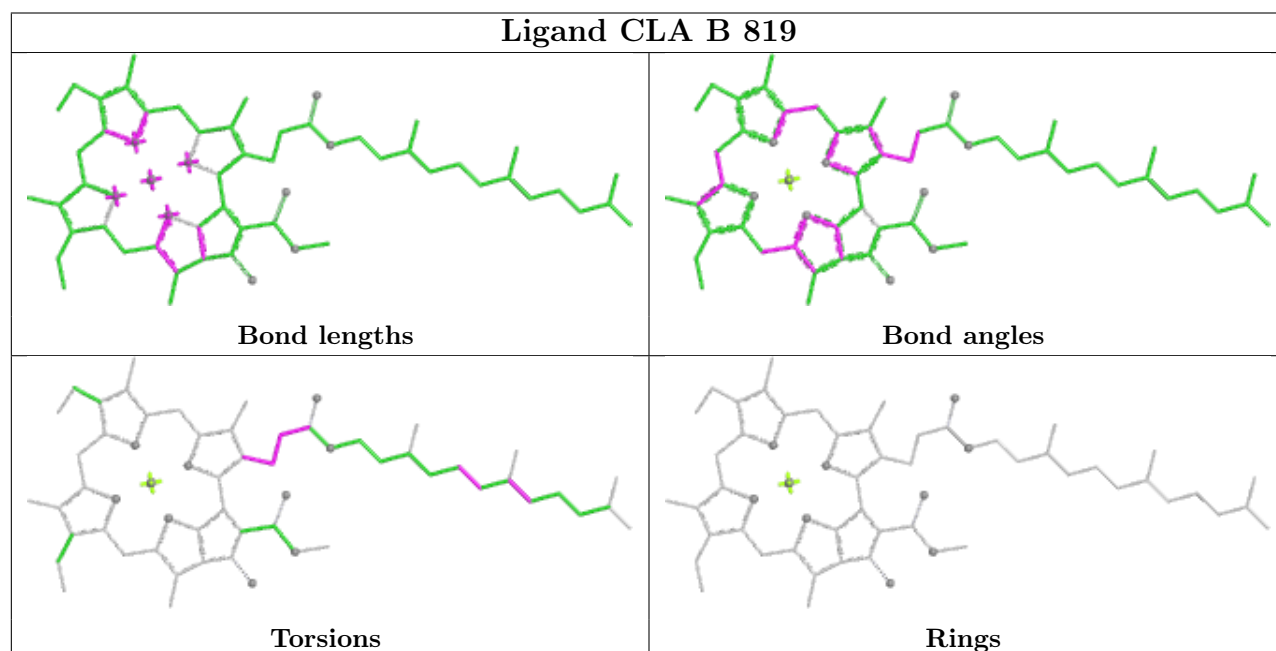
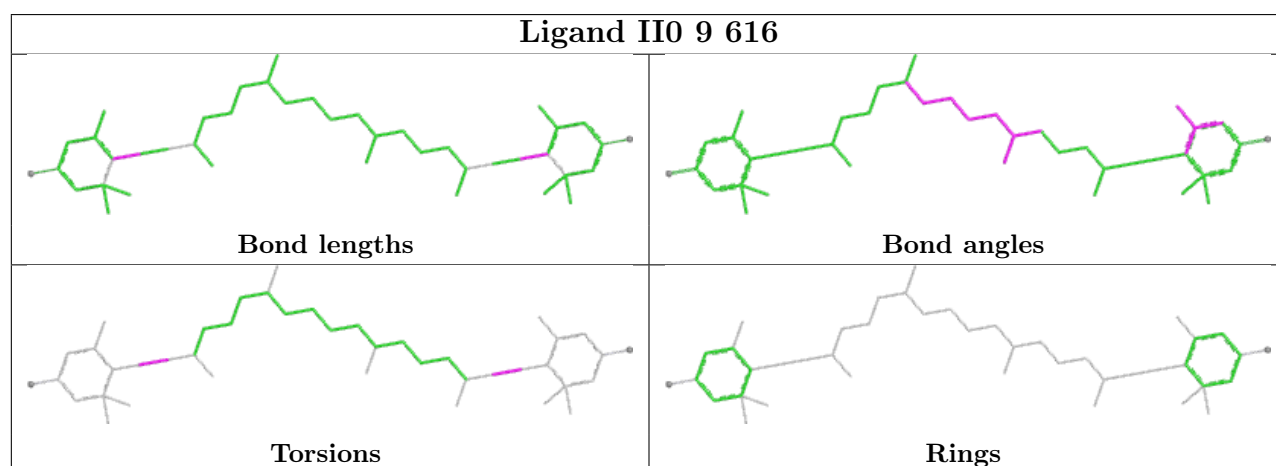
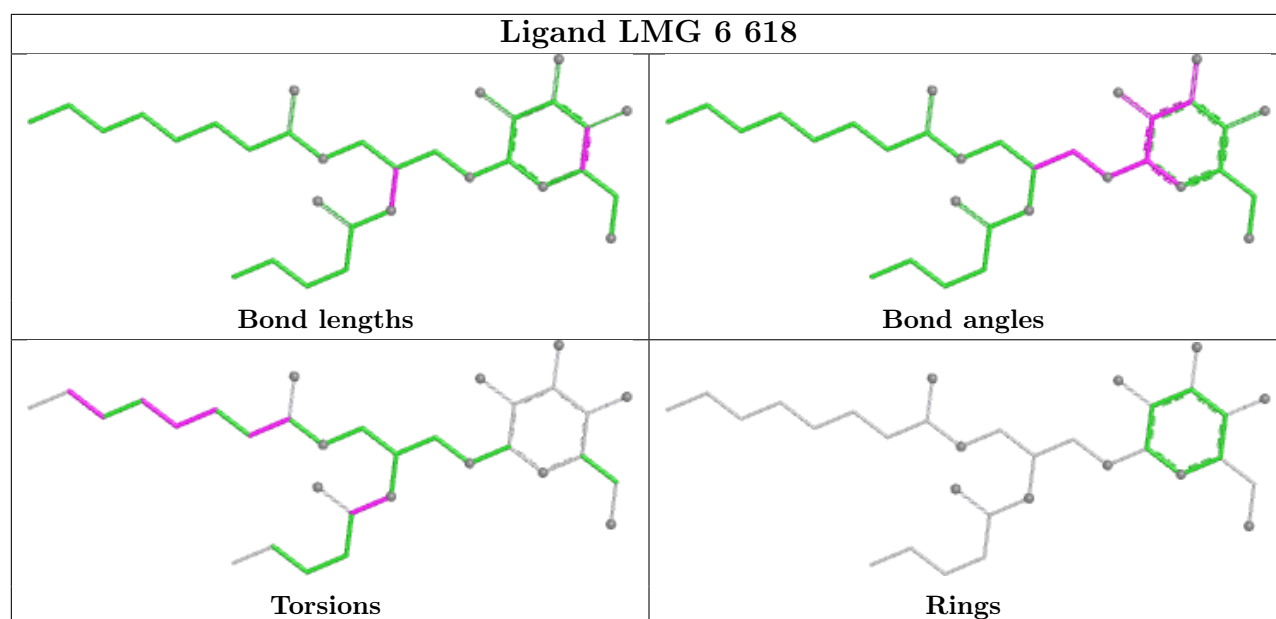
Torsions

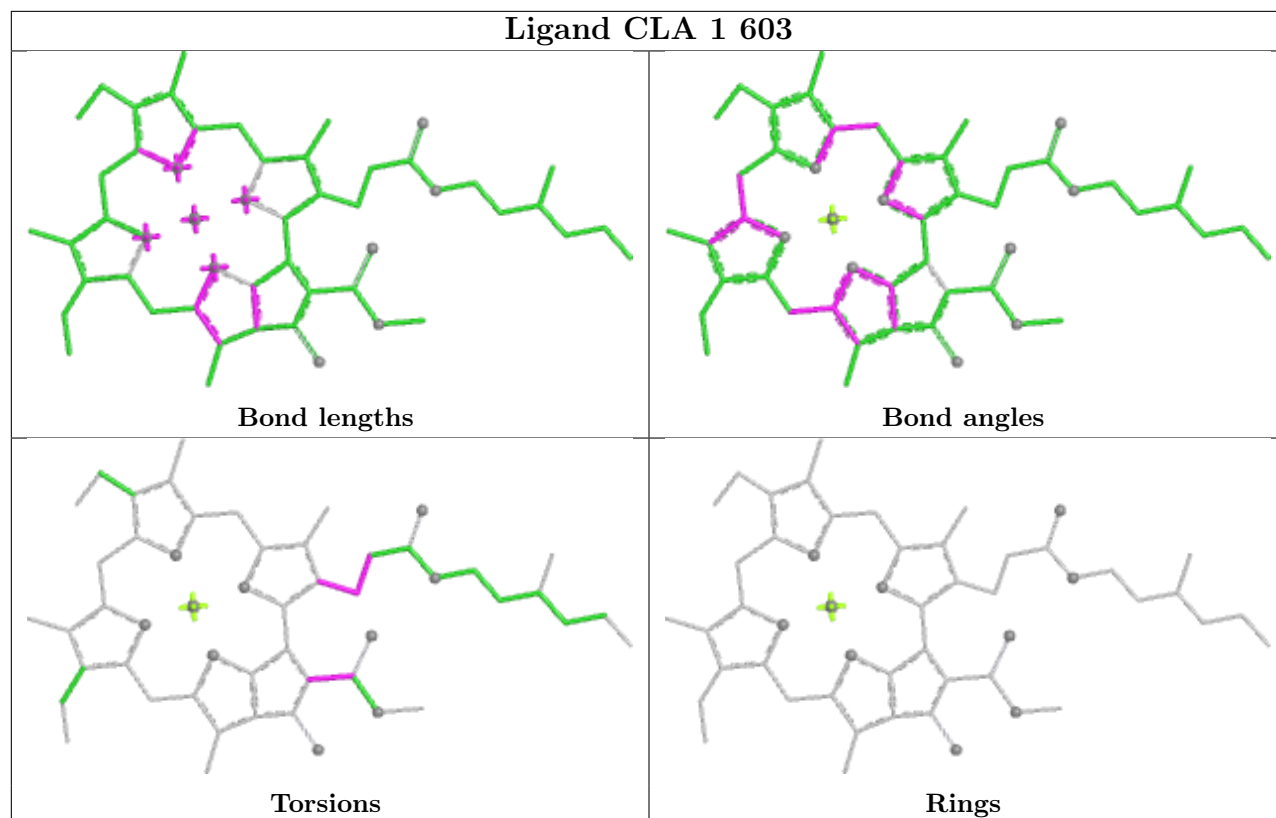
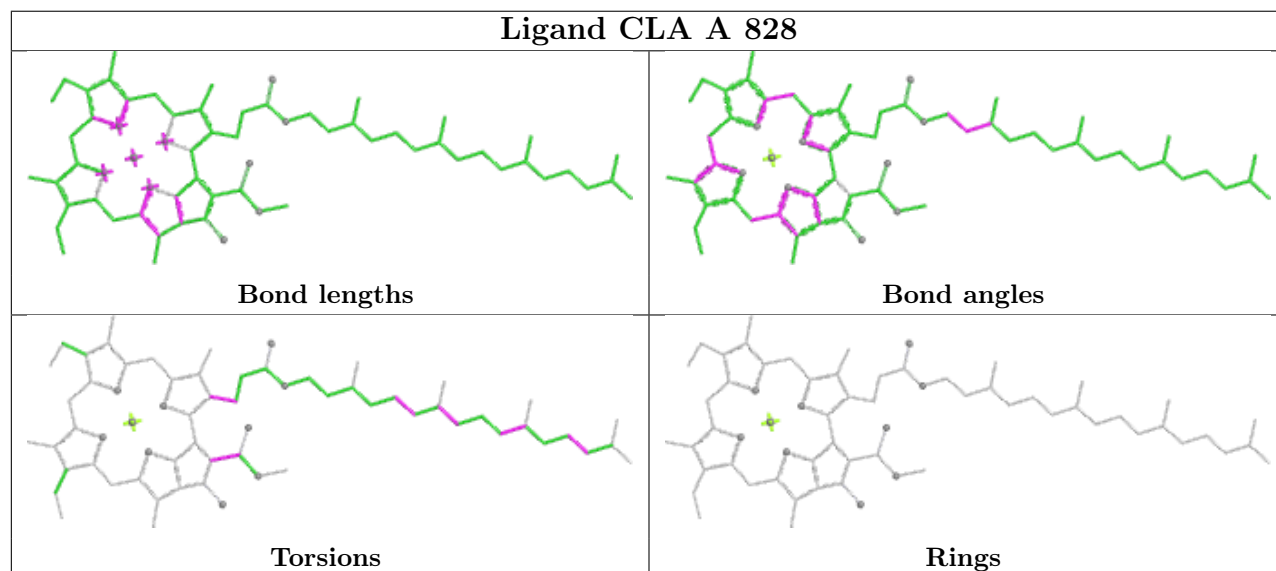


