



wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 03:18 AM JST

PDB ID : 7COY
EMDB ID : EMD-30420
Title : Structure of the far-red light utilizing photosystem I of *Acaryochloris marina*
Authors : Kawakami, K.; Yonekura, K.; Hamaguchi, T.; Kashino, Y.; Shinzawa-Itoh, K.;
Inoue-Kashino, N.; Itoh, S.; Ifuku, K.; Yamashita, E.
Deposited on : 2020-08-05
Resolution : 2.50 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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

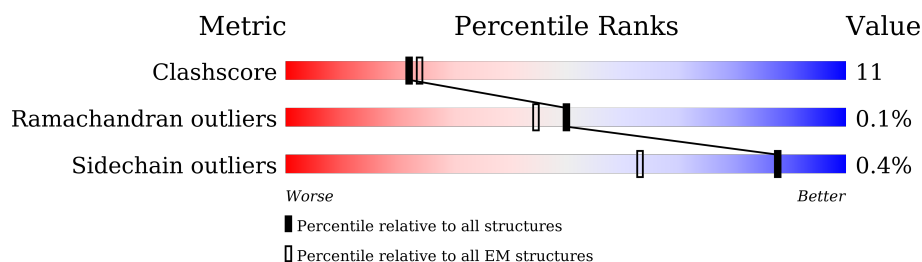
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 Å.

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



| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | aA | 753 | 19% 90% 9% |
| 1 | bA | 753 | 19% 90% 9% |
| 1 | cA | 753 | 19% 90% 9% |
| 2 | aB | 736 | 18% 89% 11% |
| 2 | bB | 736 | 18% 89% 11% |
| 2 | cB | 736 | 18% 89% 11% |
| 3 | aC | 81 | 14% 98% .. |
| 3 | bC | 81 | 19% 98% .. |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | cC | 81 | |
| 4 | aD | 139 | |
| 4 | bD | 139 | |
| 4 | cD | 139 | |
| 5 | aE | 89 | |
| 5 | bE | 89 | |
| 5 | cE | 89 | |
| 6 | aF | 167 | |
| 6 | bF | 167 | |
| 6 | cF | 167 | |
| 7 | aI | 34 | |
| 7 | bI | 34 | |
| 7 | cI | 34 | |
| 8 | aJ | 51 | |
| 8 | bJ | 51 | |
| 8 | cJ | 51 | |
| 9 | aK | 86 | |
| 9 | bK | 86 | |
| 9 | cK | 86 | |
| 10 | aL | 153 | |
| 10 | bL | 153 | |
| 10 | cL | 153 | |
| 11 | aM | 31 | |
| 11 | bM | 31 | |
| 11 | cM | 31 | |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 12 | G9R | aA | 3101 | X | - | - | - |
| 12 | G9R | cA | 3101 | X | - | - | - |
| 14 | CL7 | aA | 3103 | X | - | - | - |
| 14 | CL7 | aA | 3104 | X | - | - | - |
| 14 | CL7 | aA | 3105 | X | - | - | - |
| 14 | CL7 | aA | 3106 | X | - | - | - |
| 14 | CL7 | aA | 3107 | X | - | - | - |
| 14 | CL7 | aA | 3108 | X | - | - | - |
| 14 | CL7 | aA | 3109 | X | - | - | - |
| 14 | CL7 | aA | 3110 | X | - | - | - |
| 14 | CL7 | aA | 3111 | X | - | - | - |
| 14 | CL7 | aA | 3112 | X | - | - | - |
| 14 | CL7 | aA | 3113 | X | - | - | - |
| 14 | CL7 | aA | 3114 | X | - | - | - |
| 14 | CL7 | aA | 3115 | X | - | - | - |
| 14 | CL7 | aA | 3116 | X | - | - | - |
| 14 | CL7 | aA | 3117 | X | - | - | - |
| 14 | CL7 | aA | 3118 | X | - | - | - |
| 14 | CL7 | aA | 3119 | X | - | - | - |
| 14 | CL7 | aA | 3120 | X | - | - | - |
| 14 | CL7 | aA | 3121 | X | - | - | - |
| 14 | CL7 | aA | 3122 | X | - | - | - |
| 14 | CL7 | aA | 3123 | X | - | - | - |
| 14 | CL7 | aA | 3124 | X | - | - | - |
| 14 | CL7 | aA | 3125 | X | - | - | - |
| 14 | CL7 | aA | 3126 | X | - | - | - |
| 14 | CL7 | aA | 3127 | X | - | - | - |
| 14 | CL7 | aA | 3128 | X | - | - | - |
| 14 | CL7 | aA | 3129 | X | - | - | - |
| 14 | CL7 | aA | 3130 | X | - | - | - |
| 14 | CL7 | aA | 3131 | X | - | - | - |
| 14 | CL7 | aA | 3132 | X | - | - | - |
| 14 | CL7 | aA | 3133 | X | - | - | - |
| 14 | CL7 | aA | 3134 | X | - | - | - |
| 14 | CL7 | aA | 3140 | X | - | - | - |
| 14 | CL7 | aA | 3141 | X | - | - | - |
| 14 | CL7 | aA | 3142 | X | - | - | - |
| 14 | CL7 | aA | 3143 | X | - | - | - |
| 14 | CL7 | aA | 3146 | X | - | - | - |
| 14 | CL7 | aB | 3002 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14 | CL7 | aB | 3003 | X | - | - | - |
| 14 | CL7 | aB | 3005 | X | - | - | - |
| 14 | CL7 | aB | 3006 | X | - | - | - |
| 14 | CL7 | aB | 3007 | X | - | - | - |
| 14 | CL7 | aB | 3008 | X | - | - | - |
| 14 | CL7 | aB | 3009 | X | - | - | - |
| 14 | CL7 | aB | 3010 | X | - | - | - |
| 14 | CL7 | aB | 3011 | X | - | - | - |
| 14 | CL7 | aB | 3012 | X | - | - | - |
| 14 | CL7 | aB | 3013 | X | - | - | - |
| 14 | CL7 | aB | 3014 | X | - | - | - |
| 14 | CL7 | aB | 3015 | X | - | - | - |
| 14 | CL7 | aB | 3016 | X | - | - | - |
| 14 | CL7 | aB | 3017 | X | - | - | - |
| 14 | CL7 | aB | 3018 | X | - | - | - |
| 14 | CL7 | aB | 3019 | X | - | - | - |
| 14 | CL7 | aB | 3020 | X | - | - | - |
| 14 | CL7 | aB | 3021 | X | - | - | - |
| 14 | CL7 | aB | 3022 | X | - | - | - |
| 14 | CL7 | aB | 3023 | X | - | - | - |
| 14 | CL7 | aB | 3024 | X | - | - | - |
| 14 | CL7 | aB | 3025 | X | - | - | - |
| 14 | CL7 | aB | 3026 | X | - | - | - |
| 14 | CL7 | aB | 3030 | X | - | - | - |
| 14 | CL7 | aB | 3031 | X | - | - | - |
| 14 | CL7 | aB | 3032 | X | - | - | - |
| 14 | CL7 | aF | 201 | X | - | - | - |
| 14 | CL7 | aJ | 101 | X | - | - | - |
| 14 | CL7 | aK | 101 | X | - | - | - |
| 14 | CL7 | aL | 202 | X | - | - | - |
| 14 | CL7 | aL | 203 | X | - | - | - |
| 14 | CL7 | aL | 204 | X | - | - | - |
| 14 | CL7 | bA | 3102 | X | - | - | - |
| 14 | CL7 | bA | 3103 | X | - | - | - |
| 14 | CL7 | bA | 3104 | X | - | - | - |
| 14 | CL7 | bA | 3105 | X | - | - | - |
| 14 | CL7 | bA | 3106 | X | - | - | - |
| 14 | CL7 | bA | 3107 | X | - | - | - |
| 14 | CL7 | bA | 3108 | X | - | - | - |
| 14 | CL7 | bA | 3109 | X | - | - | - |
| 14 | CL7 | bA | 3110 | X | - | - | - |
| 14 | CL7 | bA | 3111 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14 | CL7 | bA | 3112 | X | - | - | - |
| 14 | CL7 | bA | 3113 | X | - | - | - |
| 14 | CL7 | bA | 3114 | X | - | - | - |
| 14 | CL7 | bA | 3115 | X | - | - | - |
| 14 | CL7 | bA | 3116 | X | - | - | - |
| 14 | CL7 | bA | 3117 | X | - | - | - |
| 14 | CL7 | bA | 3118 | X | - | - | - |
| 14 | CL7 | bA | 3119 | X | - | - | - |
| 14 | CL7 | bA | 3120 | X | - | - | - |
| 14 | CL7 | bA | 3121 | X | - | - | - |
| 14 | CL7 | bA | 3122 | X | - | - | - |
| 14 | CL7 | bA | 3123 | X | - | - | - |
| 14 | CL7 | bA | 3124 | X | - | - | - |
| 14 | CL7 | bA | 3125 | X | - | - | - |
| 14 | CL7 | bA | 3126 | X | - | - | - |
| 14 | CL7 | bA | 3127 | X | - | - | - |
| 14 | CL7 | bA | 3128 | X | - | - | - |
| 14 | CL7 | bA | 3129 | X | - | - | - |
| 14 | CL7 | bA | 3130 | X | - | - | - |
| 14 | CL7 | bA | 3131 | X | - | - | - |
| 14 | CL7 | bA | 3132 | X | - | - | - |
| 14 | CL7 | bA | 3133 | X | - | - | - |
| 14 | CL7 | bA | 3139 | X | - | - | - |
| 14 | CL7 | bA | 3140 | X | - | - | - |
| 14 | CL7 | bA | 3141 | X | - | - | - |
| 14 | CL7 | bA | 3142 | X | - | - | - |
| 14 | CL7 | bA | 3145 | X | - | - | - |
| 14 | CL7 | bB | 803 | X | - | - | - |
| 14 | CL7 | bB | 804 | X | - | - | - |
| 14 | CL7 | bB | 806 | X | - | - | - |
| 14 | CL7 | bB | 807 | X | - | - | - |
| 14 | CL7 | bB | 808 | X | - | - | - |
| 14 | CL7 | bB | 809 | X | - | - | - |
| 14 | CL7 | bB | 810 | X | - | - | - |
| 14 | CL7 | bB | 811 | X | - | - | - |
| 14 | CL7 | bB | 812 | X | - | - | - |
| 14 | CL7 | bB | 813 | X | - | - | - |
| 14 | CL7 | bB | 814 | X | - | - | - |
| 14 | CL7 | bB | 815 | X | - | - | - |
| 14 | CL7 | bB | 816 | X | - | - | - |
| 14 | CL7 | bB | 817 | X | - | - | - |
| 14 | CL7 | bB | 818 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14 | CL7 | bB | 819 | X | - | - | - |
| 14 | CL7 | bB | 820 | X | - | - | - |
| 14 | CL7 | bB | 821 | X | - | - | - |
| 14 | CL7 | bB | 822 | X | - | - | - |
| 14 | CL7 | bB | 823 | X | - | - | - |
| 14 | CL7 | bB | 824 | X | - | - | - |
| 14 | CL7 | bB | 825 | X | - | - | - |
| 14 | CL7 | bB | 826 | X | - | - | - |
| 14 | CL7 | bB | 827 | X | - | - | - |
| 14 | CL7 | bB | 831 | X | - | - | - |
| 14 | CL7 | bB | 832 | X | - | - | - |
| 14 | CL7 | bB | 833 | X | - | - | - |
| 14 | CL7 | bF | 201 | X | - | - | - |
| 14 | CL7 | bJ | 101 | X | - | - | - |
| 14 | CL7 | bK | 101 | X | - | - | - |
| 14 | CL7 | bL | 203 | X | - | - | - |
| 14 | CL7 | bL | 204 | X | - | - | - |
| 14 | CL7 | bL | 205 | X | - | - | - |
| 14 | CL7 | cA | 3102 | X | - | - | - |
| 14 | CL7 | cA | 3103 | X | - | - | - |
| 14 | CL7 | cA | 3104 | X | - | - | - |
| 14 | CL7 | cA | 3105 | X | - | - | - |
| 14 | CL7 | cA | 3106 | X | - | - | - |
| 14 | CL7 | cA | 3107 | X | - | - | - |
| 14 | CL7 | cA | 3108 | X | - | - | - |
| 14 | CL7 | cA | 3109 | X | - | - | - |
| 14 | CL7 | cA | 3110 | X | - | - | - |
| 14 | CL7 | cA | 3111 | X | - | - | - |
| 14 | CL7 | cA | 3112 | X | - | - | - |
| 14 | CL7 | cA | 3113 | X | - | - | - |
| 14 | CL7 | cA | 3114 | X | - | - | - |
| 14 | CL7 | cA | 3115 | X | - | - | - |
| 14 | CL7 | cA | 3116 | X | - | - | - |
| 14 | CL7 | cA | 3117 | X | - | - | - |
| 14 | CL7 | cA | 3118 | X | - | - | - |
| 14 | CL7 | cA | 3119 | X | - | - | - |
| 14 | CL7 | cA | 3120 | X | - | - | - |
| 14 | CL7 | cA | 3121 | X | - | - | - |
| 14 | CL7 | cA | 3122 | X | - | - | - |
| 14 | CL7 | cA | 3123 | X | - | - | - |
| 14 | CL7 | cA | 3124 | X | - | - | - |
| 14 | CL7 | cA | 3125 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14 | CL7 | cA | 3126 | X | - | - | - |
| 14 | CL7 | cA | 3127 | X | - | - | - |
| 14 | CL7 | cA | 3128 | X | - | - | - |
| 14 | CL7 | cA | 3129 | X | - | - | - |
| 14 | CL7 | cA | 3130 | X | - | - | - |
| 14 | CL7 | cA | 3131 | X | - | - | - |
| 14 | CL7 | cA | 3132 | X | - | - | - |
| 14 | CL7 | cA | 3133 | X | - | - | - |
| 14 | CL7 | cA | 3139 | X | - | - | - |
| 14 | CL7 | cA | 3140 | X | - | - | - |
| 14 | CL7 | cA | 3141 | X | - | - | - |
| 14 | CL7 | cA | 3142 | X | - | - | - |
| 14 | CL7 | cA | 3144 | X | - | - | - |
| 14 | CL7 | cB | 803 | X | - | - | - |
| 14 | CL7 | cB | 804 | X | - | - | - |
| 14 | CL7 | cB | 806 | X | - | - | - |
| 14 | CL7 | cB | 807 | X | - | - | - |
| 14 | CL7 | cB | 808 | X | - | - | - |
| 14 | CL7 | cB | 809 | X | - | - | - |
| 14 | CL7 | cB | 810 | X | - | - | - |
| 14 | CL7 | cB | 811 | X | - | - | - |
| 14 | CL7 | cB | 812 | X | - | - | - |
| 14 | CL7 | cB | 813 | X | - | - | - |
| 14 | CL7 | cB | 814 | X | - | - | - |
| 14 | CL7 | cB | 815 | X | - | - | - |
| 14 | CL7 | cB | 816 | X | - | - | - |
| 14 | CL7 | cB | 817 | X | - | - | - |
| 14 | CL7 | cB | 818 | X | - | - | - |
| 14 | CL7 | cB | 819 | X | - | - | - |
| 14 | CL7 | cB | 820 | X | - | - | - |
| 14 | CL7 | cB | 821 | X | - | - | - |
| 14 | CL7 | cB | 822 | X | - | - | - |
| 14 | CL7 | cB | 823 | X | - | - | - |
| 14 | CL7 | cB | 824 | X | - | - | - |
| 14 | CL7 | cB | 825 | X | - | - | - |
| 14 | CL7 | cB | 826 | X | - | - | - |
| 14 | CL7 | cB | 827 | X | - | - | - |
| 14 | CL7 | cB | 831 | X | - | - | - |
| 14 | CL7 | cB | 832 | X | - | - | - |
| 14 | CL7 | cB | 833 | X | - | - | - |
| 14 | CL7 | cF | 201 | X | - | - | - |
| 14 | CL7 | cJ | 101 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 14 | CL7 | cK | 101 | X | - | - | - |
| 14 | CL7 | cL | 203 | X | - | - | - |
| 14 | CL7 | cL | 204 | X | - | - | - |
| 14 | CL7 | cL | 205 | X | - | - | - |

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 57966 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | aA | 685 | Total | C | N | O | S | 0 | 0 |
| | | | 5203 | 3384 | 909 | 886 | 24 | | |
| 1 | bA | 685 | Total | C | N | O | S | 0 | 0 |
| | | | 5203 | 3384 | 909 | 886 | 24 | | |
| 1 | cA | 685 | Total | C | N | O | S | 0 | 0 |
| | | | 5203 | 3384 | 909 | 886 | 24 | | |

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2 | aB | 658 | Total | C | N | O | S | 0 | 0 |
| | | | 5007 | 3292 | 840 | 860 | 15 | | |
| 2 | bB | 658 | Total | C | N | O | S | 0 | 0 |
| | | | 5007 | 3292 | 840 | 860 | 15 | | |
| 2 | cB | 658 | Total | C | N | O | S | 0 | 0 |
| | | | 5007 | 3292 | 840 | 860 | 15 | | |

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 3 | aC | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 573 | 353 | 102 | 108 | 10 | | |
| 3 | bC | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 573 | 353 | 102 | 108 | 10 | | |
| 3 | cC | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 573 | 353 | 102 | 108 | 10 | | |

- Molecule 4 is a protein called Photosystem I protein PsuD.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4 | aD | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 999 | 631 | 177 | 187 | 4 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4 | bD | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 999 | 631 | 177 | 187 | 4 | | |
| 4 | cD | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 999 | 631 | 177 | 187 | 4 | | |

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|-------|
| 5 | aE | 67 | Total | C | N | O | | 0 | 0 |
| | | | 375 | 230 | 70 | 75 | | | |
| 5 | bE | 67 | Total | C | N | O | | 0 | 0 |
| | | | 375 | 230 | 70 | 75 | | | |
| 5 | cE | 67 | Total | C | N | O | | 0 | 0 |
| | | | 375 | 230 | 70 | 75 | | | |

- Molecule 6 is a protein called Photosystem I protein Psal.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6 | aF | 132 | Total | C | N | O | S | 0 | 0 |
| | | | 847 | 529 | 157 | 157 | 4 | | |
| 6 | bF | 132 | Total | C | N | O | S | 0 | 0 |
| | | | 847 | 529 | 157 | 157 | 4 | | |
| 6 | cF | 132 | Total | C | N | O | S | 0 | 0 |
| | | | 847 | 529 | 157 | 157 | 4 | | |

- Molecule 7 is a protein called Photosystem I protein Psal27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7 | aI | 30 | Total | C | N | O | S | 0 | 0 |
| | | | 225 | 151 | 33 | 39 | 2 | | |
| 7 | bI | 30 | Total | C | N | O | S | 0 | 0 |
| | | | 225 | 151 | 33 | 39 | 2 | | |
| 7 | cI | 30 | Total | C | N | O | S | 0 | 0 |
| | | | 225 | 151 | 33 | 39 | 2 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|-------|
| 8 | aJ | 35 | Total | C | N | O | | 0 | 0 |
| | | | 264 | 184 | 39 | 41 | | | |
| 8 | bJ | 35 | Total | C | N | O | | 0 | 0 |
| | | | 264 | 184 | 39 | 41 | | | |

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| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 8 | cJ | 35 | Total | C | N | O | 0 | 0 |
| | | | 264 | 184 | 39 | 41 | | |

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

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 9 | aK | 33 | Total | C | N | O | 0 | 0 |
| | | | 161 | 95 | 33 | 33 | | |
| 9 | bK | 33 | Total | C | N | O | 0 | 0 |
| | | | 161 | 95 | 33 | 33 | | |
| 9 | cK | 33 | Total | C | N | O | 0 | 0 |
| | | | 161 | 95 | 33 | 33 | | |

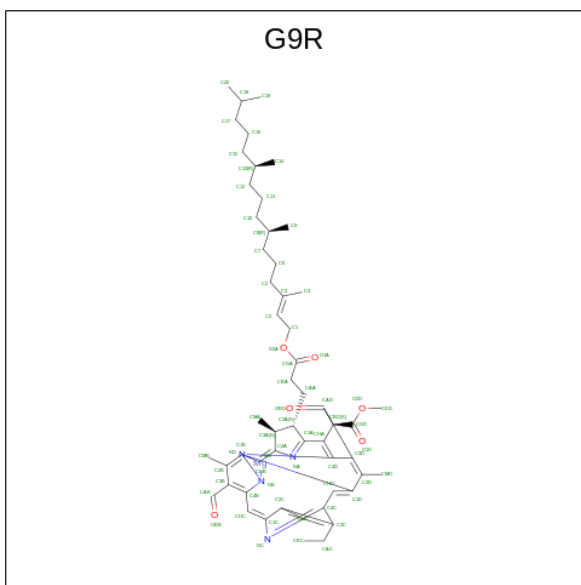
- Molecule 10 is a protein called Photosystem I protein Psal.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10 | aL | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 999 | 638 | 168 | 189 | 4 | | |
| 10 | bL | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 999 | 638 | 168 | 189 | 4 | | |
| 10 | cL | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 999 | 638 | 168 | 189 | 4 | | |

- Molecule 11 is a protein called Photosystem I protein Psam.