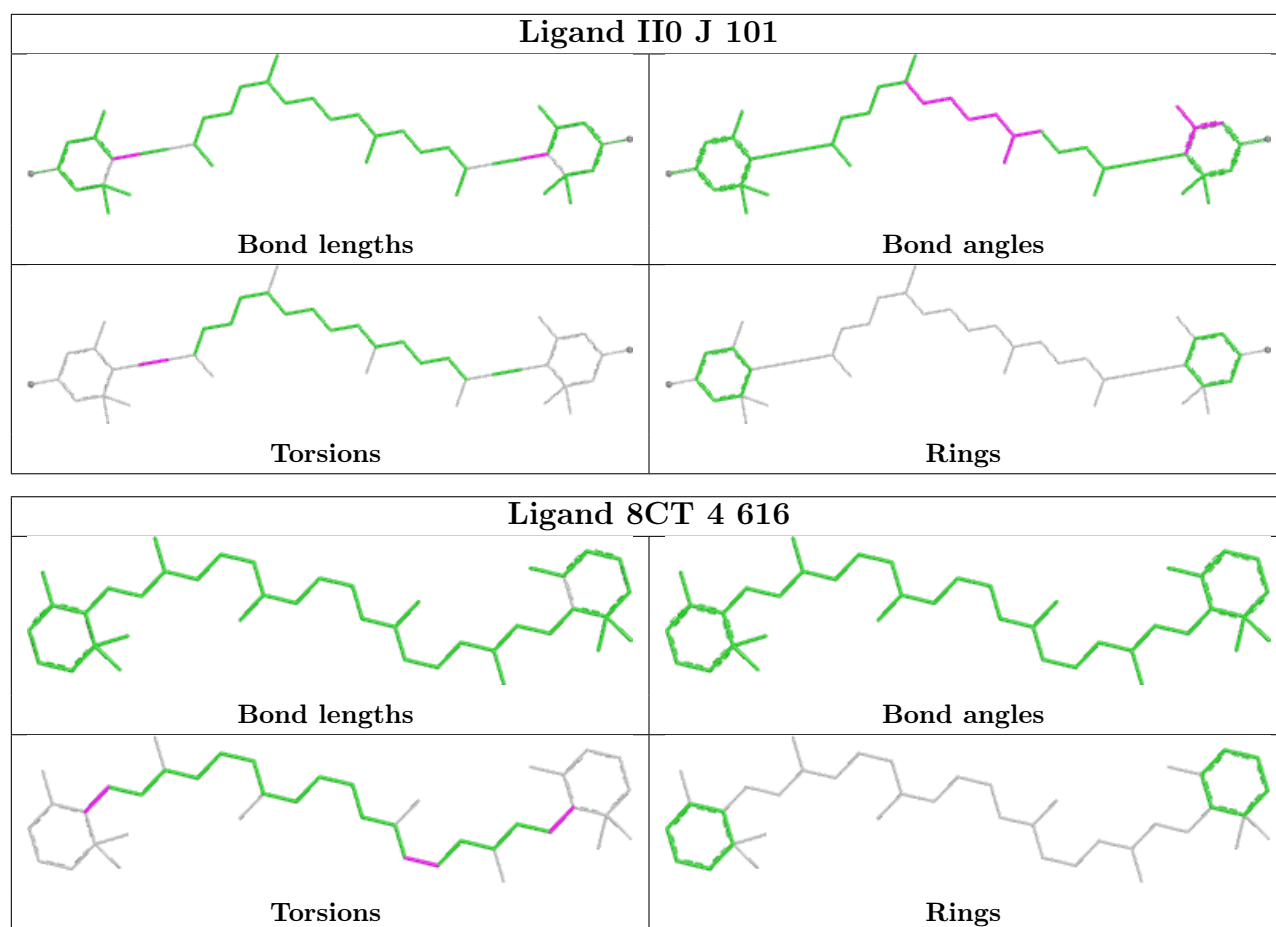
Rings



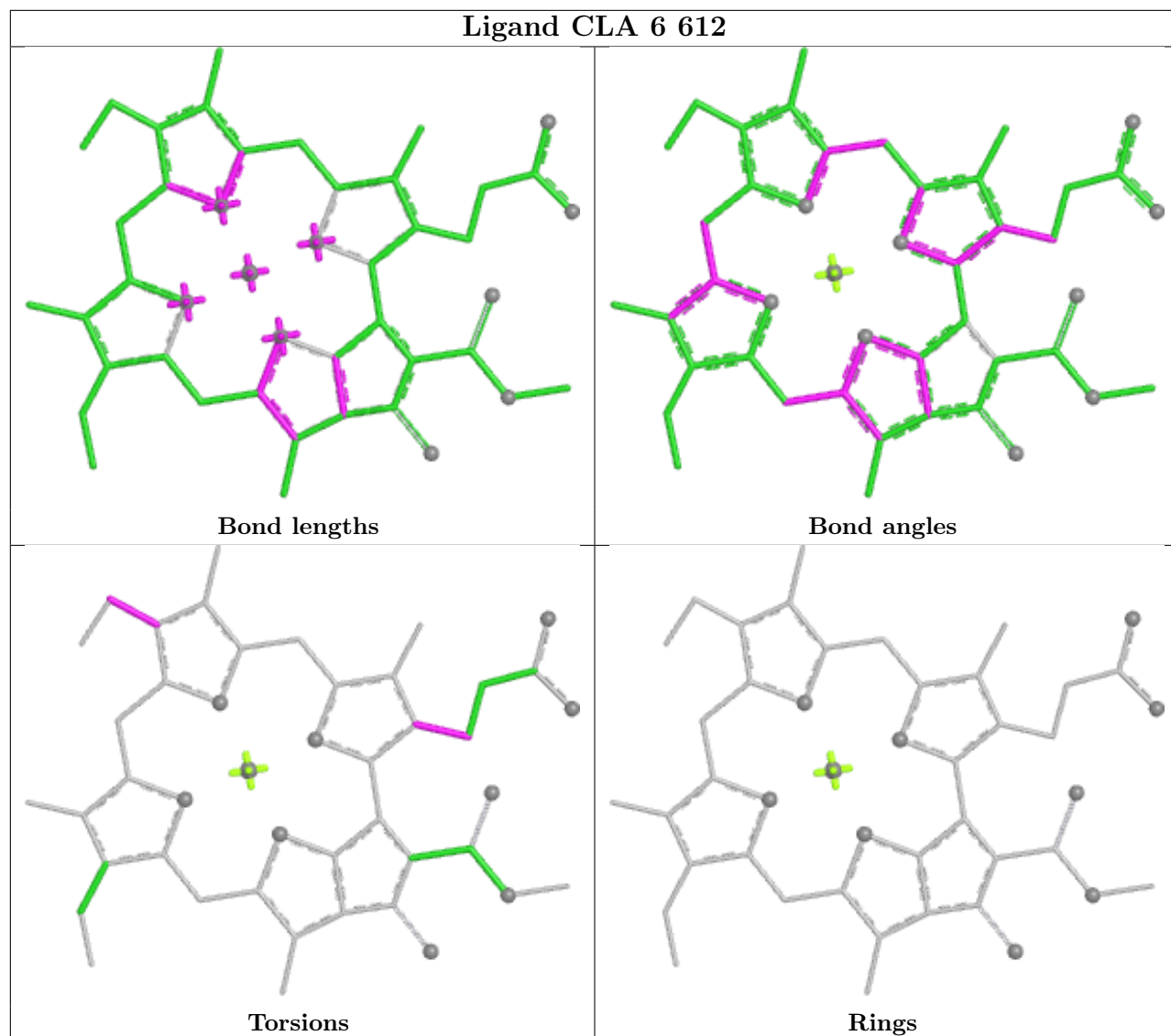


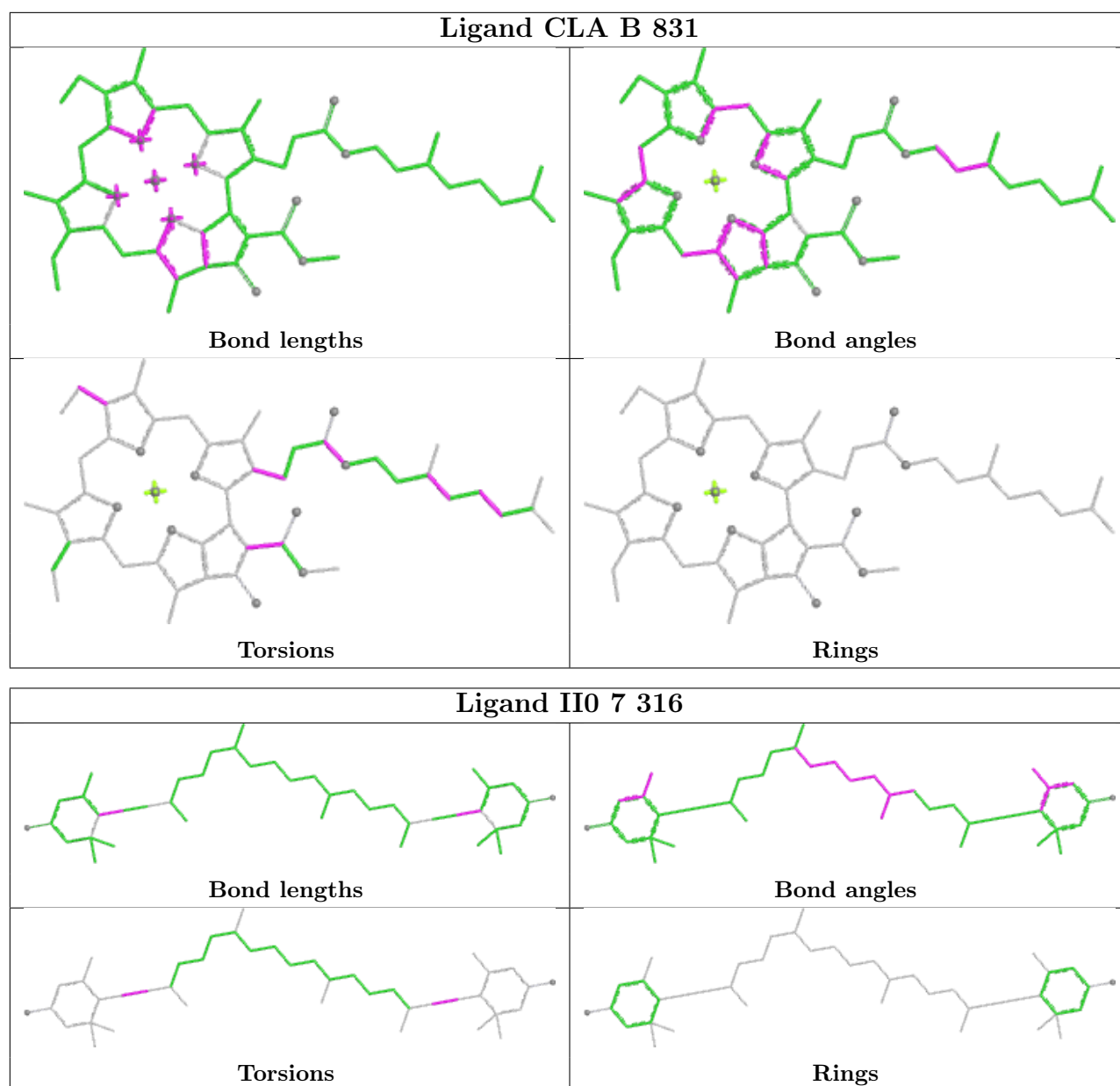


**Ligand CLA 1 603****Ligand CLA A 828**

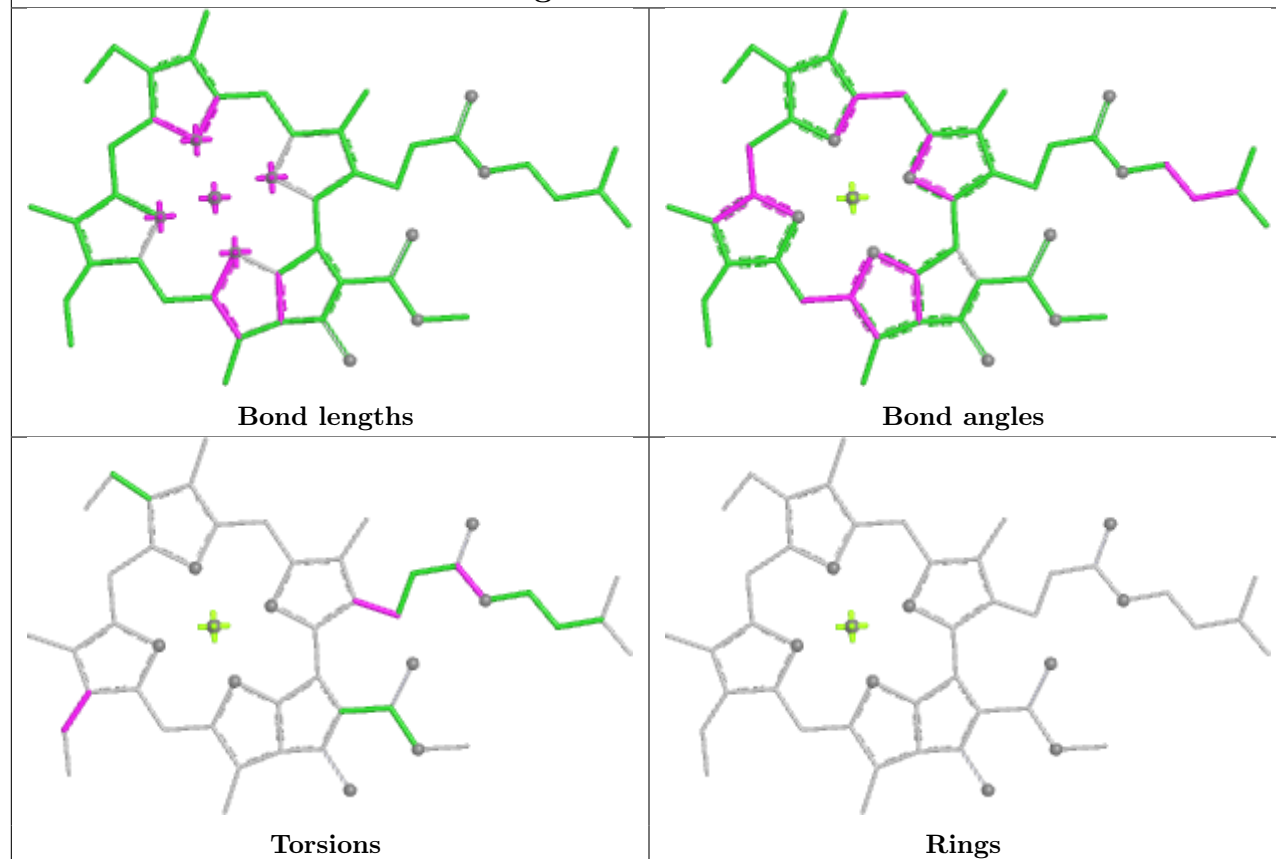


## Ligand CLA 6 612

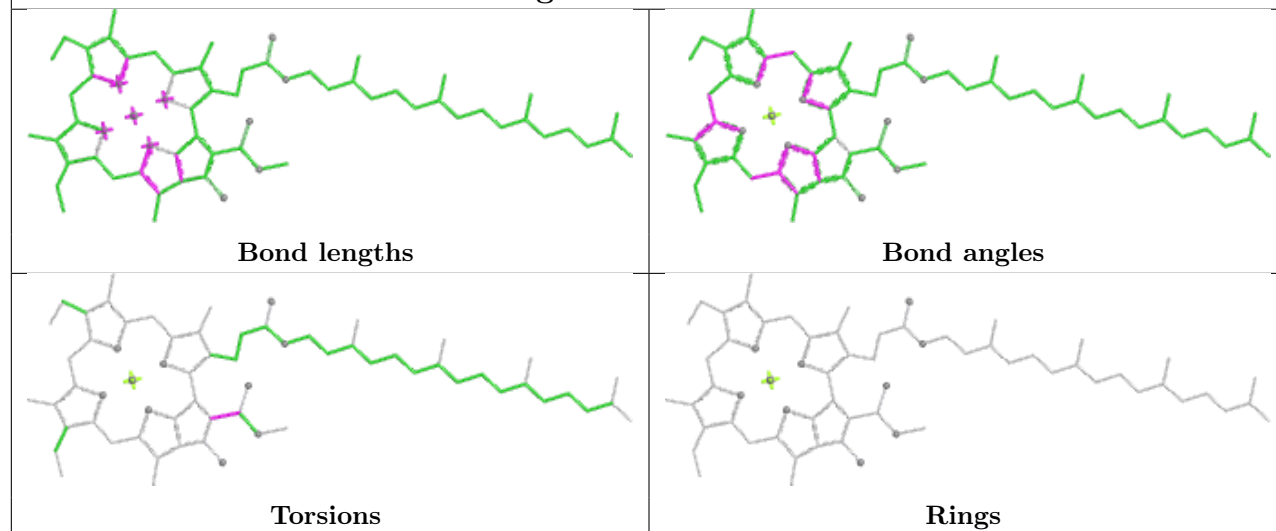


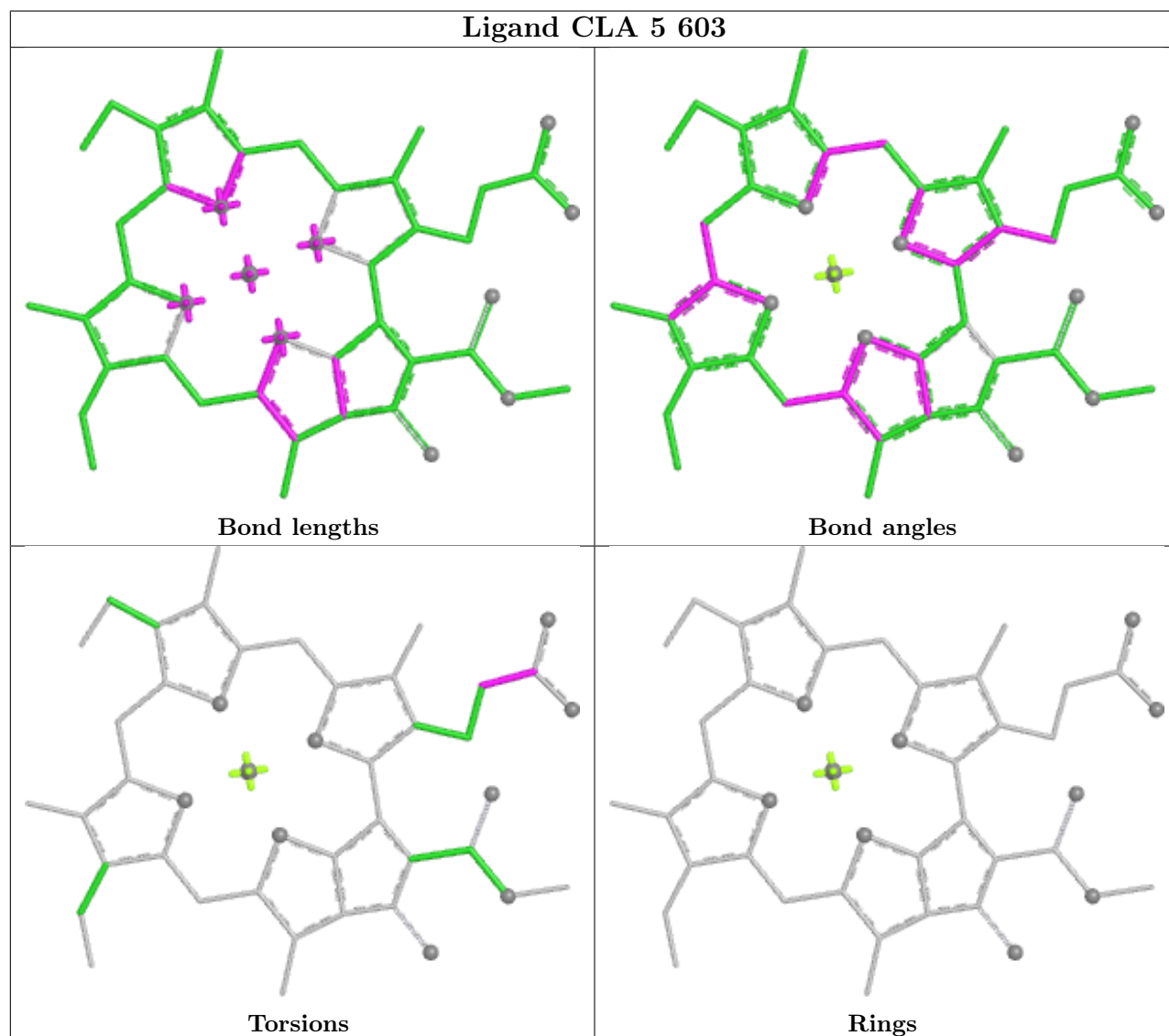
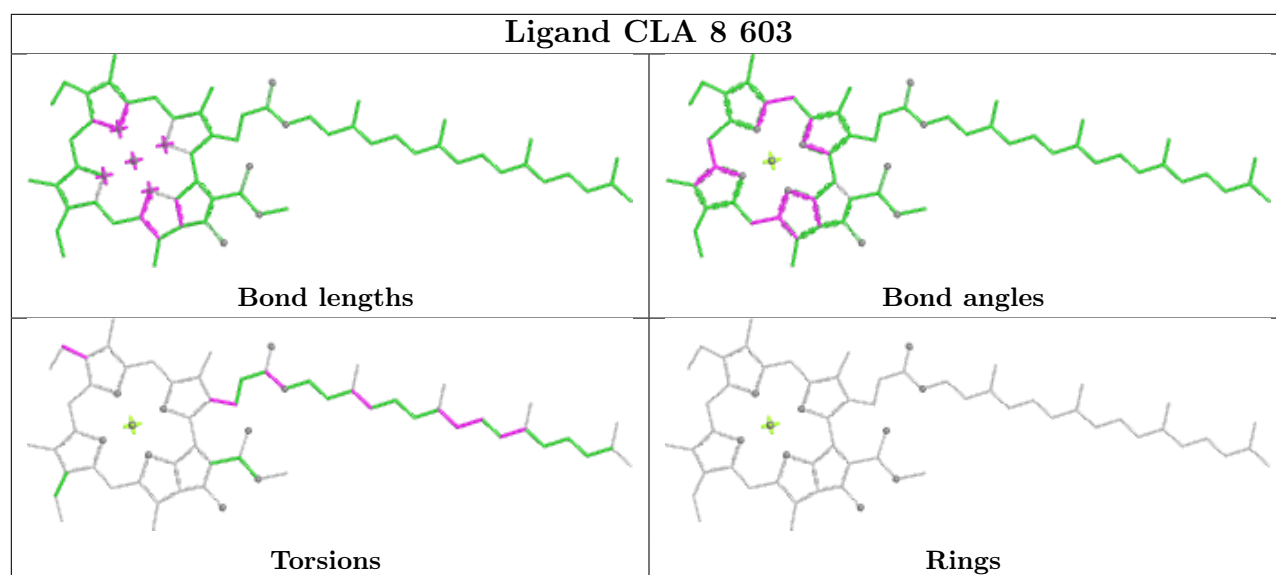


## Ligand CLA L 203



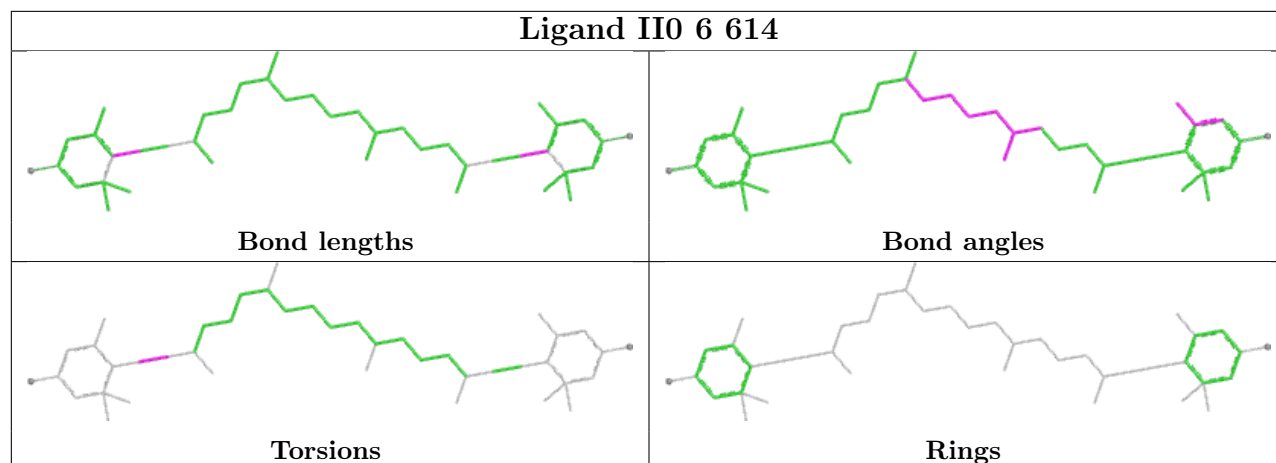
## Ligand CLA 3 604



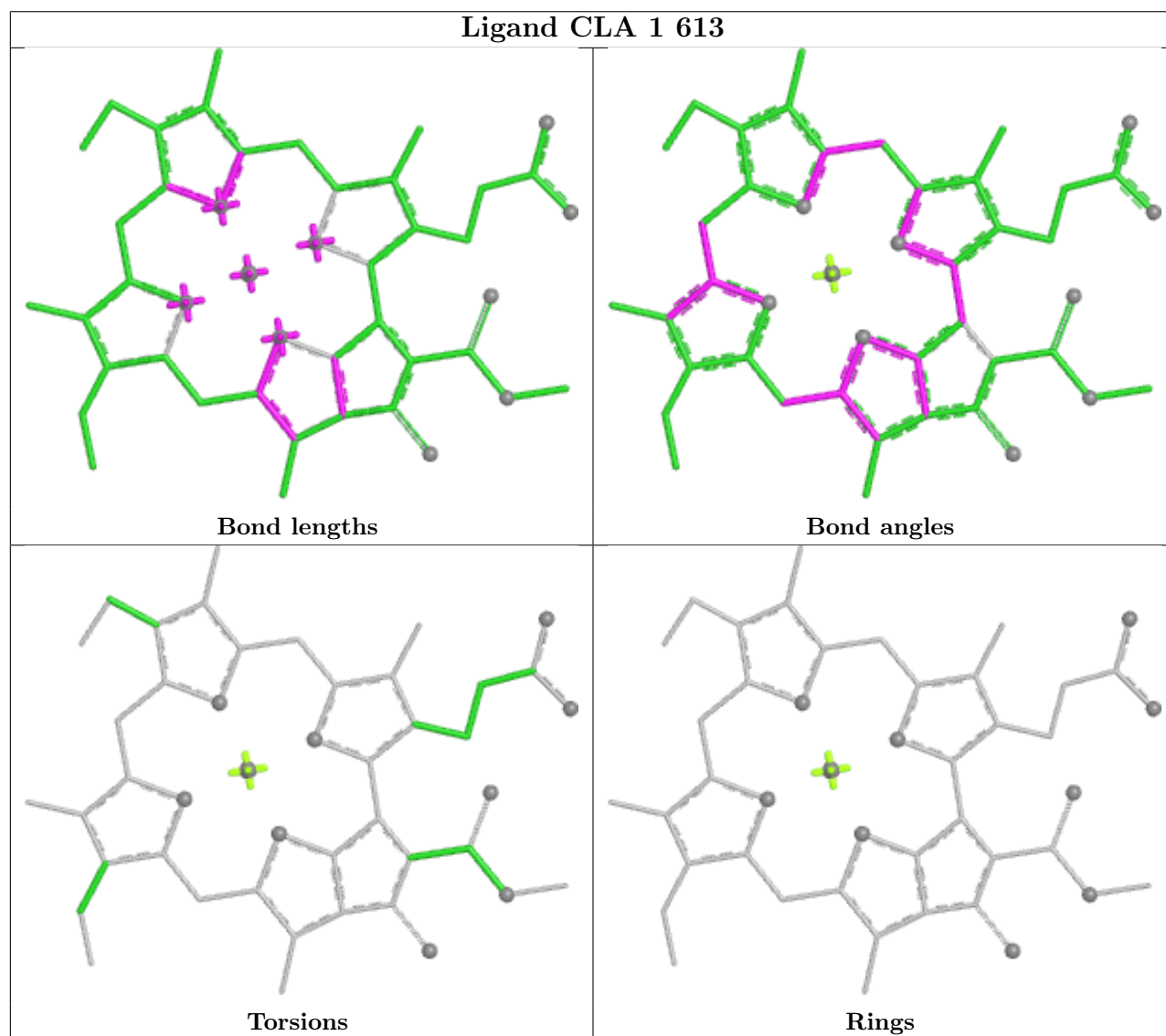




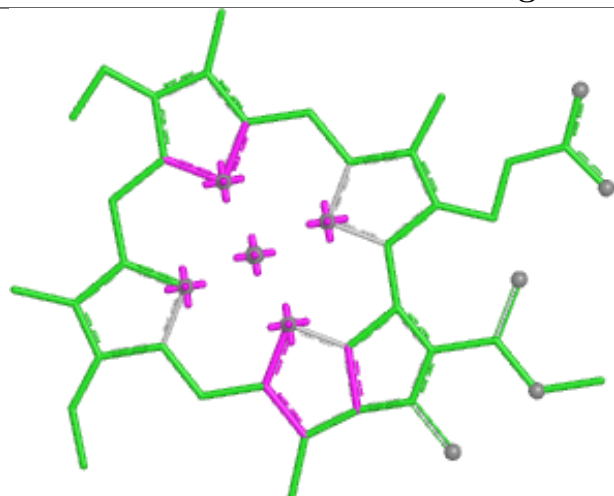
## Ligand II0 6 614



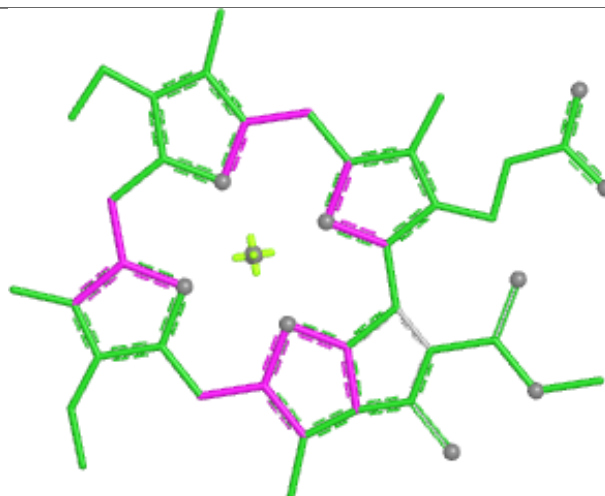
## Ligand CLA 1 613



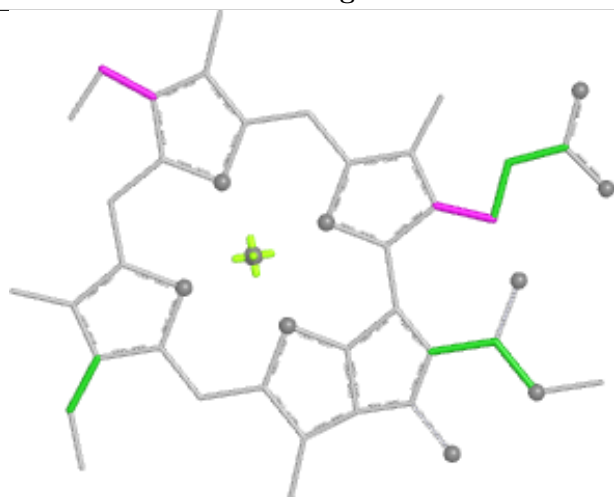