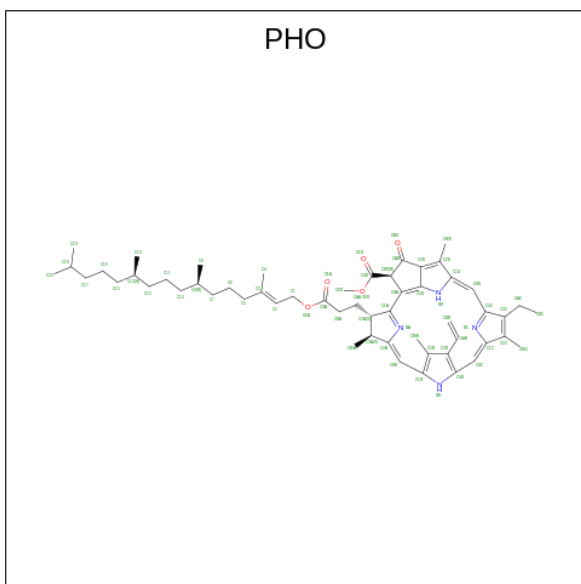
| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 11 | aM | 29 | Total | C | N | O | 0 | 0 |
| | | | 205 | 136 | 31 | 38 | | |
| 11 | bM | 29 | Total | C | N | O | 0 | 0 |
| | | | 205 | 136 | 31 | 38 | | |
| 11 | cM | 29 | Total | C | N | O | 0 | 0 |
| | | | 205 | 136 | 31 | 38 | | |

- Molecule 12 is CHLOROPHYLL D ISOMER (three-letter code: G9R) (formula: C₅₄H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



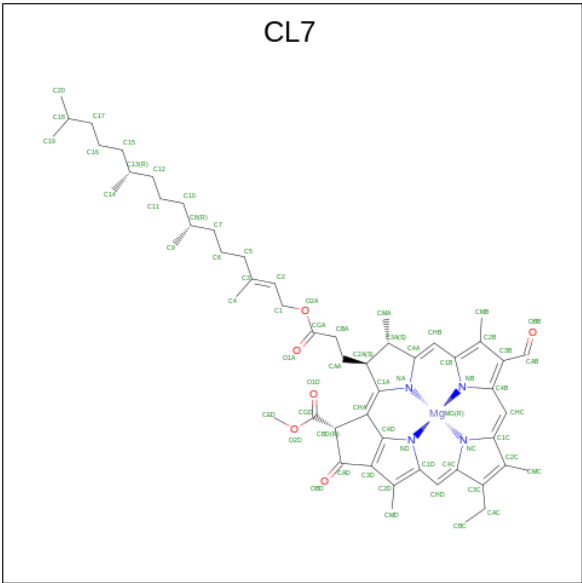
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 12 | aA | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 12 | bA | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 12 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |

- Molecule 13 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 13 | aA | 1 | Total | C | N | O | 0 |
| | | | 64 | 55 | 4 | 5 | |
| 13 | aB | 1 | Total | C | N | O | 0 |
| | | | 64 | 55 | 4 | 5 | |
| 13 | bB | 1 | Total | C | N | O | 0 |
| | | | 64 | 55 | 4 | 5 | |
| 13 | bB | 1 | Total | C | N | O | 0 |
| | | | 64 | 55 | 4 | 5 | |
| 13 | cB | 1 | Total | C | N | O | 0 |
| | | | 64 | 55 | 4 | 5 | |
| 13 | cB | 1 | Total | C | N | O | 0 |
| | | | 64 | 55 | 4 | 5 | |

- Molecule 14 is CHLOROPHYLL D (three-letter code: CL7) (formula: C₅₄H₇₀MgN₄O₆) (la-
beled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14 | aA | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | aA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | aA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | aA | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14 | aA | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aA | 1 | Total 42 | C 33 | Mg 1 | N 4 | O 4 | 0 |
| 14 | aA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | aA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | aA | 1 | Total 38 | C 31 | Mg 1 | N 4 | O 2 | 0 |
| 14 | aA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | aA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | aA | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aA | 1 | Total 38 | C 31 | Mg 1 | N 4 | O 2 | 0 |
| 14 | aA | 1 | Total 53 | C 42 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aA | 1 | Total 38 | C 31 | Mg 1 | N 4 | O 2 | 0 |
| 14 | aA | 1 | Total 38 | C 31 | Mg 1 | N 4 | O 2 | 0 |
| 14 | aA | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aA | 1 | Total 51 | C 40 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | aA | 1 | Total 50 | C 39 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aA | 1 | Total 51 | C 40 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aA | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aA | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aA | 1 | Total 53 | C 42 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aA | 1 | Total 51 | C 40 | Mg 1 | N 4 | O 6 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14 | aA | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | aA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | aA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | aA | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | aA | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aA | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aA | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aA | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | aB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aB | 1 | Total 50 | C 39 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aB | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | aB | 1 | Total 38 | C 31 | Mg 1 | N 4 | O 2 | 0 |
| 14 | aB | 1 | Total 38 | C 31 | Mg 1 | N 4 | O 2 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14 | aB | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | aB | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | aB | 1 | Total 50 | C 39 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aB | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | aB | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | aB | 1 | Total 56 | C 45 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aB | 1 | Total 38 | C 31 | Mg 1 | N 4 | O 2 | 0 |
| 14 | aB | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | aB | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | aB | 1 | Total 56 | C 45 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aB | 1 | Total 38 | C 31 | Mg 1 | N 4 | O 2 | 0 |
| 14 | aB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aB | 1 | Total 54 | C 43 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aB | 1 | Total 55 | C 44 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aF | 1 | Total 38 | C 31 | Mg 1 | N 4 | O 2 | 0 |
| 14 | aJ | 1 | Total 42 | C 33 | Mg 1 | N 4 | O 4 | 0 |
| 14 | aK | 1 | Total 37 | C 30 | Mg 1 | N 4 | O 2 | 0 |
| 14 | aL | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14 | aL | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | aL | 1 | Total 42 | C 33 | Mg 1 | N 4 | O 4 | 0 |
| 14 | bA | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | bA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | bA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | bA | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bA | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bA | 1 | Total 42 | C 33 | Mg 1 | N 4 | O 4 | 0 |
| 14 | bA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | bA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | bA | 1 | Total 38 | C 31 | Mg 1 | N 4 | O 2 | 0 |
| 14 | bA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | bA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | bA | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bA | 1 | Total 38 | C 31 | Mg 1 | N 4 | O 2 | 0 |
| 14 | bA | 1 | Total 53 | C 42 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bA | 1 | Total 38 | C 31 | Mg 1 | N 4 | O 2 | 0 |
| 14 | bA | 1 | Total 38 | C 31 | Mg 1 | N 4 | O 2 | 0 |
| 14 | bA | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bA | 1 | Total 51 | C 40 | Mg 1 | N 4 | O 6 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14 | bA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | bA | 1 | Total 50 | C 39 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bA | 1 | Total 51 | C 40 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bA | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bA | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bA | 1 | Total 53 | C 42 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bA | 1 | Total 51 | C 40 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bA | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | bA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | bA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | bA | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | bA | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bA | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bA | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | bB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14 | bB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bB | 1 | Total 50 | C 39 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bB | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | bB | 1 | Total 38 | C 31 | Mg 1 | N 4 | O 2 | 0 |
| 14 | bB | 1 | Total 38 | C 31 | Mg 1 | N 4 | O 2 | 0 |
| 14 | bB | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | bB | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | bB | 1 | Total 50 | C 39 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bB | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | bB | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | bB | 1 | Total 56 | C 45 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bB | 1 | Total 38 | C 31 | Mg 1 | N 4 | O 2 | 0 |
| 14 | bB | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | bB | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | bB | 1 | Total 56 | C 45 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bB | 1 | Total 38 | C 31 | Mg 1 | N 4 | O 2 | 0 |
| 14 | bB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | bB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14 | bB | 1 | Total | C | Mg | N | O | 0 |
| | | | 54 | 43 | 1 | 4 | 6 | |
| 14 | bB | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 14 | bB | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 44 | 1 | 4 | 6 | |
| 14 | bF | 1 | Total | C | Mg | N | O | 0 |
| | | | 38 | 31 | 1 | 4 | 2 | |
| 14 | bJ | 1 | Total | C | Mg | N | O | 0 |
| | | | 42 | 33 | 1 | 4 | 4 | |
| 14 | bK | 1 | Total | C | Mg | N | O | 0 |
| | | | 37 | 30 | 1 | 4 | 2 | |
| 14 | bL | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 14 | bL | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 14 | bL | 1 | Total | C | Mg | N | O | 0 |
| | | | 42 | 33 | 1 | 4 | 4 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 32 | 1 | 4 | 4 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 32 | 1 | 4 | 4 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 32 | 1 | 4 | 4 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 42 | 33 | 1 | 4 | 4 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 32 | 1 | 4 | 4 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 32 | 1 | 4 | 4 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 38 | 31 | 1 | 4 | 2 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 32 | 1 | 4 | 4 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 32 | 1 | 4 | 4 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 38 | 31 | 1 | 4 | 2 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 53 | 42 | 1 | 4 | 6 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 38 | 31 | 1 | 4 | 2 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 38 | 31 | 1 | 4 | 2 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 51 | 40 | 1 | 4 | 6 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 32 | 1 | 4 | 4 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 39 | 1 | 4 | 6 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 51 | 40 | 1 | 4 | 6 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 53 | 42 | 1 | 4 | 6 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 51 | 40 | 1 | 4 | 6 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 32 | 1 | 4 | 4 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 32 | 1 | 4 | 4 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 32 | 1 | 4 | 4 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 32 | 1 | 4 | 4 | |
| 14 | cA | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14 | cA | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | cA | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | cA | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | cA | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | cB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | cB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | cB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | cB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | cB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | cB | 1 | Total 50 | C 39 | Mg 1 | N 4 | O 6 | 0 |
| 14 | cB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 14 | cB | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | cB | 1 | Total 38 | C 31 | Mg 1 | N 4 | O 2 | 0 |
| 14 | cB | 1 | Total 38 | C 31 | Mg 1 | N 4 | O 2 | 0 |
| 14 | cB | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | cB | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | cB | 1 | Total 50 | C 39 | Mg 1 | N 4 | O 6 | 0 |
| 14 | cB | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | cB | 1 | Total 41 | C 32 | Mg 1 | N 4 | O 4 | 0 |
| 14 | cB | 1 | Total 56 | C 45 | Mg 1 | N 4 | O 6 | 0 |
| 14 | cB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14 | cB | 1 | Total | C | Mg | N | O | 0 |
| | | | 38 | 31 | 1 | 4 | 2 | |
| 14 | cB | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 32 | 1 | 4 | 4 | |
| 14 | cB | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 32 | 1 | 4 | 4 | |
| 14 | cB | 1 | Total | C | Mg | N | O | 0 |
| | | | 56 | 45 | 1 | 4 | 6 | |
| 14 | cB | 1 | Total | C | Mg | N | O | 0 |
| | | | 38 | 31 | 1 | 4 | 2 | |
| 14 | cB | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 14 | cB | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 14 | cB | 1 | Total | C | Mg | N | O | 0 |
| | | | 54 | 43 | 1 | 4 | 6 | |
| 14 | cB | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 14 | cB | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 44 | 1 | 4 | 6 | |
| 14 | cF | 1 | Total | C | Mg | N | O | 0 |
| | | | 38 | 31 | 1 | 4 | 2 | |
| 14 | cJ | 1 | Total | C | Mg | N | O | 0 |
| | | | 42 | 33 | 1 | 4 | 4 | |
| 14 | cK | 1 | Total | C | Mg | N | O | 0 |
| | | | 37 | 30 | 1 | 4 | 2 | |
| 14 | cL | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 14 | cL | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 14 | cL | 1 | Total | C | Mg | N | O | 0 |
| | | | 42 | 33 | 1 | 4 | 4 | |

- Molecule 15 is UNKNOWN LIGAND (three-letter code: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

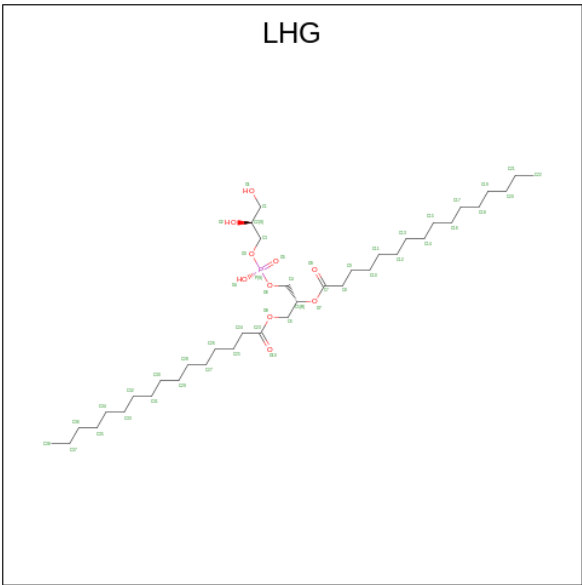
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|-----|---------|
| 15 | aA | 4 | Total | C | 0 |
| | | | 150 | 150 | |
| 15 | aB | 3 | Total | C | 0 |
| | | | 120 | 120 | |
| 15 | aI | 2 | Total | C | 0 |
| | | | 80 | 80 | |

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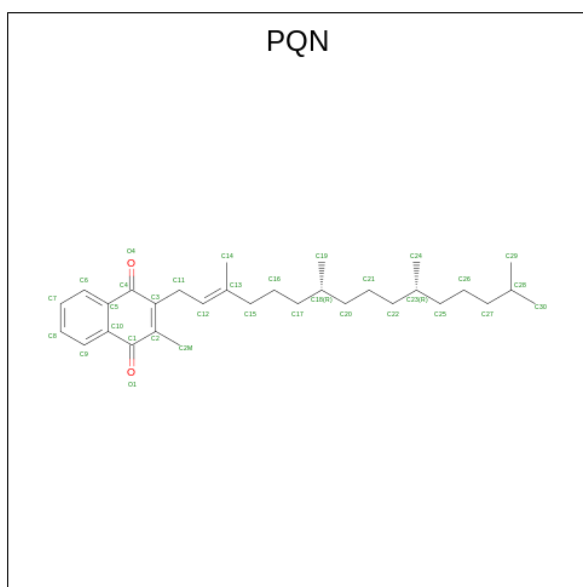
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|--------------|----------|---------|
| 15 | aJ | 1 | Total 40 | C 40 | 0 |
| 15 | aL | 2 | Total 80 | C 80 | 0 |
| 15 | bA | 4 | Total 150 | C 150 | 0 |
| 15 | bB | 3 | Total 120 | C 120 | 0 |
| 15 | bI | 2 | Total 80 | C 80 | 0 |
| 15 | bJ | 1 | Total 40 | C 40 | 0 |
| 15 | bL | 2 | Total 80 | C 80 | 0 |
| 15 | cA | 3 | Total 110 | C 110 | 0 |
| 15 | cB | 3 | Total 120 | C 120 | 0 |
| 15 | cF | 1 | Total 40 | C 40 | 0 |
| 15 | cI | 2 | Total 80 | C 80 | 0 |
| 15 | cJ | 1 | Total 40 | C 40 | 0 |
| 15 | cL | 2 | Total 80 | C 80 | 0 |

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



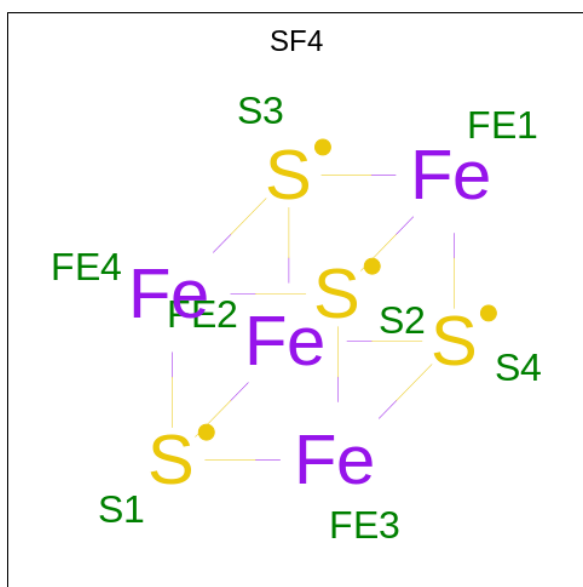
| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 16 | aA | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |
| 16 | aA | 1 | Total | C | O | P | 0 |
| | | | 21 | 12 | 8 | 1 | |
| 16 | bA | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |
| 16 | bA | 1 | Total | C | O | P | 0 |
| | | | 21 | 12 | 8 | 1 | |
| 16 | cA | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |
| 16 | cA | 1 | Total | C | O | P | 0 |
| | | | 21 | 12 | 8 | 1 | |

- Molecule 17 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



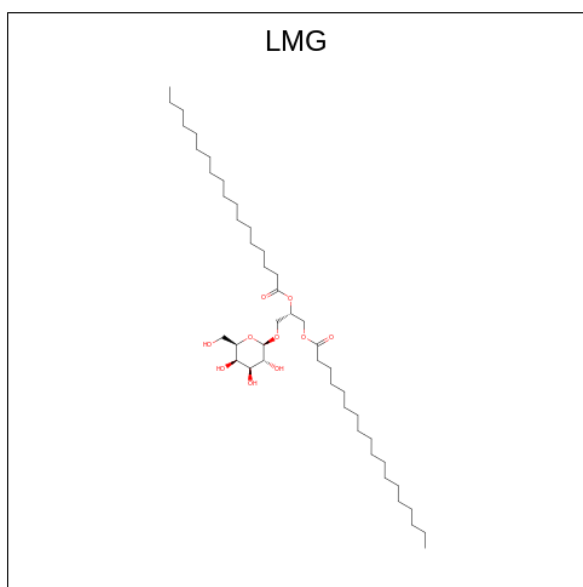
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 17 | aA | 1 | Total | C | O | 0 |
| | | | 33 | 31 | 2 | |
| 17 | aB | 1 | Total | C | O | 0 |
| | | | 33 | 31 | 2 | |
| 17 | bA | 1 | Total | C | O | 0 |
| | | | 33 | 31 | 2 | |
| 17 | bB | 1 | Total | C | O | 0 |
| | | | 33 | 31 | 2 | |
| 17 | cA | 1 | Total | C | O | 0 |
| | | | 33 | 31 | 2 | |
| 17 | cB | 1 | Total | C | O | 0 |
| | | | 33 | 31 | 2 | |

- Molecule 18 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 18 | aB | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 18 | aC | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 18 | aC | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 18 | bB | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 18 | bC | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 18 | bC | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 18 | cB | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 18 | cC | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 18 | cC | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |

- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 19 | aB | 1 | Total | C | O | 0 |
| | | | 52 | 42 | 10 | |
| 19 | bB | 1 | Total | C | O | 0 |
| | | | 52 | 42 | 10 | |
| 19 | cB | 1 | Total | C | O | 0 |
| | | | 52 | 42 | 10 | |

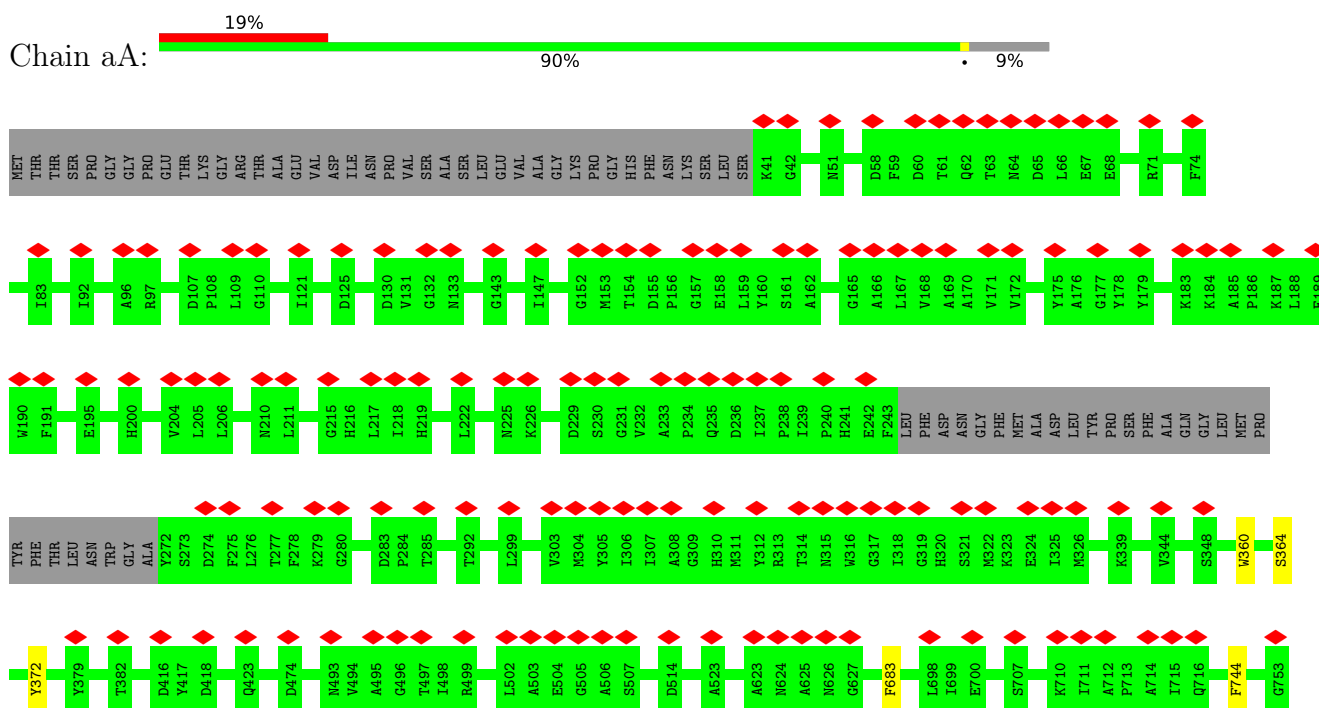
- Molecule 20 is water.

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 20 | aA | 13 | Total | O | 0 |
| | | | 13 | 13 | |
| 20 | aB | 12 | Total | O | 0 |
| | | | 12 | 12 | |
| 20 | aL | 3 | Total | O | 0 |
| | | | 3 | 3 | |
| 20 | bA | 12 | Total | O | 0 |
| | | | 12 | 12 | |
| 20 | bB | 13 | Total | O | 0 |
| | | | 13 | 13 | |
| 20 | bL | 3 | Total | O | 0 |
| | | | 3 | 3 | |
| 20 | cA | 13 | Total | O | 0 |
| | | | 13 | 13 | |
| 20 | cB | 12 | Total | O | 0 |
| | | | 12 | 12 | |
| 20 | cL | 3 | Total | O | 0 |
| | | | 3 | 3 | |

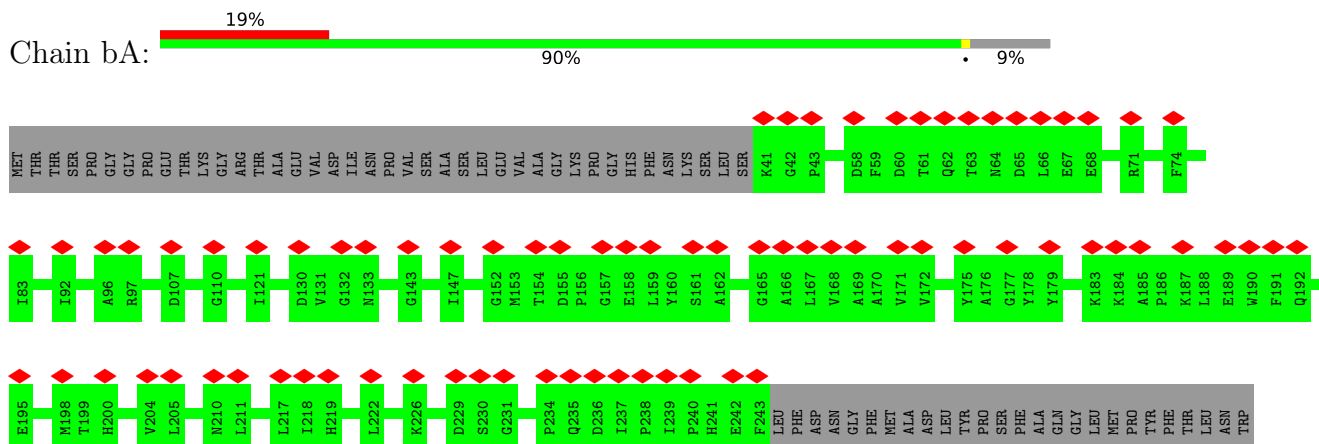
3 Residue-property plots

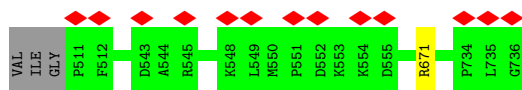
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



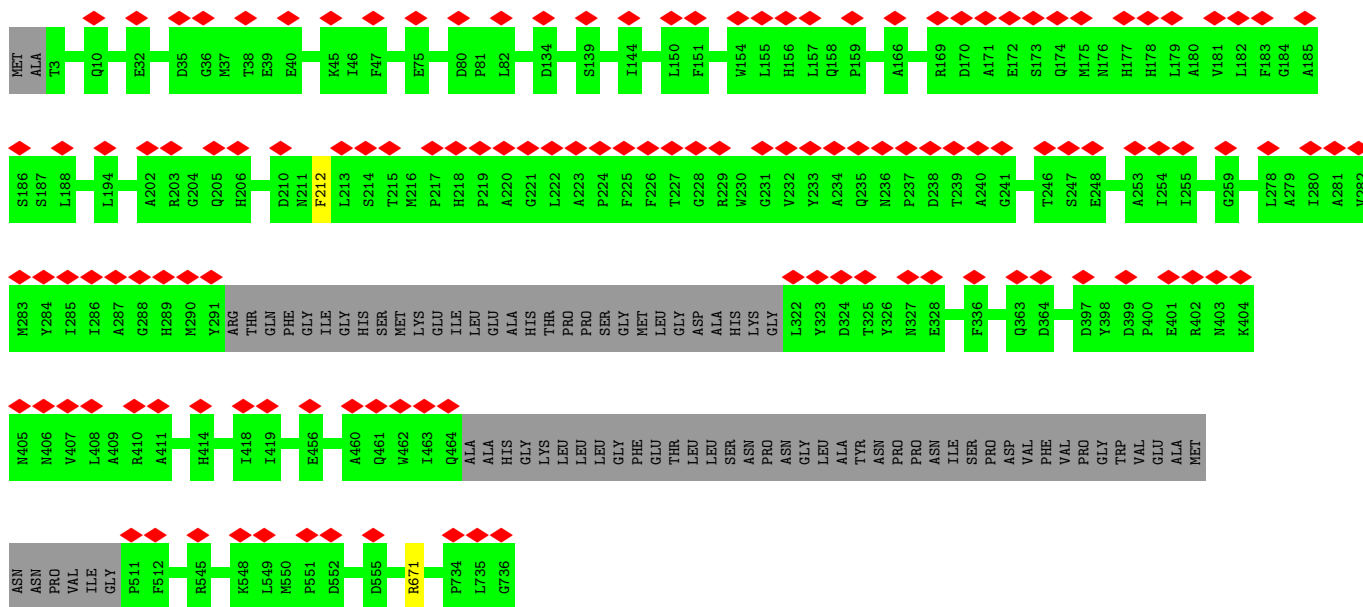
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