## Ligand CLA 5 612



Bond lengths



Bond angles

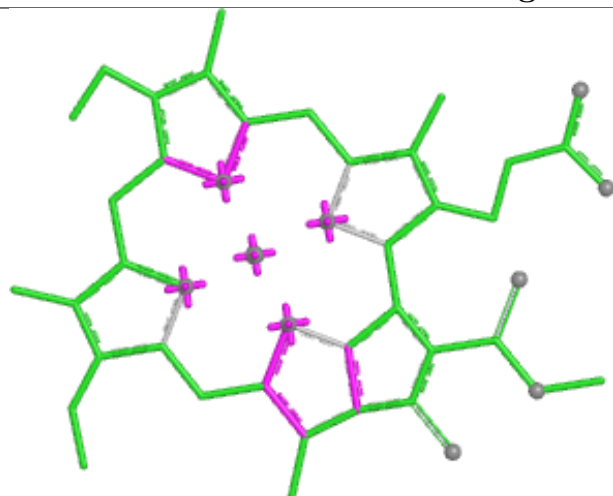


Torsions

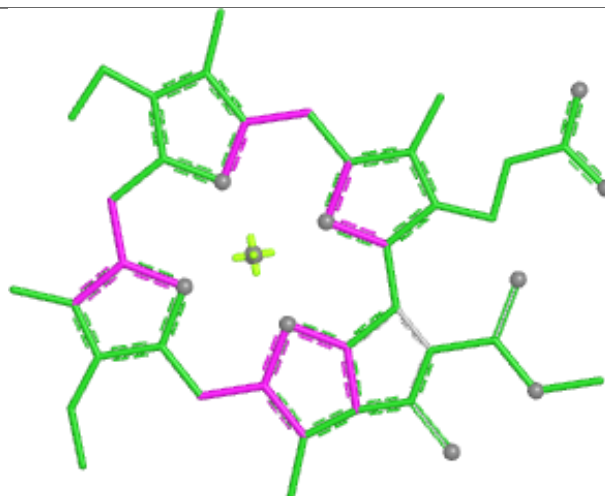


Rings

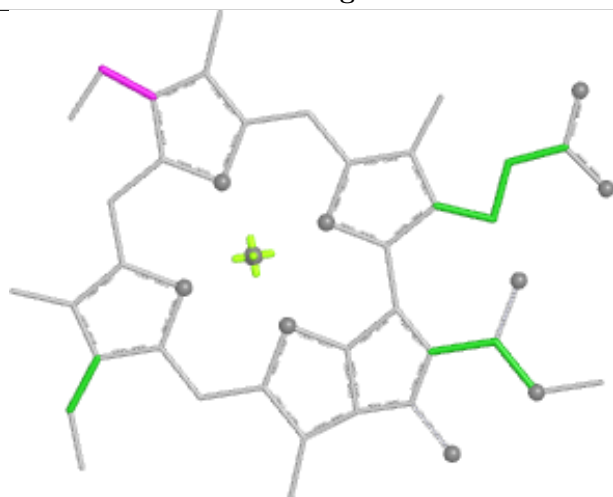
## Ligand CLA 5 607



Bond lengths



Bond angles

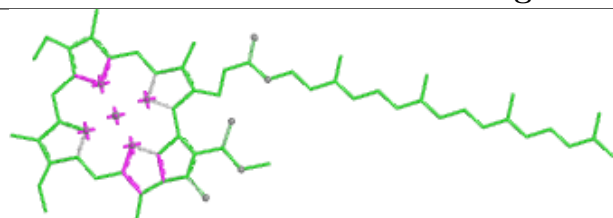


Torsions

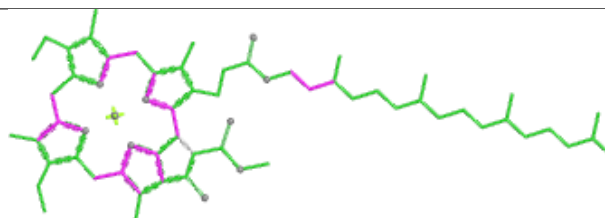


Rings

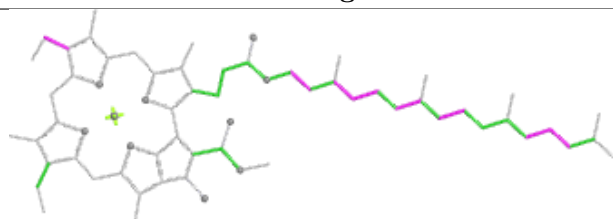
## Ligand CLA B 823



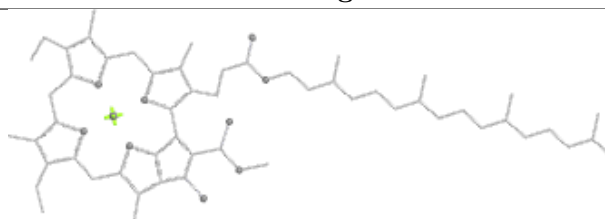
Bond lengths



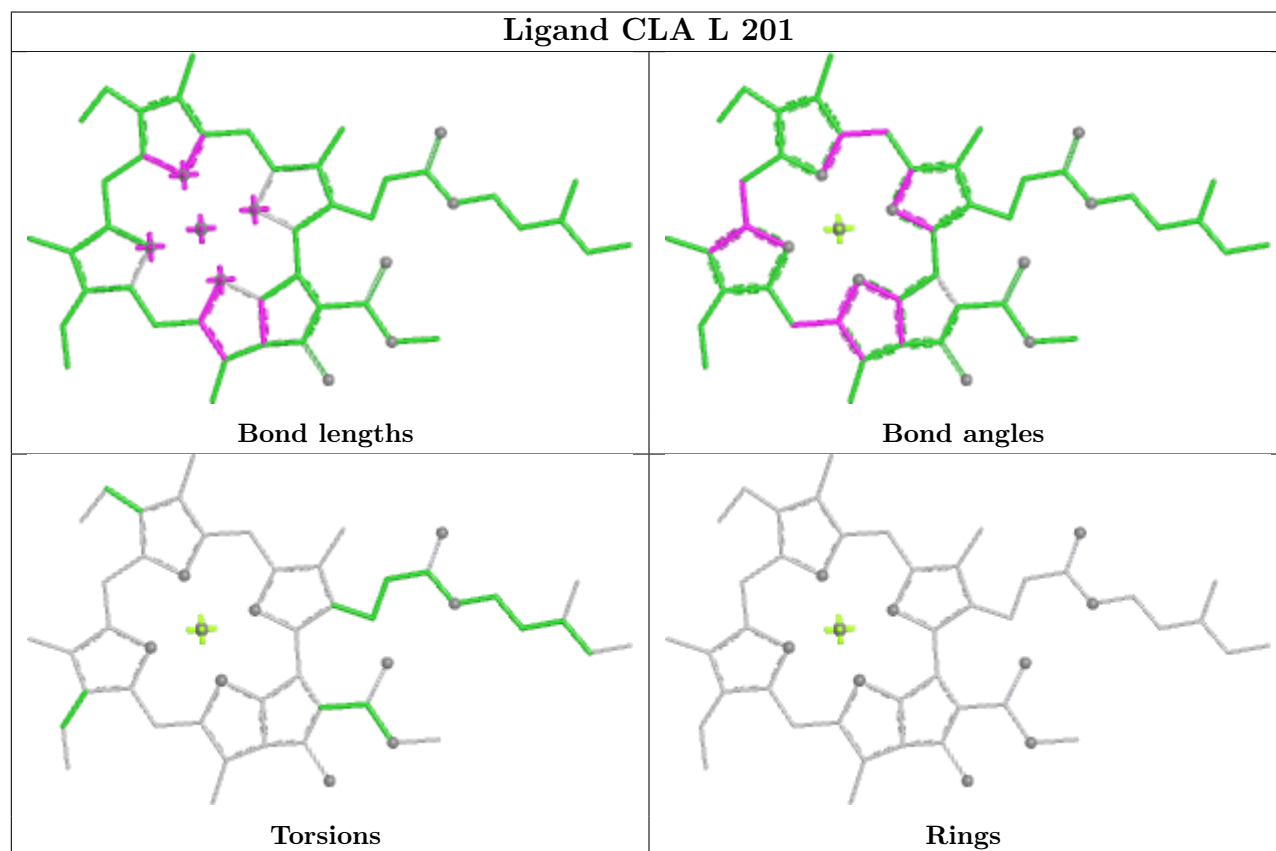
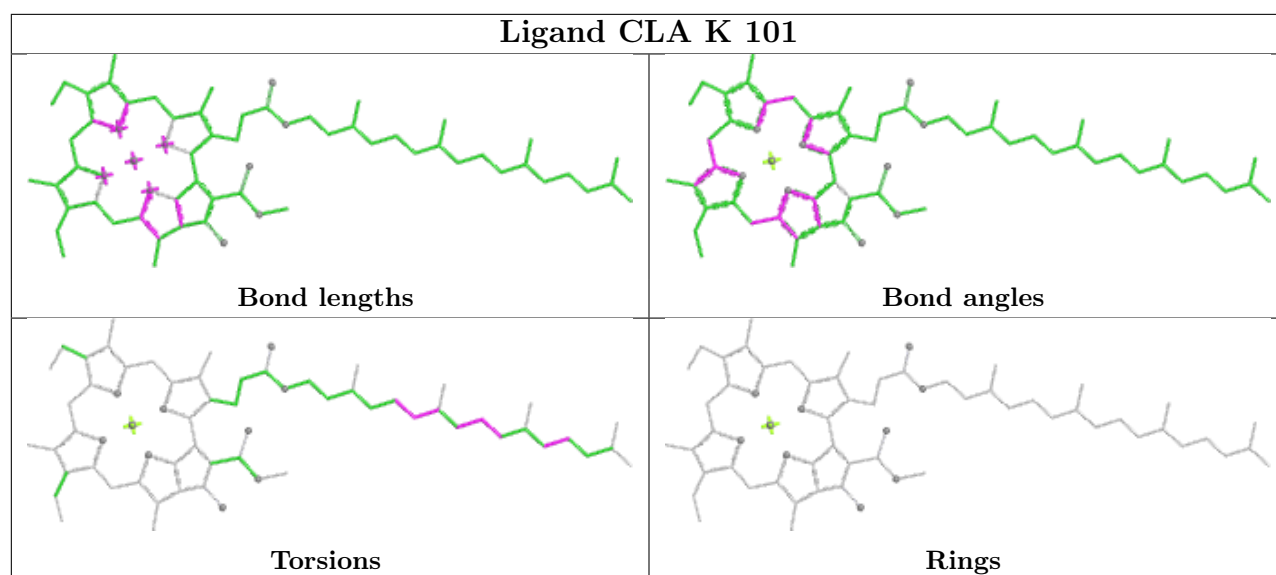
Bond angles

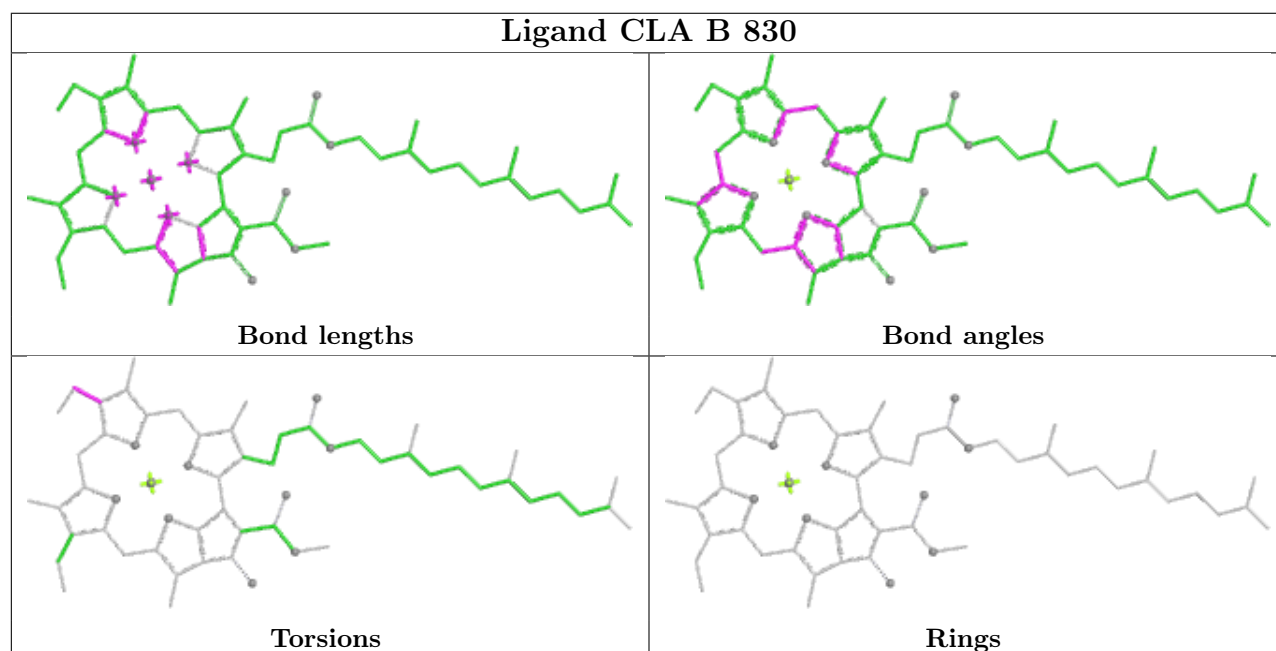
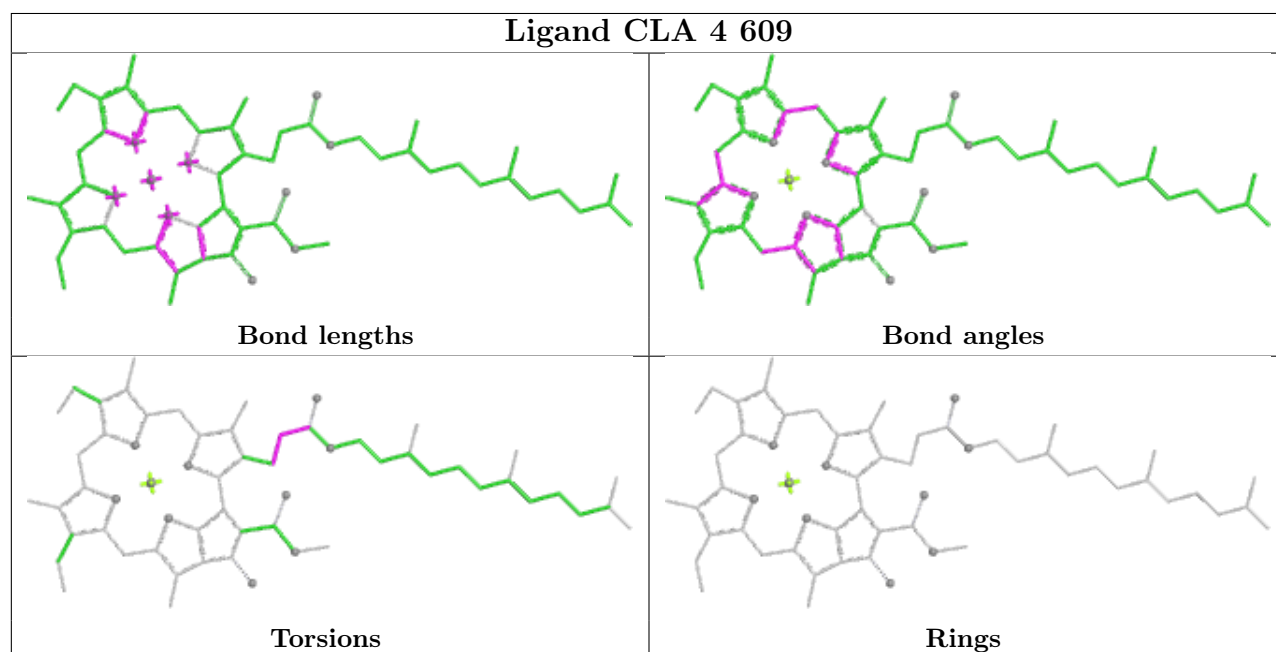
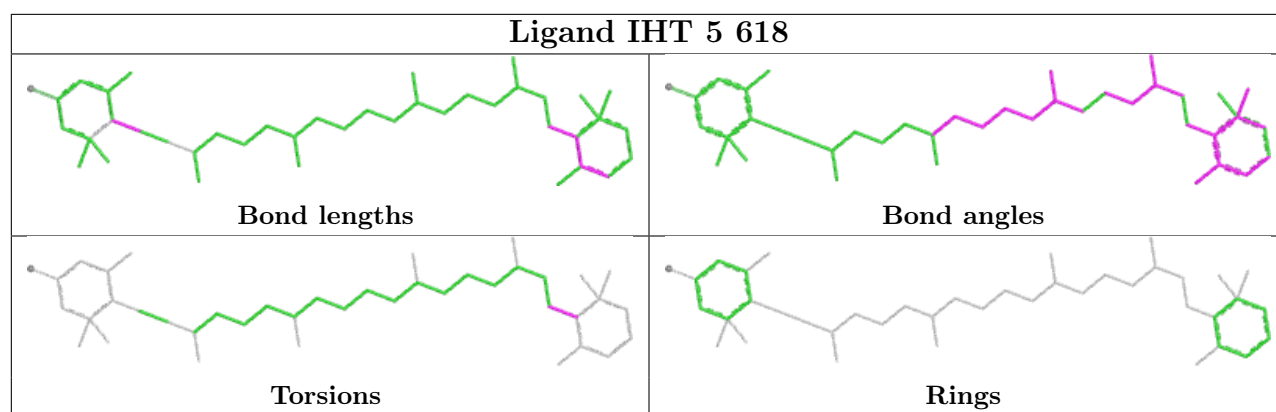