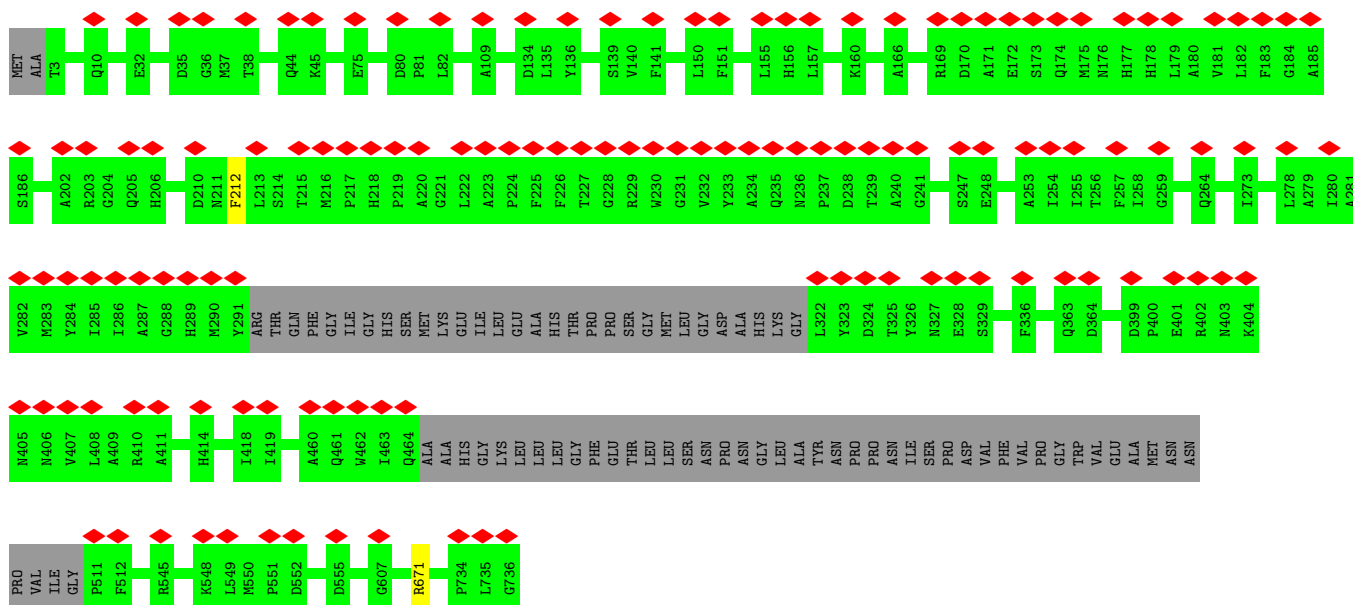
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain bB: 18% 89% 11%

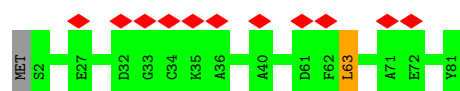


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

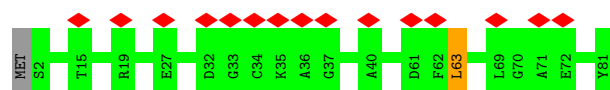
Chain cB: 18% 89% 11%



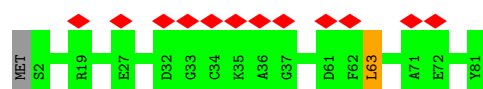
- Molecule 3: Photosystem I iron-sulfur center



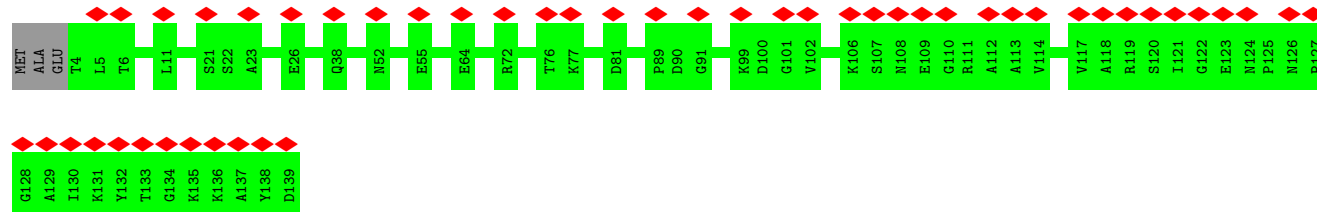
- Molecule 3: Photosystem I iron-sulfur center



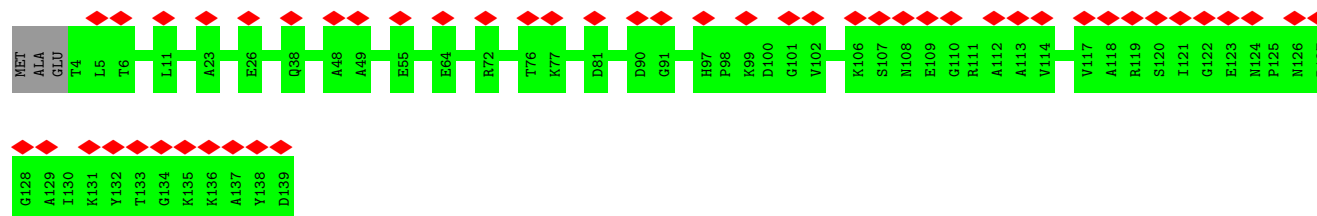
- Molecule 3: Photosystem I iron-sulfur center



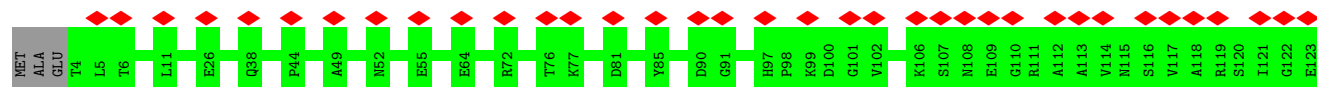
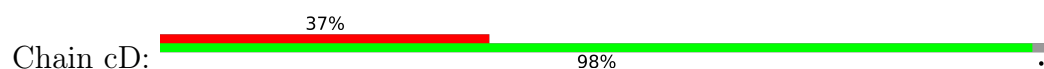
- Molecule 4: Photosystem I protein PsaD

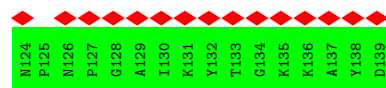


- Molecule 4: Photosystem I protein PsaD

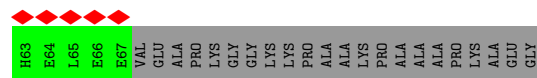
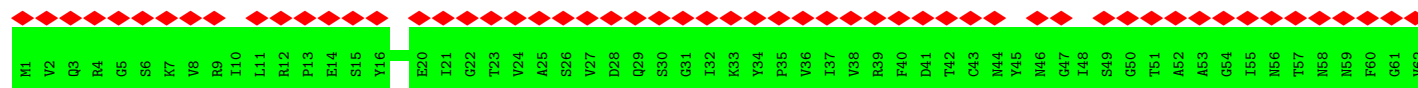
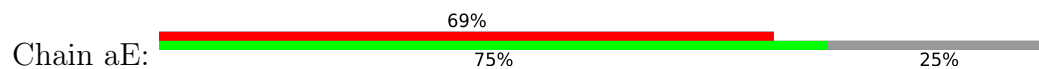


- Molecule 4: Photosystem I protein PsaD

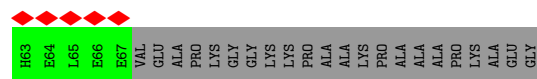
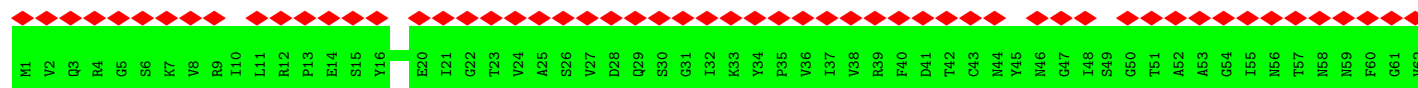
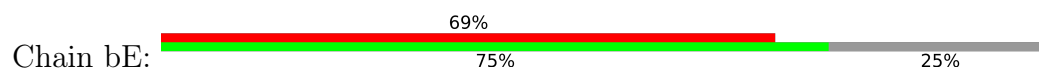




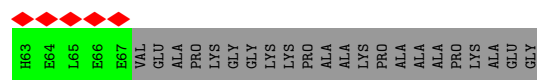
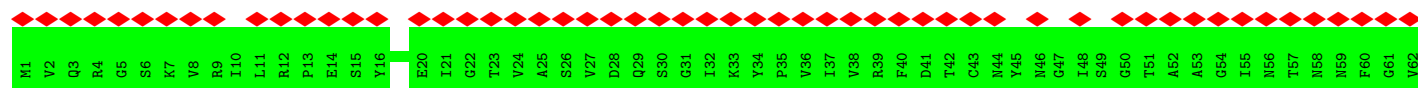
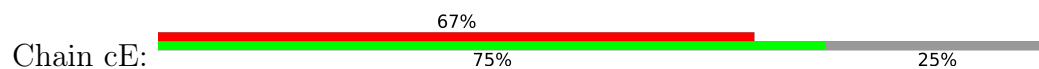
• Molecule 5: Photosystem I reaction center subunit IV



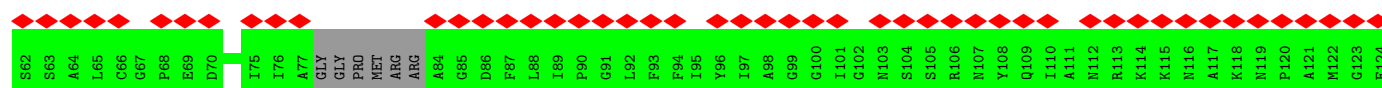
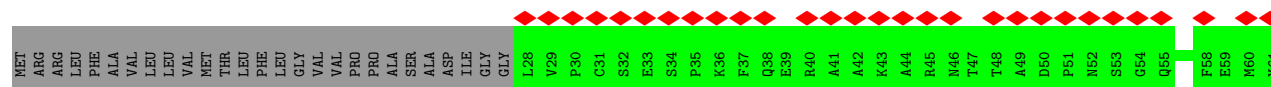
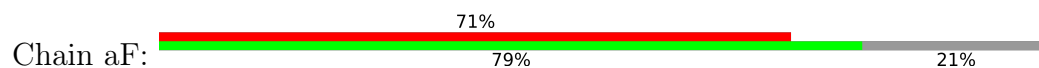
• Molecule 5: Photosystem I reaction center subunit IV

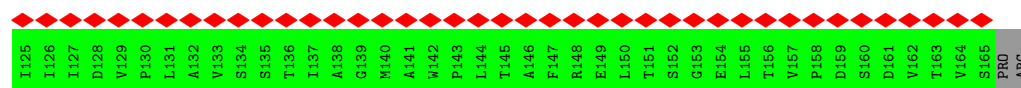


• Molecule 5: Photosystem I reaction center subunit IV

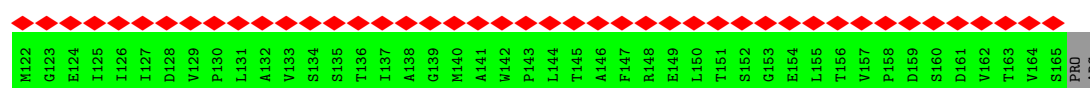
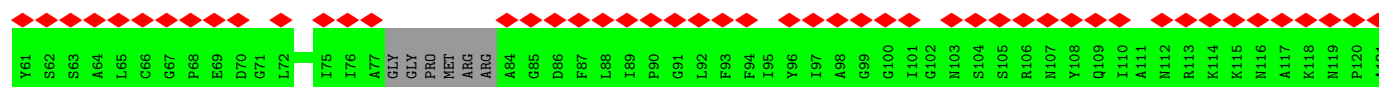
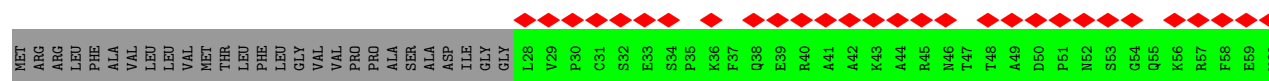
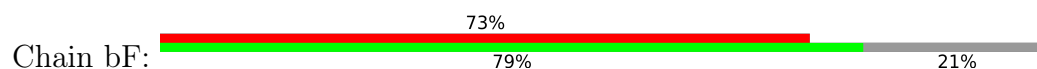


• Molecule 6: Photosystem I protein PsaF

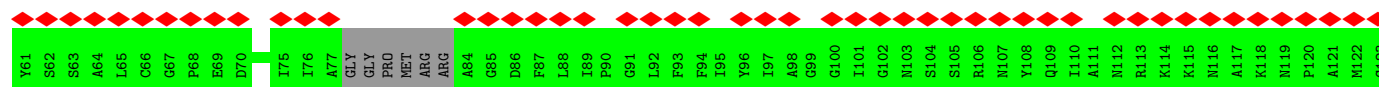
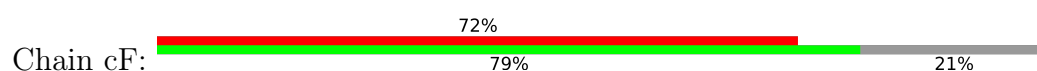




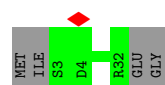
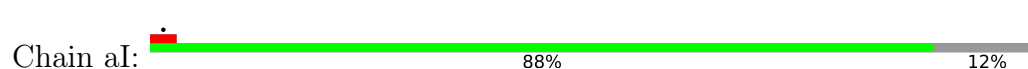
- Molecule 6: Photosystem I protein Psaf



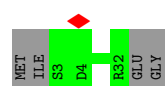
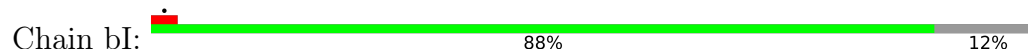
- Molecule 6: Photosystem I protein Psaf




- Molecule 7: Photosystem I protein Psaf27

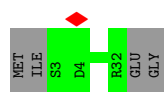


- Molecule 7: Photosystem I protein Psaf27



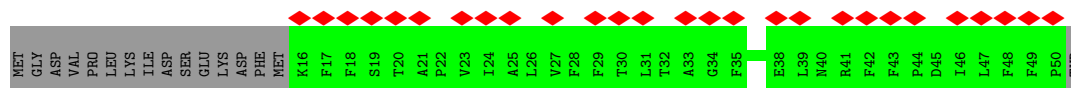
- Molecule 7: Photosystem I protein Psaf27

Chain cI:  88% 12%



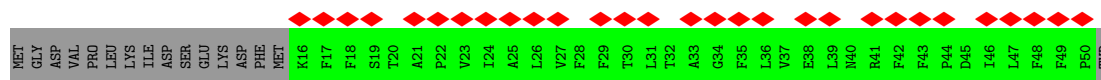
- Molecule 8: Photosystem I reaction center subunit IX

Chain aJ:  53% 69% 31%



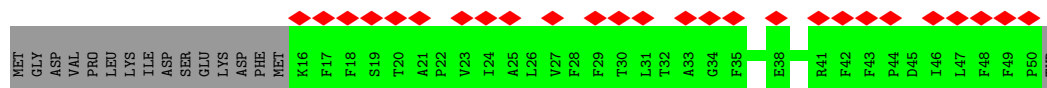
- Molecule 8: Photosystem I reaction center subunit IX

Chain bJ:  57% 69% 31%




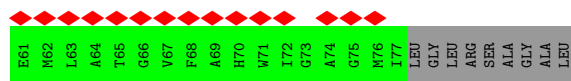
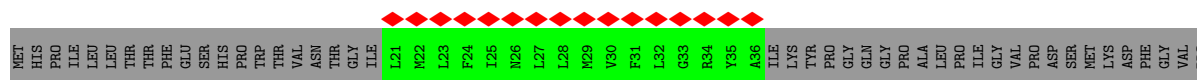
- Molecule 8: Photosystem I reaction center subunit IX

Chain cJ:  51% 69% 31%



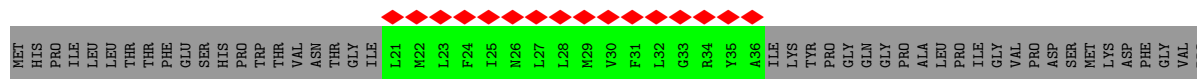
- Molecule 9: Photosystem I reaction center subunit PsaK

Chain aK:  36% 38% 62%

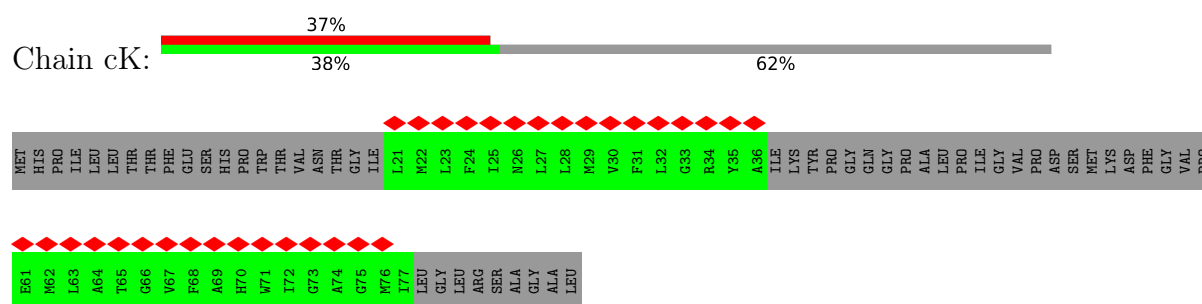


- Molecule 9: Photosystem I reaction center subunit PsaK

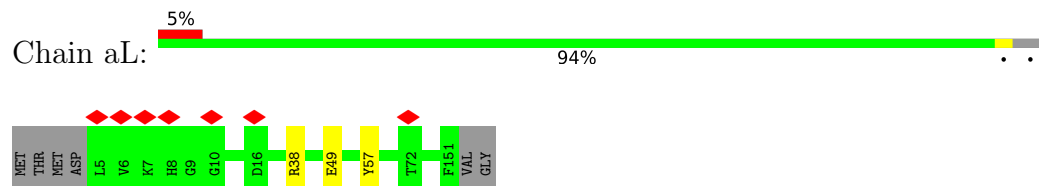
Chain bK:  37% 38% 62%



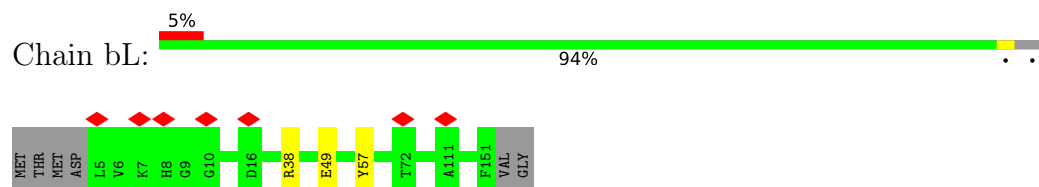
- Molecule 9: Photosystem I reaction center subunit PsaK



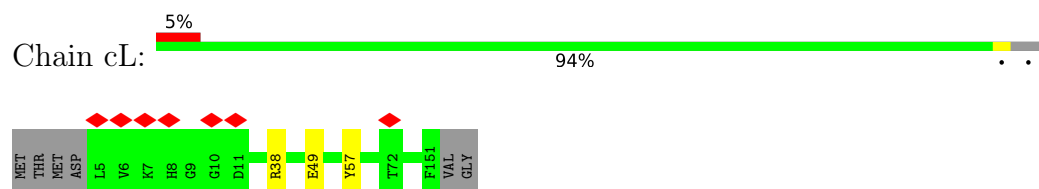
- Molecule 10: Photosystem I protein PsaL



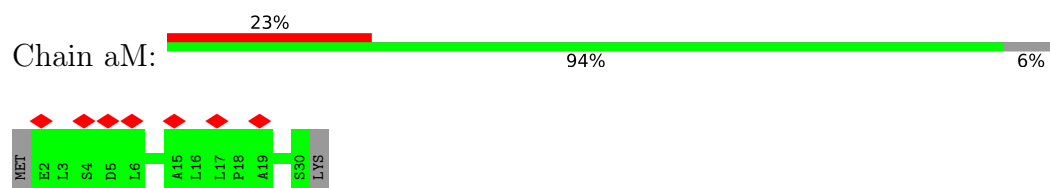
- Molecule 10: Photosystem I protein PsaL



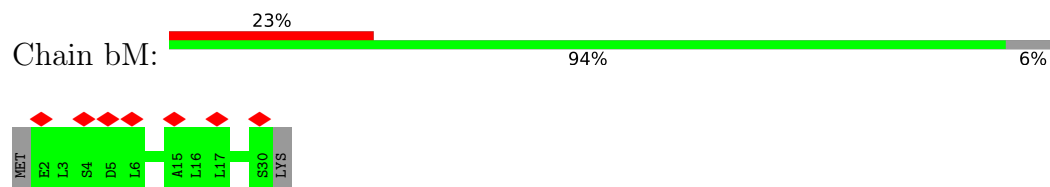
- Molecule 10: Photosystem I protein PsaL



- Molecule 11: Photosystem I protein PsaM

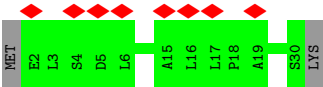


- Molecule 11: Photosystem I protein PsaM



- Molecule 11: Photosystem I protein PsaM





4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 86419 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | JEOL CRYO ARM 300 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 85.7 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 0.075 | Depositor |
| Minimum map value | -0.047 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.001 | Depositor |
| Recommended contour level | 0.00637 | Depositor |
| Map size (\AA) | 356.40002, 356.40002, 356.40002 | wwPDB |
| Map dimensions | 330, 330, 330 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 1.08, 1.08, 1.08 | 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: G9R, PQN, SF4, PHO, CL7, LHG, UNL, LMG

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 | aA | 0.77 | 2/5369 (0.0%) | 0.78 | 0/7326 |
| 1 | bA | 0.77 | 2/5369 (0.0%) | 0.78 | 0/7326 |
| 1 | cA | 0.77 | 2/5369 (0.0%) | 0.78 | 0/7326 |
| 2 | aB | 0.74 | 1/5185 (0.0%) | 0.75 | 1/7107 (0.0%) |
| 2 | bB | 0.74 | 1/5185 (0.0%) | 0.76 | 1/7107 (0.0%) |
| 2 | cB | 0.74 | 1/5185 (0.0%) | 0.76 | 1/7107 (0.0%) |
| 3 | aC | 0.70 | 0/582 | 0.79 | 0/792 |
| 3 | bC | 0.70 | 0/582 | 0.78 | 0/792 |
| 3 | cC | 0.70 | 0/582 | 0.78 | 0/792 |
| 4 | aD | 0.62 | 0/1018 | 0.68 | 0/1379 |
| 4 | bD | 0.62 | 0/1018 | 0.68 | 0/1379 |
| 4 | cD | 0.62 | 0/1018 | 0.68 | 0/1379 |
| 5 | aE | 0.77 | 0/379 | 0.67 | 0/524 |
| 5 | bE | 0.75 | 0/379 | 0.67 | 0/524 |
| 5 | cE | 0.77 | 0/379 | 0.67 | 0/524 |
| 6 | aF | 0.67 | 0/863 | 0.66 | 0/1183 |
| 6 | bF | 0.66 | 0/863 | 0.65 | 0/1183 |
| 6 | cF | 0.66 | 0/863 | 0.66 | 0/1183 |
| 7 | aI | 0.67 | 0/230 | 0.79 | 0/313 |
| 7 | bI | 0.68 | 0/230 | 0.79 | 0/313 |
| 7 | cI | 0.68 | 0/230 | 0.79 | 0/313 |
| 8 | aJ | 0.57 | 0/273 | 0.59 | 0/373 |
| 8 | bJ | 0.58 | 0/273 | 0.59 | 0/373 |
| 8 | cJ | 0.57 | 0/273 | 0.59 | 0/373 |
| 9 | aK | 0.81 | 0/159 | 0.69 | 0/217 |
| 9 | bK | 0.81 | 0/159 | 0.69 | 0/217 |
| 9 | cK | 0.81 | 0/159 | 0.69 | 0/217 |
| 10 | aL | 0.82 | 1/1020 (0.1%) | 0.79 | 1/1394 (0.1%) |
| 10 | bL | 0.82 | 1/1020 (0.1%) | 0.79 | 1/1394 (0.1%) |
| 10 | cL | 0.81 | 1/1020 (0.1%) | 0.79 | 1/1394 (0.1%) |
| 11 | aM | 0.66 | 0/205 | 0.70 | 0/281 |
| 11 | bM | 0.66 | 0/205 | 0.71 | 0/281 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 11 | cM | 0.66 | 0/205 | 0.71 | 0/281 |
| All | All | 0.74 | 12/45849 (0.0%) | 0.75 | 6/62667 (0.0%) |

The worst 5 of 12 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | cB | 212 | PHE | C-N | 8.20 | 1.52 | 1.34 |
| 2 | bB | 212 | PHE | C-N | 8.20 | 1.52 | 1.34 |
| 2 | aB | 212 | PHE | C-N | 8.12 | 1.52 | 1.34 |
| 10 | aL | 49 | GLU | CD-OE2 | -5.71 | 1.19 | 1.25 |
| 10 | bL | 49 | GLU | CD-OE2 | -5.43 | 1.19 | 1.25 |

The worst 5 of 6 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | cB | 671 | ARG | NE-CZ-NH2 | -6.26 | 117.17 | 120.30 |
| 2 | aB | 671 | ARG | NE-CZ-NH2 | -6.25 | 117.18 | 120.30 |
| 2 | bB | 671 | ARG | NE-CZ-NH2 | -6.14 | 117.23 | 120.30 |
| 10 | cL | 38 | ARG | NE-CZ-NH2 | -5.34 | 117.63 | 120.30 |
| 10 | bL | 38 | ARG | NE-CZ-NH2 | -5.29 | 117.66 | 120.30 |

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 | aA | 5203 | 0 | 4894 | 0 | 0 |
| 1 | bA | 5203 | 0 | 4894 | 0 | 0 |
| 1 | cA | 5203 | 0 | 4894 | 0 | 0 |
| 2 | aB | 5007 | 0 | 4607 | 0 | 0 |
| 2 | bB | 5007 | 0 | 4607 | 0 | 0 |
| 2 | cB | 5007 | 0 | 4607 | 0 | 0 |
| 3 | aC | 573 | 0 | 543 | 0 | 0 |
| 3 | bC | 573 | 0 | 543 | 0 | 0 |
| 3 | cC | 573 | 0 | 543 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | aD | 999 | 0 | 981 | 0 | 0 |
| 4 | bD | 999 | 0 | 981 | 0 | 0 |
| 4 | cD | 999 | 0 | 981 | 0 | 0 |
| 5 | aE | 375 | 0 | 218 | 0 | 0 |
| 5 | bE | 375 | 0 | 218 | 0 | 0 |
| 5 | cE | 375 | 0 | 218 | 0 | 0 |
| 6 | aF | 847 | 0 | 707 | 0 | 0 |
| 6 | bF | 847 | 0 | 707 | 0 | 0 |
| 6 | cF | 847 | 0 | 707 | 0 | 0 |
| 7 | aI | 225 | 0 | 231 | 0 | 0 |
| 7 | bI | 225 | 0 | 231 | 0 | 0 |
| 7 | cI | 225 | 0 | 231 | 0 | 0 |
| 8 | aJ | 264 | 0 | 237 | 0 | 0 |
| 8 | bJ | 264 | 0 | 237 | 0 | 0 |
| 8 | cJ | 264 | 0 | 237 | 0 | 0 |
| 9 | aK | 161 | 0 | 80 | 0 | 0 |
| 9 | bK | 161 | 0 | 80 | 0 | 0 |
| 9 | cK | 161 | 0 | 80 | 0 | 0 |
| 10 | aL | 999 | 0 | 976 | 0 | 0 |
| 10 | bL | 999 | 0 | 976 | 0 | 0 |
| 10 | cL | 999 | 0 | 976 | 0 | 0 |
| 11 | aM | 205 | 0 | 232 | 0 | 0 |
| 11 | bM | 205 | 0 | 232 | 0 | 0 |
| 11 | cM | 205 | 0 | 232 | 0 | 0 |
| 12 | aA | 65 | 0 | 0 | 0 | 0 |
| 12 | bA | 65 | 0 | 0 | 0 | 0 |
| 12 | cA | 65 | 0 | 0 | 0 | 0 |
| 13 | aA | 64 | 0 | 74 | 0 | 0 |
| 13 | aB | 64 | 0 | 74 | 0 | 0 |
| 13 | bB | 128 | 0 | 148 | 0 | 0 |
| 13 | cB | 128 | 0 | 148 | 0 | 0 |
| 14 | aA | 1862 | 0 | 1586 | 0 | 0 |
| 14 | aB | 1410 | 0 | 1250 | 0 | 0 |
| 14 | aF | 38 | 0 | 24 | 0 | 0 |
| 14 | aJ | 42 | 0 | 28 | 0 | 0 |
| 14 | aK | 37 | 0 | 23 | 0 | 0 |
| 14 | aL | 172 | 0 | 169 | 0 | 0 |
| 14 | bA | 1862 | 0 | 1586 | 0 | 0 |
| 14 | bB | 1410 | 0 | 1250 | 0 | 0 |
| 14 | bF | 38 | 0 | 24 | 0 | 0 |
| 14 | bJ | 42 | 0 | 28 | 0 | 0 |
| 14 | bK | 37 | 0 | 23 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 14 | bL | 172 | 0 | 169 | 0 | 0 |
| 14 | cA | 1862 | 0 | 1586 | 0 | 0 |
| 14 | cB | 1410 | 0 | 1250 | 0 | 0 |
| 14 | cF | 38 | 0 | 24 | 0 | 0 |
| 14 | cJ | 42 | 0 | 28 | 0 | 0 |
| 14 | cK | 37 | 0 | 23 | 0 | 0 |
| 14 | cL | 172 | 0 | 169 | 0 | 0 |
| 15 | aA | 150 | 0 | 0 | 0 | 0 |
| 15 | aB | 120 | 0 | 0 | 0 | 0 |
| 15 | aI | 80 | 0 | 0 | 0 | 0 |
| 15 | aJ | 40 | 0 | 0 | 0 | 0 |
| 15 | aL | 80 | 0 | 0 | 0 | 0 |
| 15 | bA | 150 | 0 | 0 | 0 | 0 |
| 15 | bB | 120 | 0 | 0 | 0 | 0 |
| 15 | bI | 80 | 0 | 0 | 0 | 0 |
| 15 | bJ | 40 | 0 | 0 | 0 | 0 |
| 15 | bL | 80 | 0 | 0 | 0 | 0 |
| 15 | cA | 110 | 0 | 0 | 0 | 0 |
| 15 | cB | 120 | 0 | 0 | 0 | 0 |
| 15 | cF | 40 | 0 | 0 | 0 | 0 |
| 15 | cI | 80 | 0 | 0 | 0 | 0 |
| 15 | cJ | 40 | 0 | 0 | 0 | 0 |
| 15 | cL | 80 | 0 | 0 | 0 | 0 |
| 16 | aA | 70 | 0 | 91 | 0 | 0 |
| 16 | bA | 70 | 0 | 90 | 0 | 0 |
| 16 | cA | 70 | 0 | 90 | 0 | 0 |
| 17 | aA | 33 | 0 | 46 | 0 | 0 |
| 17 | aB | 33 | 0 | 46 | 0 | 0 |
| 17 | bA | 33 | 0 | 46 | 0 | 0 |
| 17 | bB | 33 | 0 | 46 | 0 | 0 |
| 17 | cA | 33 | 0 | 46 | 0 | 0 |
| 17 | cB | 33 | 0 | 46 | 0 | 0 |
| 18 | aB | 8 | 0 | 0 | 0 | 0 |
| 18 | aC | 16 | 0 | 0 | 0 | 0 |
| 18 | bB | 8 | 0 | 0 | 0 | 0 |
| 18 | bC | 16 | 0 | 0 | 0 | 0 |
| 18 | cB | 8 | 0 | 0 | 0 | 0 |
| 18 | cC | 16 | 0 | 0 | 0 | 0 |
| 19 | aB | 52 | 0 | 77 | 0 | 0 |
| 19 | bB | 52 | 0 | 77 | 0 | 0 |
| 19 | cB | 52 | 0 | 77 | 0 | 0 |
| 20 | aA | 13 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 20 | aB | 12 | 0 | 0 | 0 | 0 |
| 20 | aL | 3 | 0 | 0 | 0 | 0 |
| 20 | bA | 12 | 0 | 0 | 0 | 0 |
| 20 | bB | 13 | 0 | 0 | 0 | 0 |
| 20 | bL | 3 | 0 | 0 | 0 | 0 |
| 20 | cA | 13 | 0 | 0 | 0 | 0 |
| 20 | cB | 12 | 0 | 0 | 0 | 0 |
| 20 | cL | 3 | 0 | 0 | 0 | 0 |
| All | All | 57966 | 0 | 51580 | 0 | 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 11.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1 | aA | 681/753 (90%) | 637 (94%) | 44 (6%) | 0 | 100 | 100 |
| 1 | bA | 681/753 (90%) | 635 (93%) | 46 (7%) | 0 | 100 | 100 |
| 1 | cA | 681/753 (90%) | 637 (94%) | 44 (6%) | 0 | 100 | 100 |
| 2 | aB | 652/736 (89%) | 616 (94%) | 36 (6%) | 0 | 100 | 100 |
| 2 | bB | 652/736 (89%) | 616 (94%) | 36 (6%) | 0 | 100 | 100 |
| 2 | cB | 652/736 (89%) | 616 (94%) | 36 (6%) | 0 | 100 | 100 |
| 3 | aC | 78/81 (96%) | 72 (92%) | 5 (6%) | 1 (1%) | 10 | 19 |
| 3 | bC | 78/81 (96%) | 72 (92%) | 5 (6%) | 1 (1%) | 10 | 19 |
| 3 | cC | 78/81 (96%) | 72 (92%) | 5 (6%) | 1 (1%) | 10 | 19 |
| 4 | aD | 134/139 (96%) | 126 (94%) | 8 (6%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 4 | bD | 134/139 (96%) | 126 (94%) | 8 (6%) | 0 | 100 | 100 |
| 4 | cD | 134/139 (96%) | 126 (94%) | 8 (6%) | 0 | 100 | 100 |
| 5 | aE | 65/89 (73%) | 61 (94%) | 4 (6%) | 0 | 100 | 100 |
| 5 | bE | 65/89 (73%) | 61 (94%) | 4 (6%) | 0 | 100 | 100 |
| 5 | cE | 65/89 (73%) | 61 (94%) | 4 (6%) | 0 | 100 | 100 |
| 6 | aF | 128/167 (77%) | 120 (94%) | 8 (6%) | 0 | 100 | 100 |
| 6 | bF | 128/167 (77%) | 120 (94%) | 8 (6%) | 0 | 100 | 100 |
| 6 | cF | 128/167 (77%) | 119 (93%) | 9 (7%) | 0 | 100 | 100 |
| 7 | aI | 28/34 (82%) | 27 (96%) | 1 (4%) | 0 | 100 | 100 |
| 7 | bI | 28/34 (82%) | 27 (96%) | 1 (4%) | 0 | 100 | 100 |
| 7 | cI | 28/34 (82%) | 27 (96%) | 1 (4%) | 0 | 100 | 100 |
| 8 | aJ | 33/51 (65%) | 31 (94%) | 2 (6%) | 0 | 100 | 100 |
| 8 | bJ | 33/51 (65%) | 31 (94%) | 2 (6%) | 0 | 100 | 100 |
| 8 | cJ | 33/51 (65%) | 31 (94%) | 2 (6%) | 0 | 100 | 100 |
| 9 | aK | 29/86 (34%) | 29 (100%) | 0 | 0 | 100 | 100 |
| 9 | bK | 29/86 (34%) | 29 (100%) | 0 | 0 | 100 | 100 |
| 9 | cK | 29/86 (34%) | 29 (100%) | 0 | 0 | 100 | 100 |
| 10 | aL | 145/153 (95%) | 142 (98%) | 3 (2%) | 0 | 100 | 100 |
| 10 | bL | 145/153 (95%) | 142 (98%) | 3 (2%) | 0 | 100 | 100 |
| 10 | cL | 145/153 (95%) | 142 (98%) | 3 (2%) | 0 | 100 | 100 |
| 11 | aM | 27/31 (87%) | 27 (100%) | 0 | 0 | 100 | 100 |
| 11 | bM | 27/31 (87%) | 27 (100%) | 0 | 0 | 100 | 100 |
| 11 | cM | 27/31 (87%) | 27 (100%) | 0 | 0 | 100 | 100 |
| All | All | 6000/6960 (86%) | 5661 (94%) | 336 (6%) | 3 (0%) | 50 | 69 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | aC | 63 | LEU |
| 3 | cC | 63 | LEU |
| 3 | bC | 63 | LEU |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1 | aA | 500/606 (82%) | 497 (99%) | 3 (1%) | 84 | 94 |
| 1 | bA | 500/606 (82%) | 497 (99%) | 3 (1%) | 84 | 94 |
| 1 | cA | 500/606 (82%) | 497 (99%) | 3 (1%) | 84 | 94 |
| 2 | aB | 471/594 (79%) | 471 (100%) | 0 | 100 | 100 |
| 2 | bB | 471/594 (79%) | 471 (100%) | 0 | 100 | 100 |
| 2 | cB | 471/594 (79%) | 471 (100%) | 0 | 100 | 100 |
| 3 | aC | 60/69 (87%) | 59 (98%) | 1 (2%) | 56 | 79 |
| 3 | bC | 60/69 (87%) | 59 (98%) | 1 (2%) | 56 | 79 |
| 3 | cC | 60/69 (87%) | 59 (98%) | 1 (2%) | 56 | 79 |
| 4 | aD | 99/112 (88%) | 99 (100%) | 0 | 100 | 100 |
| 4 | bD | 99/112 (88%) | 99 (100%) | 0 | 100 | 100 |
| 4 | cD | 99/112 (88%) | 99 (100%) | 0 | 100 | 100 |
| 5 | aE | 11/69 (16%) | 11 (100%) | 0 | 100 | 100 |
| 5 | bE | 11/69 (16%) | 11 (100%) | 0 | 100 | 100 |
| 5 | cE | 11/69 (16%) | 11 (100%) | 0 | 100 | 100 |
| 6 | aF | 62/133 (47%) | 62 (100%) | 0 | 100 | 100 |
| 6 | bF | 62/133 (47%) | 62 (100%) | 0 | 100 | 100 |
| 6 | cF | 62/133 (47%) | 62 (100%) | 0 | 100 | 100 |
| 7 | aI | 23/26 (88%) | 23 (100%) | 0 | 100 | 100 |
| 7 | bI | 23/26 (88%) | 23 (100%) | 0 | 100 | 100 |
| 7 | cI | 23/26 (88%) | 23 (100%) | 0 | 100 | 100 |
| 8 | aJ | 23/46 (50%) | 23 (100%) | 0 | 100 | 100 |
| 8 | bJ | 23/46 (50%) | 23 (100%) | 0 | 100 | 100 |
| 8 | cJ | 23/46 (50%) | 23 (100%) | 0 | 100 | 100 |
| 10 | aL | 96/112 (86%) | 95 (99%) | 1 (1%) | 73 | 88 |
| 10 | bL | 96/112 (86%) | 95 (99%) | 1 (1%) | 73 | 88 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 10 | cL | 96/112 (86%) | 95 (99%) | 1 (1%) | 73 | 88 |
| 11 | aM | 23/25 (92%) | 23 (100%) | 0 | 100 | 100 |
| 11 | bM | 23/25 (92%) | 23 (100%) | 0 | 100 | 100 |
| 11 | cM | 23/25 (92%) | 23 (100%) | 0 | 100 | 100 |
| All | All | 4104/5376 (76%) | 4089 (100%) | 15 (0%) | 88 | 96 |