Torsions

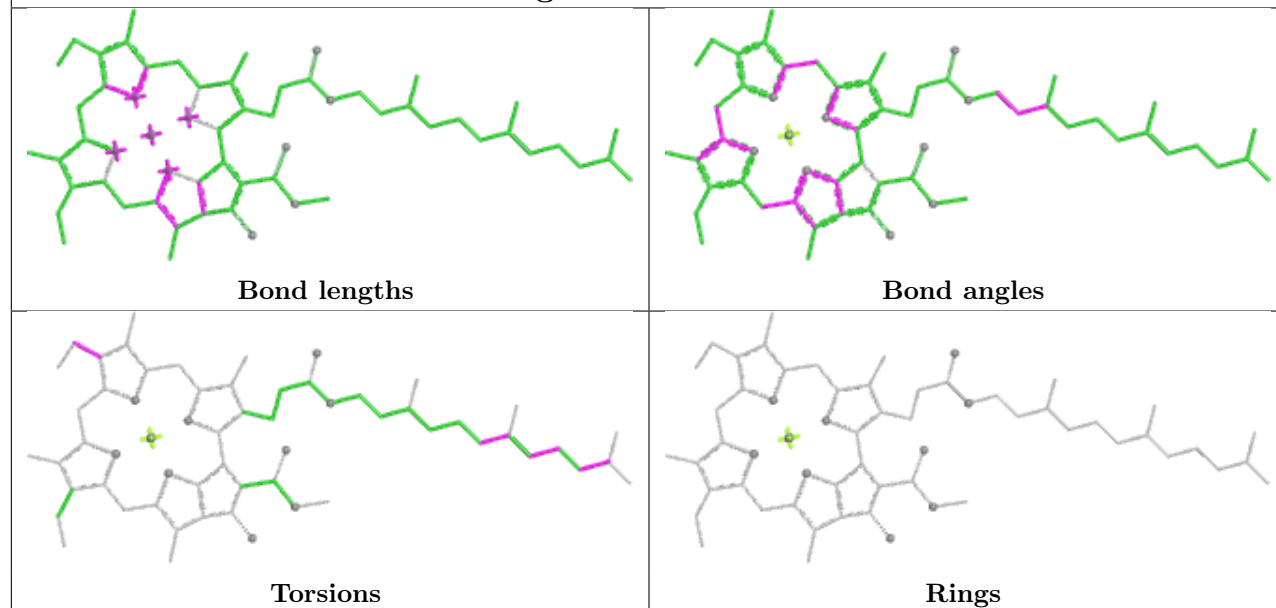


Rings

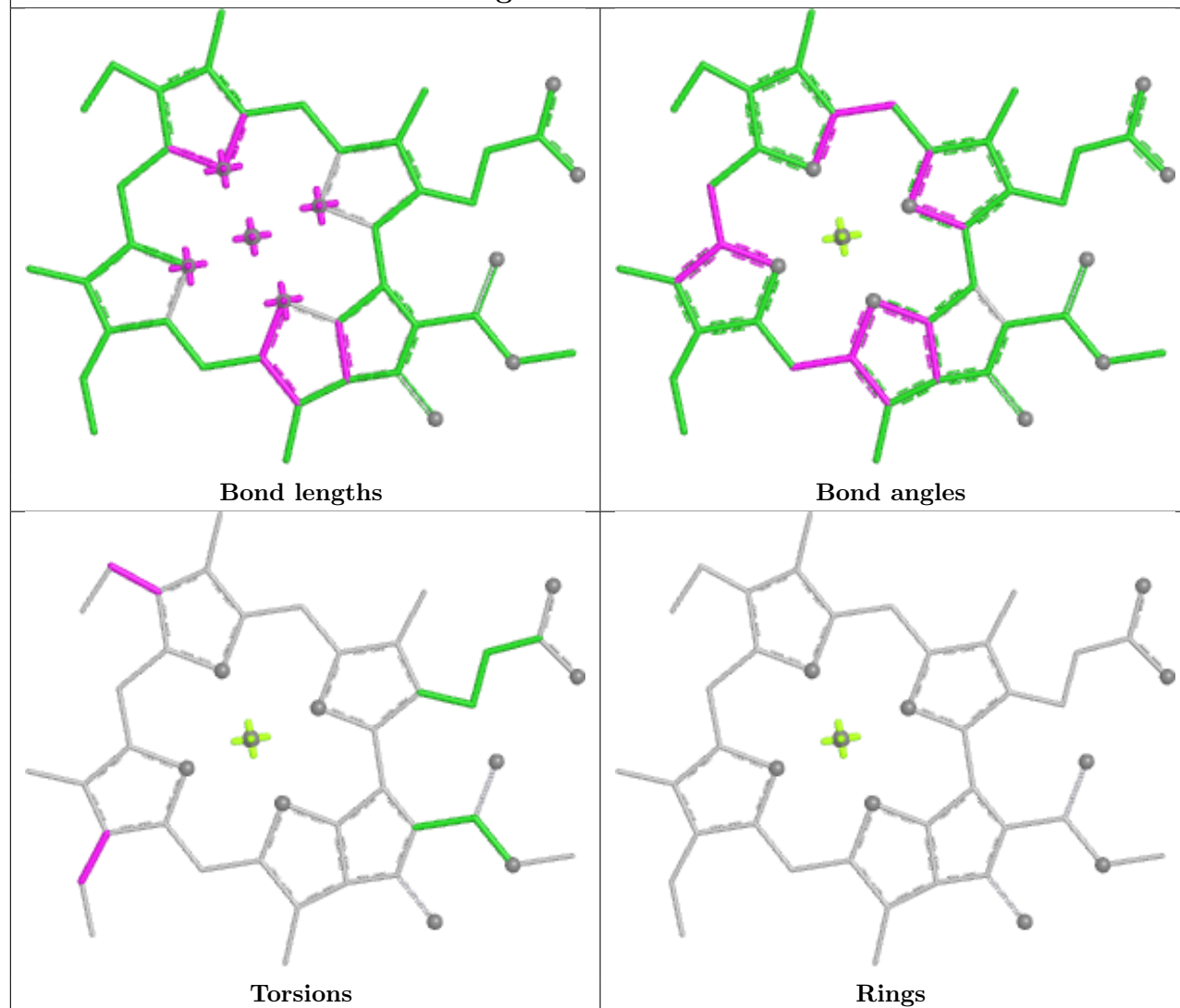




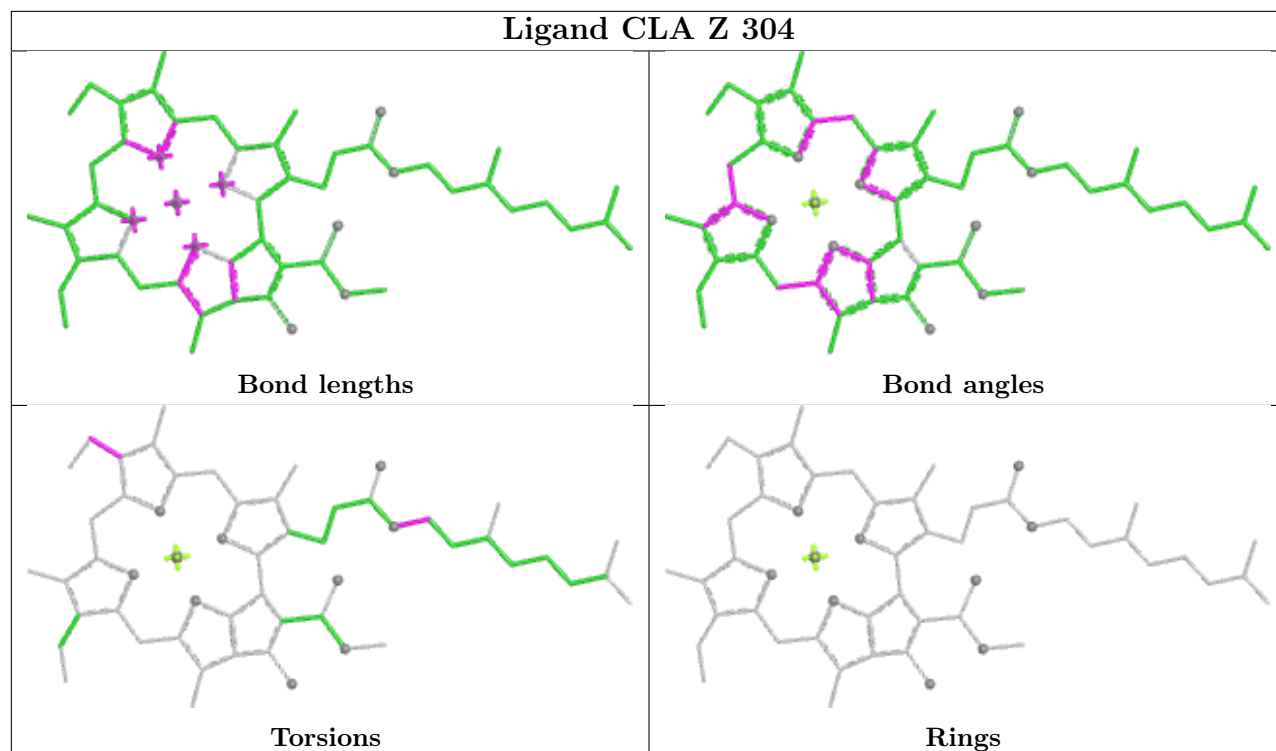
## Ligand CLA 1 612



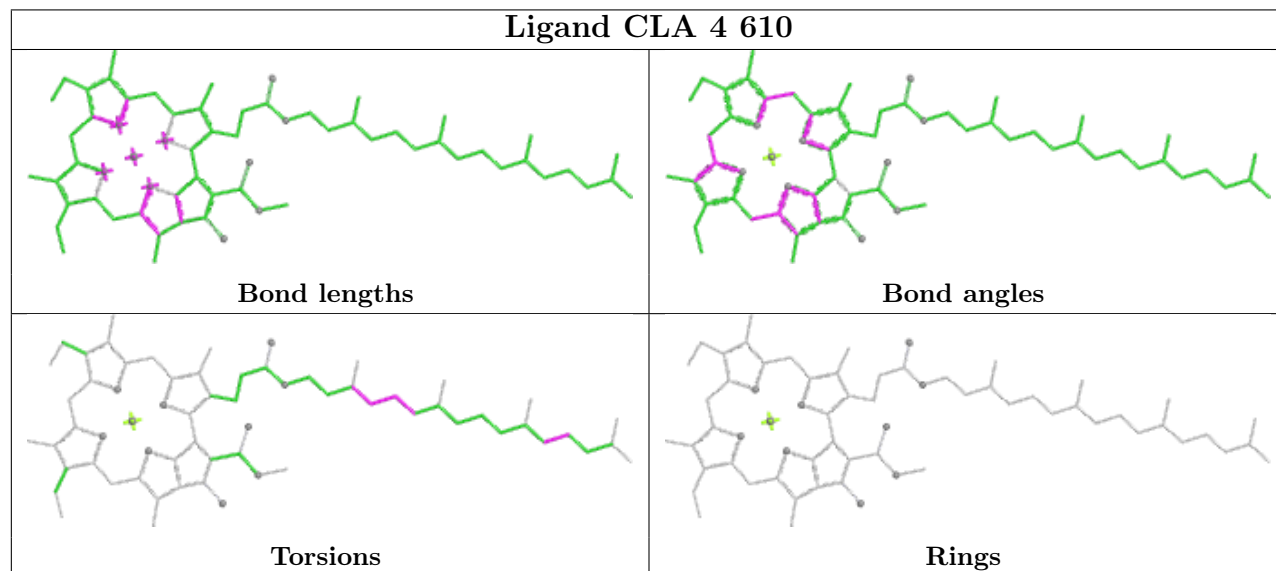
## Ligand CLA 6 601

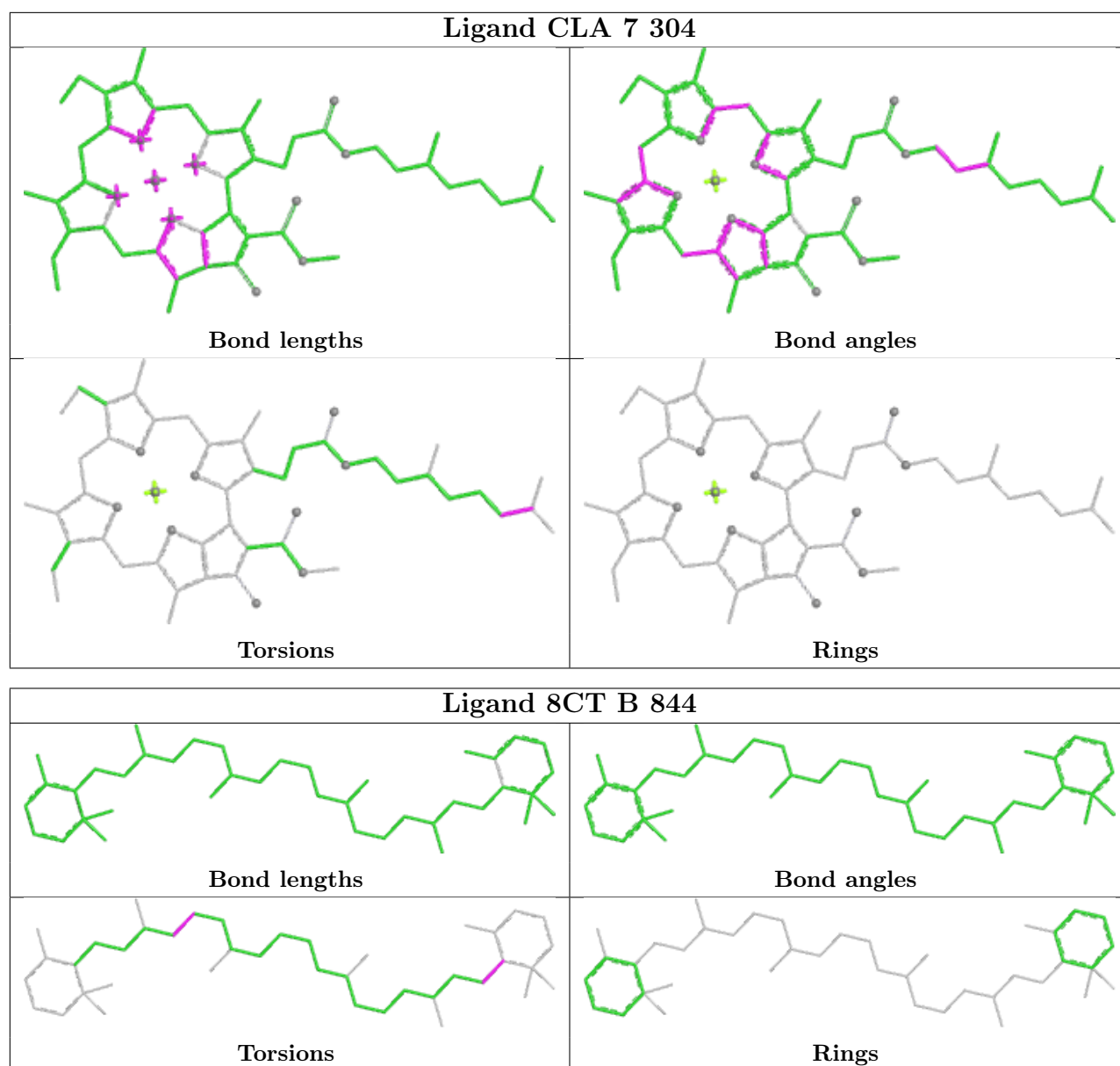


## Ligand CLA Z 304



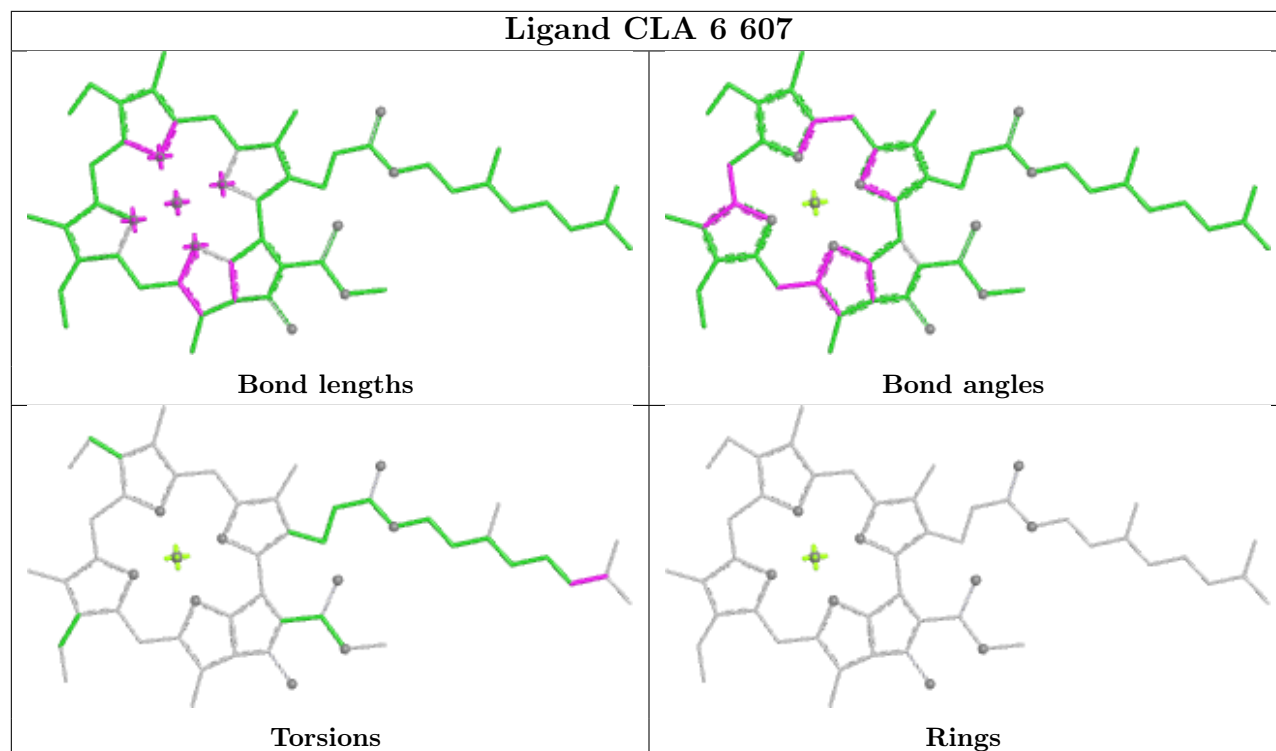
## Ligand CLA 4 610



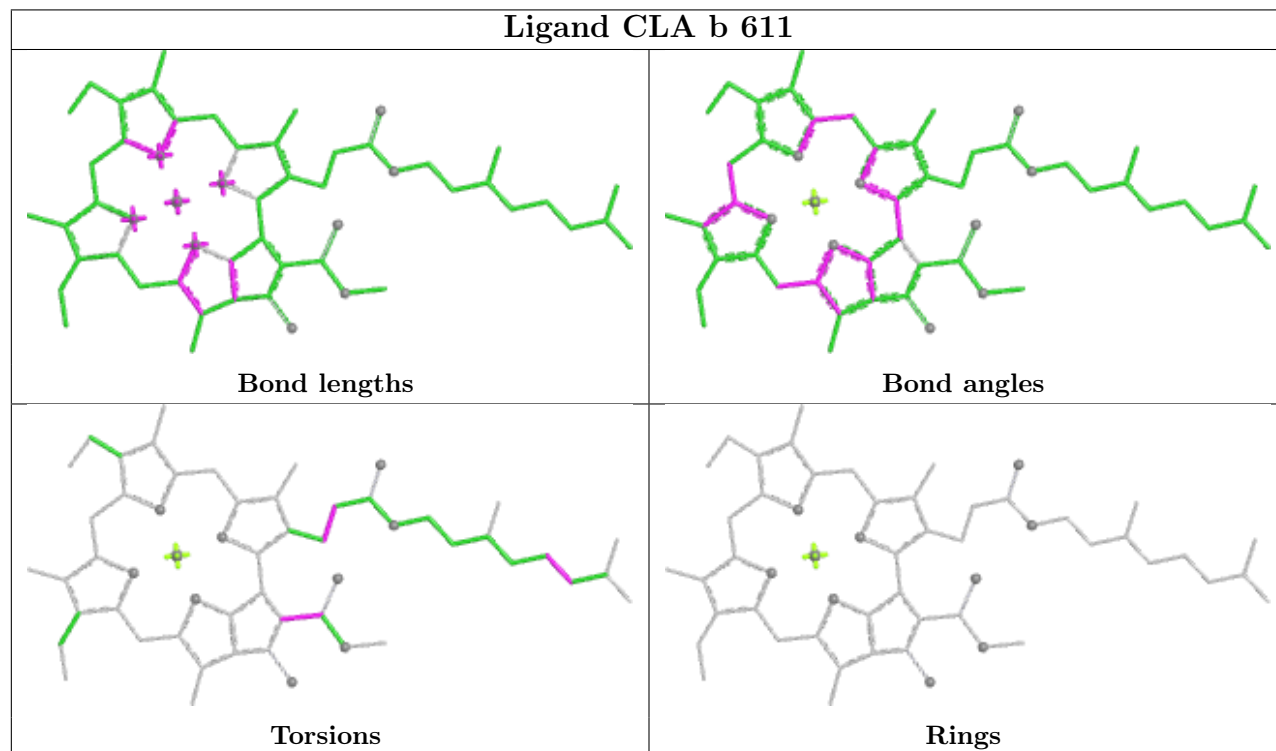




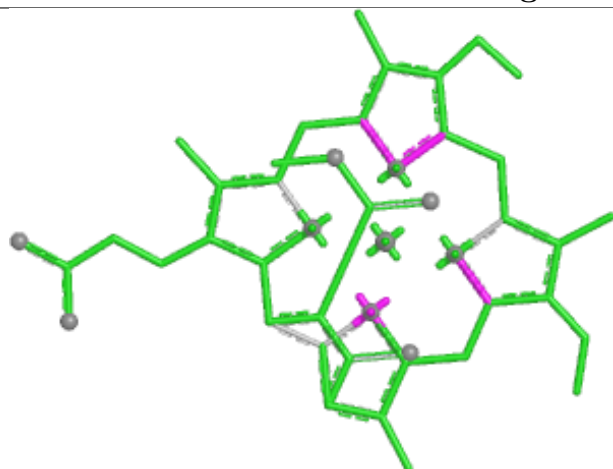
## Ligand CLA 6 607



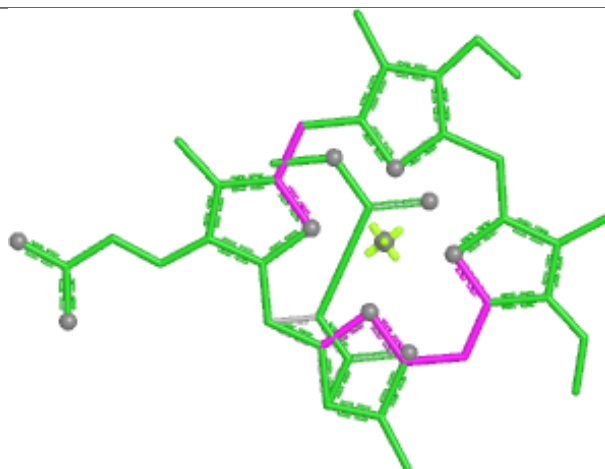
## Ligand CLA b 611



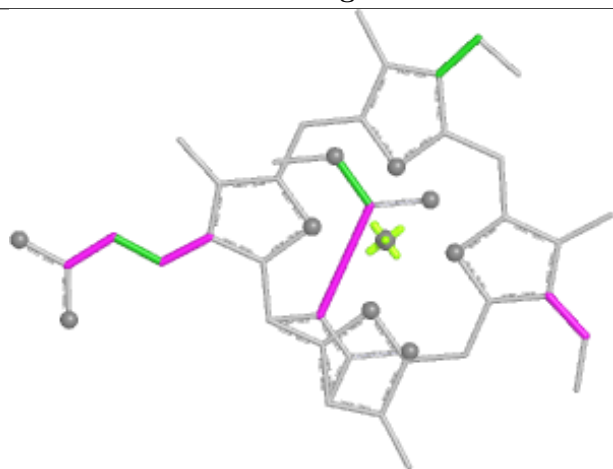
## Ligand KC2 7 311



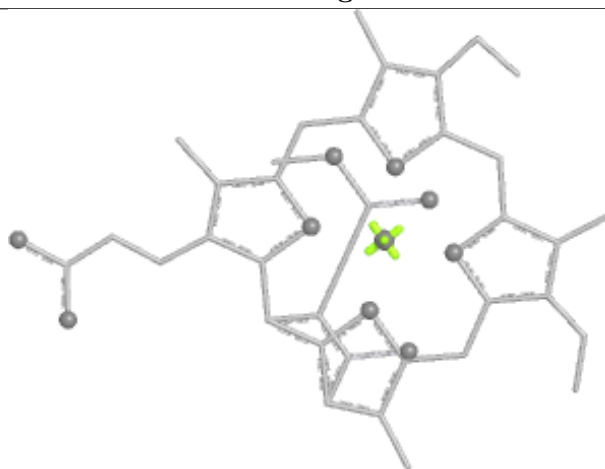
Bond lengths



Bond angles

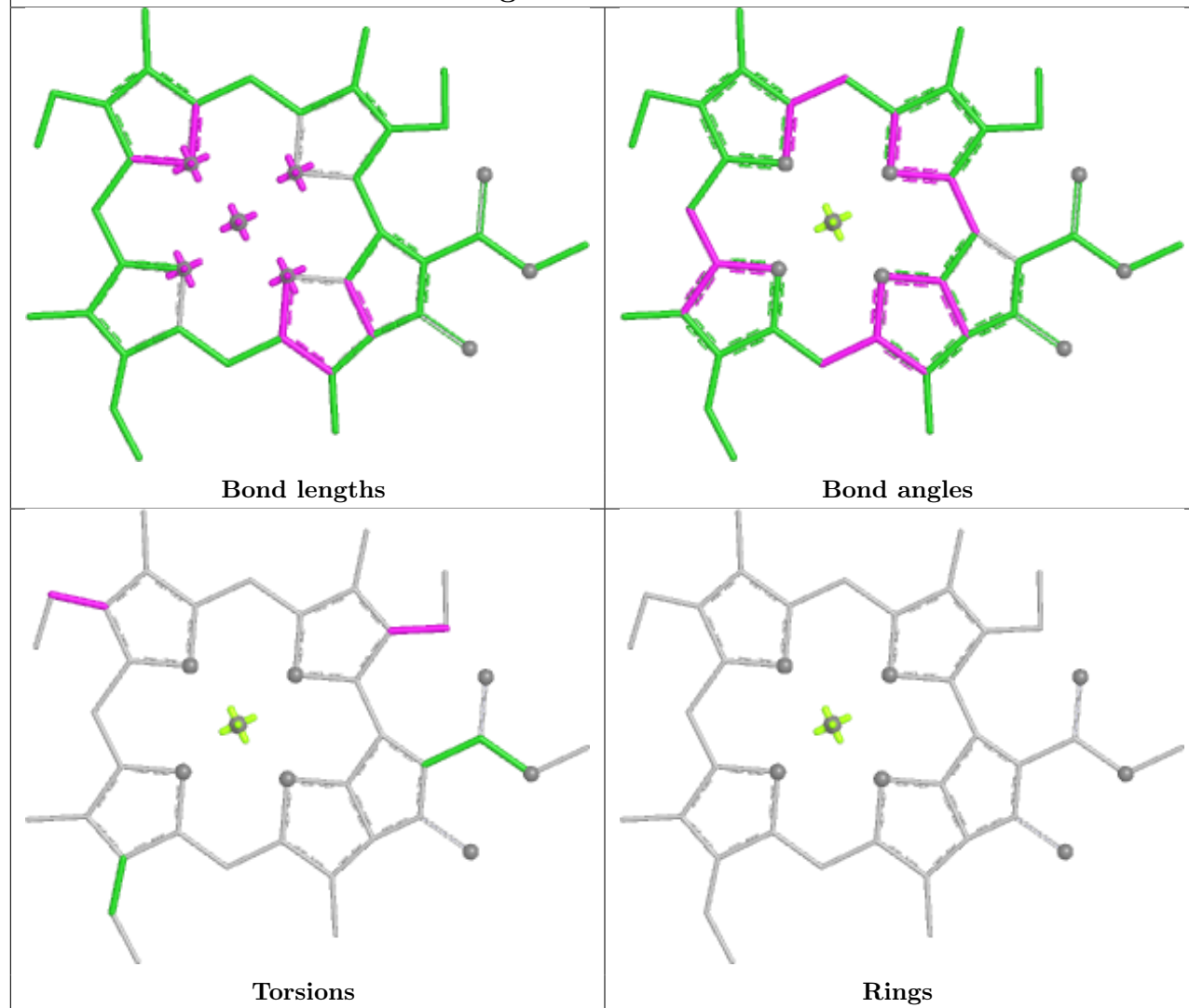


Torsions

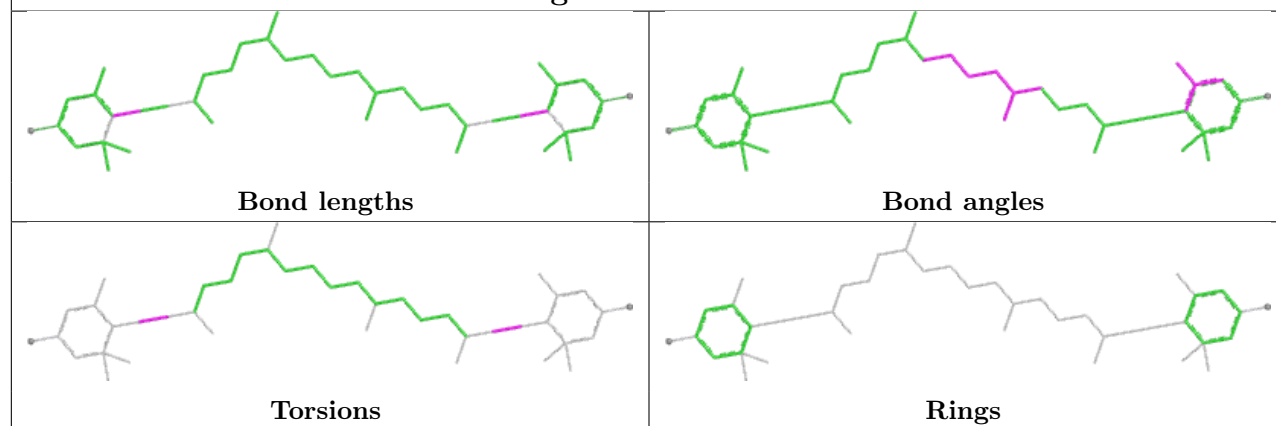


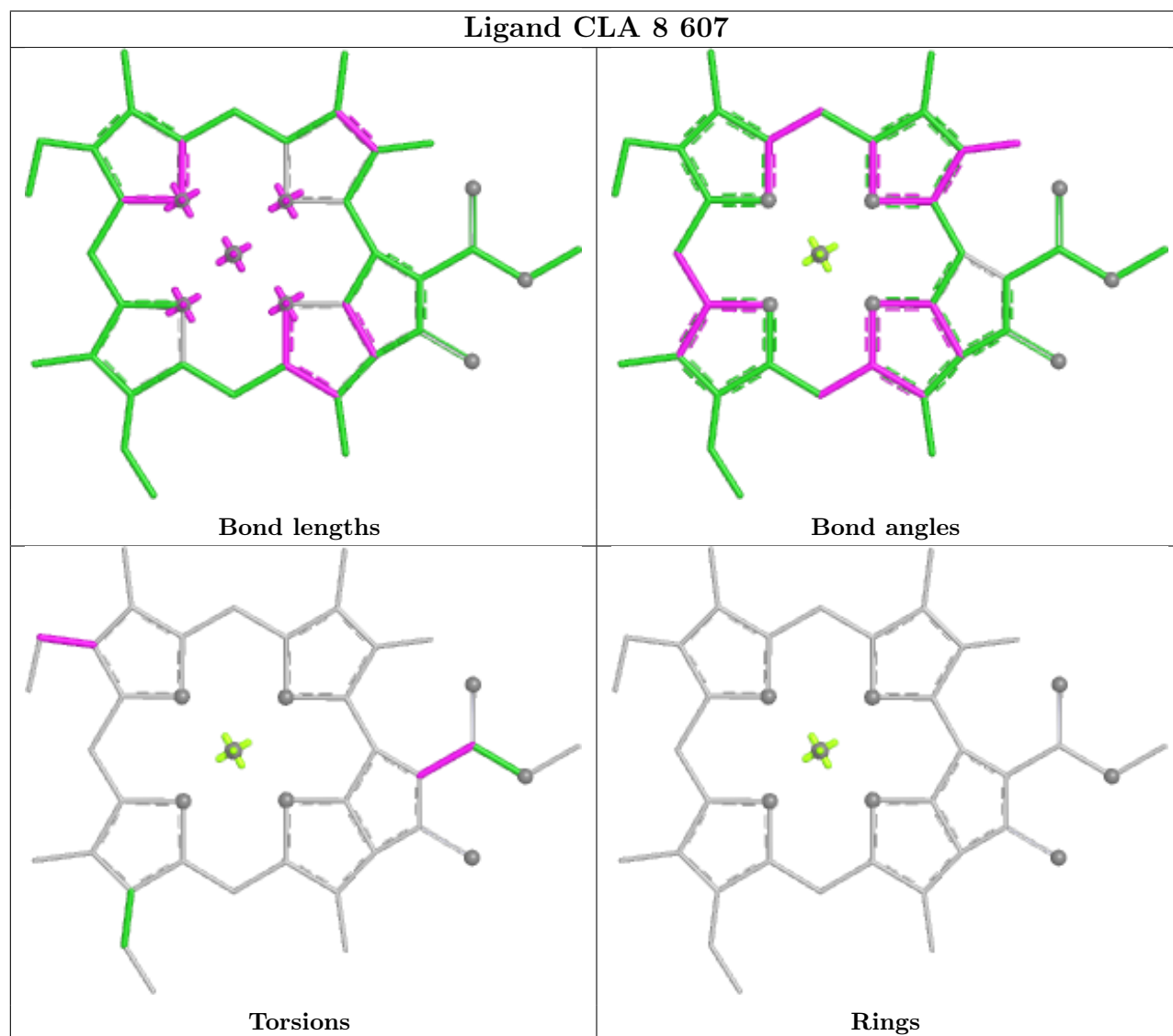
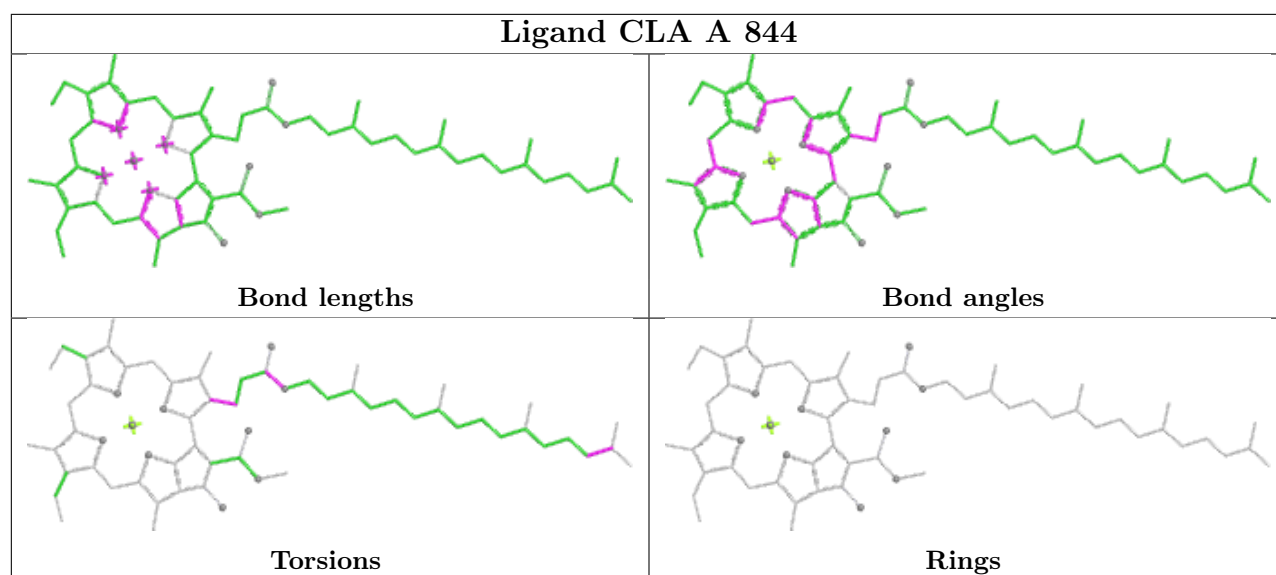
Rings

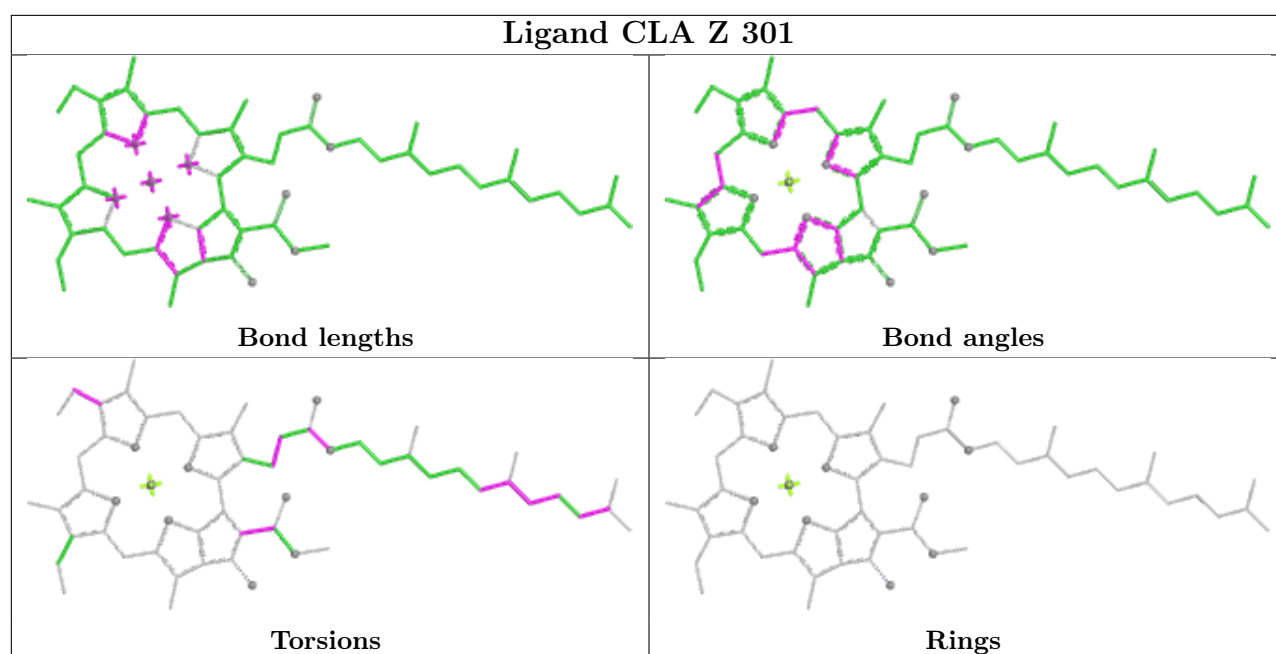
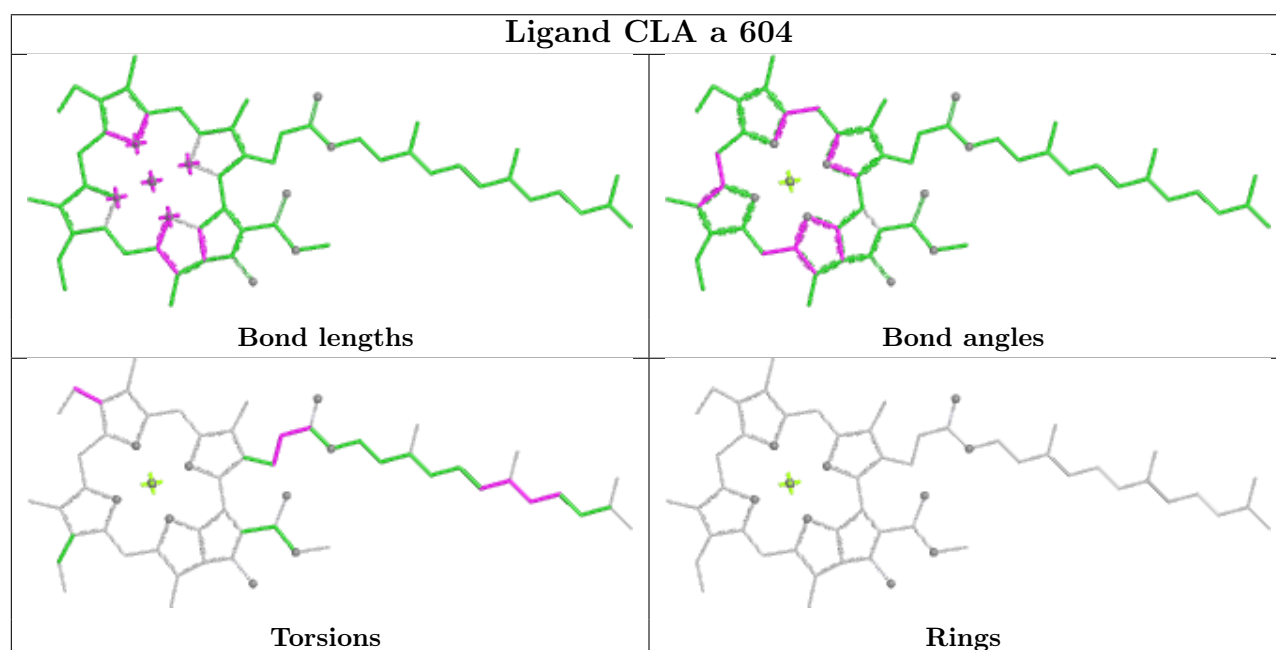
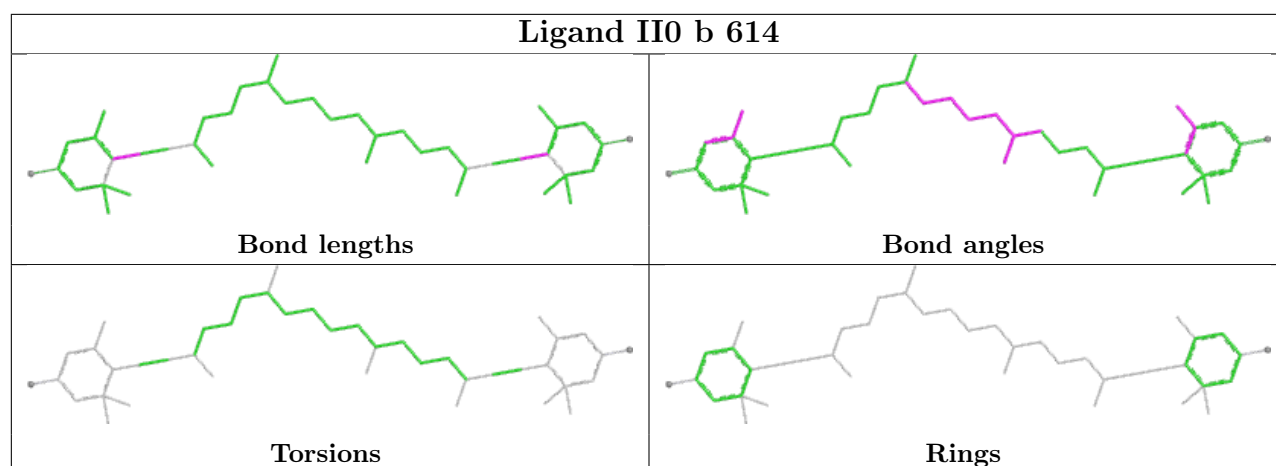
## Ligand CLA 2 601