5 of 15 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | bA | 744 | PHE |
| 3 | cC | 63 | LEU |
| 3 | bC | 63 | LEU |
| 10 | cL | 57 | TYR |
| 1 | cA | 372 | TYR |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | bA | 608 | ASN |
| 3 | bC | 38 | GLN |
| 2 | cB | 337 | HIS |
| 2 | bB | 685 | HIS |
| 1 | cA | 94 | HIS |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 279 ligands modelled in this entry, 36 are unknown - leaving 243 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 14 | CL7 | cA | 3105 | - | 42,49,73 | 2.90 | 15 (35%) | 36,84,113 | 2.18 | 14 (38%) |
| 14 | CL7 | cB | 816 | - | 51,58,73 | 2.70 | 21 (41%) | 47,95,113 | 1.97 | 12 (25%) |
| 14 | CL7 | aA | 3117 | - | 54,61,73 | 2.35 | 18 (33%) | 50,98,113 | 1.84 | 14 (28%) |
| 14 | CL7 | bA | 3116 | - | 54,61,73 | 2.41 | 19 (35%) | 50,98,113 | 1.91 | 13 (26%) |
| 14 | CL7 | aB | 3032 | - | 56,63,73 | 2.51 | 20 (35%) | 53,101,113 | 1.69 | 12 (22%) |
| 14 | CL7 | aA | 3123 | - | 51,58,73 | 2.36 | 17 (33%) | 47,95,113 | 2.23 | 15 (31%) |
| 18 | SF4 | bC | 102 | 3 | 0,12,12 | - | - | - | - | - |
| 14 | CL7 | aA | 3121 | - | 52,59,73 | 2.40 | 16 (30%) | 48,96,113 | 2.00 | 12 (25%) |
| 14 | CL7 | aA | 3109 | 1 | 43,50,73 | 2.71 | 17 (39%) | 36,85,113 | 1.73 | 9 (25%) |
| 14 | CL7 | bA | 3118 | - | 39,46,73 | 2.77 | 19 (48%) | 30,80,113 | 1.67 | 5 (16%) |
| 14 | CL7 | bA | 3107 | - | 66,73,73 | 2.31 | 19 (28%) | 65,113,113 | 1.59 | 10 (15%) |
| 14 | CL7 | cA | 3114 | - | 66,73,73 | 2.15 | 17 (25%) | 65,113,113 | 1.88 | 20 (30%) |
| 14 | CL7 | aK | 101 | - | 38,45,73 | 2.85 | 14 (36%) | 31,78,113 | 1.61 | 6 (19%) |
| 14 | CL7 | cA | 3126 | 1 | 54,61,73 | 2.48 | 16 (29%) | 51,97,113 | 1.63 | 9 (17%) |
| 14 | CL7 | aB | 3022 | - | 42,49,73 | 2.64 | 15 (35%) | 36,84,113 | 2.03 | 12 (33%) |
| 14 | CL7 | aA | 3129 | - | 66,73,73 | 2.23 | 16 (24%) | 65,113,113 | 1.79 | 17 (26%) |
| 14 | CL7 | aB | 3031 | - | 66,73,73 | 2.29 | 20 (30%) | 65,113,113 | 1.93 | 14 (21%) |
| 14 | CL7 | cB | 811 | - | 42,49,73 | 2.73 | 16 (38%) | 36,84,113 | 1.77 | 7 (19%) |
| 14 | CL7 | aA | 3122 | - | 42,49,73 | 2.70 | 19 (45%) | 36,84,113 | 1.96 | 6 (16%) |
| 14 | CL7 | cA | 3111 | - | 39,46,73 | 2.79 | 16 (41%) | 30,80,113 | 1.38 | 3 (10%) |
| 14 | CL7 | cA | 3123 | - | 52,59,73 | 2.74 | 22 (42%) | 48,96,113 | 2.44 | 16 (33%) |
| 14 | CL7 | cB | 833 | - | 56,63,73 | 2.52 | 19 (33%) | 53,101,113 | 1.73 | 12 (22%) |
| 14 | CL7 | cJ | 101 | 8 | 43,50,73 | 2.60 | 17 (39%) | 35,85,113 | 1.31 | 3 (8%) |
| 14 | CL7 | aB | 3002 | - | 66,73,73 | 2.40 | 19 (28%) | 65,113,113 | 1.84 | 12 (18%) |
| 14 | CL7 | aB | 3026 | - | 66,73,73 | 2.65 | 27 (40%) | 65,113,113 | 1.97 | 19 (29%) |
| 14 | CL7 | cA | 3107 | - | 66,73,73 | 2.31 | 18 (27%) | 65,113,113 | 1.55 | 10 (15%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 18 | SF4 | cC | 101 | 3 | 0,12,12 | - | - | - | | |
| 14 | CL7 | cA | 3113 | - | 42,49,73 | 2.72 | 15 (35%) | 36,84,113 | 1.78 | 10 (27%) |
| 14 | CL7 | cA | 3128 | - | 66,73,73 | 2.37 | 21 (31%) | 65,113,113 | 1.83 | 19 (29%) |
| 17 | PQN | aA | 3144 | - | 34,34,34 | 2.03 | 11 (32%) | 42,45,45 | 1.34 | 5 (11%) |
| 12 | G9R | aA | 3101 | - | 65,71,71 | 2.56 | 20 (30%) | 71,104,104 | 2.95 | 31 (43%) |
| 14 | CL7 | aA | 3119 | - | 39,46,73 | 2.73 | 18 (46%) | 30,80,113 | 1.68 | 6 (20%) |
| 14 | CL7 | bB | 827 | - | 66,73,73 | 2.53 | 25 (37%) | 65,113,113 | 2.10 | 24 (36%) |
| 14 | CL7 | aA | 3128 | - | 52,59,73 | 2.63 | 17 (32%) | 48,96,113 | 1.87 | 15 (31%) |
| 14 | CL7 | cA | 3102 | - | 66,73,73 | 2.64 | 20 (30%) | 65,113,113 | 2.29 | 21 (32%) |
| 14 | CL7 | bA | 3120 | - | 52,59,73 | 2.49 | 16 (30%) | 48,96,113 | 1.91 | 14 (29%) |
| 14 | CL7 | bB | 804 | - | 66,73,73 | 2.79 | 27 (40%) | 65,113,113 | 1.84 | 18 (27%) |
| 14 | CL7 | bA | 3127 | - | 52,59,73 | 2.63 | 16 (30%) | 48,96,113 | 2.03 | 17 (35%) |
| 14 | CL7 | bL | 203 | 10 | 66,73,73 | 2.29 | 17 (25%) | 65,113,113 | 1.80 | 17 (26%) |
| 14 | CL7 | aB | 3013 | - | 42,49,73 | 2.56 | 15 (35%) | 36,84,113 | 1.71 | 9 (25%) |
| 14 | CL7 | cB | 815 | - | 42,49,73 | 2.72 | 16 (38%) | 36,84,113 | 1.77 | 8 (22%) |
| 14 | CL7 | bB | 826 | - | 66,73,73 | 2.56 | 21 (31%) | 65,113,113 | 1.49 | 14 (21%) |
| 14 | CL7 | cA | 3112 | - | 42,49,73 | 2.68 | 15 (35%) | 36,84,113 | 1.74 | 9 (25%) |
| 18 | SF4 | cC | 102 | 3 | 0,12,12 | - | - | - | | |
| 14 | CL7 | bB | 831 | - | 55,62,73 | 2.35 | 17 (30%) | 51,99,113 | 1.62 | 12 (23%) |
| 18 | SF4 | aC | 101 | 3 | 0,12,12 | - | - | - | | |
| 18 | SF4 | bB | 802 | 1,2 | 0,12,12 | - | - | - | | |
| 14 | CL7 | cB | 821 | - | 39,46,73 | 2.72 | 15 (38%) | 30,80,113 | 1.29 | 2 (6%) |
| 14 | CL7 | cA | 3117 | - | 39,46,73 | 2.71 | 16 (41%) | 30,80,113 | 1.57 | 6 (20%) |
| 14 | CL7 | bB | 822 | - | 42,49,73 | 2.58 | 15 (35%) | 36,84,113 | 1.83 | 7 (19%) |
| 14 | CL7 | aB | 3015 | - | 51,58,73 | 2.70 | 24 (47%) | 47,95,113 | 1.92 | 8 (17%) |
| 14 | CL7 | aB | 3009 | - | 66,73,73 | 2.35 | 22 (33%) | 65,113,113 | 1.76 | 18 (27%) |
| 12 | G9R | bA | 3101 | - | 65,71,71 | 2.73 | 23 (35%) | 71,104,104 | 3.11 | 32 (45%) |
| 14 | CL7 | cA | 3130 | - | 42,49,73 | 2.71 | 18 (42%) | 36,84,113 | 1.63 | 7 (19%) |
| 14 | CL7 | bB | 820 | - | 66,73,73 | 2.32 | 23 (34%) | 65,113,113 | 1.69 | 12 (18%) |
| 14 | CL7 | cB | 832 | - | 66,73,73 | 2.28 | 20 (30%) | 65,113,113 | 1.82 | 15 (23%) |
| 14 | CL7 | cA | 3121 | - | 42,49,73 | 2.76 | 19 (45%) | 36,84,113 | 1.96 | 9 (25%) |
| 14 | CL7 | bB | 812 | - | 39,46,73 | 2.79 | 17 (43%) | 30,80,113 | 1.43 | 3 (10%) |
| 14 | CL7 | aB | 3016 | - | 42,49,73 | 2.64 | 17 (40%) | 36,84,113 | 1.88 | 8 (22%) |
| 14 | CL7 | bA | 3105 | - | 42,49,73 | 2.91 | 17 (40%) | 36,84,113 | 2.24 | 15 (41%) |
| 14 | CL7 | cA | 3132 | - | 66,73,73 | 2.48 | 24 (36%) | 65,113,113 | 1.99 | 21 (32%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | CL7 | bB | 817 | - | 42,49,73 | 2.65 | 17 (40%) | 36,84,113 | 1.86 | 8 (22%) |
| 12 | G9R | cA | 3101 | - | 65,71,71 | 2.77 | 19 (29%) | 71,104,104 | 2.86 | 31 (43%) |
| 14 | CL7 | bB | 819 | - | 57,64,73 | 3.14 | 21 (36%) | 54,102,113 | 1.84 | 14 (25%) |
| 14 | CL7 | bK | 101 | - | 38,45,73 | 2.93 | 17 (44%) | 31,78,113 | 1.68 | 6 (19%) |
| 14 | CL7 | cA | 3116 | - | 54,61,73 | 2.41 | 19 (35%) | 50,98,113 | 1.99 | 15 (30%) |
| 13 | PHO | bB | 801 | - | 51,69,69 | 3.70 | 13 (25%) | 47,99,99 | 1.70 | 8 (17%) |
| 13 | PHO | cB | 801 | - | 51,69,69 | 3.70 | 13 (25%) | 47,99,99 | 1.74 | 8 (17%) |
| 14 | CL7 | bA | 3110 | - | 42,49,73 | 2.64 | 14 (33%) | 36,84,113 | 1.64 | 6 (16%) |
| 19 | LMG | bB | 830 | - | 52,52,55 | 0.97 | 3 (5%) | 60,60,63 | 1.28 | 6 (10%) |
| 14 | CL7 | bA | 3114 | - | 66,73,73 | 2.17 | 16 (24%) | 65,113,113 | 1.89 | 17 (26%) |
| 13 | PHO | cB | 805 | - | 51,69,69 | 2.98 | 21 (41%) | 47,99,99 | 2.21 | 12 (25%) |
| 19 | LMG | cB | 830 | - | 52,52,55 | 0.92 | 3 (5%) | 60,60,63 | 1.35 | 7 (11%) |
| 14 | CL7 | bA | 3106 | - | 66,73,73 | 2.28 | 20 (30%) | 65,113,113 | 1.74 | 16 (24%) |
| 14 | CL7 | cF | 201 | - | 39,46,73 | 2.77 | 17 (43%) | 30,80,113 | 1.55 | 4 (13%) |
| 16 | LHG | aA | 3139 | 14 | 20,20,48 | 1.51 | 3 (15%) | 22,25,54 | 1.28 | 3 (13%) |
| 14 | CL7 | aB | 3008 | 2 | 51,58,73 | 2.62 | 19 (37%) | 47,95,113 | 2.04 | 16 (34%) |
| 14 | CL7 | aB | 3017 | - | 42,49,73 | 2.65 | 14 (33%) | 36,84,113 | 1.70 | 8 (22%) |
| 19 | LMG | aB | 3029 | - | 52,52,55 | 0.86 | 1 (1%) | 60,60,63 | 1.22 | 7 (11%) |
| 14 | CL7 | bA | 3124 | - | 66,73,73 | 2.51 | 23 (34%) | 65,113,113 | 2.12 | 16 (24%) |
| 14 | CL7 | cA | 3119 | - | 47,54,73 | 2.82 | 19 (40%) | 42,90,113 | 2.28 | 11 (26%) |
| 14 | CL7 | bA | 3130 | - | 42,49,73 | 2.70 | 18 (42%) | 36,84,113 | 1.58 | 7 (19%) |
| 14 | CL7 | cB | 807 | - | 66,73,73 | 2.19 | 18 (27%) | 65,113,113 | 1.74 | 17 (26%) |
| 14 | CL7 | cA | 3129 | - | 42,49,73 | 3.28 | 19 (45%) | 36,84,113 | 2.51 | 18 (50%) |
| 14 | CL7 | aA | 3126 | - | 66,73,73 | 2.31 | 18 (27%) | 65,113,113 | 1.78 | 17 (26%) |
| 14 | CL7 | aB | 3014 | - | 42,49,73 | 2.67 | 17 (40%) | 36,84,113 | 1.60 | 7 (19%) |
| 14 | CL7 | bB | 813 | - | 39,46,73 | 2.74 | 16 (41%) | 30,80,113 | 1.43 | 4 (13%) |
| 14 | CL7 | cB | 824 | - | 57,64,73 | 2.37 | 15 (26%) | 54,102,113 | 1.65 | 11 (20%) |
| 14 | CL7 | bA | 3109 | - | 42,49,73 | 2.64 | 15 (35%) | 36,84,113 | 1.68 | 9 (25%) |
| 14 | CL7 | bL | 204 | - | 66,73,73 | 2.30 | 18 (27%) | 65,113,113 | 2.02 | 18 (27%) |
| 14 | CL7 | aA | 3107 | - | 66,73,73 | 2.18 | 21 (31%) | 65,113,113 | 1.69 | 15 (23%) |
| 14 | CL7 | aB | 3025 | - | 66,73,73 | 2.56 | 21 (31%) | 65,113,113 | 1.67 | 15 (23%) |
| 17 | PQN | cA | 3143 | - | 34,34,34 | 2.07 | 10 (29%) | 42,45,45 | 1.62 | 6 (14%) |
| 14 | CL7 | bA | 3133 | 16 | 42,49,73 | 2.56 | 15 (35%) | 36,84,113 | 1.82 | 6 (16%) |
| 14 | CL7 | aA | 3143 | - | 66,73,73 | 2.39 | 19 (28%) | 65,113,113 | 1.55 | 10 (15%) |
| 14 | CL7 | aB | 3010 | - | 42,49,73 | 2.72 | 17 (40%) | 36,84,113 | 1.97 | 10 (27%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | CL7 | aF | 201 | - | 39,46,73 | 2.76 | 17 (43%) | 30,80,113 | 1.58 | 2 (6%) |
| 14 | CL7 | cA | 3104 | - | 42,49,73 | 2.62 | 14 (33%) | 36,84,113 | 1.72 | 7 (19%) |
| 17 | PQN | aB | 3027 | - | 34,34,34 | 2.53 | 14 (41%) | 42,45,45 | 1.47 | 6 (14%) |
| 14 | CL7 | aA | 3125 | - | 66,73,73 | 2.39 | 25 (37%) | 65,113,113 | 1.92 | 16 (24%) |
| 14 | CL7 | aB | 3020 | - | 39,46,73 | 2.72 | 16 (41%) | 30,80,113 | 1.27 | 2 (6%) |
| 14 | CL7 | aA | 3140 | - | 66,73,73 | 2.17 | 16 (24%) | 65,113,113 | 1.36 | 5 (7%) |
| 14 | CL7 | bB | 821 | - | 39,46,73 | 2.69 | 16 (41%) | 30,80,113 | 1.27 | 2 (6%) |
| 14 | CL7 | aB | 3012 | - | 39,46,73 | 2.75 | 17 (43%) | 30,80,113 | 1.44 | 5 (16%) |
| 14 | CL7 | cB | 814 | - | 42,49,73 | 2.56 | 16 (38%) | 36,84,113 | 1.69 | 9 (25%) |
| 14 | CL7 | cA | 3110 | - | 42,49,73 | 2.63 | 15 (35%) | 36,84,113 | 1.67 | 5 (13%) |
| 14 | CL7 | cA | 3141 | - | 66,73,73 | 2.15 | 15 (22%) | 65,113,113 | 1.71 | 10 (15%) |
| 14 | CL7 | aA | 3103 | - | 66,73,73 | 2.50 | 21 (31%) | 65,113,113 | 2.16 | 17 (26%) |
| 14 | CL7 | aL | 202 | 10 | 66,73,73 | 2.26 | 17 (25%) | 65,113,113 | 1.79 | 15 (23%) |
| 14 | CL7 | aB | 3018 | - | 57,64,73 | 3.14 | 20 (35%) | 54,102,113 | 1.92 | 14 (25%) |
| 14 | CL7 | aA | 3114 | - | 42,49,73 | 2.66 | 15 (35%) | 36,84,113 | 1.64 | 7 (19%) |
| 14 | CL7 | aA | 3108 | - | 66,73,73 | 2.27 | 18 (27%) | 65,113,113 | 1.52 | 10 (15%) |
| 14 | CL7 | cB | 823 | - | 42,49,73 | 2.65 | 15 (35%) | 36,84,113 | 2.05 | 12 (33%) |
| 14 | CL7 | cA | 3125 | - | 66,73,73 | 2.38 | 21 (31%) | 65,113,113 | 2.12 | 20 (30%) |
| 14 | CL7 | bB | 823 | - | 42,49,73 | 2.63 | 13 (30%) | 36,84,113 | 2.07 | 12 (33%) |
| 14 | CL7 | bA | 3140 | - | 66,73,73 | 2.32 | 20 (30%) | 65,113,113 | 1.80 | 14 (21%) |
| 16 | LHG | bA | 3138 | 14 | 20,20,48 | 1.64 | 4 (20%) | 22,25,54 | 1.25 | 2 (9%) |
| 14 | CL7 | bA | 3139 | - | 66,73,73 | 2.22 | 18 (27%) | 65,113,113 | 1.52 | 8 (12%) |
| 14 | CL7 | bA | 3112 | - | 42,49,73 | 2.69 | 15 (35%) | 36,84,113 | 1.75 | 9 (25%) |
| 14 | CL7 | aA | 3133 | - | 66,73,73 | 2.47 | 24 (36%) | 65,113,113 | 1.91 | 19 (29%) |
| 13 | PHO | aA | 3102 | - | 51,69,69 | 3.64 | 14 (27%) | 47,99,99 | 1.74 | 8 (17%) |
| 14 | CL7 | aA | 3115 | - | 66,73,73 | 2.07 | 15 (22%) | 65,113,113 | 1.73 | 18 (27%) |
| 14 | CL7 | aA | 3118 | - | 39,46,73 | 2.70 | 16 (41%) | 30,80,113 | 1.44 | 5 (16%) |
| 14 | CL7 | aA | 3113 | - | 42,49,73 | 2.63 | 15 (35%) | 36,84,113 | 1.75 | 8 (22%) |
| 14 | CL7 | cA | 3140 | - | 66,73,73 | 2.33 | 20 (30%) | 65,113,113 | 1.78 | 16 (24%) |
| 14 | CL7 | cB | 822 | - | 42,49,73 | 2.54 | 16 (38%) | 36,84,113 | 2.03 | 7 (19%) |
| 14 | CL7 | cA | 3131 | - | 42,49,73 | 2.74 | 16 (38%) | 36,84,113 | 1.76 | 10 (27%) |
| 14 | CL7 | cA | 3103 | - | 42,49,73 | 2.65 | 16 (38%) | 36,84,113 | 1.64 | 8 (22%) |
| 14 | CL7 | bA | 3126 | 1 | 54,61,73 | 2.44 | 15 (27%) | 51,97,113 | 1.32 | 7 (13%) |
| 14 | CL7 | bB | 814 | - | 42,49,73 | 2.56 | 16 (38%) | 36,84,113 | 1.68 | 9 (25%) |
| 18 | SF4 | bC | 101 | 3 | 0,12,12 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | CL7 | cK | 101 | - | 38,45,73 | 2.86 | 17 (44%) | 31,78,113 | 1.44 | 4 (12%) |
| 14 | CL7 | cB | 827 | - | 66,73,73 | 2.51 | 26 (39%) | 65,113,113 | 1.97 | 19 (29%) |
| 14 | CL7 | bA | 3111 | - | 39,46,73 | 2.80 | 16 (41%) | 30,80,113 | 1.35 | 3 (10%) |
| 14 | CL7 | aA | 3127 | 1 | 54,61,73 | 2.43 | 16 (29%) | 51,97,113 | 1.28 | 7 (13%) |
| 14 | CL7 | bA | 3141 | - | 66,73,73 | 2.15 | 17 (25%) | 65,113,113 | 1.63 | 11 (16%) |
| 14 | CL7 | aA | 3142 | - | 66,73,73 | 2.11 | 17 (25%) | 65,113,113 | 1.55 | 12 (18%) |
| 14 | CL7 | bA | 3128 | - | 66,73,73 | 2.44 | 22 (33%) | 65,113,113 | 1.94 | 22 (33%) |
| 14 | CL7 | cB | 820 | - | 66,73,73 | 2.29 | 21 (31%) | 65,113,113 | 1.64 | 10 (15%) |
| 14 | CL7 | aB | 3023 | - | 57,64,73 | 2.40 | 16 (28%) | 54,102,113 | 1.60 | 11 (20%) |
| 14 | CL7 | bA | 3103 | - | 42,49,73 | 2.64 | 17 (40%) | 36,84,113 | 1.69 | 9 (25%) |
| 14 | CL7 | cA | 3106 | - | 66,73,73 | 2.31 | 20 (30%) | 65,113,113 | 1.75 | 15 (23%) |
| 14 | CL7 | bB | 807 | - | 66,73,73 | 2.20 | 19 (28%) | 65,113,113 | 1.76 | 16 (24%) |
| 14 | CL7 | bB | 803 | - | 66,73,73 | 2.45 | 20 (30%) | 65,113,113 | 2.11 | 14 (21%) |
| 14 | CL7 | bB | 832 | - | 66,73,73 | 2.25 | 19 (28%) | 65,113,113 | 1.83 | 14 (21%) |
| 14 | CL7 | cB | 818 | - | 42,49,73 | 2.64 | 16 (38%) | 36,84,113 | 1.56 | 6 (16%) |
| 14 | CL7 | cB | 817 | - | 42,49,73 | 2.67 | 17 (40%) | 36,84,113 | 1.85 | 8 (22%) |
| 14 | CL7 | aA | 3104 | - | 42,49,73 | 2.62 | 16 (38%) | 36,84,113 | 1.62 | 8 (22%) |
| 14 | CL7 | bB | 810 | - | 66,73,73 | 2.38 | 22 (33%) | 65,113,113 | 1.69 | 15 (23%) |
| 14 | CL7 | aA | 3124 | - | 52,59,73 | 2.66 | 19 (36%) | 48,96,113 | 2.15 | 17 (35%) |
| 14 | CL7 | bB | 825 | - | 39,46,73 | 2.69 | 15 (38%) | 30,80,113 | 1.50 | 3 (10%) |
| 17 | PQN | bA | 3143 | - | 34,34,34 | 2.06 | 12 (35%) | 42,45,45 | 1.67 | 6 (14%) |
| 14 | CL7 | cA | 3120 | - | 52,59,73 | 2.50 | 18 (34%) | 48,96,113 | 1.87 | 13 (27%) |
| 14 | CL7 | cA | 3139 | - | 66,73,73 | 2.20 | 16 (24%) | 65,113,113 | 1.54 | 8 (12%) |
| 14 | CL7 | cL | 205 | - | 43,50,73 | 2.99 | 21 (48%) | 36,85,113 | 1.78 | 8 (22%) |
| 14 | CL7 | bB | 816 | - | 51,58,73 | 2.68 | 22 (43%) | 47,95,113 | 2.05 | 11 (23%) |
| 14 | CL7 | cA | 3142 | - | 66,73,73 | 2.41 | 19 (28%) | 65,113,113 | 1.65 | 12 (18%) |
| 14 | CL7 | bA | 3102 | - | 66,73,73 | 2.65 | 21 (31%) | 65,113,113 | 2.24 | 19 (29%) |
| 14 | CL7 | aA | 3141 | - | 66,73,73 | 2.19 | 19 (28%) | 65,113,113 | 1.57 | 14 (21%) |
| 14 | CL7 | bA | 3104 | - | 42,49,73 | 2.62 | 14 (33%) | 36,84,113 | 1.71 | 8 (22%) |
| 14 | CL7 | bA | 3117 | - | 39,46,73 | 2.71 | 16 (41%) | 30,80,113 | 1.58 | 6 (20%) |
| 14 | CL7 | cA | 3144 | - | 42,49,73 | 2.59 | 15 (35%) | 36,84,113 | 1.60 | 6 (16%) |
| 14 | CL7 | aB | 3030 | - | 55,62,73 | 2.34 | 17 (30%) | 51,99,113 | 1.56 | 11 (21%) |
| 14 | CL7 | bF | 201 | - | 39,46,73 | 2.74 | 18 (46%) | 30,80,113 | 1.57 | 5 (16%) |
| 14 | CL7 | cA | 3108 | 1 | 43,50,73 | 2.69 | 17 (39%) | 36,85,113 | 1.98 | 13 (36%) |
| 14 | CL7 | bA | 3131 | - | 42,49,73 | 2.75 | 17 (40%) | 36,84,113 | 1.76 | 9 (25%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | CL7 | cL | 204 | - | 66,73,73 | 2.35 | 21 (31%) | 65,113,113 | 1.93 | 20 (30%) |
| 14 | CL7 | bA | 3123 | - | 52,59,73 | 2.67 | 19 (36%) | 48,96,113 | 2.26 | 16 (33%) |
| 14 | CL7 | aB | 3007 | - | 66,73,73 | 2.28 | 19 (28%) | 65,113,113 | 1.86 | 15 (23%) |
| 14 | CL7 | cB | 812 | - | 39,46,73 | 2.78 | 17 (43%) | 30,80,113 | 1.46 | 5 (16%) |
| 14 | CL7 | cA | 3127 | - | 52,59,73 | 2.68 | 18 (34%) | 48,96,113 | 1.99 | 15 (31%) |
| 16 | LHG | aA | 3138 | - | 48,48,48 | 0.97 | 4 (8%) | 51,54,54 | 0.95 | 3 (5%) |
| 14 | CL7 | cB | 825 | - | 39,46,73 | 2.73 | 15 (38%) | 30,80,113 | 1.54 | 5 (16%) |
| 14 | CL7 | bB | 809 | 2 | 51,58,73 | 2.71 | 20 (39%) | 47,95,113 | 2.13 | 15 (31%) |
| 14 | CL7 | cB | 826 | - | 66,73,73 | 2.59 | 21 (31%) | 65,113,113 | 1.50 | 16 (24%) |
| 14 | CL7 | cB | 813 | - | 39,46,73 | 2.75 | 16 (41%) | 30,80,113 | 1.45 | 3 (10%) |
| 17 | PQN | cB | 828 | - | 34,34,34 | 2.55 | 13 (38%) | 42,45,45 | 1.51 | 6 (14%) |
| 14 | CL7 | bB | 818 | - | 42,49,73 | 2.65 | 15 (35%) | 36,84,113 | 1.76 | 8 (22%) |
| 14 | CL7 | bJ | 101 | 8 | 43,50,73 | 2.64 | 15 (34%) | 35,85,113 | 1.35 | 3 (8%) |
| 14 | CL7 | bA | 3121 | - | 42,49,73 | 2.77 | 24 (57%) | 36,84,113 | 2.00 | 9 (25%) |
| 14 | CL7 | cL | 203 | 10 | 66,73,73 | 2.24 | 19 (28%) | 65,113,113 | 1.74 | 12 (18%) |
| 14 | CL7 | aA | 3111 | - | 42,49,73 | 2.60 | 14 (33%) | 36,84,113 | 1.66 | 5 (13%) |
| 14 | CL7 | aB | 3019 | - | 66,73,73 | 2.31 | 21 (31%) | 65,113,113 | 1.72 | 13 (20%) |
| 16 | LHG | cA | 3138 | 14 | 20,20,48 | 1.60 | 4 (20%) | 22,25,54 | 1.17 | 2 (9%) |
| 14 | CL7 | bB | 806 | - | 66,73,73 | 2.45 | 20 (30%) | 65,113,113 | 1.53 | 11 (16%) |
| 14 | CL7 | bA | 3108 | - | 43,50,73 | 2.78 | 19 (44%) | 36,85,113 | 1.81 | 11 (30%) |
| 14 | CL7 | cA | 3118 | - | 39,46,73 | 2.75 | 18 (46%) | 30,80,113 | 1.69 | 6 (20%) |
| 14 | CL7 | cA | 3109 | - | 42,49,73 | 2.62 | 15 (35%) | 36,84,113 | 1.67 | 9 (25%) |
| 14 | CL7 | bA | 3119 | - | 47,54,73 | 2.79 | 15 (31%) | 42,90,113 | 2.23 | 11 (26%) |
| 14 | CL7 | cB | 819 | - | 57,64,73 | 3.21 | 22 (38%) | 54,102,113 | 1.89 | 12 (22%) |
| 14 | CL7 | bA | 3129 | - | 42,49,73 | 3.24 | 23 (54%) | 36,84,113 | 2.39 | 17 (47%) |
| 14 | CL7 | aL | 203 | - | 66,73,73 | 2.30 | 19 (28%) | 65,113,113 | 1.97 | 20 (30%) |
| 14 | CL7 | bA | 3122 | - | 51,58,73 | 2.38 | 16 (31%) | 47,95,113 | 2.29 | 15 (31%) |
| 14 | CL7 | aA | 3105 | - | 42,49,73 | 2.61 | 14 (33%) | 36,84,113 | 1.71 | 8 (22%) |
| 14 | CL7 | aB | 3024 | - | 39,46,73 | 2.72 | 16 (41%) | 30,80,113 | 1.54 | 6 (20%) |
| 14 | CL7 | bB | 824 | - | 57,64,73 | 2.37 | 15 (26%) | 54,102,113 | 1.63 | 12 (22%) |
| 14 | CL7 | bB | 833 | - | 56,63,73 | 2.53 | 20 (35%) | 53,101,113 | 1.69 | 14 (26%) |
| 14 | CL7 | cA | 3124 | - | 66,73,73 | 2.48 | 24 (36%) | 65,113,113 | 2.15 | 18 (27%) |
| 16 | LHG | bA | 3137 | - | 48,48,48 | 1.08 | 5 (10%) | 51,54,54 | 0.97 | 3 (5%) |
| 14 | CL7 | bB | 815 | - | 42,49,73 | 2.71 | 15 (35%) | 36,84,113 | 1.78 | 9 (25%) |
| 14 | CL7 | bA | 3113 | - | 42,49,73 | 2.72 | 15 (35%) | 36,84,113 | 1.72 | 8 (22%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | CL7 | aB | 3021 | - | 42,49,73 | 2.59 | 15 (35%) | 36,84,113 | 1.88 | 9 (25%) |
| 14 | CL7 | cA | 3122 | - | 51,58,73 | 2.42 | 16 (31%) | 47,95,113 | 2.29 | 14 (29%) |
| 14 | CL7 | cB | 809 | 2 | 51,58,73 | 2.63 | 19 (37%) | 47,95,113 | 2.08 | 13 (27%) |
| 18 | SF4 | aB | 3001 | 1,2 | 0,12,12 | - | - | - | - | - |
| 14 | CL7 | cB | 803 | - | 66,73,73 | 2.46 | 20 (30%) | 65,113,113 | 2.11 | 17 (26%) |
| 14 | CL7 | aA | 3120 | - | 47,54,73 | 2.67 | 17 (36%) | 42,90,113 | 2.06 | 11 (26%) |
| 14 | CL7 | aA | 3131 | - | 42,49,73 | 2.68 | 18 (42%) | 36,84,113 | 1.63 | 7 (19%) |
| 14 | CL7 | cA | 3133 | 16 | 42,49,73 | 2.55 | 14 (33%) | 36,84,113 | 1.79 | 8 (22%) |
| 14 | CL7 | bA | 3132 | - | 66,73,73 | 2.53 | 24 (36%) | 65,113,113 | 1.89 | 18 (27%) |
| 18 | SF4 | aC | 102 | 3 | 0,12,12 | - | - | - | - | - |
| 14 | CL7 | aA | 3130 | - | 42,49,73 | 3.10 | 21 (50%) | 36,84,113 | 2.30 | 16 (44%) |
| 14 | CL7 | aB | 3006 | - | 66,73,73 | 2.19 | 20 (30%) | 65,113,113 | 1.78 | 18 (27%) |
| 14 | CL7 | aA | 3132 | - | 42,49,73 | 2.68 | 15 (35%) | 36,84,113 | 1.83 | 9 (25%) |
| 14 | CL7 | aB | 3011 | - | 39,46,73 | 2.81 | 17 (43%) | 30,80,113 | 1.41 | 3 (10%) |
| 14 | CL7 | aL | 204 | - | 43,50,73 | 2.98 | 21 (48%) | 36,85,113 | 1.74 | 8 (22%) |
| 14 | CL7 | cB | 810 | - | 66,73,73 | 2.38 | 24 (36%) | 65,113,113 | 1.76 | 16 (24%) |
| 14 | CL7 | aA | 3146 | - | 42,49,73 | 2.60 | 15 (35%) | 36,84,113 | 1.77 | 7 (19%) |
| 18 | SF4 | cB | 802 | 1,2 | 0,12,12 | - | - | - | - | - |
| 14 | CL7 | aA | 3134 | 16 | 42,49,73 | 2.57 | 15 (35%) | 36,84,113 | 1.70 | 6 (16%) |
| 13 | PHO | aB | 3004 | - | 51,69,69 | 2.99 | 19 (37%) | 47,99,99 | 2.30 | 12 (25%) |
| 14 | CL7 | aB | 3005 | - | 66,73,73 | 2.45 | 20 (30%) | 65,113,113 | 1.61 | 13 (20%) |
| 14 | CL7 | cB | 804 | - | 66,73,73 | 2.74 | 29 (43%) | 65,113,113 | 1.80 | 15 (23%) |
| 14 | CL7 | bA | 3115 | - | 39,46,73 | 2.68 | 17 (43%) | 30,80,113 | 1.40 | 6 (20%) |
| 14 | CL7 | aA | 3116 | - | 39,46,73 | 2.66 | 17 (43%) | 30,80,113 | 1.41 | 6 (20%) |
| 14 | CL7 | aB | 3003 | - | 66,73,73 | 2.63 | 28 (42%) | 65,113,113 | 1.78 | 15 (23%) |
| 14 | CL7 | bA | 3125 | - | 66,73,73 | 2.41 | 21 (31%) | 65,113,113 | 2.14 | 18 (27%) |
| 14 | CL7 | bL | 205 | - | 43,50,73 | 2.99 | 22 (51%) | 36,85,113 | 1.73 | 9 (25%) |
| 14 | CL7 | cA | 3115 | - | 39,46,73 | 2.66 | 17 (43%) | 30,80,113 | 1.39 | 5 (16%) |
| 14 | CL7 | cB | 808 | - | 66,73,73 | 2.23 | 19 (28%) | 65,113,113 | 1.86 | 13 (20%) |
| 14 | CL7 | cB | 831 | - | 55,62,73 | 2.30 | 16 (29%) | 51,99,113 | 1.63 | 12 (23%) |
| 13 | PHO | bB | 805 | - | 51,69,69 | 2.96 | 19 (37%) | 47,99,99 | 2.14 | 11 (23%) |
| 14 | CL7 | aA | 3110 | - | 42,49,73 | 2.57 | 14 (33%) | 36,84,113 | 1.65 | 8 (22%) |
| 14 | CL7 | aJ | 101 | 8 | 43,50,73 | 2.63 | 16 (37%) | 35,85,113 | 1.31 | 3 (8%) |
| 16 | LHG | cA | 3137 | - | 48,48,48 | 0.97 | 5 (10%) | 51,54,54 | 1.02 | 3 (5%) |
| 17 | PQN | bB | 828 | - | 34,34,34 | 2.48 | 13 (38%) | 42,45,45 | 1.55 | 6 (14%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | CL7 | bA | 3145 | - | 42,49,73 | 2.62 | 16 (38%) | 36,84,113 | 1.61 | 4 (11%) |
| 14 | CL7 | bB | 811 | - | 42,49,73 | 2.75 | 18 (42%) | 36,84,113 | 1.93 | 9 (25%) |
| 14 | CL7 | aA | 3112 | - | 39,46,73 | 2.77 | 17 (43%) | 30,80,113 | 1.34 | 2 (6%) |
| 14 | CL7 | bA | 3142 | - | 66,73,73 | 2.42 | 19 (28%) | 65,113,113 | 1.63 | 11 (16%) |
| 14 | CL7 | cB | 806 | - | 66,73,73 | 2.42 | 20 (30%) | 65,113,113 | 1.64 | 12 (18%) |
| 14 | CL7 | aA | 3106 | - | 42,49,73 | 2.84 | 16 (38%) | 36,84,113 | 2.11 | 12 (33%) |
| 14 | CL7 | bB | 808 | - | 66,73,73 | 2.29 | 18 (27%) | 65,113,113 | 1.85 | 13 (20%) |

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 |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CL7 | cA | 3105 | - | 2/2/10/20 | 3/8/86/115 | - |
| 14 | CL7 | cB | 816 | - | 2/2/12/20 | 6/19/97/115 | - |
| 14 | CL7 | aA | 3117 | - | 2/2/12/20 | 8/23/101/115 | - |
| 14 | CL7 | bA | 3116 | - | 2/2/12/20 | 9/23/101/115 | - |
| 14 | CL7 | aB | 3032 | - | 2/2/13/20 | 10/25/103/115 | - |
| 14 | CL7 | aA | 3123 | - | 2/2/12/20 | 7/19/97/115 | - |
| 18 | SF4 | bC | 102 | 3 | - | - | 0/6/5/5 |
| 14 | CL7 | aA | 3121 | - | 2/2/12/20 | 6/21/99/115 | - |
| 14 | CL7 | aA | 3109 | 1 | 1/1/10/20 | 3/10/88/115 | - |
| 14 | CL7 | bA | 3118 | - | 2/2/9/20 | 0/2/80/115 | - |
| 14 | CL7 | bA | 3107 | - | 1/1/15/20 | 14/37/115/115 | - |
| 14 | CL7 | cA | 3114 | - | 1/1/15/20 | 19/37/115/115 | - |
| 14 | CL7 | aK | 101 | - | 2/2/8/20 | 0/2/76/115 | - |
| 14 | CL7 | cA | 3126 | 1 | 2/2/11/20 | 10/24/98/115 | - |
| 14 | CL7 | aB | 3022 | - | 2/2/10/20 | 4/8/86/115 | - |
| 14 | CL7 | aA | 3129 | - | 2/2/15/20 | 18/37/115/115 | - |
| 14 | CL7 | aB | 3031 | - | 2/2/15/20 | 15/37/115/115 | - |
| 14 | CL7 | cB | 811 | - | 2/2/10/20 | 4/8/86/115 | - |
| 14 | CL7 | aA | 3122 | - | 1/1/10/20 | 2/8/86/115 | - |
| 14 | CL7 | cA | 3111 | - | 2/2/9/20 | 0/2/80/115 | - |
| 14 | CL7 | cA | 3123 | - | 2/2/12/20 | 5/21/99/115 | - |
| 14 | CL7 | cB | 833 | - | 2/2/13/20 | 11/25/103/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CL7 | cJ | 101 | 8 | 1/1/10/20 | 2/7/85/115 | - |
| 14 | CL7 | aB | 3002 | - | 2/2/15/20 | 19/37/115/115 | - |
| 14 | CL7 | aB | 3026 | - | 2/2/15/20 | 18/37/115/115 | - |
| 14 | CL7 | cA | 3107 | - | 1/1/15/20 | 13/37/115/115 | - |
| 18 | SF4 | cC | 101 | 3 | - | - | 0/6/5/5 |
| 14 | CL7 | cA | 3113 | - | 1/1/10/20 | 0/8/86/115 | - |
| 14 | CL7 | cA | 3128 | - | 2/2/15/20 | 19/37/115/115 | - |
| 17 | PQN | aA | 3144 | - | - | 14/23/43/43 | 0/2/2/2 |
| 12 | G9R | aA | 3101 | - | 1/1/17/22 | 5/48/107/107 | - |
| 14 | CL7 | aA | 3119 | - | 1/1/9/20 | 0/2/80/115 | - |
| 14 | CL7 | bB | 827 | - | 2/2/15/20 | 15/37/115/115 | - |
| 14 | CL7 | aA | 3128 | - | 2/2/12/20 | 10/21/99/115 | - |
| 14 | CL7 | cA | 3102 | - | 1/1/15/20 | 8/37/115/115 | - |
| 14 | CL7 | bA | 3120 | - | 2/2/12/20 | 7/21/99/115 | - |
| 14 | CL7 | bB | 804 | - | 2/2/15/20 | 7/37/115/115 | - |
| 14 | CL7 | bA | 3127 | - | 2/2/12/20 | 8/21/99/115 | - |
| 14 | CL7 | bL | 203 | 10 | 2/2/15/20 | 21/37/115/115 | - |
| 14 | CL7 | aB | 3013 | - | 1/1/10/20 | 3/8/86/115 | - |
| 14 | CL7 | cB | 815 | - | 2/2/10/20 | 1/8/86/115 | - |
| 14 | CL7 | bB | 826 | - | 2/2/15/20 | 15/37/115/115 | - |
| 14 | CL7 | cA | 3112 | - | 2/2/10/20 | 4/8/86/115 | - |
| 18 | SF4 | cC | 102 | 3 | - | - | 0/6/5/5 |
| 14 | CL7 | bB | 831 | - | 2/2/12/20 | 6/24/102/115 | - |
| 18 | SF4 | aC | 101 | 3 | - | - | 0/6/5/5 |
| 18 | SF4 | bB | 802 | 1,2 | - | - | 0/6/5/5 |
| 14 | CL7 | cB | 821 | - | 1/1/9/20 | 0/2/80/115 | - |
| 14 | CL7 | cA | 3117 | - | 2/2/9/20 | 0/2/80/115 | - |
| 14 | CL7 | bB | 822 | - | 1/1/10/20 | 2/8/86/115 | - |
| 14 | CL7 | aB | 3015 | - | 2/2/12/20 | 6/19/97/115 | - |
| 14 | CL7 | aB | 3009 | - | 2/2/15/20 | 18/37/115/115 | - |
| 14 | CL7 | cA | 3130 | - | 2/2/10/20 | 4/8/86/115 | - |
| 14 | CL7 | cB | 832 | - | 2/2/15/20 | 18/37/115/115 | - |
| 14 | CL7 | bB | 820 | - | 2/2/15/20 | 12/37/115/115 | - |
| 12 | G9R | bA | 3101 | - | - | 12/48/107/107 | - |
| 14 | CL7 | cA | 3121 | - | 2/2/10/20 | 1/8/86/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CL7 | bB | 812 | - | 2/2/9/20 | 0/2/80/115 | - |
| 14 | CL7 | aB | 3016 | - | 2/2/10/20 | 4/8/86/115 | - |
| 14 | CL7 | bA | 3105 | - | 2/2/10/20 | 2/8/86/115 | - |
| 14 | CL7 | cA | 3132 | - | 2/2/15/20 | 18/37/115/115 | - |
| 14 | CL7 | bB | 817 | - | 2/2/10/20 | 4/8/86/115 | - |
| 12 | G9R | cA | 3101 | - | 1/1/17/22 | 7/48/107/107 | - |
| 14 | CL7 | bB | 819 | - | 2/2/13/20 | 9/27/105/115 | - |
| 14 | CL7 | bK | 101 | - | 2/2/8/20 | 0/2/76/115 | - |
| 14 | CL7 | cA | 3116 | - | 2/2/12/20 | 8/23/101/115 | - |
| 14 | CL7 | bA | 3110 | - | 2/2/10/20 | 3/8/86/115 | - |
| 13 | PHO | bB | 801 | - | - | 12/37/103/103 | 0/5/6/6 |
| 13 | PHO | cB | 801 | - | - | 10/37/103/103 | 0/5/6/6 |
| 19 | LMG | bB | 830 | - | - | 18/47/67/70 | 0/1/1/1 |
| 14 | CL7 | bA | 3114 | - | 2/2/15/20 | 19/37/115/115 | - |
| 13 | PHO | cB | 805 | - | - | 18/37/103/103 | 0/5/6/6 |
| 19 | LMG | cB | 830 | - | - | 18/47/67/70 | 0/1/1/1 |
| 14 | CL7 | bA | 3106 | - | 2/2/15/20 | 20/37/115/115 | - |
| 14 | CL7 | cF | 201 | - | 2/2/9/20 | 0/2/80/115 | - |
| 16 | LHG | aA | 3139 | 14 | - | 9/23/23/53 | - |
| 14 | CL7 | aB | 3008 | 2 | 2/2/12/20 | 4/19/97/115 | - |
| 14 | CL7 | aB | 3017 | - | 2/2/10/20 | 6/8/86/115 | - |
| 19 | LMG | aB | 3029 | - | - | 20/47/67/70 | 0/1/1/1 |
| 14 | CL7 | bA | 3124 | - | 2/2/15/20 | 9/37/115/115 | - |
| 14 | CL7 | cA | 3119 | - | 2/2/11/20 | 3/15/93/115 | - |
| 14 | CL7 | bA | 3130 | - | 2/2/10/20 | 4/8/86/115 | - |
| 14 | CL7 | cB | 807 | - | 1/1/15/20 | 14/37/115/115 | - |
| 14 | CL7 | cA | 3129 | - | 1/1/10/20 | 2/8/86/115 | - |
| 14 | CL7 | aA | 3126 | - | 2/2/15/20 | 11/37/115/115 | - |
| 14 | CL7 | aB | 3014 | - | 1/1/10/20 | 1/8/86/115 | - |
| 14 | CL7 | bB | 813 | - | 2/2/9/20 | 0/2/80/115 | - |
| 14 | CL7 | cB | 824 | - | 2/2/13/20 | 13/27/105/115 | - |
| 14 | CL7 | bA | 3109 | - | 2/2/10/20 | 2/8/86/115 | - |
| 14 | CL7 | bL | 204 | - | 2/2/15/20 | 11/37/115/115 | - |
| 14 | CL7 | aA | 3107 | - | 2/2/15/20 | 21/37/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CL7 | aB | 3025 | - | 2/2/15/20 | 14/37/115/115 | - |
| 17 | PQN | cA | 3143 | - | - | 13/23/43/43 | 0/2/2/2 |
| 14 | CL7 | bA | 3133 | 16 | 2/2/10/20 | 3/8/86/115 | - |
| 14 | CL7 | aA | 3143 | - | 1/1/15/20 | 18/37/115/115 | - |
| 14 | CL7 | aB | 3010 | - | 2/2/10/20 | 3/8/86/115 | - |
| 14 | CL7 | aF | 201 | - | 2/2/9/20 | 0/2/80/115 | - |
| 14 | CL7 | cA | 3104 | - | 2/2/10/20 | 4/8/86/115 | - |
| 17 | PQN | aB | 3027 | - | - | 8/23/43/43 | 0/2/2/2 |
| 14 | CL7 | aA | 3125 | - | 2/2/15/20 | 7/37/115/115 | - |
| 14 | CL7 | aB | 3020 | - | 1/1/9/20 | 0/2/80/115 | - |
| 14 | CL7 | aA | 3140 | - | 2/2/15/20 | 18/37/115/115 | - |
| 14 | CL7 | bB | 821 | - | 1/1/9/20 | 0/2/80/115 | - |
| 14 | CL7 | aB | 3012 | - | 2/2/9/20 | 0/2/80/115 | - |
| 14 | CL7 | cB | 814 | - | 1/1/10/20 | 2/8/86/115 | - |
| 14 | CL7 | cA | 3110 | - | 1/1/10/20 | 2/8/86/115 | - |
| 14 | CL7 | cA | 3141 | - | 2/2/15/20 | 16/37/115/115 | - |
| 14 | CL7 | aA | 3103 | - | 1/1/15/20 | 8/37/115/115 | - |
| 14 | CL7 | aL | 202 | 10 | 2/2/15/20 | 19/37/115/115 | - |
| 14 | CL7 | aB | 3018 | - | 2/2/13/20 | 9/27/105/115 | - |
| 14 | CL7 | aA | 3114 | - | 2/2/10/20 | 0/8/86/115 | - |
| 14 | CL7 | aA | 3108 | - | 1/1/15/20 | 14/37/115/115 | - |
| 14 | CL7 | cB | 823 | - | 2/2/10/20 | 5/8/86/115 | - |
| 14 | CL7 | cA | 3125 | - | 2/2/15/20 | 9/37/115/115 | - |
| 14 | CL7 | bB | 823 | - | 2/2/10/20 | 5/8/86/115 | - |
| 14 | CL7 | bA | 3140 | - | 2/2/15/20 | 15/37/115/115 | - |
| 16 | LHG | bA | 3138 | 14 | - | 11/23/23/53 | - |
| 14 | CL7 | bA | 3139 | - | 2/2/15/20 | 17/37/115/115 | - |
| 14 | CL7 | bA | 3112 | - | 2/2/10/20 | 3/8/86/115 | - |
| 14 | CL7 | aA | 3133 | - | 2/2/15/20 | 16/37/115/115 | - |
| 14 | CL7 | aA | 3115 | - | 2/2/15/20 | 17/37/115/115 | - |
| 14 | CL7 | aA | 3118 | - | 2/2/9/20 | 0/2/80/115 | - |
| 13 | PHO | aA | 3102 | - | - | 9/37/103/103 | 0/5/6/6 |
| 14 | CL7 | aA | 3113 | - | 2/2/10/20 | 3/8/86/115 | - |
| 14 | CL7 | cA | 3140 | - | 2/2/15/20 | 15/37/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CL7 | cB | 822 | - | 1/1/10/20 | 3/8/86/115 | - |
| 14 | CL7 | cA | 3131 | - | 2/2/10/20 | 5/8/86/115 | - |
| 14 | CL7 | cA | 3103 | - | 2/2/10/20 | 3/8/86/115 | - |
| 14 | CL7 | bA | 3126 | 1 | 1/1/11/20 | 10/24/98/115 | - |
| 14 | CL7 | bB | 814 | - | 1/1/10/20 | 3/8/86/115 | - |
| 18 | SF4 | bC | 101 | 3 | - | - | 0/6/5/5 |
| 14 | CL7 | cK | 101 | - | 2/2/8/20 | 0/2/76/115 | - |
| 14 | CL7 | cB | 827 | - | 1/1/15/20 | 18/37/115/115 | - |
| 14 | CL7 | bA | 3111 | - | 2/2/9/20 | 0/2/80/115 | - |
| 14 | CL7 | aA | 3127 | 1 | 1/1/11/20 | 11/24/98/115 | - |
| 14 | CL7 | bA | 3141 | - | 2/2/15/20 | 13/37/115/115 | - |
| 14 | CL7 | aA | 3142 | - | 2/2/15/20 | 16/37/115/115 | - |
| 14 | CL7 | bA | 3128 | - | 2/2/15/20 | 17/37/115/115 | - |
| 14 | CL7 | cB | 820 | - | 2/2/15/20 | 15/37/115/115 | - |
| 14 | CL7 | aB | 3023 | - | 2/2/13/20 | 14/27/105/115 | - |
| 14 | CL7 | bA | 3103 | - | 2/2/10/20 | 2/8/86/115 | - |
| 14 | CL7 | cA | 3106 | - | 2/2/15/20 | 18/37/115/115 | - |
| 14 | CL7 | bB | 807 | - | 1/1/15/20 | 13/37/115/115 | - |
| 14 | CL7 | bB | 803 | - | 2/2/15/20 | 11/37/115/115 | - |
| 14 | CL7 | bB | 832 | - | 2/2/15/20 | 16/37/115/115 | - |
| 14 | CL7 | cB | 818 | - | 2/2/10/20 | 3/8/86/115 | - |
| 14 | CL7 | cB | 817 | - | 2/2/10/20 | 4/8/86/115 | - |
| 14 | CL7 | aA | 3104 | - | 2/2/10/20 | 2/8/86/115 | - |
| 14 | CL7 | bB | 810 | - | 2/2/15/20 | 20/37/115/115 | - |
| 14 | CL7 | aA | 3124 | - | 2/2/12/20 | 4/21/99/115 | - |
| 14 | CL7 | bB | 825 | - | 2/2/9/20 | 0/2/80/115 | - |
| 17 | PQN | bA | 3143 | - | - | 15/23/43/43 | 0/2/2/2 |
| 14 | CL7 | cA | 3120 | - | 2/2/12/20 | 5/21/99/115 | - |
| 14 | CL7 | cA | 3139 | - | 2/2/15/20 | 16/37/115/115 | - |
| 14 | CL7 | cL | 205 | - | 2/2/10/20 | 2/10/88/115 | - |
| 14 | CL7 | bB | 816 | - | 1/1/12/20 | 3/19/97/115 | - |
| 14 | CL7 | cA | 3142 | - | 2/2/15/20 | 17/37/115/115 | - |
| 14 | CL7 | bA | 3102 | - | 1/1/15/20 | 6/37/115/115 | - |
| 14 | CL7 | aA | 3141 | - | 2/2/15/20 | 16/37/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CL7 | bA | 3104 | - | 2/2/10/20 | 4/8/86/115 | - |
| 14 | CL7 | bA | 3117 | - | 2/2/9/20 | 0/2/80/115 | - |
| 14 | CL7 | cA | 3144 | - | 2/2/10/20 | 3/8/86/115 | - |
| 14 | CL7 | aB | 3030 | - | 2/2/12/20 | 7/24/102/115 | - |
| 14 | CL7 | bF | 201 | - | 2/2/9/20 | 0/2/80/115 | - |
| 14 | CL7 | cA | 3108 | 1 | 1/1/10/20 | 4/10/88/115 | - |
| 14 | CL7 | bA | 3131 | - | 2/2/10/20 | 4/8/86/115 | - |
| 14 | CL7 | cL | 204 | - | 2/2/15/20 | 17/37/115/115 | - |
| 14 | CL7 | bA | 3123 | - | 2/2/12/20 | 6/21/99/115 | - |
| 14 | CL7 | aB | 3007 | - | 2/2/15/20 | 13/37/115/115 | - |
| 14 | CL7 | cB | 812 | - | 2/2/9/20 | 0/2/80/115 | - |
| 14 | CL7 | cA | 3127 | - | 2/2/12/20 | 9/21/99/115 | - |
| 16 | LHG | aA | 3138 | - | - | 16/53/53/53 | - |
| 14 | CL7 | cB | 825 | - | 2/2/9/20 | 0/2/80/115 | - |
| 14 | CL7 | bB | 809 | 2 | 2/2/12/20 | 5/19/97/115 | - |
| 14 | CL7 | cB | 826 | - | 2/2/15/20 | 16/37/115/115 | - |
| 14 | CL7 | cB | 813 | - | 2/2/9/20 | 0/2/80/115 | - |
| 17 | PQN | cB | 828 | - | - | 8/23/43/43 | 0/2/2/2 |
| 14 | CL7 | bB | 818 | - | 2/2/10/20 | 6/8/86/115 | - |
| 14 | CL7 | bJ | 101 | 8 | 1/1/10/20 | 4/7/85/115 | - |
| 14 | CL7 | bA | 3121 | - | 2/2/10/20 | 3/8/86/115 | - |
| 14 | CL7 | cL | 203 | 10 | 2/2/15/20 | 21/37/115/115 | - |
| 14 | CL7 | aA | 3111 | - | 1/1/10/20 | 2/8/86/115 | - |
| 14 | CL7 | aB | 3019 | - | 2/2/15/20 | 16/37/115/115 | - |
| 16 | LHG | cA | 3138 | 14 | - | 12/23/23/53 | - |
| 14 | CL7 | bB | 806 | - | 2/2/15/20 | 15/37/115/115 | - |
| 14 | CL7 | bA | 3108 | - | 1/1/10/20 | 4/10/88/115 | - |
| 14 | CL7 | cA | 3118 | - | 1/1/9/20 | 0/2/80/115 | - |
| 14 | CL7 | cA | 3109 | - | 2/2/10/20 | 1/8/86/115 | - |
| 14 | CL7 | bA | 3119 | - | 2/2/11/20 | 2/15/93/115 | - |
| 14 | CL7 | cB | 819 | - | 2/2/13/20 | 9/27/105/115 | - |
| 14 | CL7 | bA | 3129 | - | 1/1/10/20 | 2/8/86/115 | - |
| 14 | CL7 | aL | 203 | - | 2/2/15/20 | 14/37/115/115 | - |
| 14 | CL7 | bA | 3122 | - | 2/2/12/20 | 7/19/97/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CL7 | aA | 3105 | - | 2/2/10/20 | 3/8/86/115 | - |
| 14 | CL7 | aB | 3024 | - | 2/2/9/20 | 0/2/80/115 | - |
| 14 | CL7 | bB | 824 | - | 2/2/13/20 | 10/27/105/115 | - |
| 14 | CL7 | bB | 833 | - | 2/2/13/20 | 11/25/103/115 | - |
| 14 | CL7 | cA | 3124 | - | 2/2/15/20 | 9/37/115/115 | - |
| 16 | LHG | bA | 3137 | - | - | 17/53/53/53 | - |
| 14 | CL7 | bB | 815 | - | 2/2/10/20 | 1/8/86/115 | - |
| 14 | CL7 | bA | 3113 | - | 1/1/10/20 | 0/8/86/115 | - |
| 14 | CL7 | aB | 3021 | - | 1/1/10/20 | 3/8/86/115 | - |
| 14 | CL7 | cA | 3122 | - | 2/2/12/20 | 8/19/97/115 | - |
| 14 | CL7 | cB | 809 | 2 | 2/2/12/20 | 4/19/97/115 | - |
| 18 | SF4 | aB | 3001 | 1,2 | - | - | 0/6/5/5 |
| 14 | CL7 | cB | 803 | - | 2/2/15/20 | 13/37/115/115 | - |
| 14 | CL7 | aA | 3120 | - | 2/2/11/20 | 3/15/93/115 | - |
| 14 | CL7 | aA | 3131 | - | 1/1/10/20 | 3/8/86/115 | - |
| 14 | CL7 | cA | 3133 | 16 | 2/2/10/20 | 2/8/86/115 | - |
| 14 | CL7 | bA | 3132 | - | 2/2/15/20 | 16/37/115/115 | - |
| 18 | SF4 | aC | 102 | 3 | - | - | 0/6/5/5 |
| 14 | CL7 | aA | 3130 | - | 1/1/10/20 | 3/8/86/115 | - |
| 14 | CL7 | aB | 3006 | - | 1/1/15/20 | 13/37/115/115 | - |
| 14 | CL7 | aA | 3132 | - | 2/2/10/20 | 5/8/86/115 | - |
| 14 | CL7 | aB | 3011 | - | 2/2/9/20 | 0/2/80/115 | - |
| 14 | CL7 | aL | 204 | - | 2/2/10/20 | 0/10/88/115 | - |
| 14 | CL7 | cB | 810 | - | 2/2/15/20 | 17/37/115/115 | - |
| 14 | CL7 | aA | 3146 | - | 2/2/10/20 | 5/8/86/115 | - |
| 18 | SF4 | cB | 802 | 1,2 | - | - | 0/6/5/5 |
| 14 | CL7 | aA | 3134 | 16 | 2/2/10/20 | 6/8/86/115 | - |
| 13 | PHO | aB | 3004 | - | - | 20/37/103/103 | 0/5/6/6 |
| 14 | CL7 | aB | 3005 | - | 2/2/15/20 | 8/37/115/115 | - |
| 14 | CL7 | cB | 804 | - | 1/1/15/20 | 6/37/115/115 | - |
| 14 | CL7 | bA | 3115 | - | 1/1/9/20 | 2/2/80/115 | - |
| 14 | CL7 | aA | 3116 | - | 1/1/9/20 | 2/2/80/115 | - |
| 14 | CL7 | aB | 3003 | - | 2/2/15/20 | 4/37/115/115 | - |
| 14 | CL7 | bA | 3125 | - | 2/2/15/20 | 7/37/115/115 | - |
| 14 | CL7 | bL | 205 | - | 2/2/10/20 | 1/10/88/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CL7 | cA | 3115 | - | 1/1/9/20 | 2/2/80/115 | - |
| 14 | CL7 | cB | 808 | - | 2/2/15/20 | 16/37/115/115 | - |
| 14 | CL7 | cB | 831 | - | 2/2/12/20 | 7/24/102/115 | - |
| 14 | CL7 | aJ | 101 | 8 | 1/1/10/20 | 2/7/85/115 | - |
| 14 | CL7 | aA | 3110 | - | 2/2/10/20 | 0/8/86/115 | - |
| 13 | PHO | bB | 805 | - | - | 18/37/103/103 | 0/5/6/6 |
| 16 | LHG | cA | 3137 | - | - | 15/53/53/53 | - |
| 17 | PQN | bB | 828 | - | - | 7/23/43/43 | 0/2/2/2 |
| 14 | CL7 | bA | 3145 | - | 2/2/10/20 | 3/8/86/115 | - |
| 14 | CL7 | bB | 811 | - | 2/2/10/20 | 1/8/86/115 | - |
| 14 | CL7 | aA | 3112 | - | 2/2/9/20 | 0/2/80/115 | - |
| 14 | CL7 | bA | 3142 | - | 2/2/15/20 | 14/37/115/115 | - |
| 14 | CL7 | cB | 806 | - | 2/2/15/20 | 13/37/115/115 | - |
| 14 | CL7 | aA | 3106 | - | 2/2/10/20 | 3/8/86/115 | - |
| 14 | CL7 | bB | 808 | - | 2/2/15/20 | 13/37/115/115 | - |