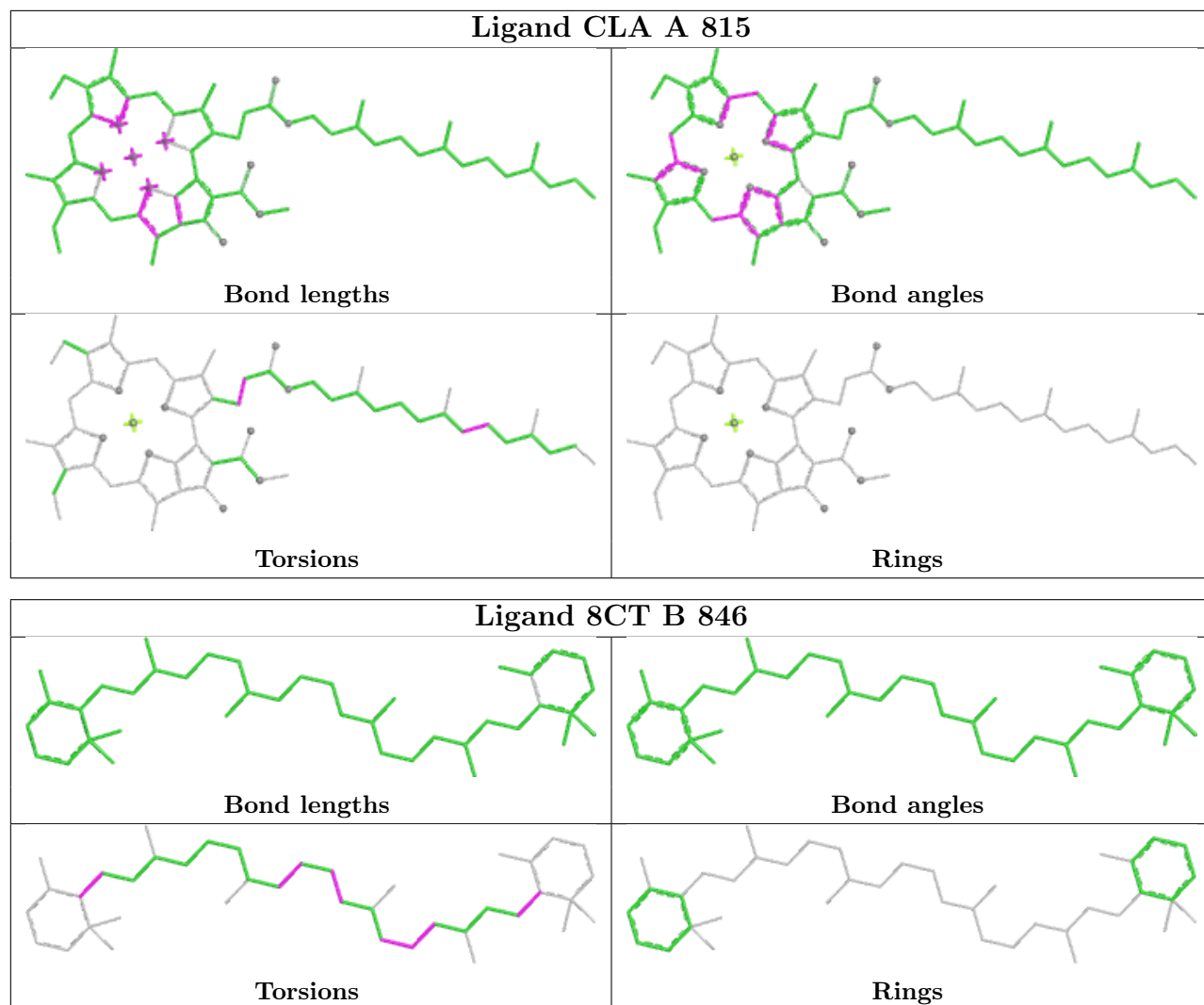


## Ligand II0 5 614

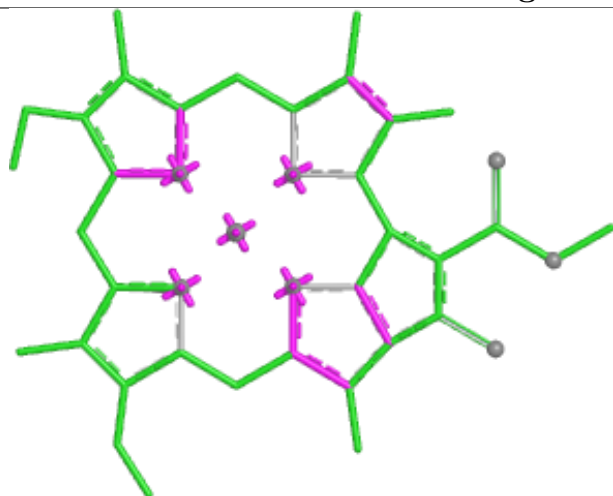




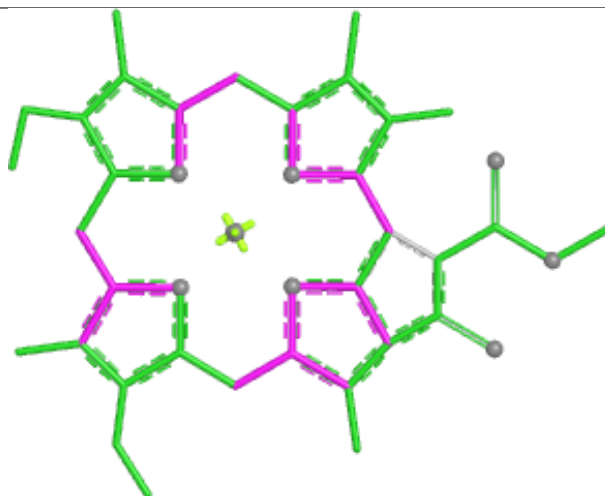




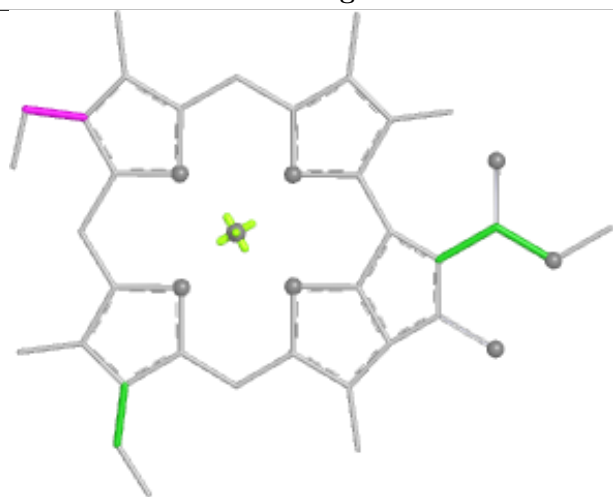
## Ligand CLA 9 614



Bond lengths



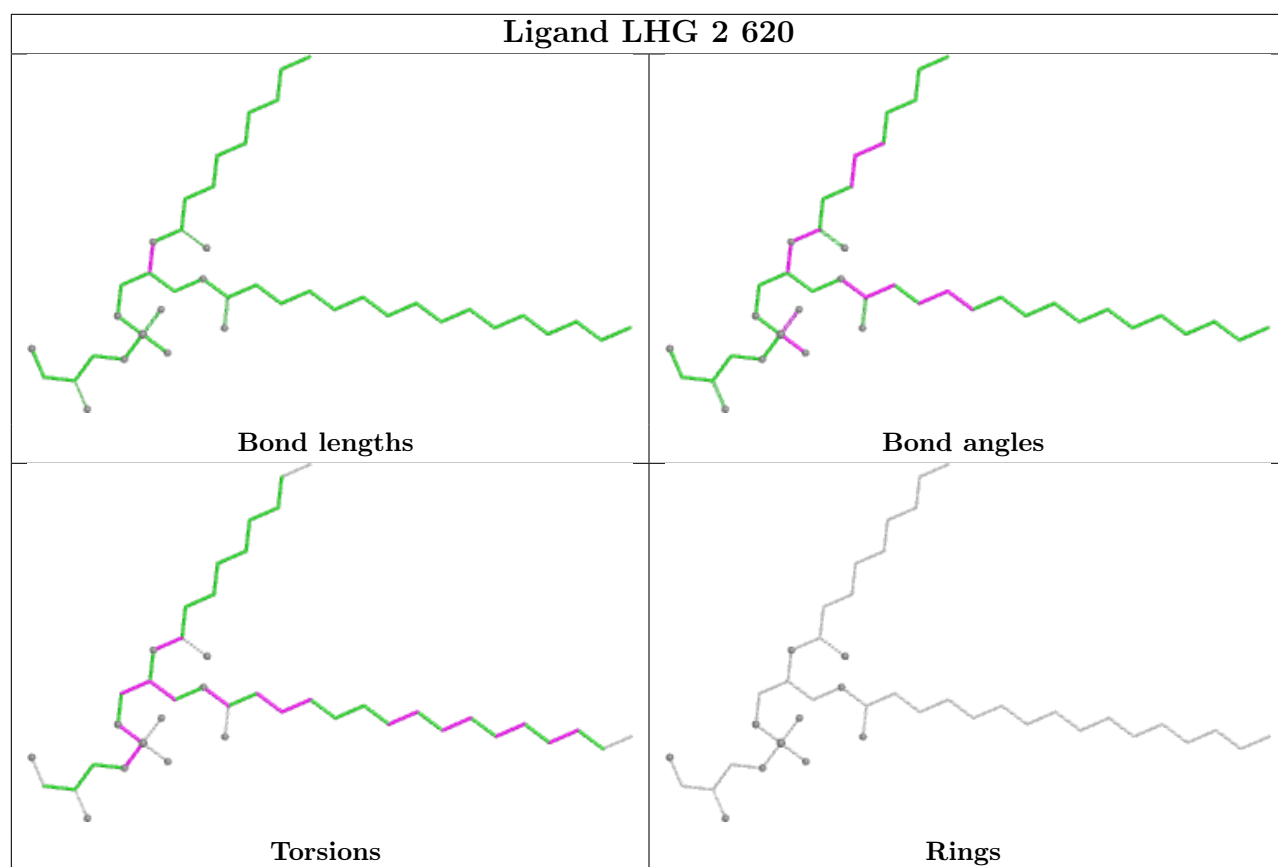
Bond angles



Torsions

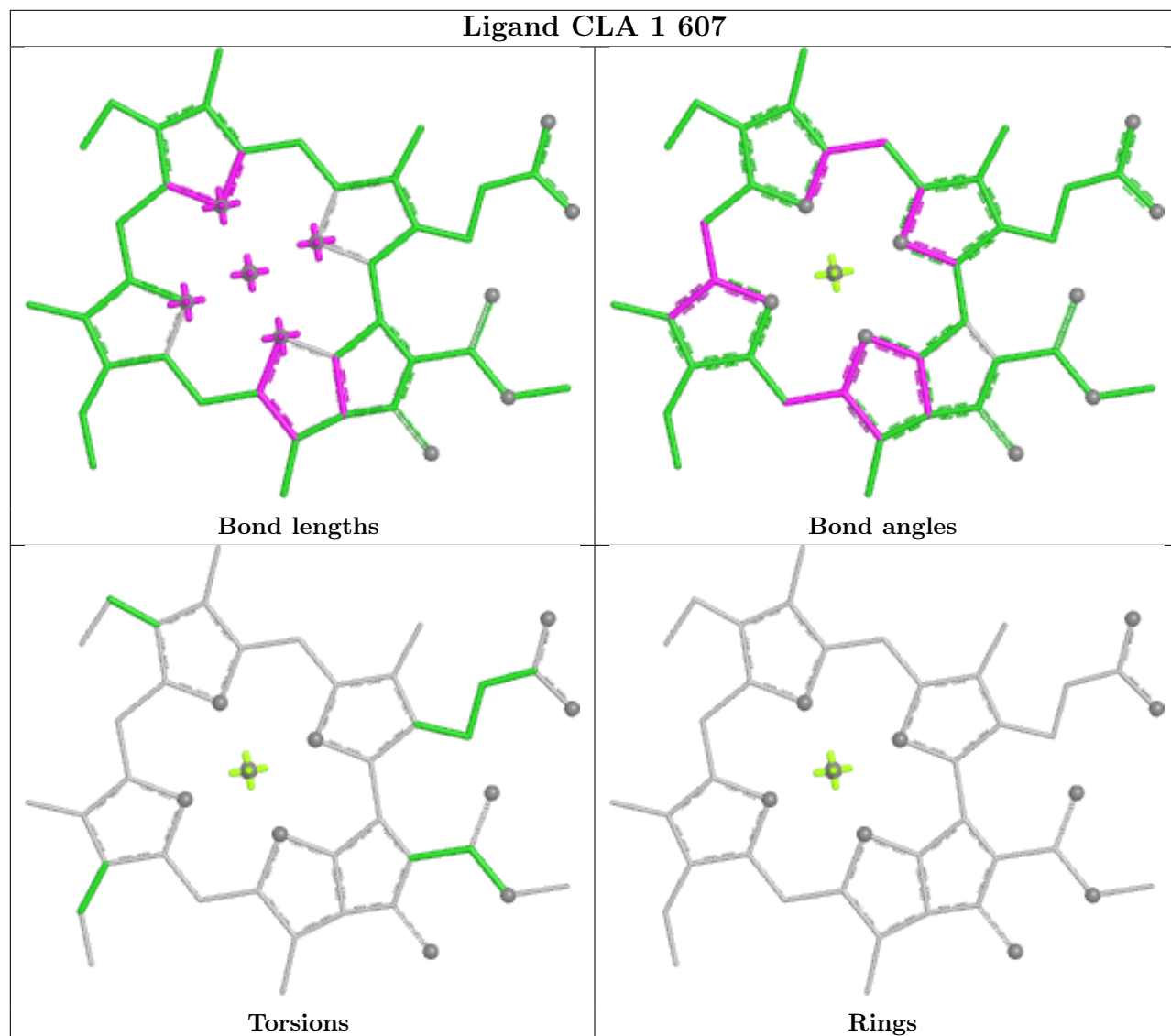


Rings

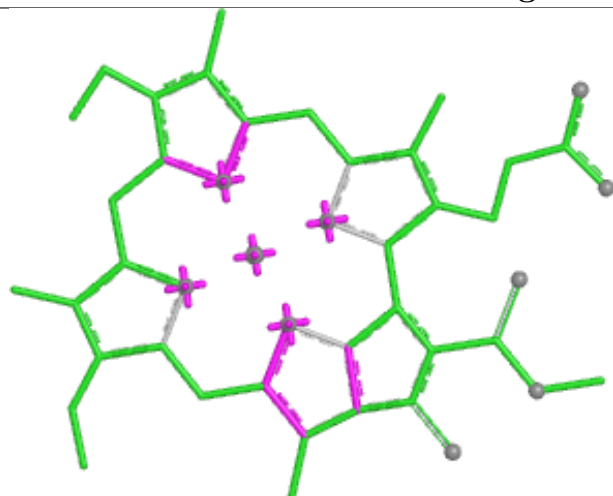




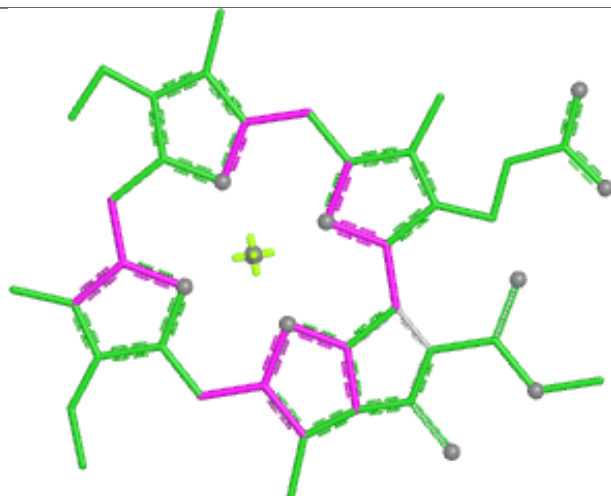
## Ligand CLA 1 607



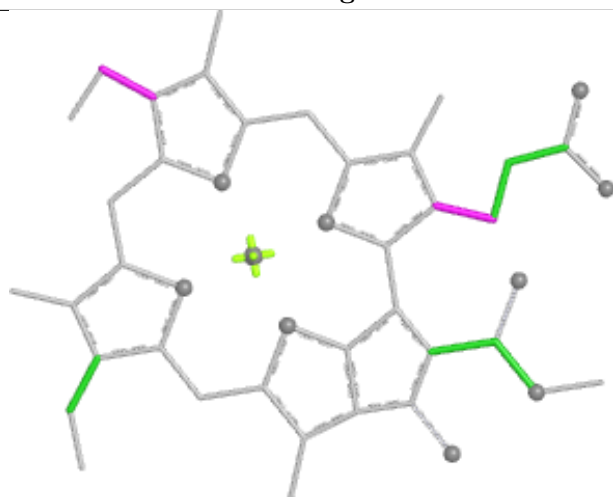
## Ligand CLA 1 601



Bond lengths



Bond angles

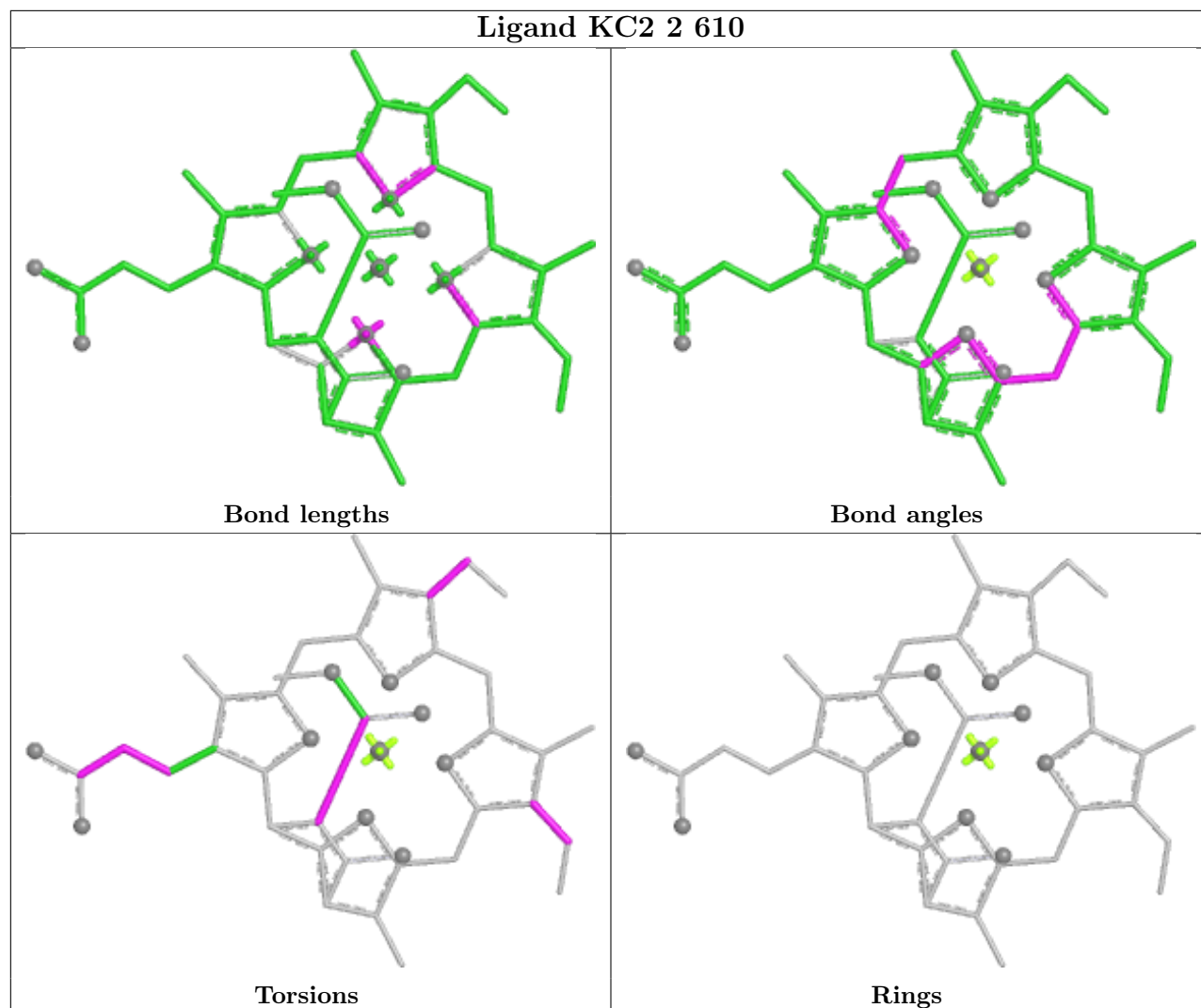


Torsions

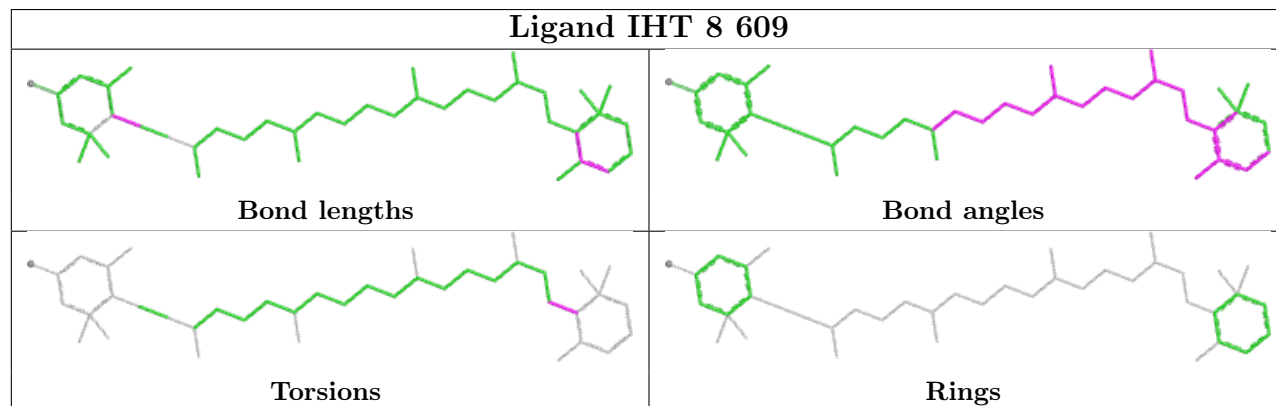


Rings

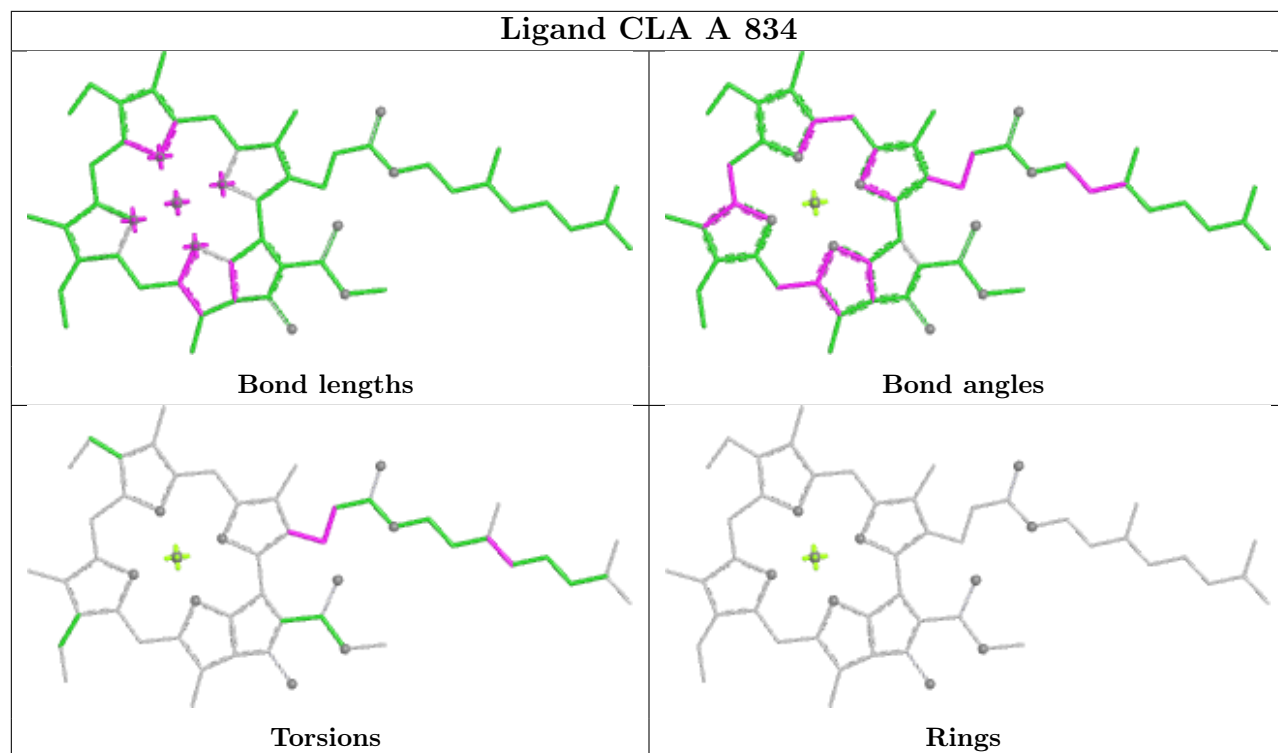
## Ligand KC2 2 610



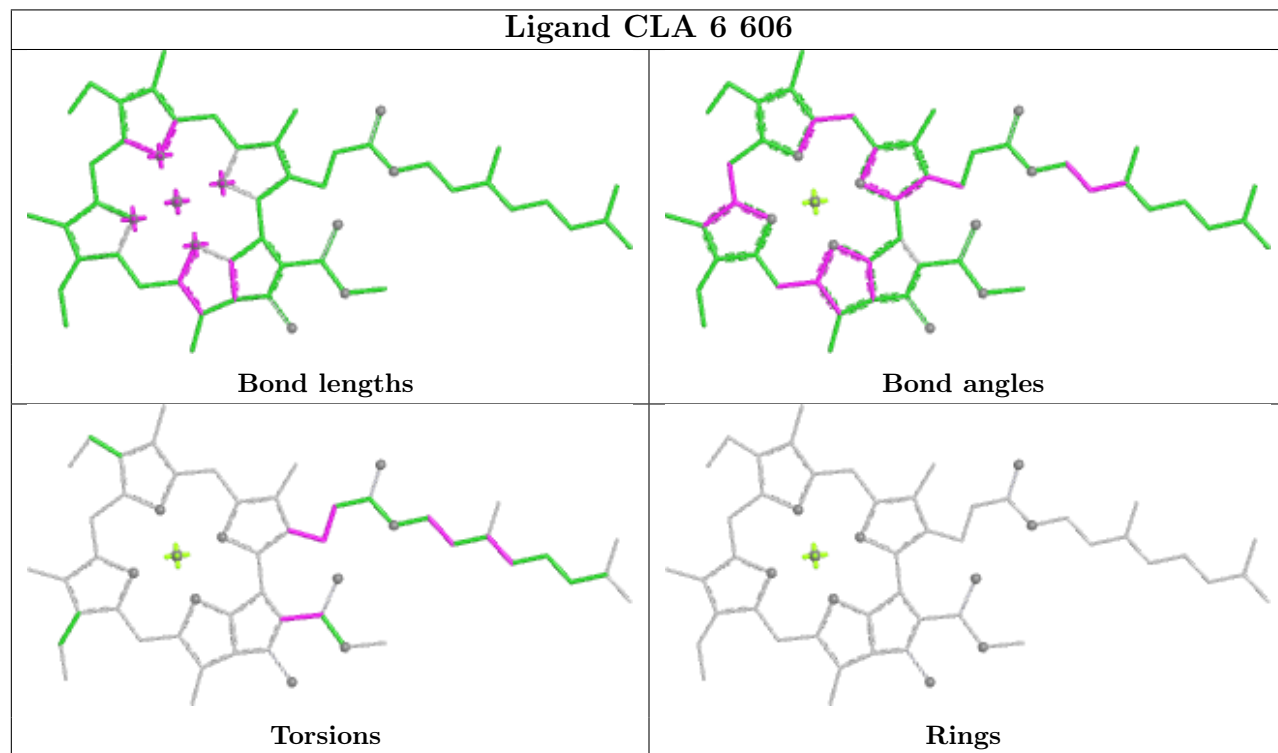
## Ligand IHT 8 609

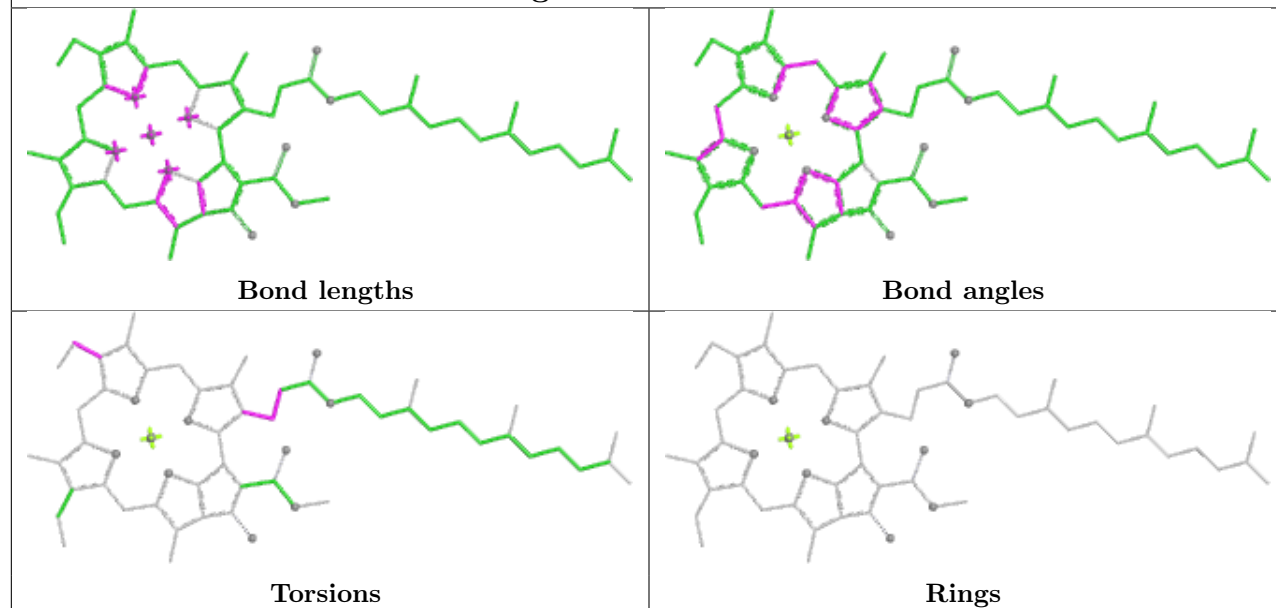
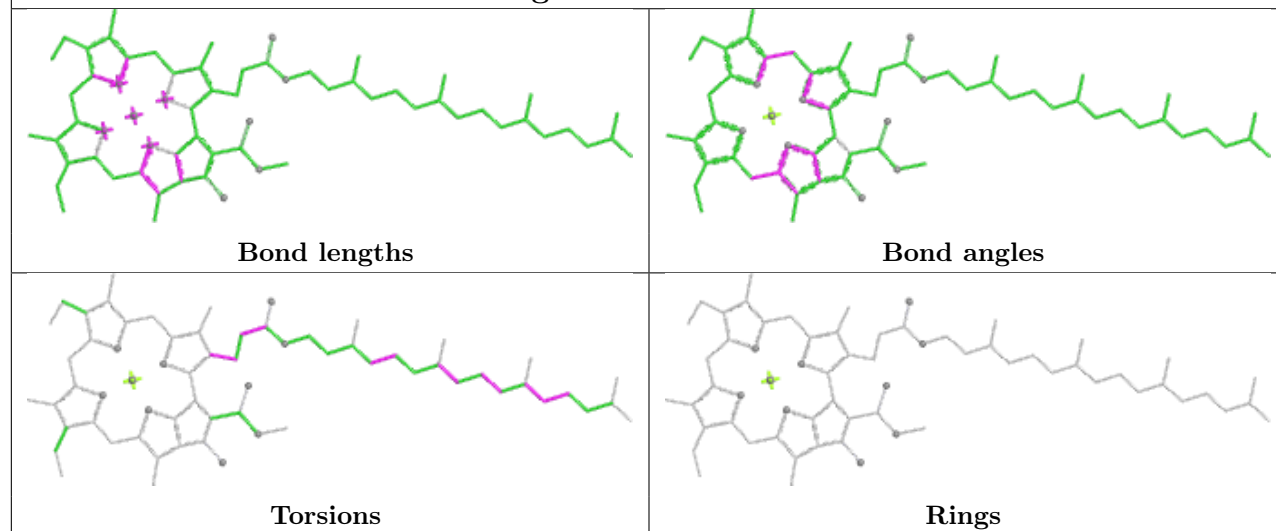


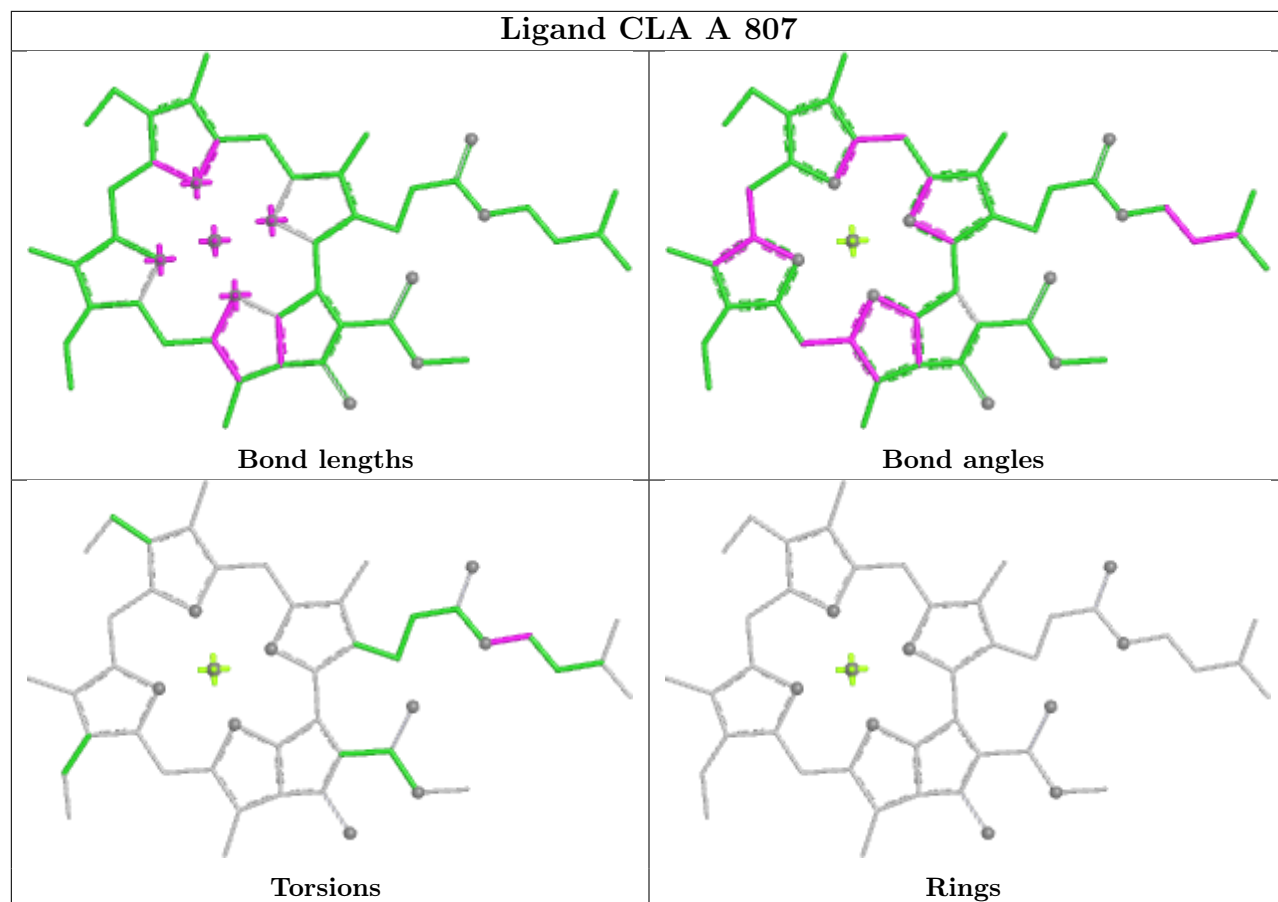
## Ligand CLA A 834



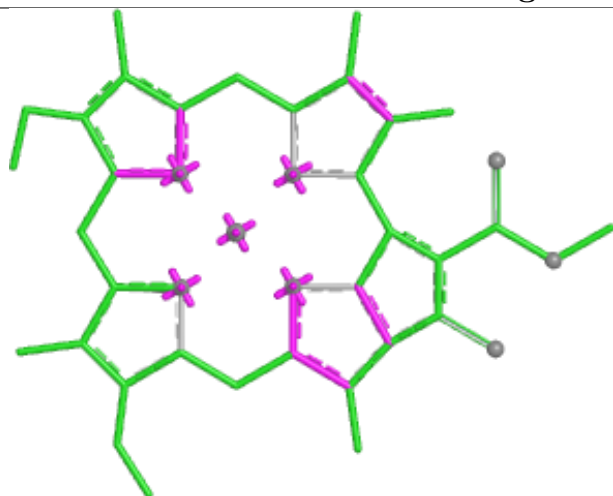
## Ligand CLA 6 606



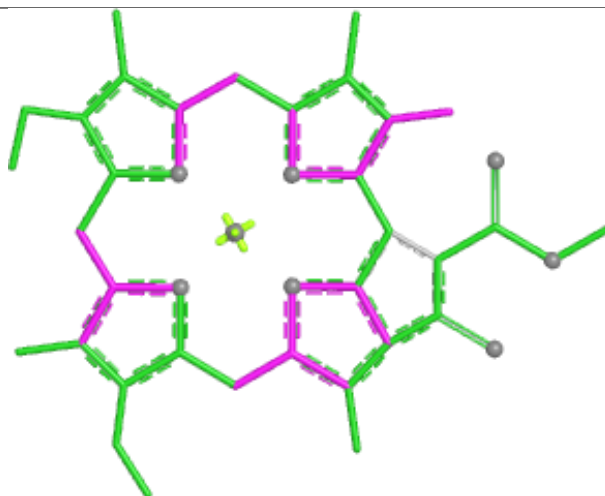
**Ligand CLA A 809****Ligand CLA A 811**



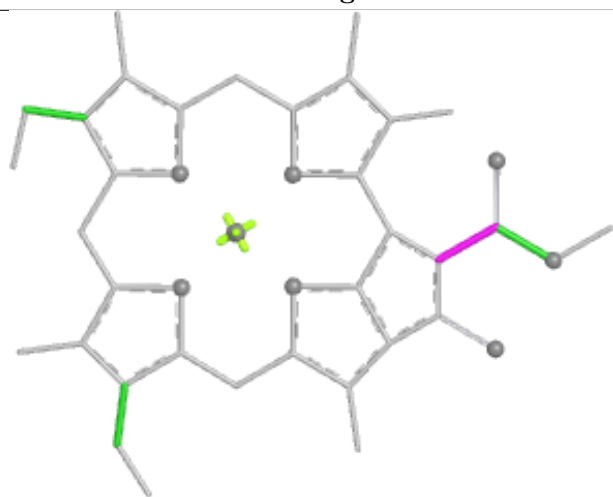
## Ligand CLA 9 611



Bond lengths



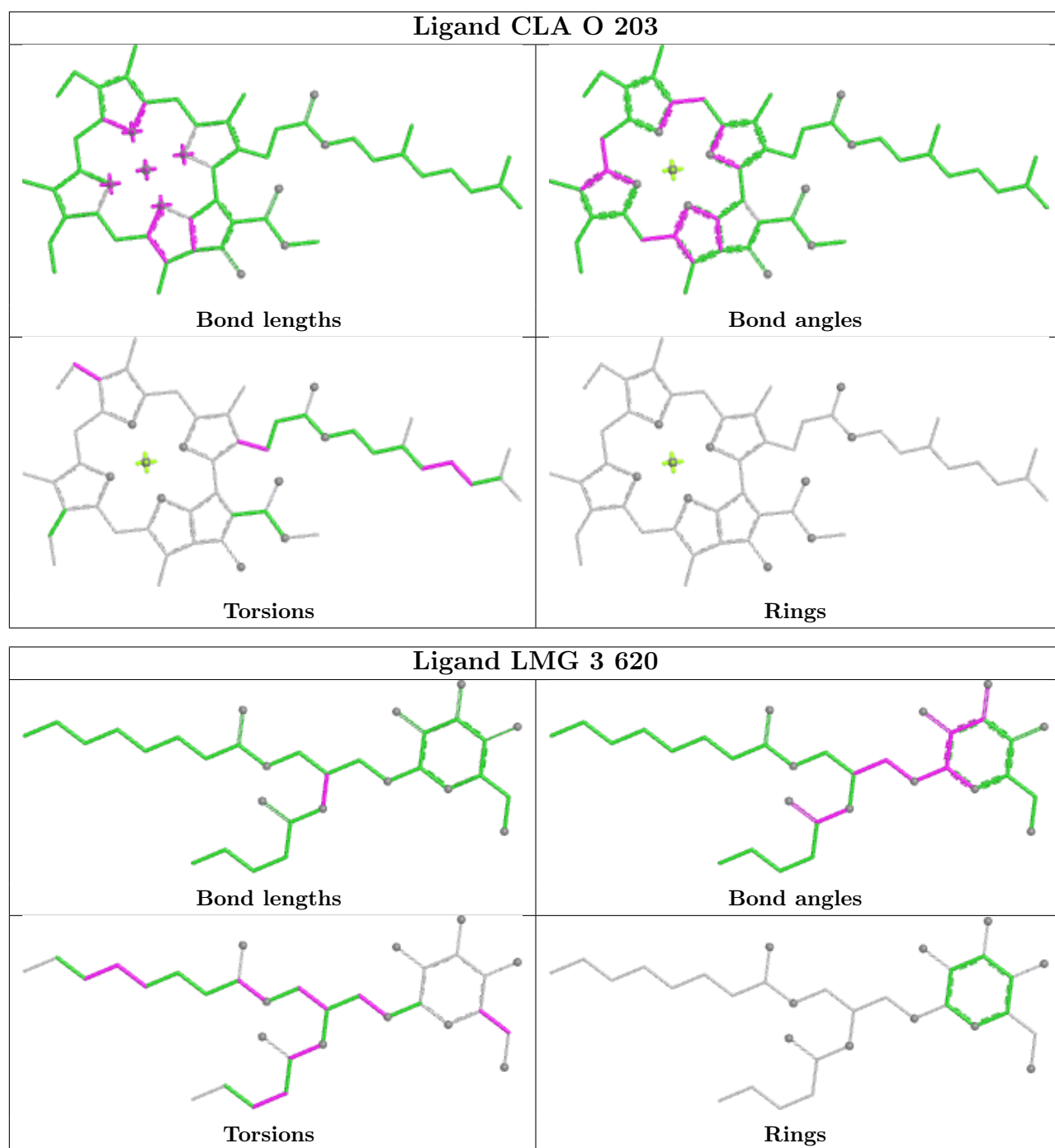
Bond angles



Torsions

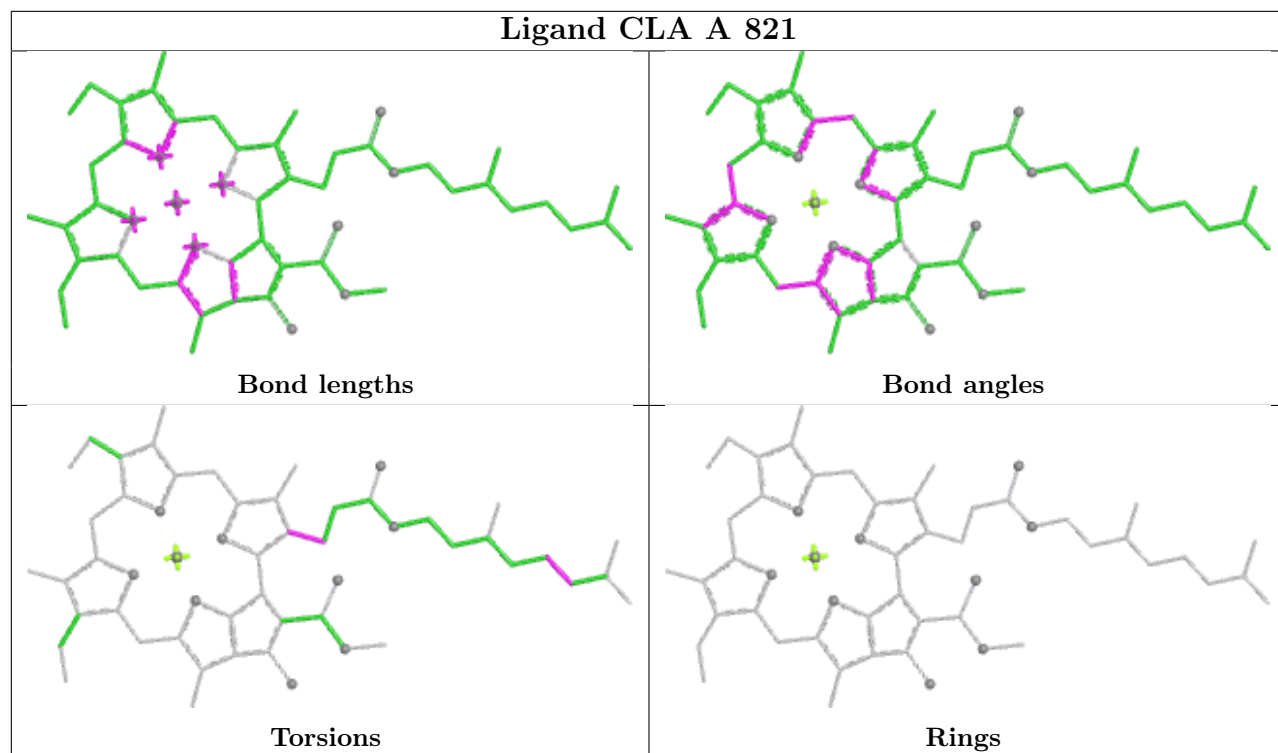


Rings

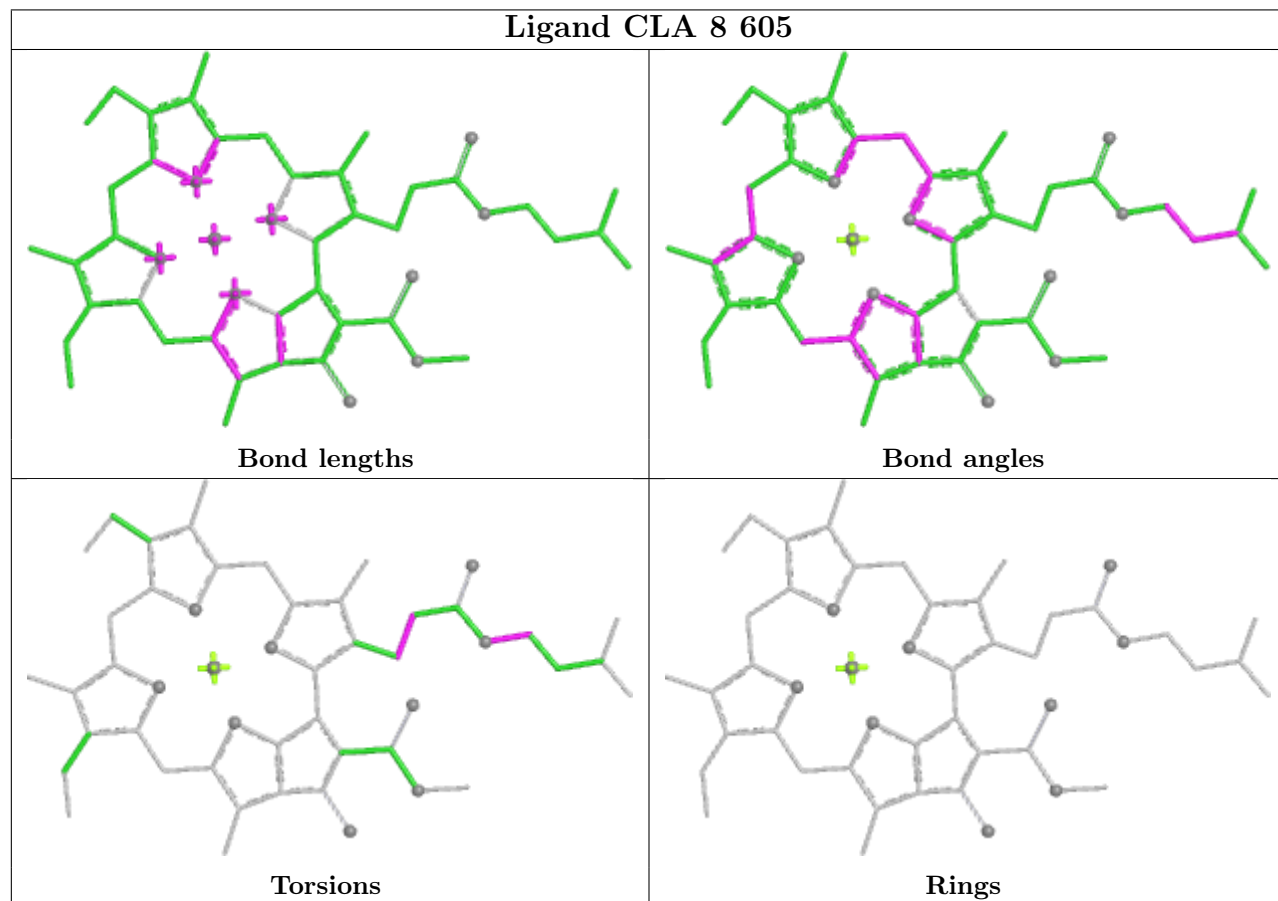


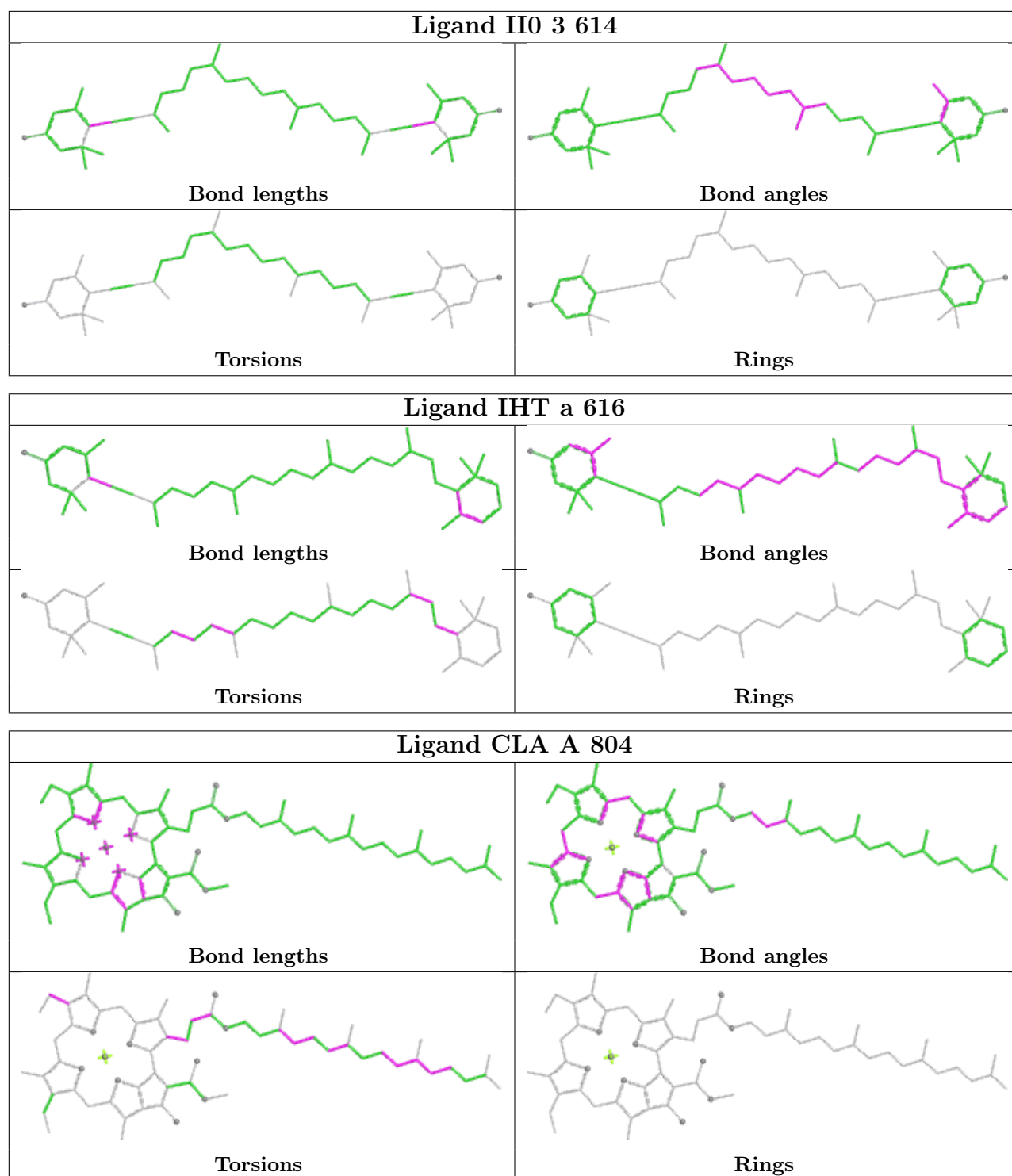


## Ligand CLA A 821

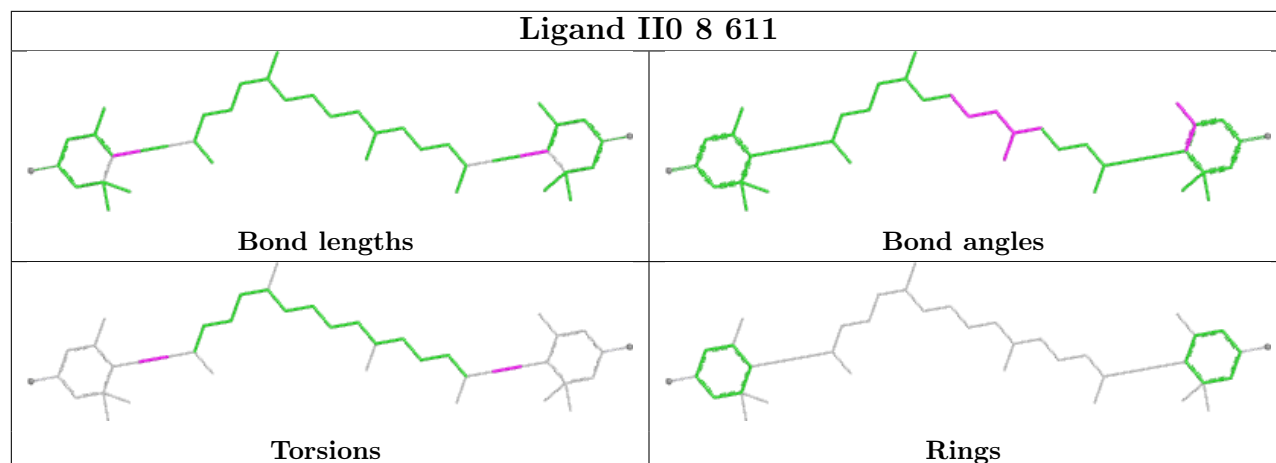


## Ligand CLA 8 605

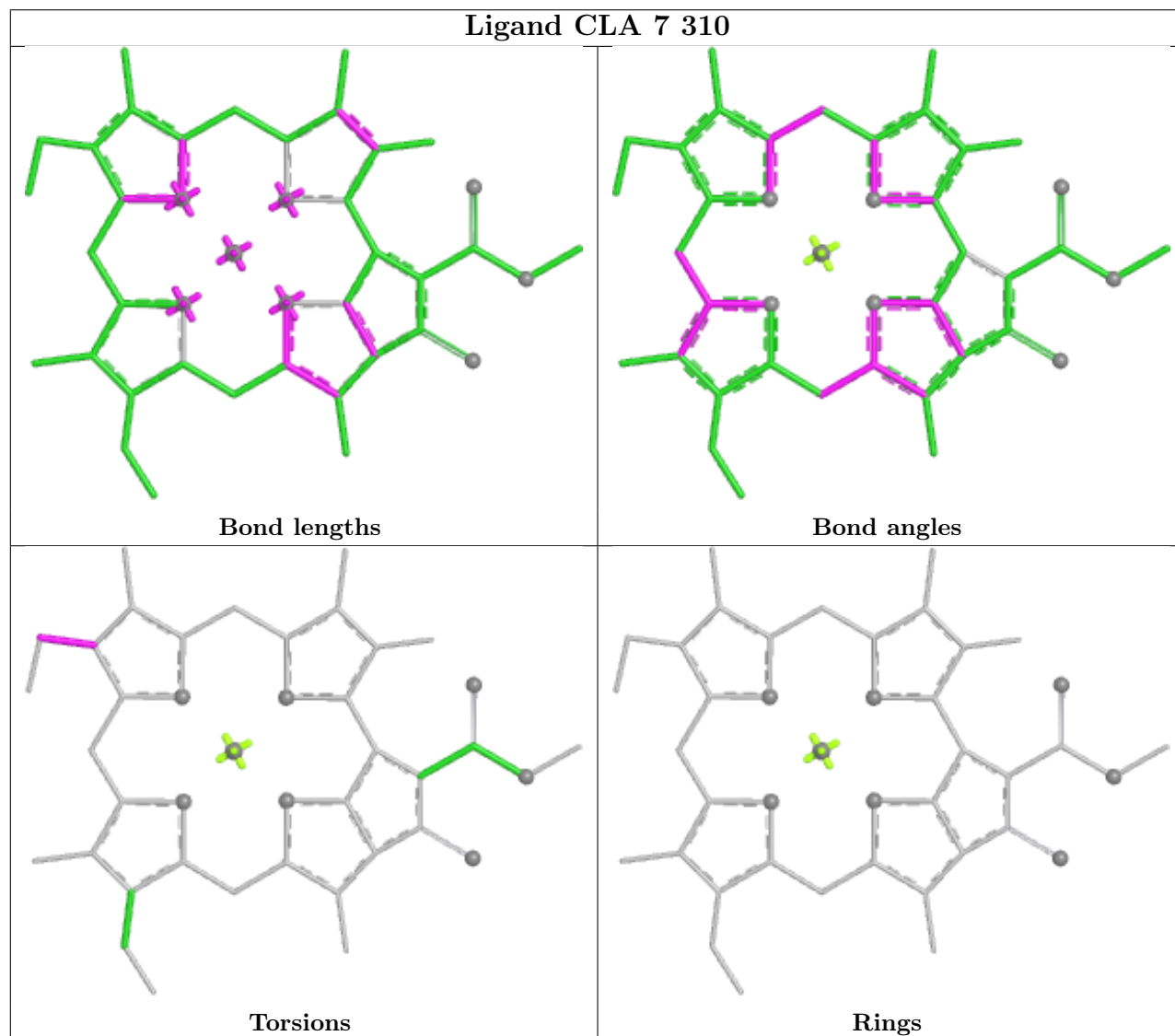


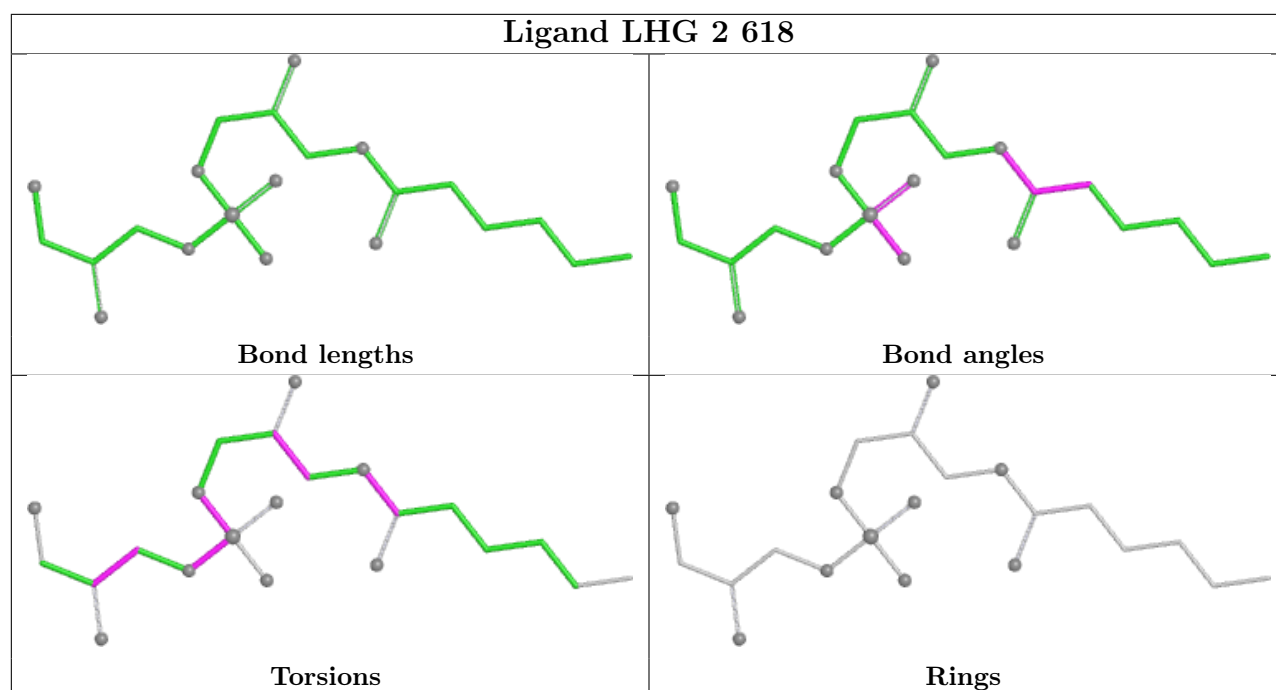


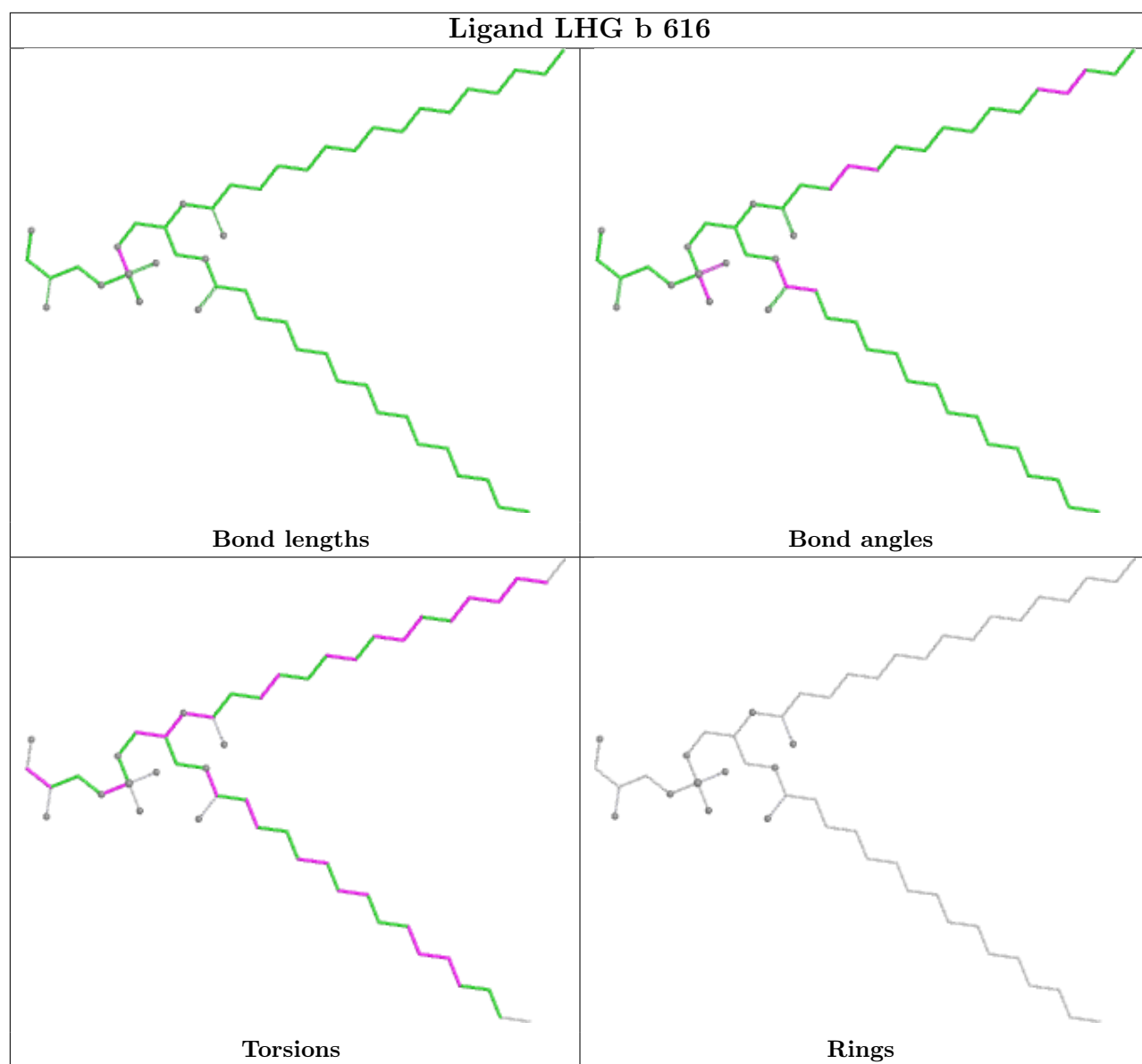
## Ligand II0 8 611

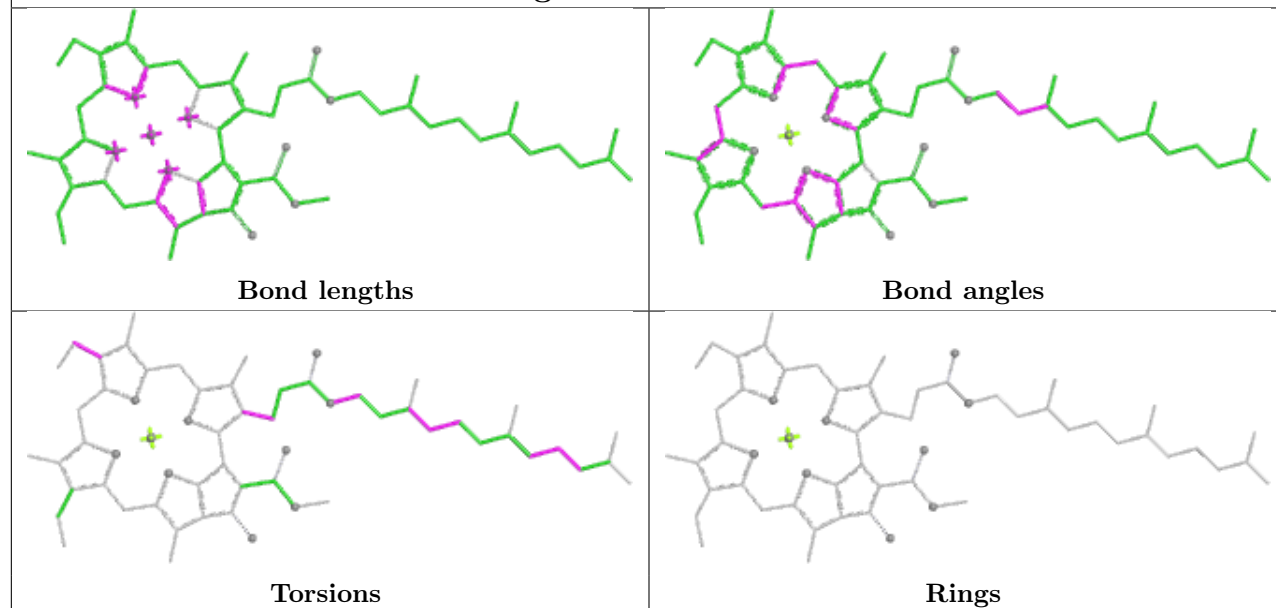
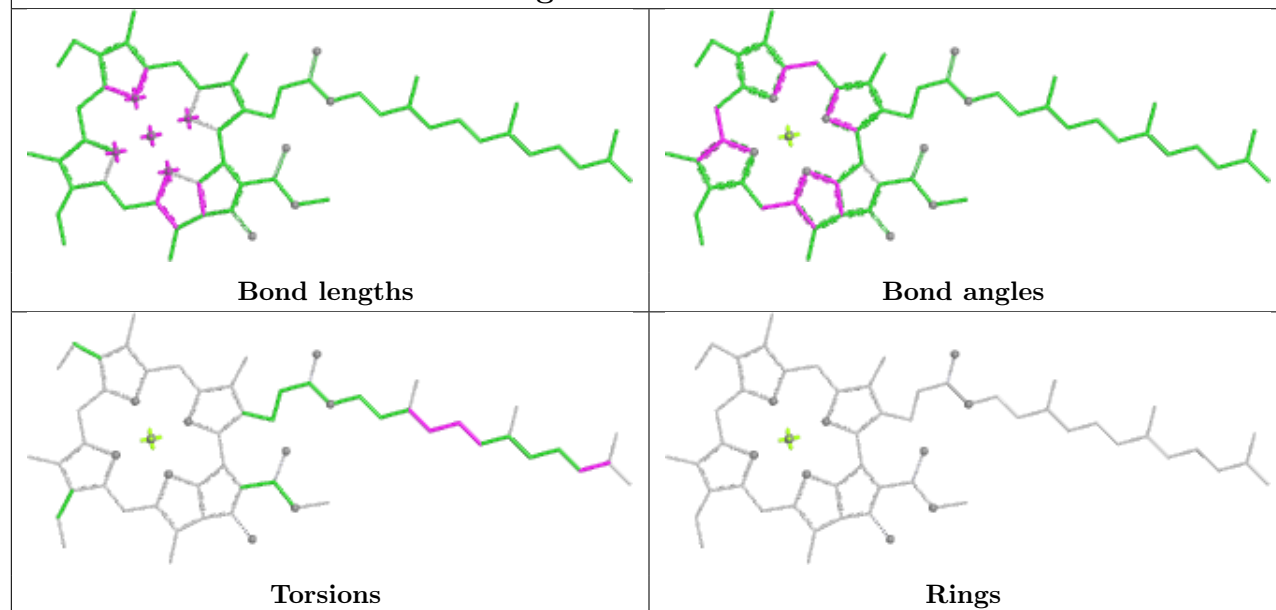