The worst 5 of 4062 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 12 | bA | 3101 | G9R | CHC-C1C | 15.30 | 1.47 | 1.35 |
| 12 | cA | 3101 | G9R | CHC-C1C | 15.15 | 1.47 | 1.35 |
| 13 | cB | 801 | PHO | C3A-C2A | -14.42 | 1.41 | 1.54 |
| 13 | bB | 801 | PHO | C3A-C2A | -14.37 | 1.41 | 1.54 |
| 13 | aA | 3102 | PHO | C3A-C2A | -13.81 | 1.42 | 1.54 |

The worst 5 of 2539 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 12 | bA | 3101 | G9R | C1D-ND-C4D | -12.65 | 96.34 | 106.41 |
| 12 | aA | 3101 | G9R | C1D-ND-C4D | -11.65 | 97.13 | 106.41 |
| 12 | cA | 3101 | G9R | C1D-ND-C4D | -9.58 | 98.78 | 106.41 |
| 14 | cA | 3124 | CL7 | O2D-CGD-O1D | -9.45 | 105.36 | 123.84 |
| 14 | cA | 3119 | CL7 | C1A-NA-C4A | -9.09 | 100.80 | 106.30 |

5 of 376 chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 12 | aA | 3101 | G9R | ND |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 12 | cA | 3101 | G9R | ND |
| 14 | aA | 3103 | CL7 | NC |
| 14 | aA | 3104 | CL7 | NA |
| 14 | aA | 3104 | CL7 | NC |

5 of 1852 torsion outliers are listed below:

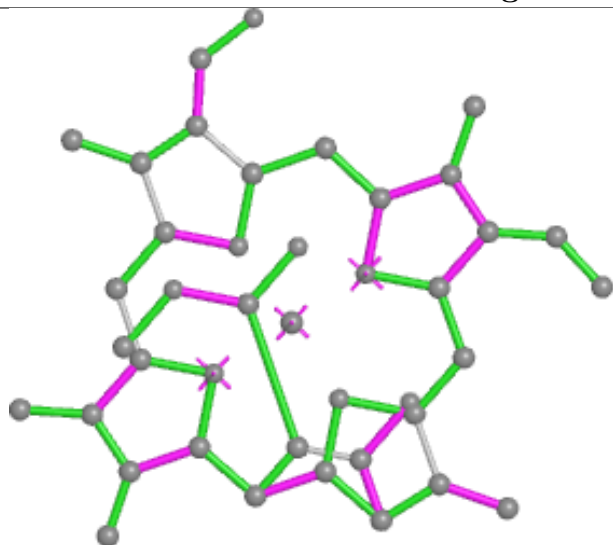
| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|----------------|
| 12 | bA | 3101 | G9R | NB-C4B-CHC-C1C |
| 12 | bA | 3101 | G9R | NC-C1C-CHC-C4B |
| 13 | aA | 3102 | PHO | CBA-CGA-O2A-C1 |
| 13 | aA | 3102 | PHO | O1A-CGA-O2A-C1 |
| 13 | bB | 801 | PHO | CBA-CGA-O2A-C1 |

There are no ring outliers.

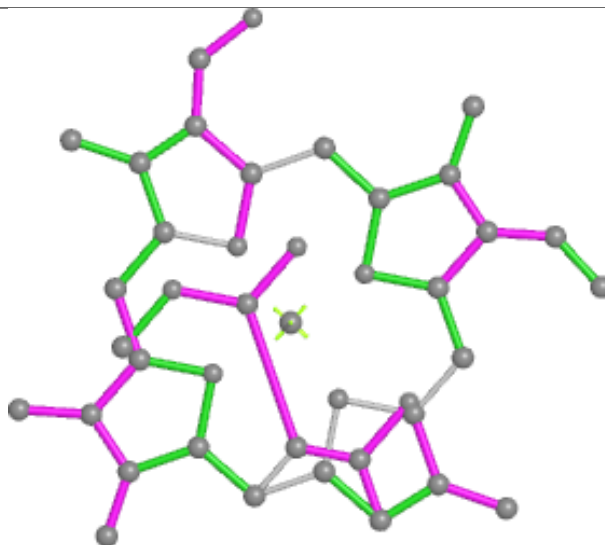
No monomer is involved in short contacts.

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.

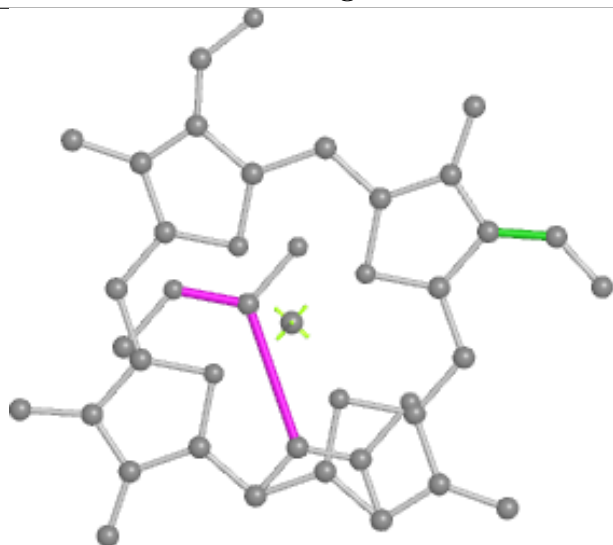
Ligand CL7 cA 3105



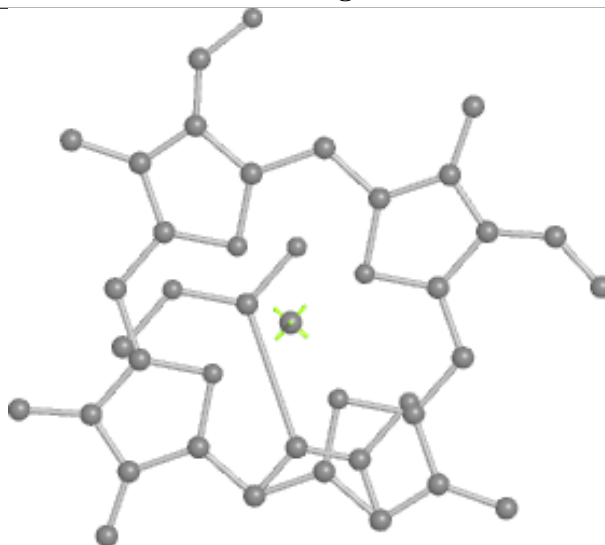
Bond lengths



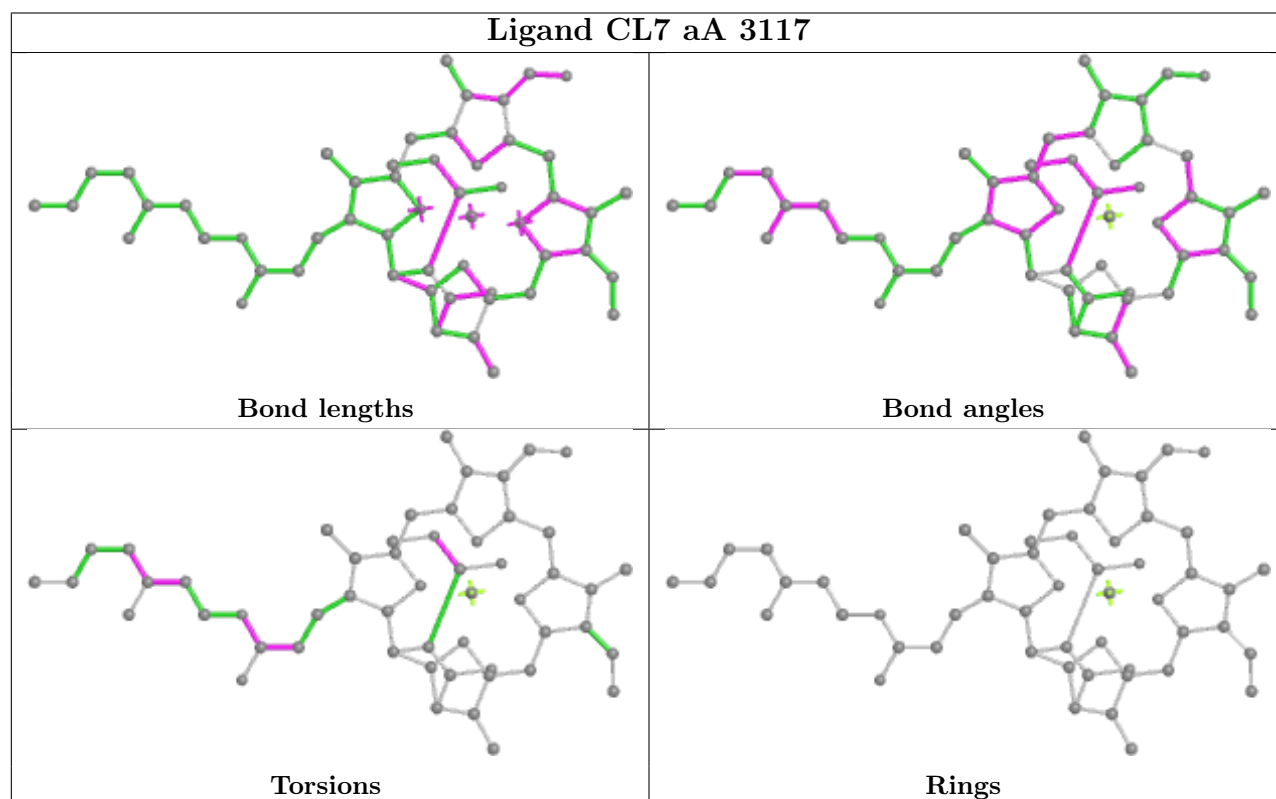
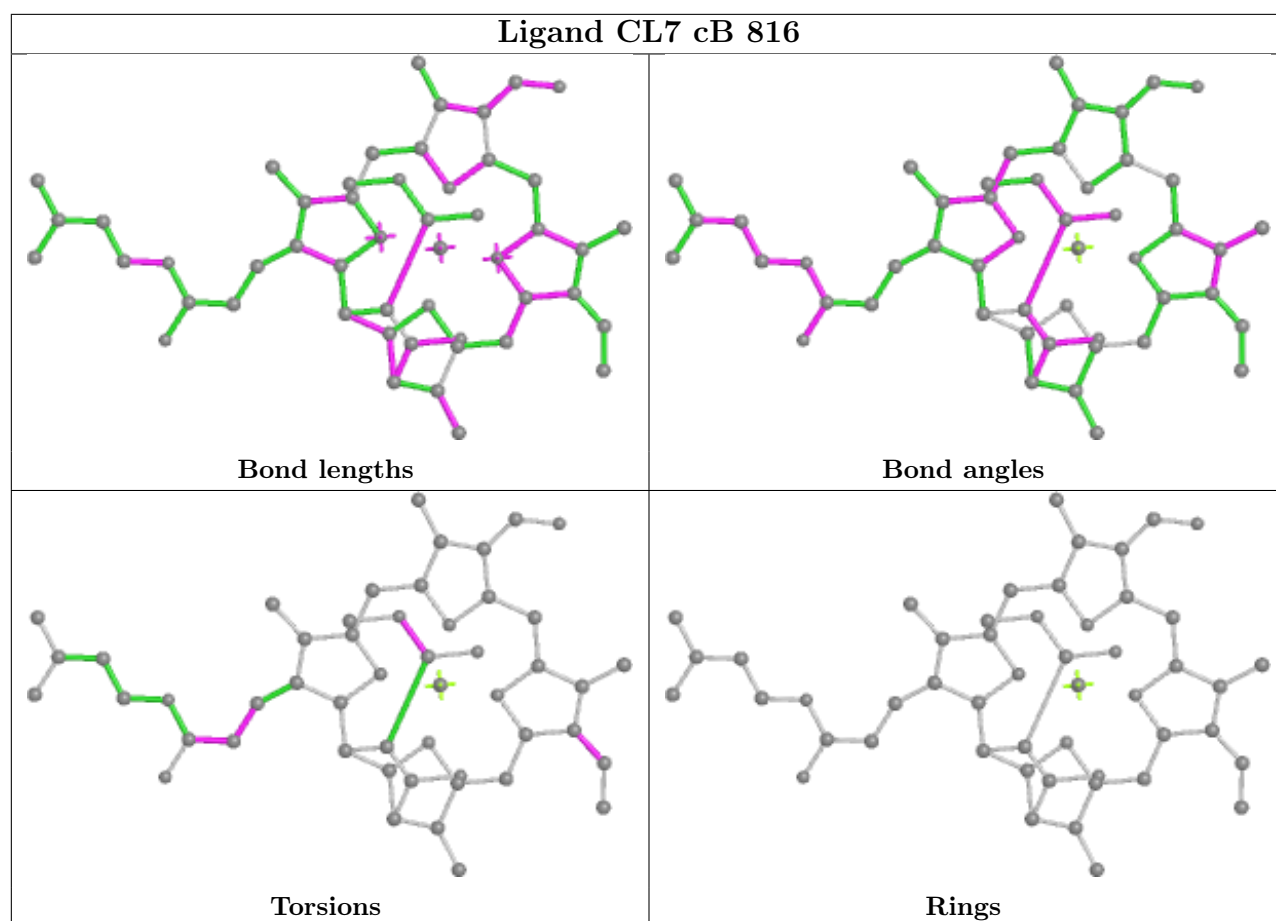
Bond angles

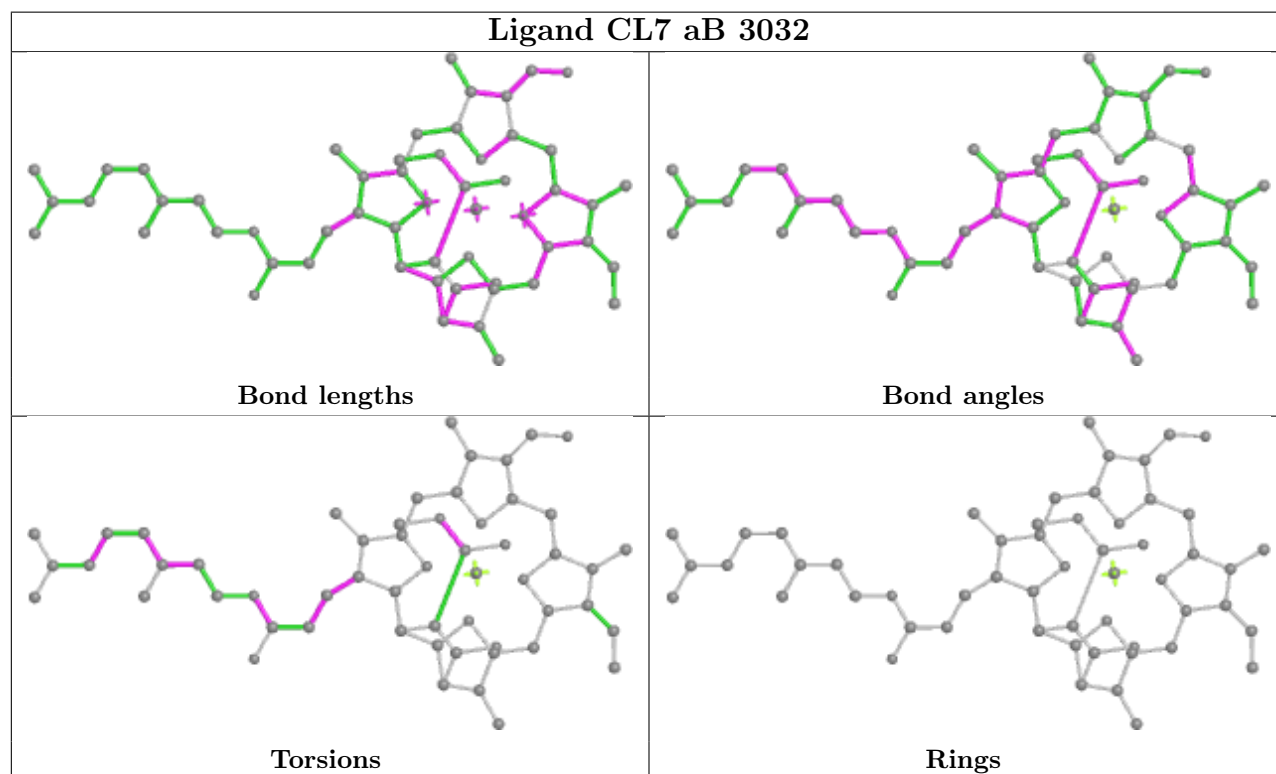
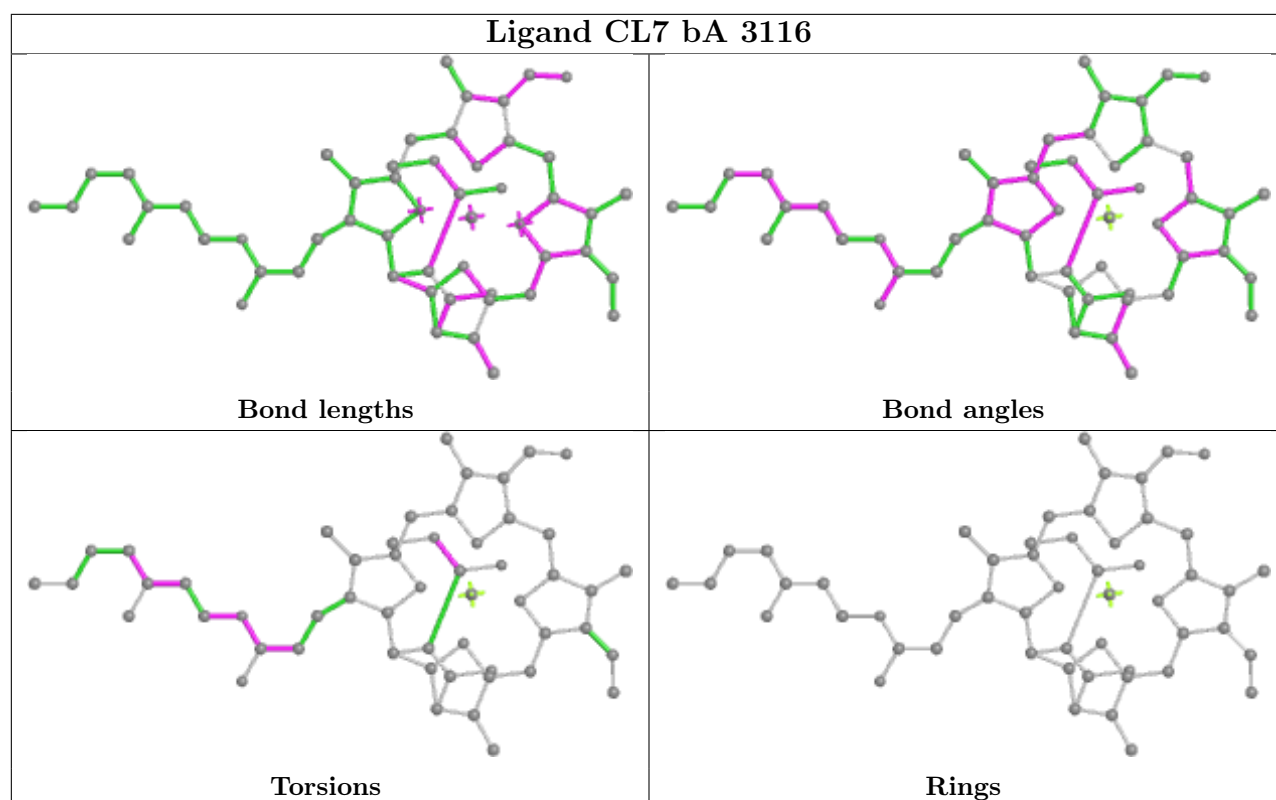