## Ligand CLA 7 310

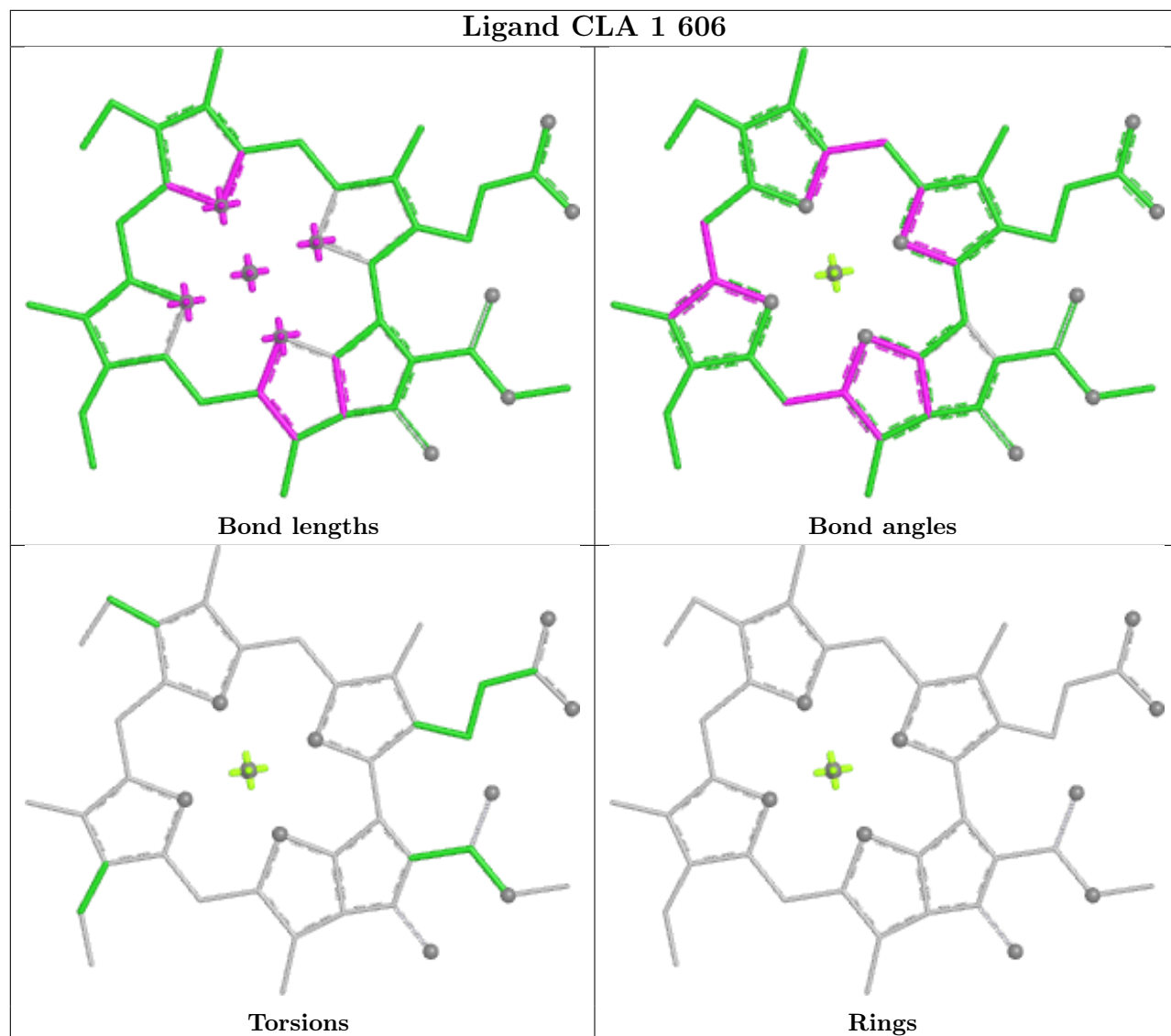




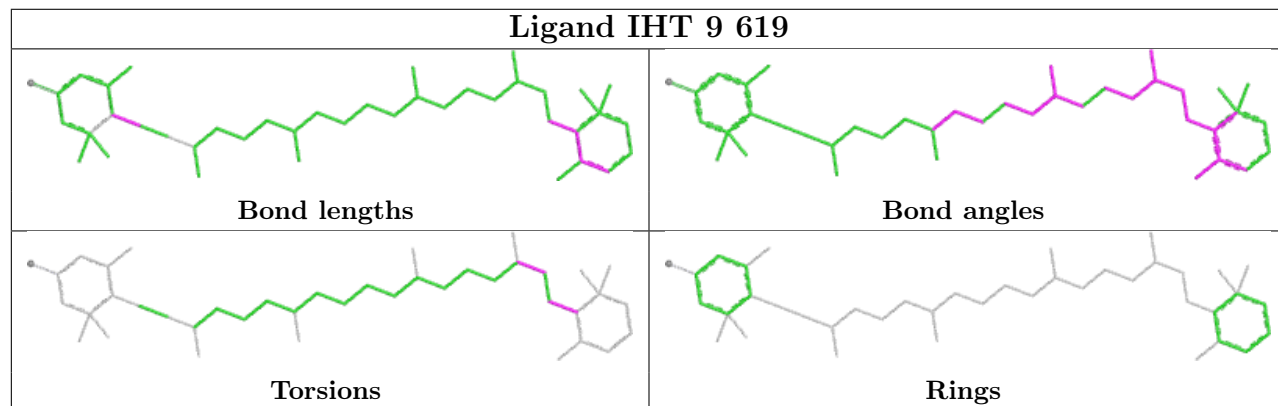


**Ligand CLA F 202****Ligand CLA 3 607**

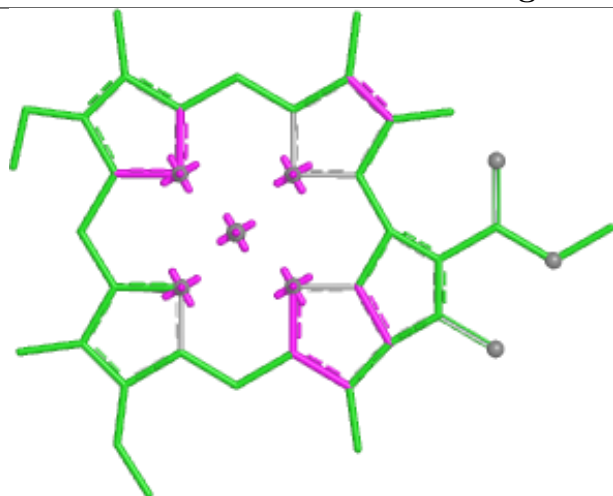
## Ligand CLA 1 606



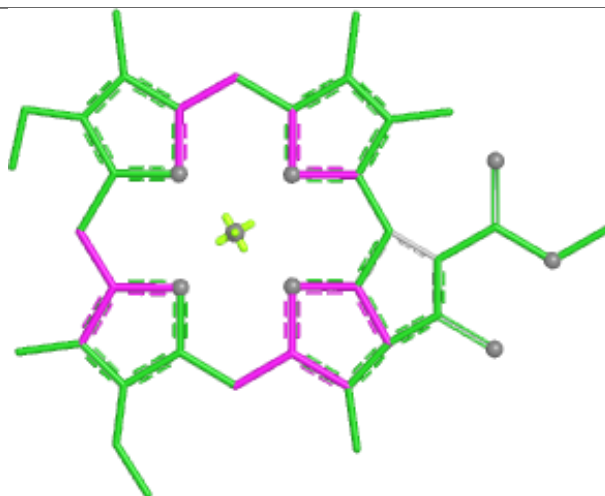
## Ligand IHT 9 619



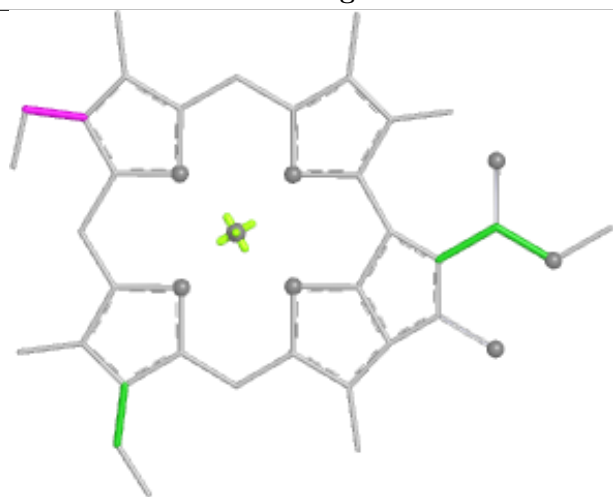
## Ligand CLA 1 609



Bond lengths



Bond angles

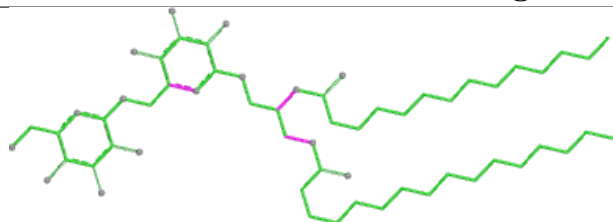


Torsions

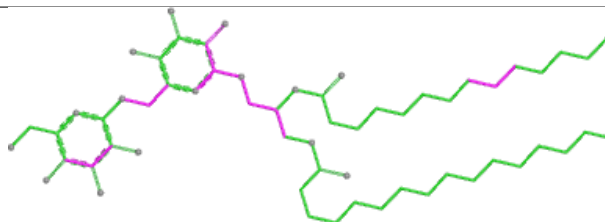


Rings

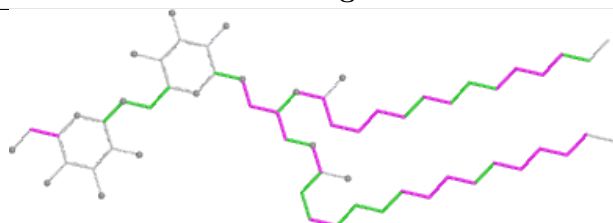
## Ligand DGD Z 303



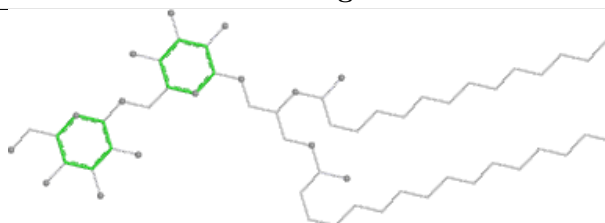
Bond lengths



Bond angles



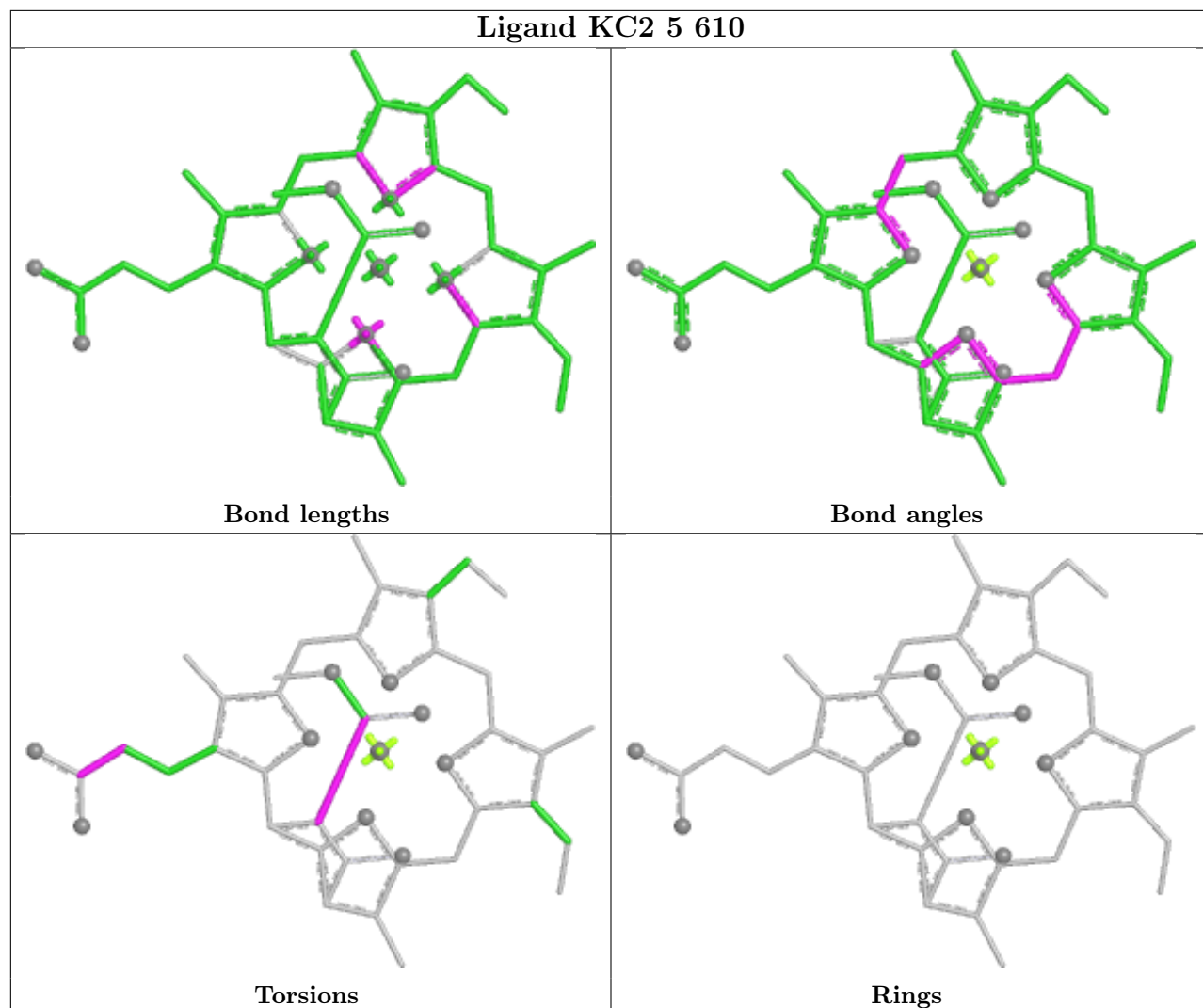
Torsions



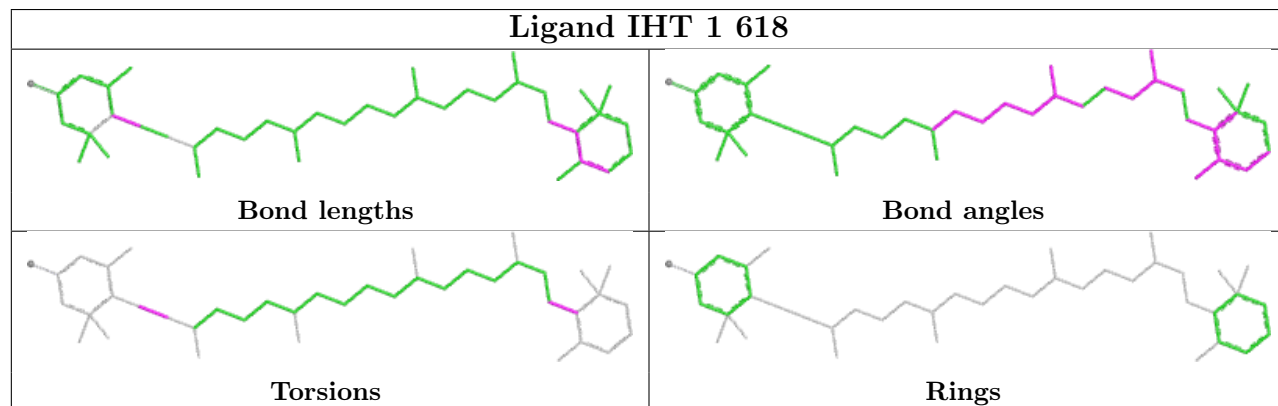
Rings

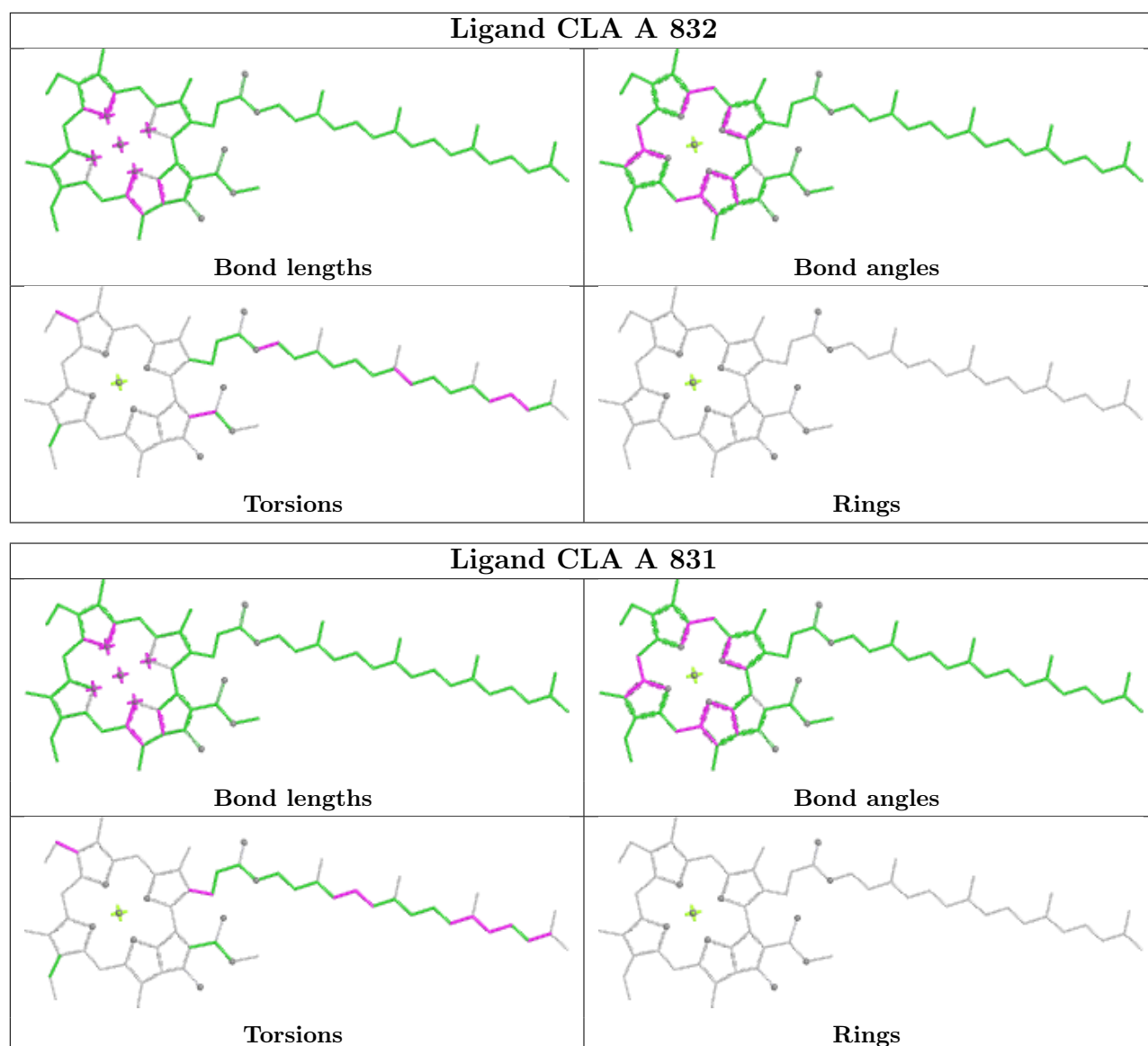


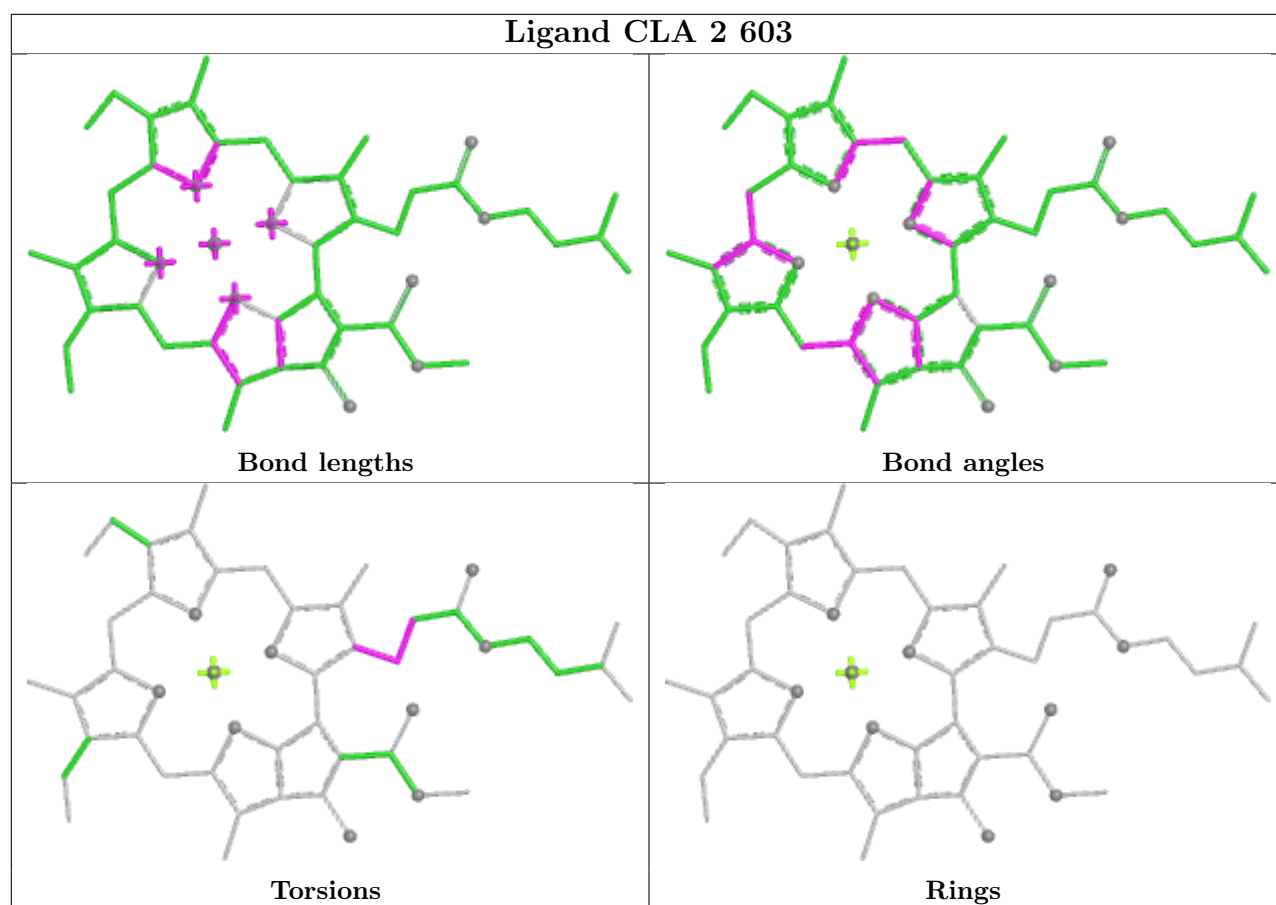
## Ligand KC2 5 610



## Ligand IHT 1 618







## 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.

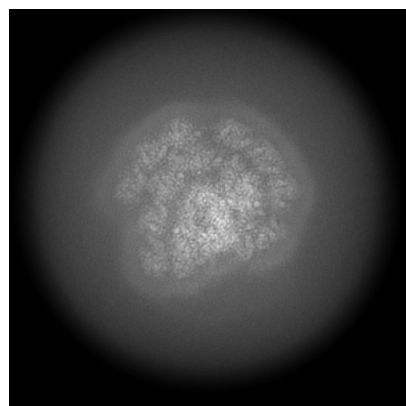
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33683. These allow visual inspection of the internal detail of the map and identification of artifacts.

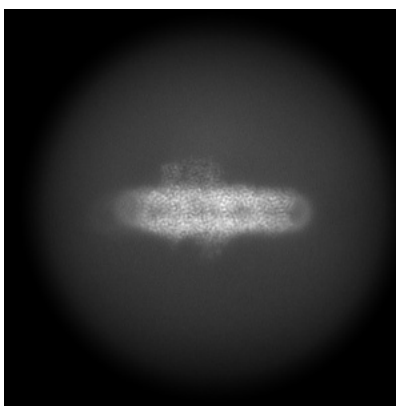
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

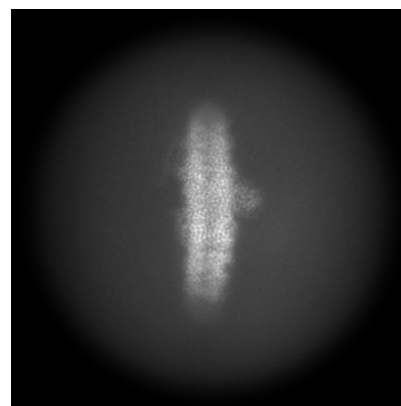
#### 6.1.1 Primary map



X

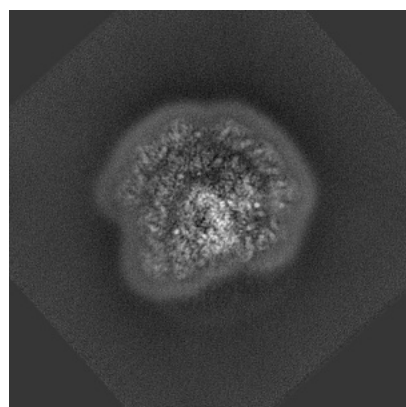


Y

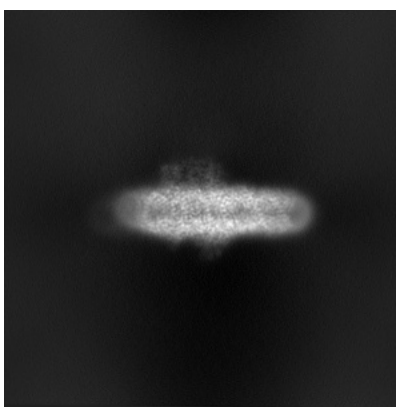


Z

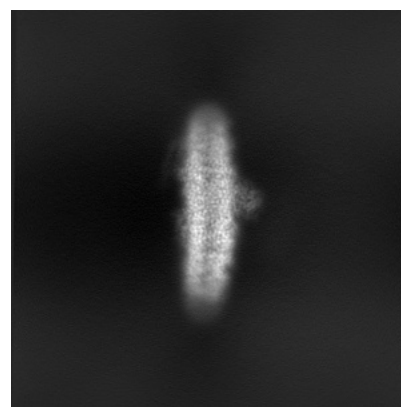
#### 6.1.2 Raw map



X



Y

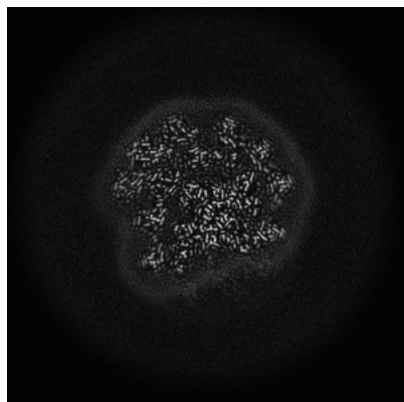


Z

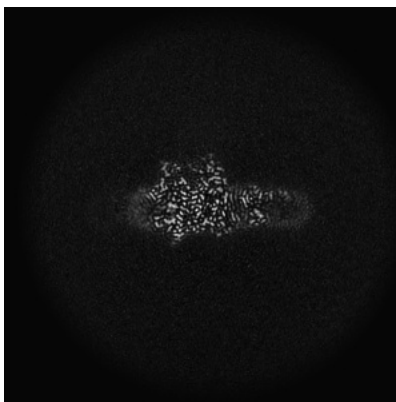
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

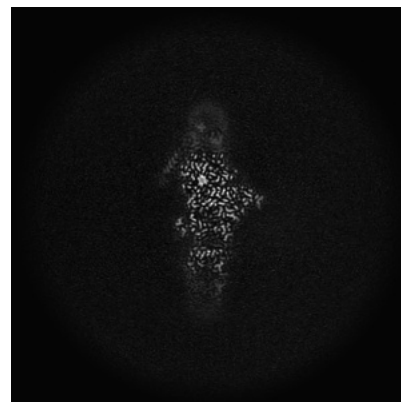
### 6.2.1 Primary map



X Index: 200

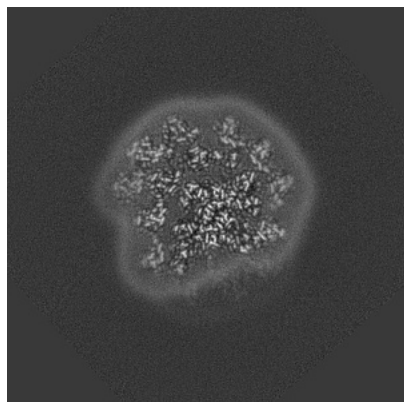


Y Index: 200

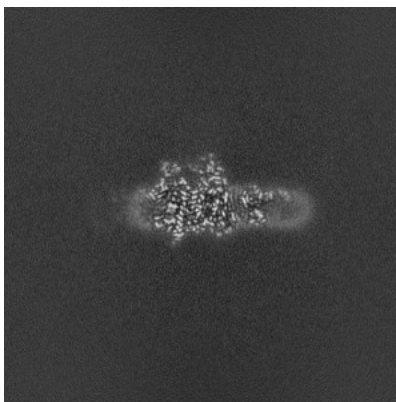


Z Index: 200

### 6.2.2 Raw map



X Index: 200



Y Index: 200

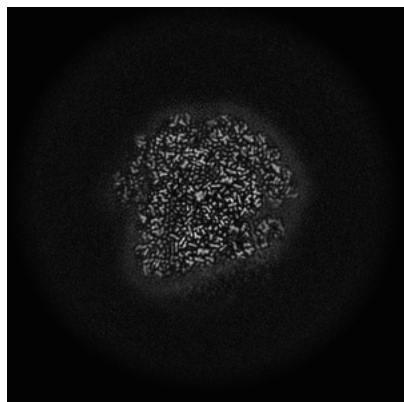


Z Index: 200

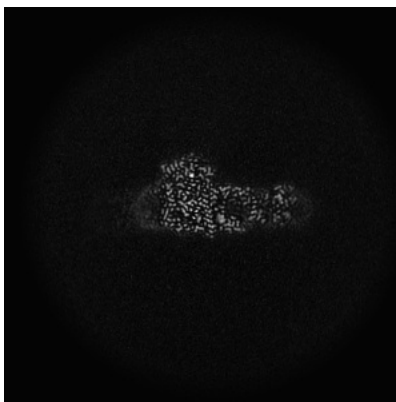
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

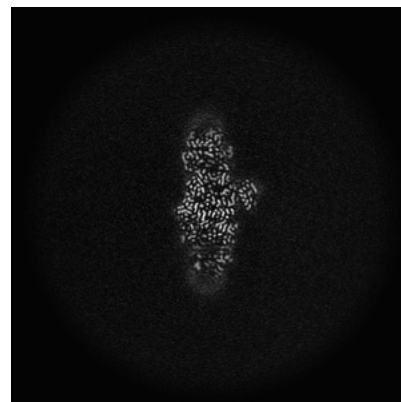
### 6.3.1 Primary map



X Index: 210

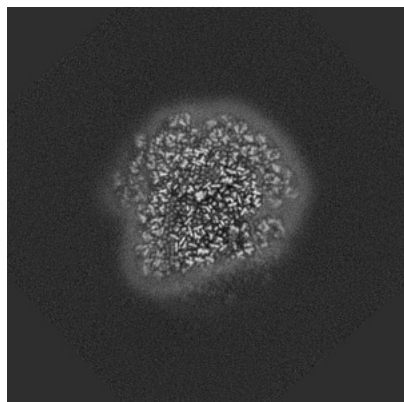


Y Index: 212

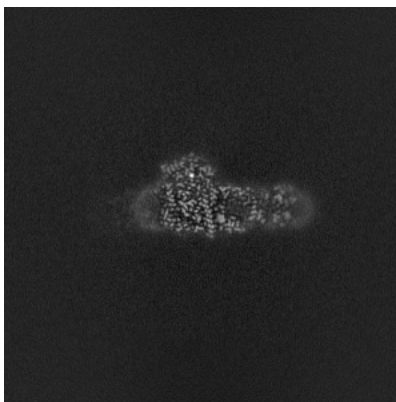


Z Index: 174

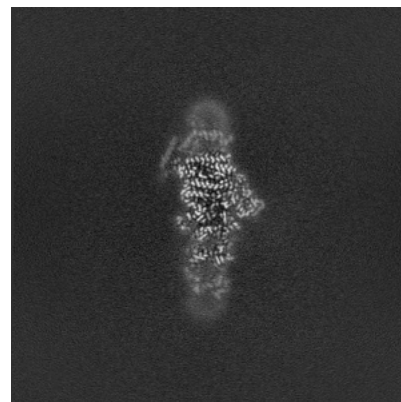
### 6.3.2 Raw map



X Index: 210



Y Index: 212



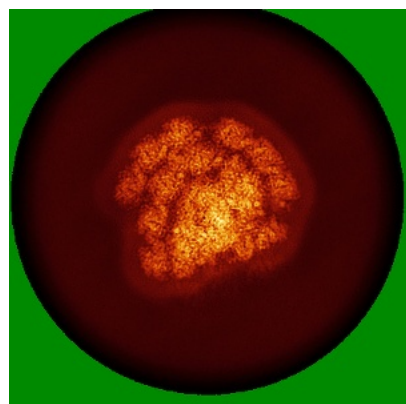
Z Index: 206

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

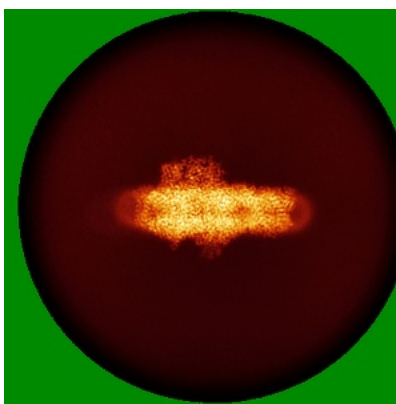


## 6.4 Orthogonal standard-deviation projections (False-color) ⓘ

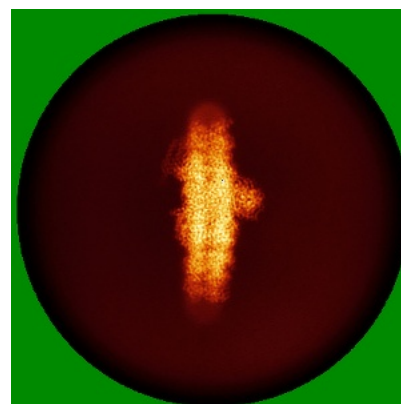
### 6.4.1 Primary map



X

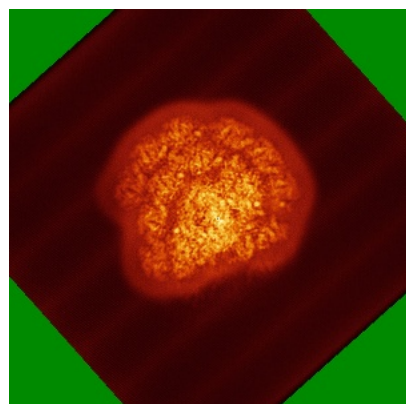


Y

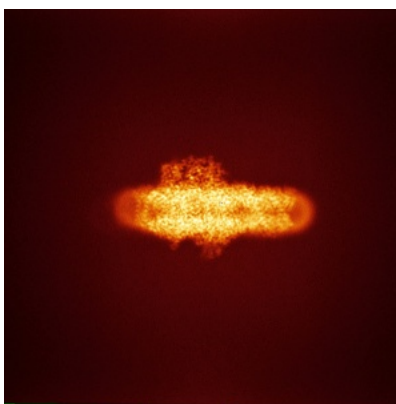


Z

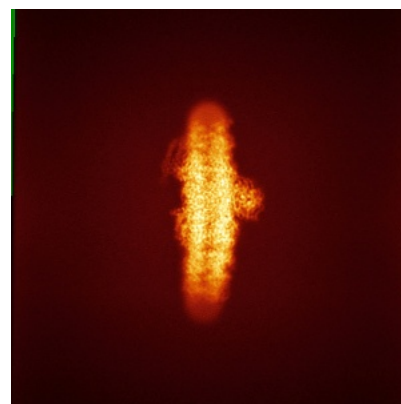
### 6.4.2 Raw map



X



Y

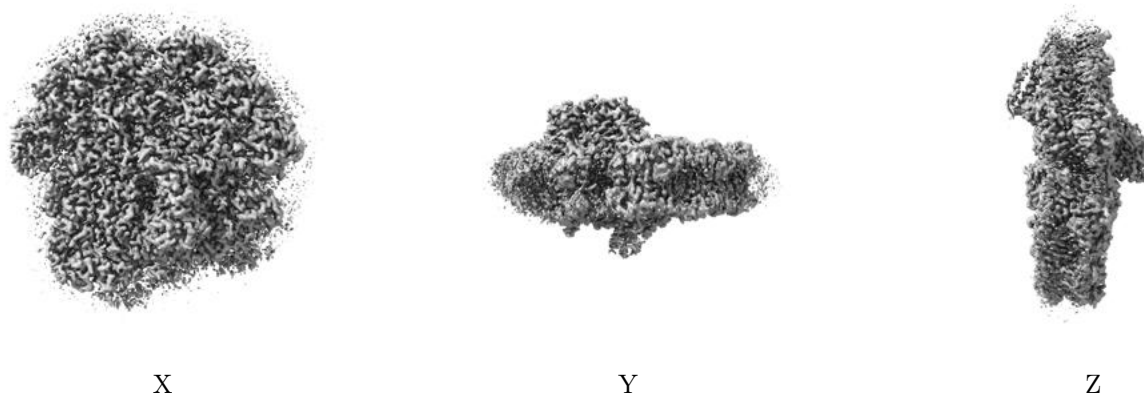


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

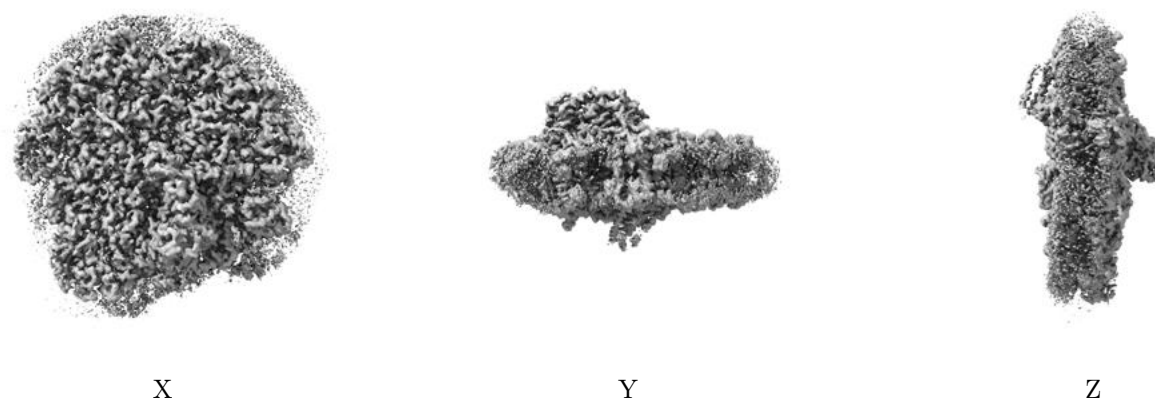
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

## 6.6 Mask visualisation [i](#)

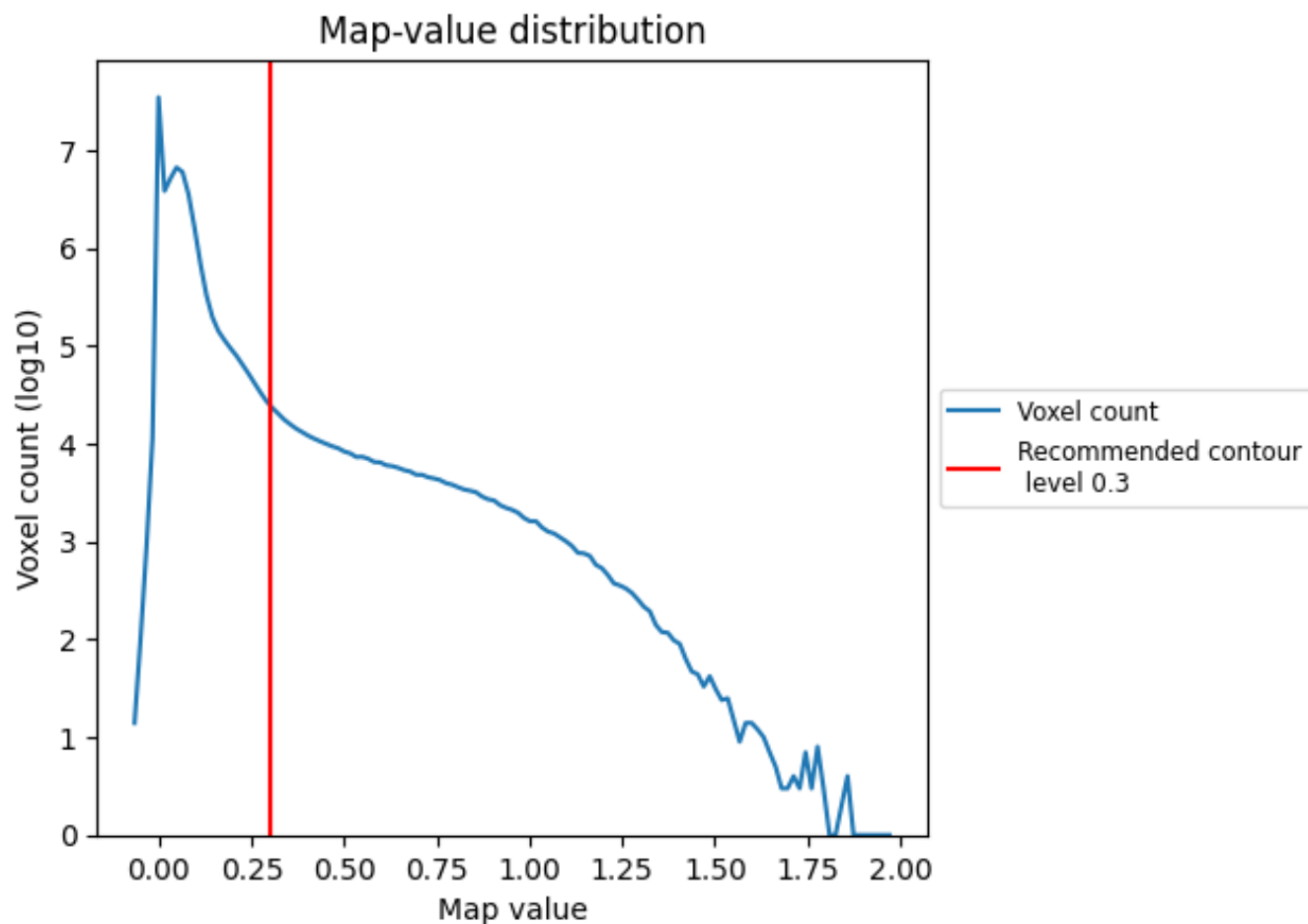
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

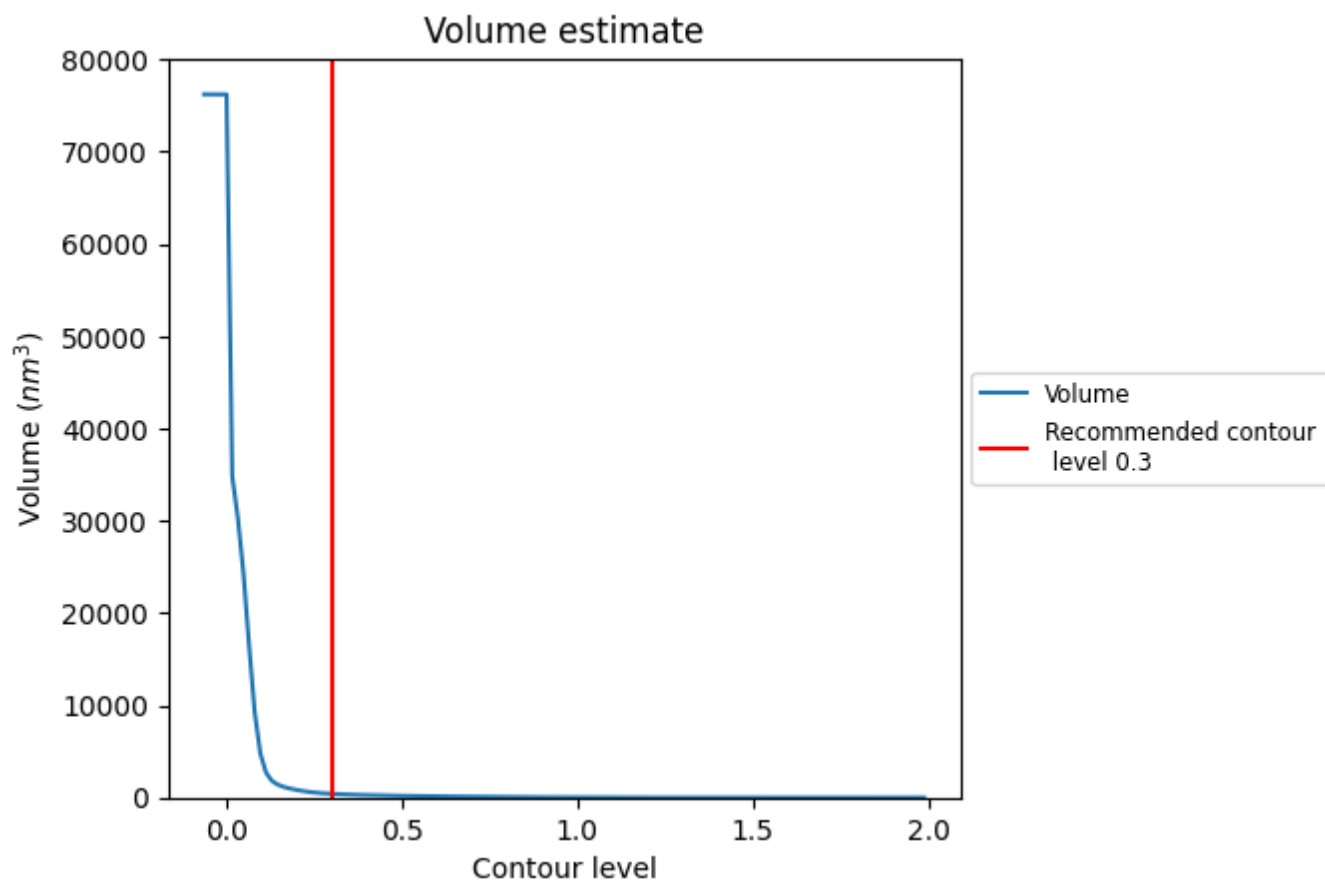
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

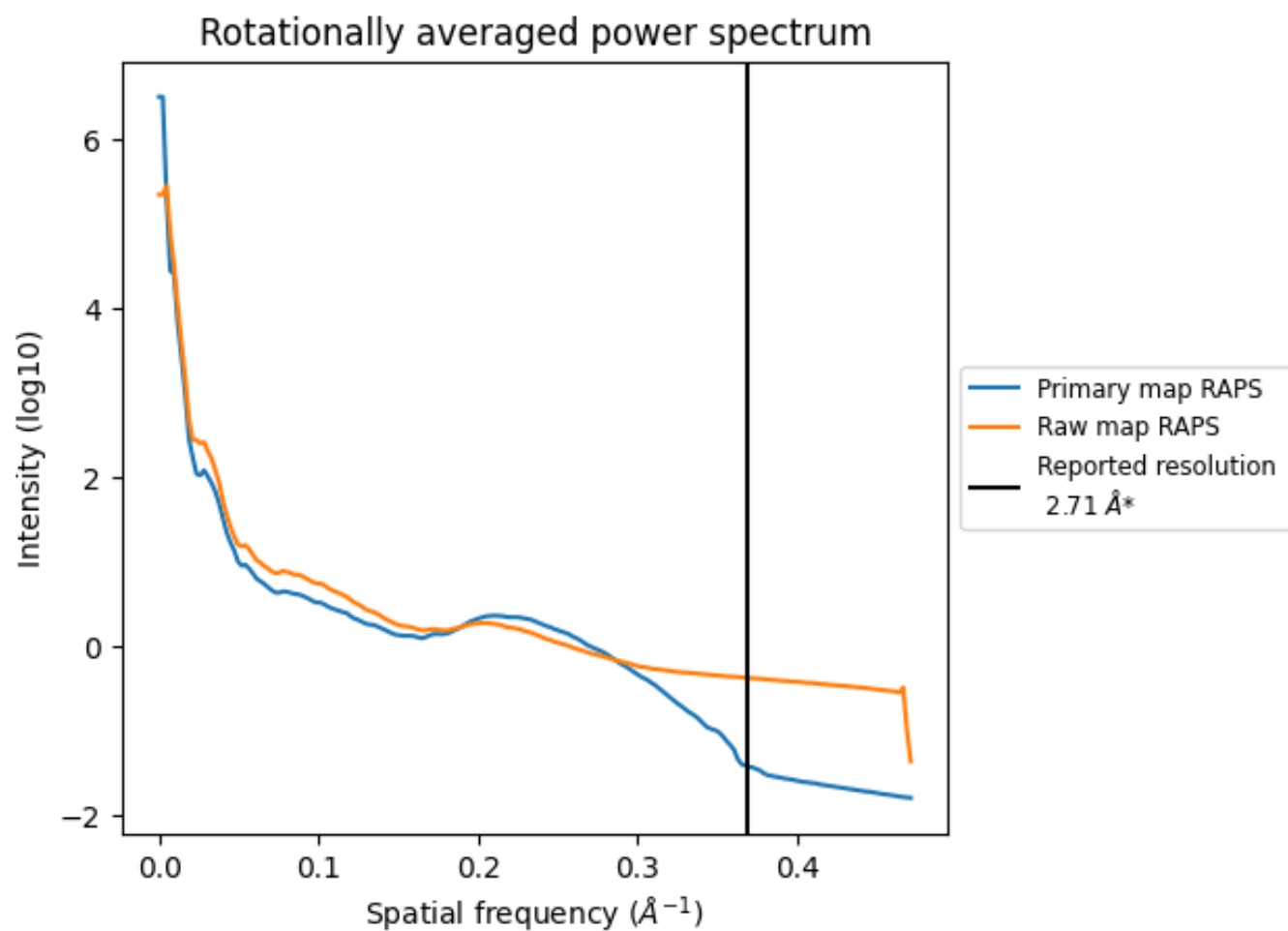
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 402 nm<sup>3</sup>; this corresponds to an approximate mass of 363 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 ⓘ

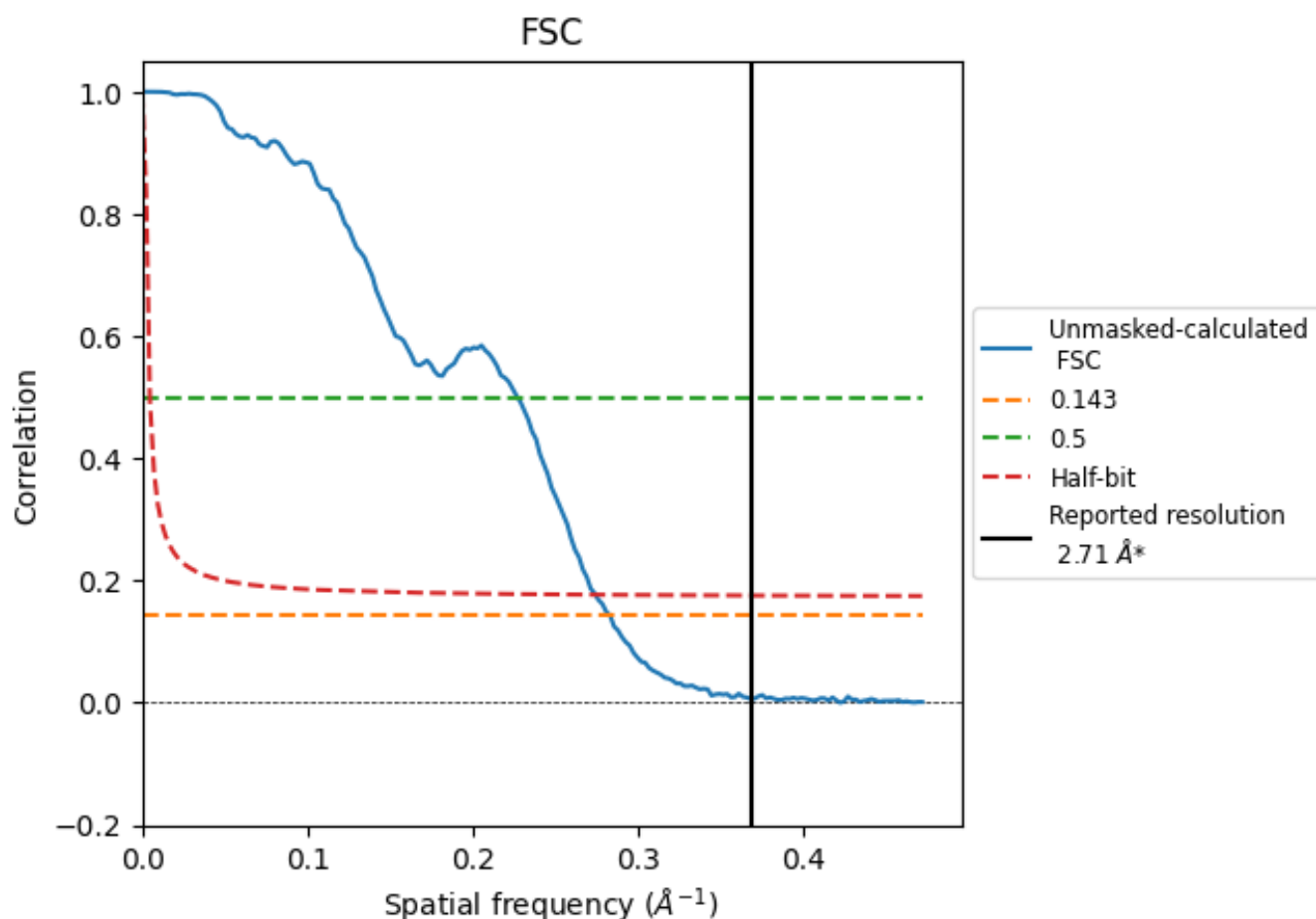


\*Reported resolution corresponds to spatial frequency of 0.369 Å<sup>-1</sup>

## 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 0.369 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

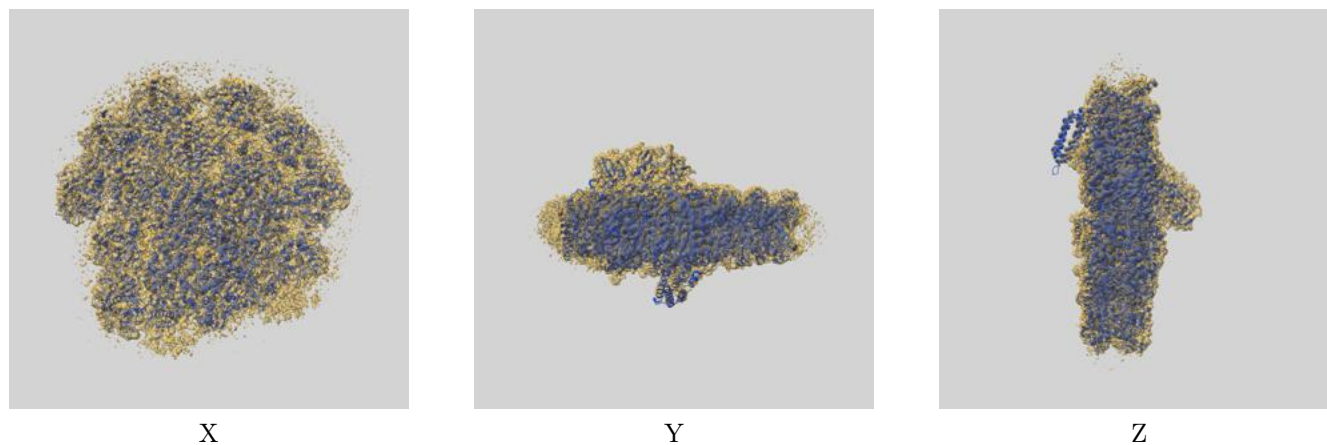
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.71                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 3.54                               | 4.41 | 3.65     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.54 differs from the reported value 2.71 by more than 10 %

## 9 Map-model fit [i](#)

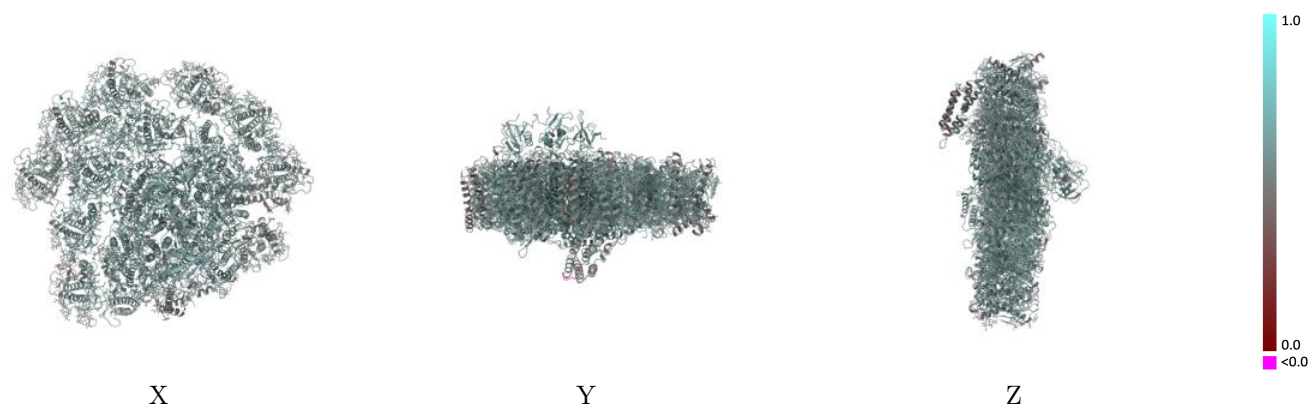
This section contains information regarding the fit between EMDB map EMD-33683 and PDB model 7Y8A. Per-residue inclusion information can be found in [section 3](#) on [page 38](#).

### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

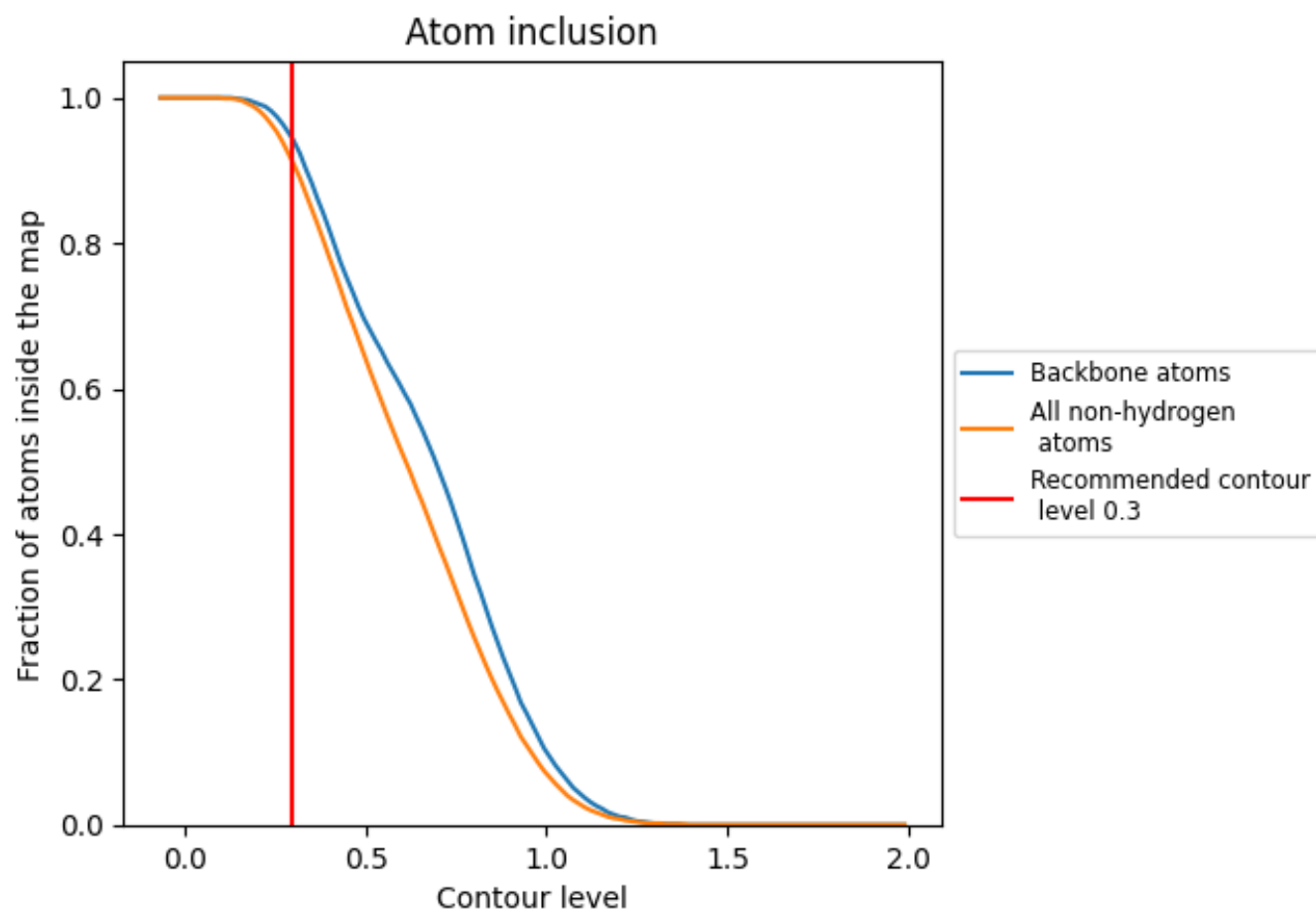


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 91% 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 (0.3) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9110   |  0.5810   |
| 1     |  0.8440   |  0.5270   |
| 2     |  0.9210   |  0.5810   |
| 3     |  0.9450   |  0.6080   |
| 4     |  0.9400   |  0.5980   |
| 5     |  0.8730   |  0.5370   |
| 6     |  0.9080   |  0.5580   |
| 7     |  0.8780   |  0.5340   |
| 8     |  0.8870   |  0.5560   |
| 9     |  0.7800   |  0.5420   |
| A     |  0.9690   |  0.6140   |
| B     |  0.9730   |  0.6220   |
| C     |  0.9680   |  0.6020   |
| D     |  0.9470   |  0.5840   |
| E     |  0.8740  |  0.5850  |
| F     |  0.9230 |  0.5960 |
| I     |  0.9760 |  0.6120 |
| J     |  0.9610 |  0.6110 |
| K     |  0.8740 |  0.5370 |
| L     |  0.8760 |  0.5640 |
| M     |  0.9430 |  0.5940 |
| O     |  0.5870 |  0.4700 |
| R     |  0.9360 |  0.5890 |
| X     |  0.5590 |  0.4670 |
| Z     |  0.8960 |  0.5790 |
| a     |  0.9040 |  0.5640 |
| b     |  0.9200 |  0.5640 |