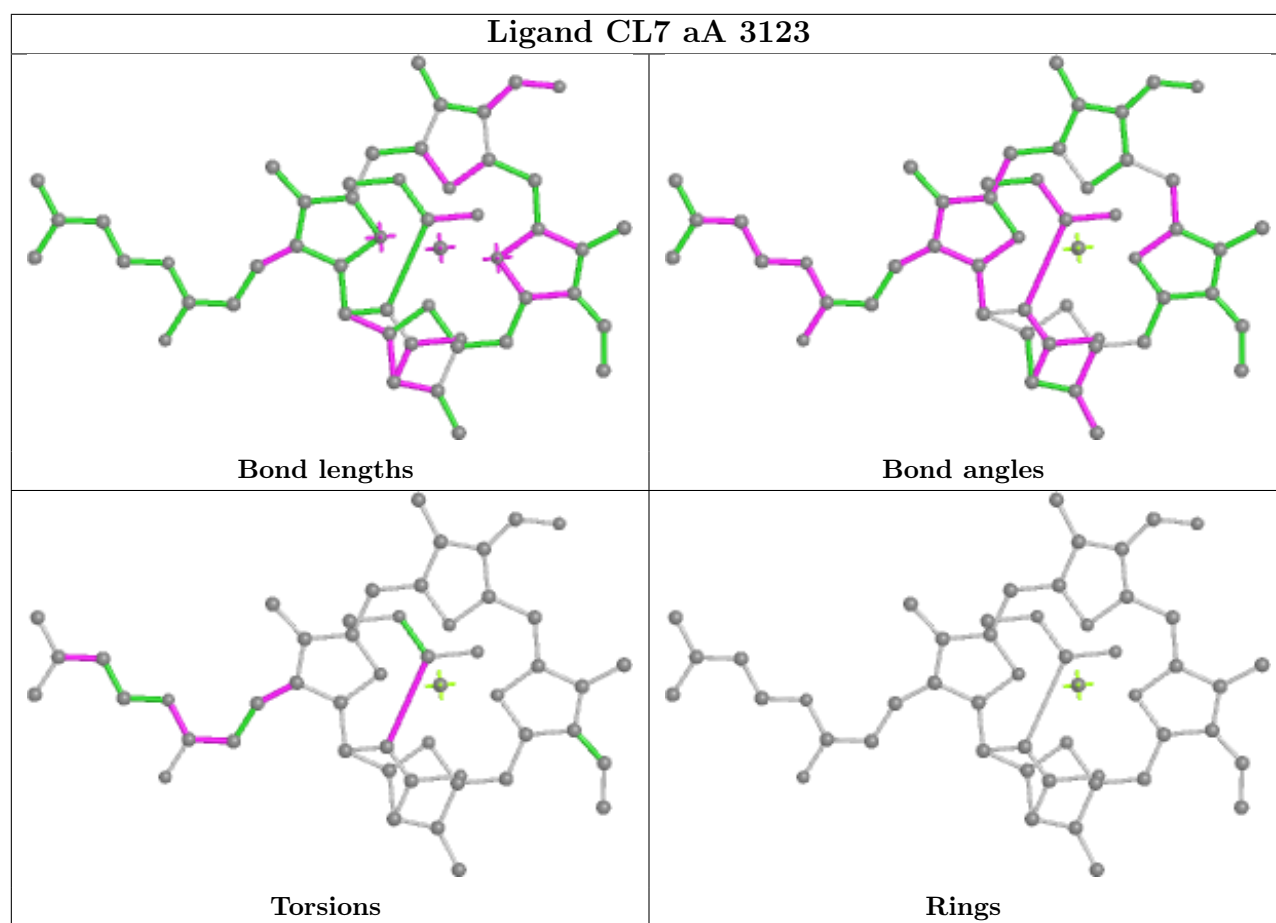
Torsions

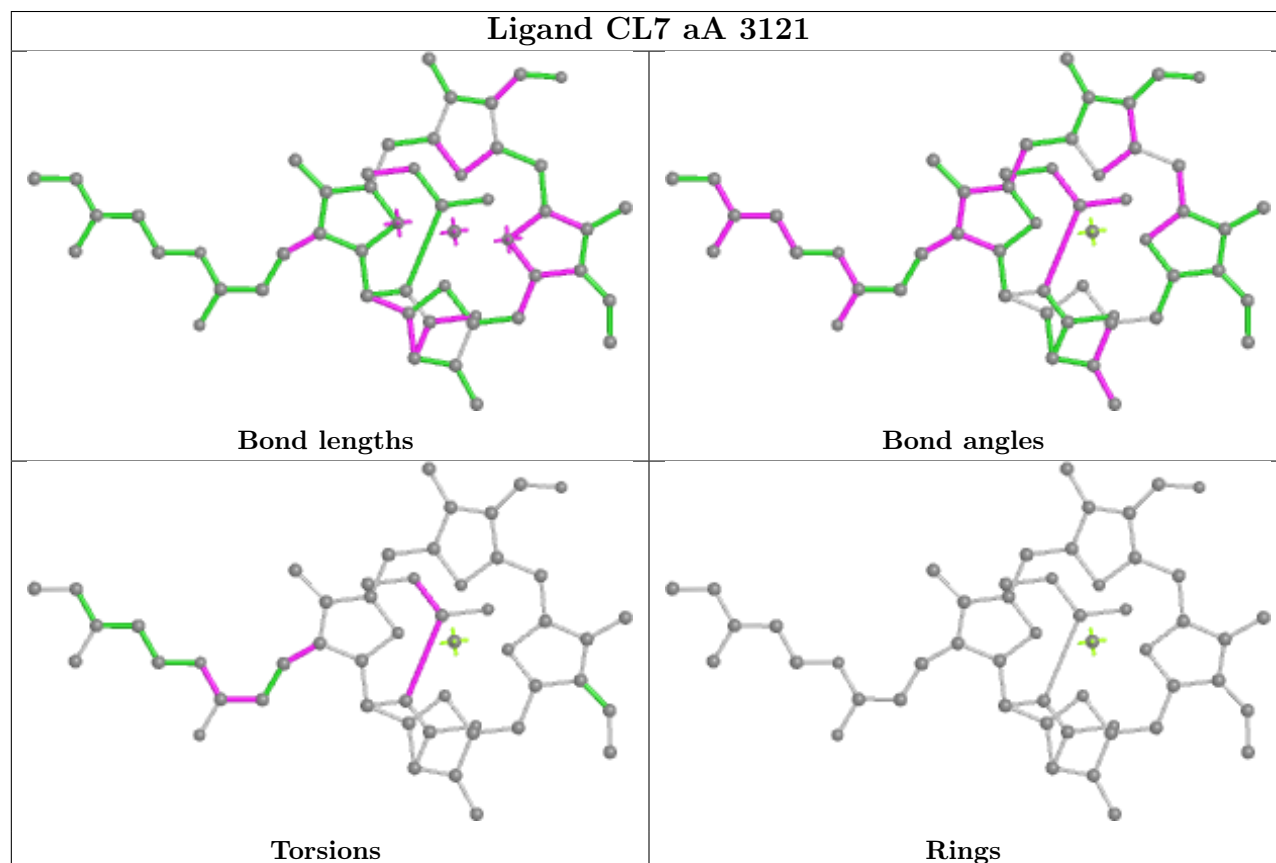
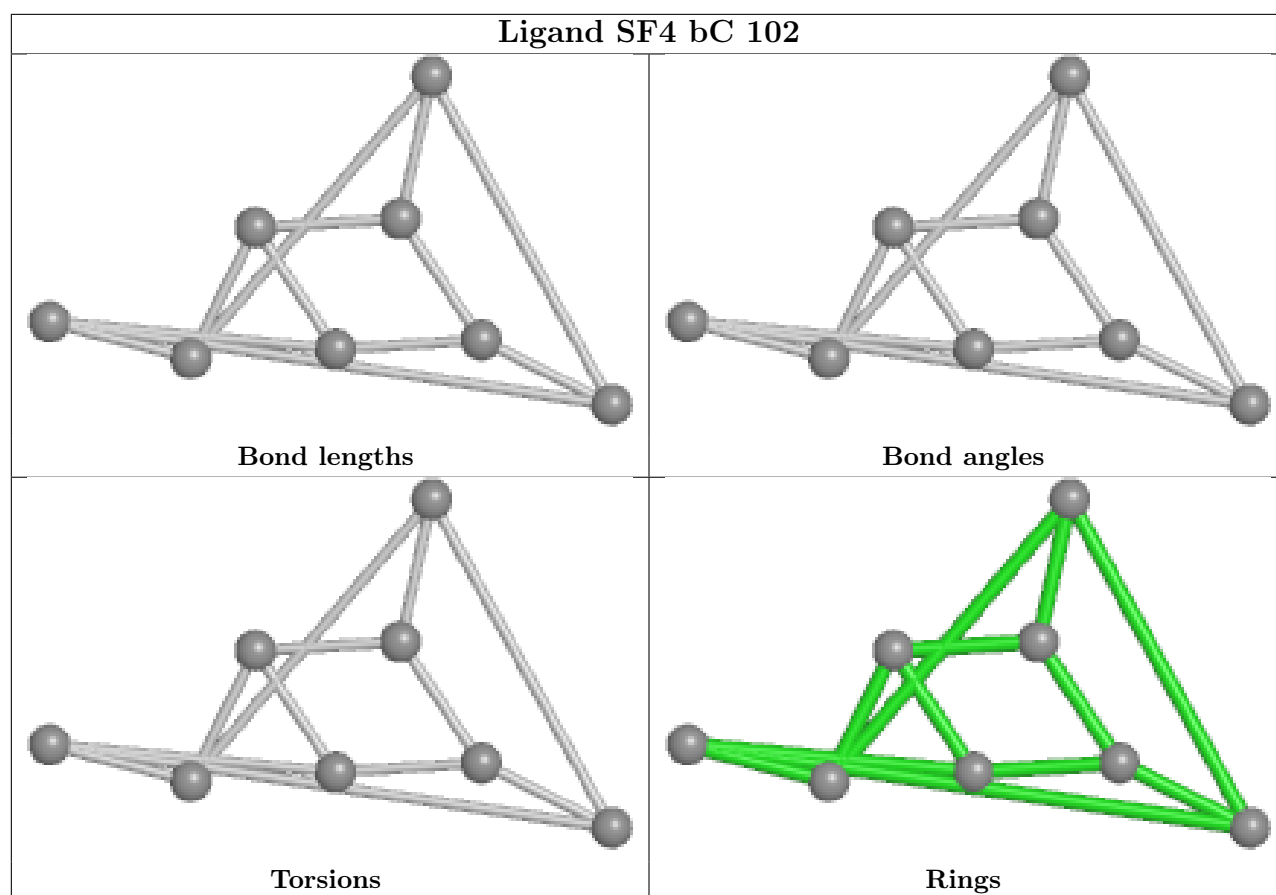


Rings

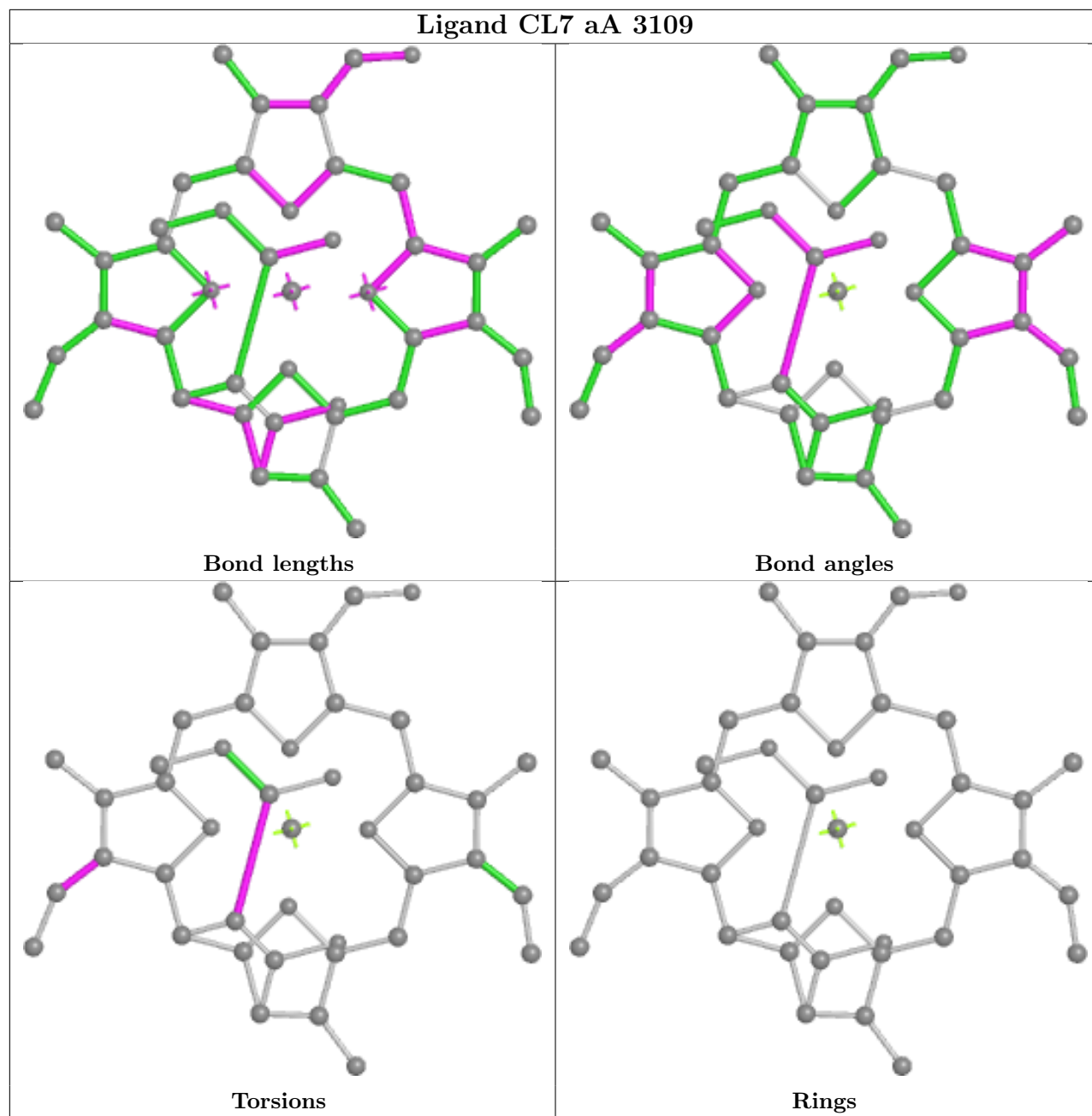




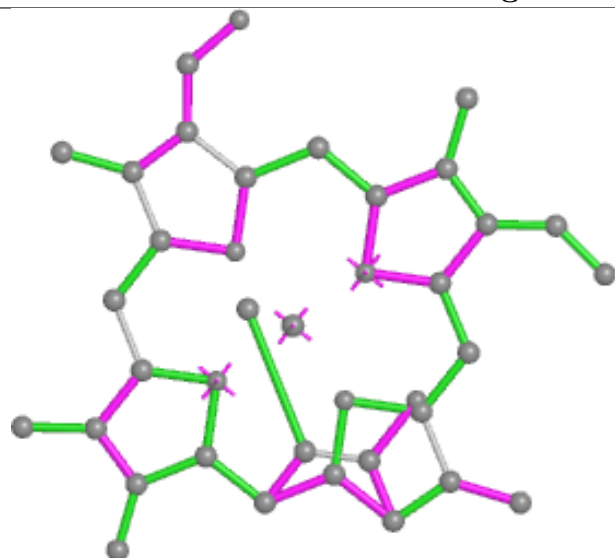




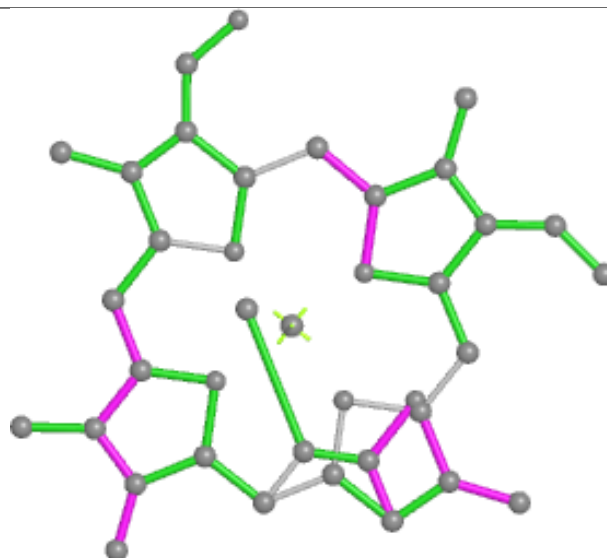
Ligand CL7 aA 3109



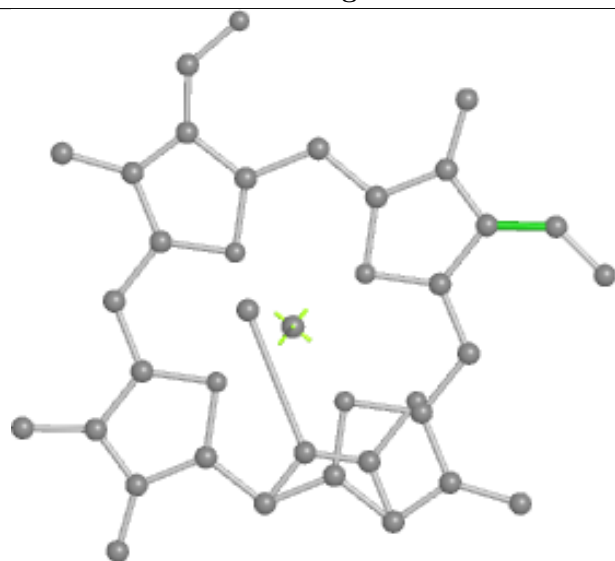
Ligand CL7 bA 3118



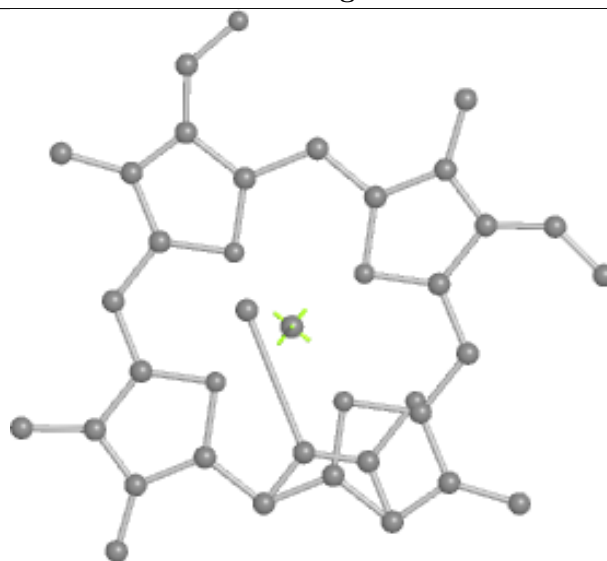
Bond lengths



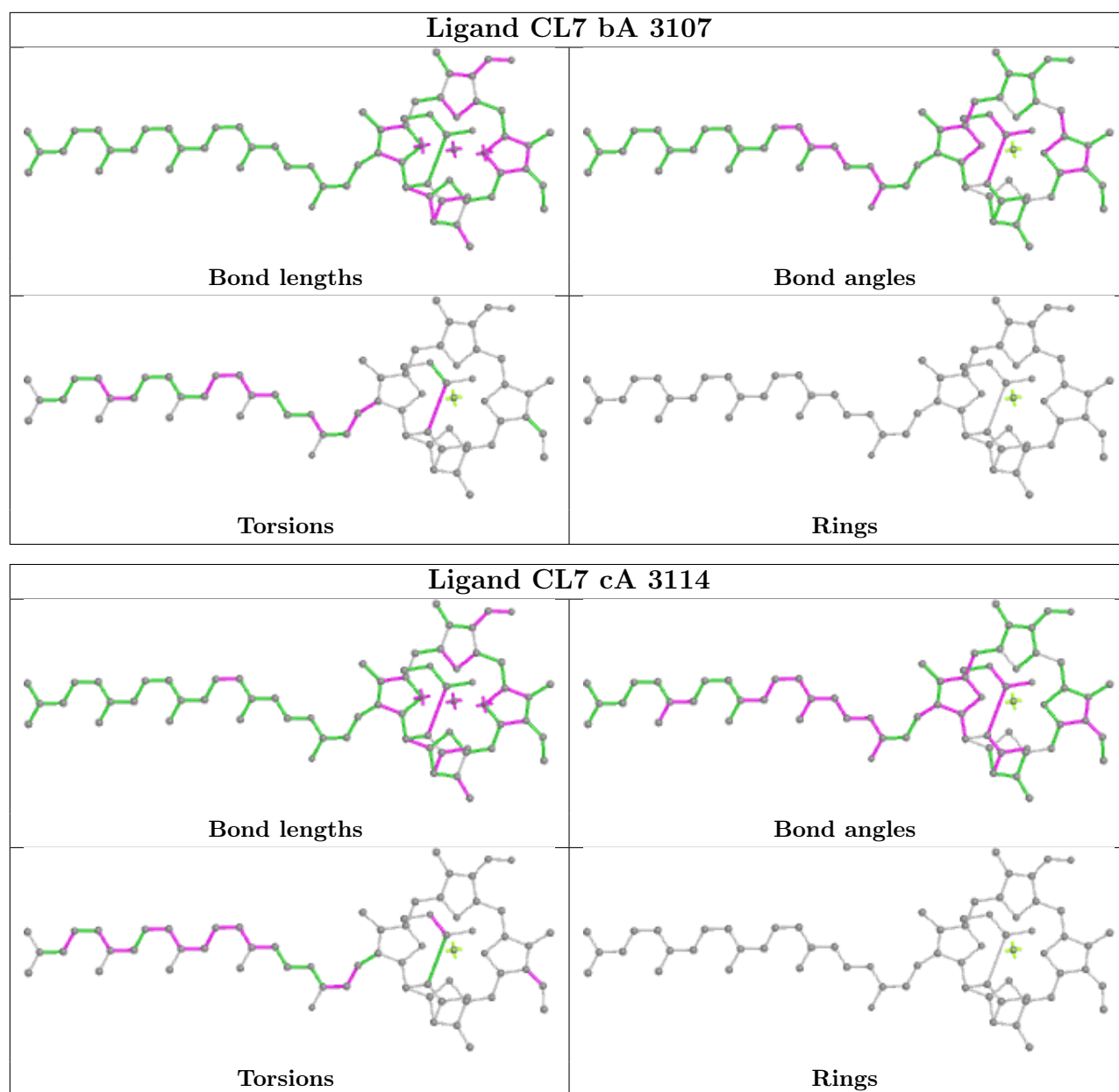
Bond angles

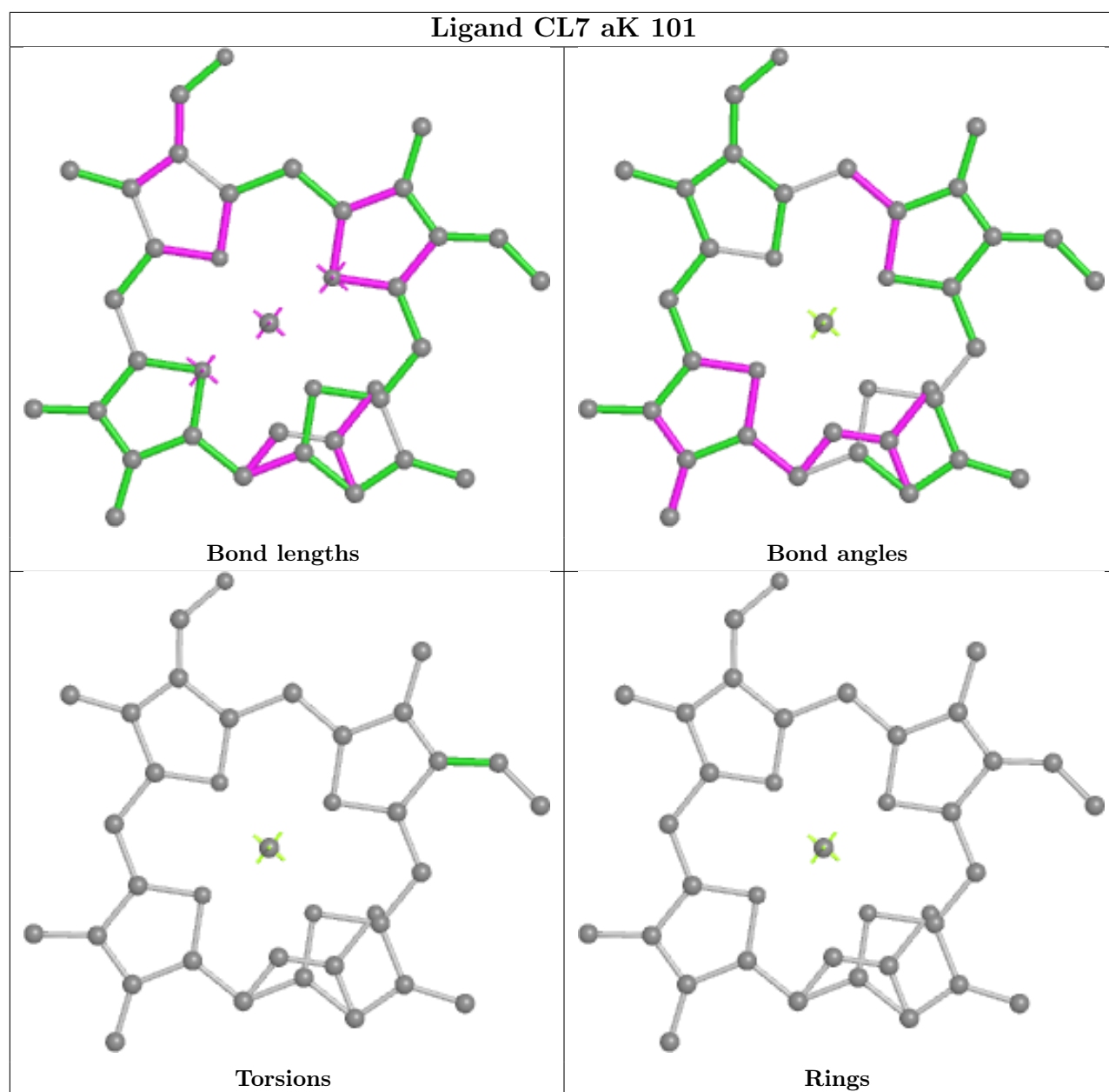


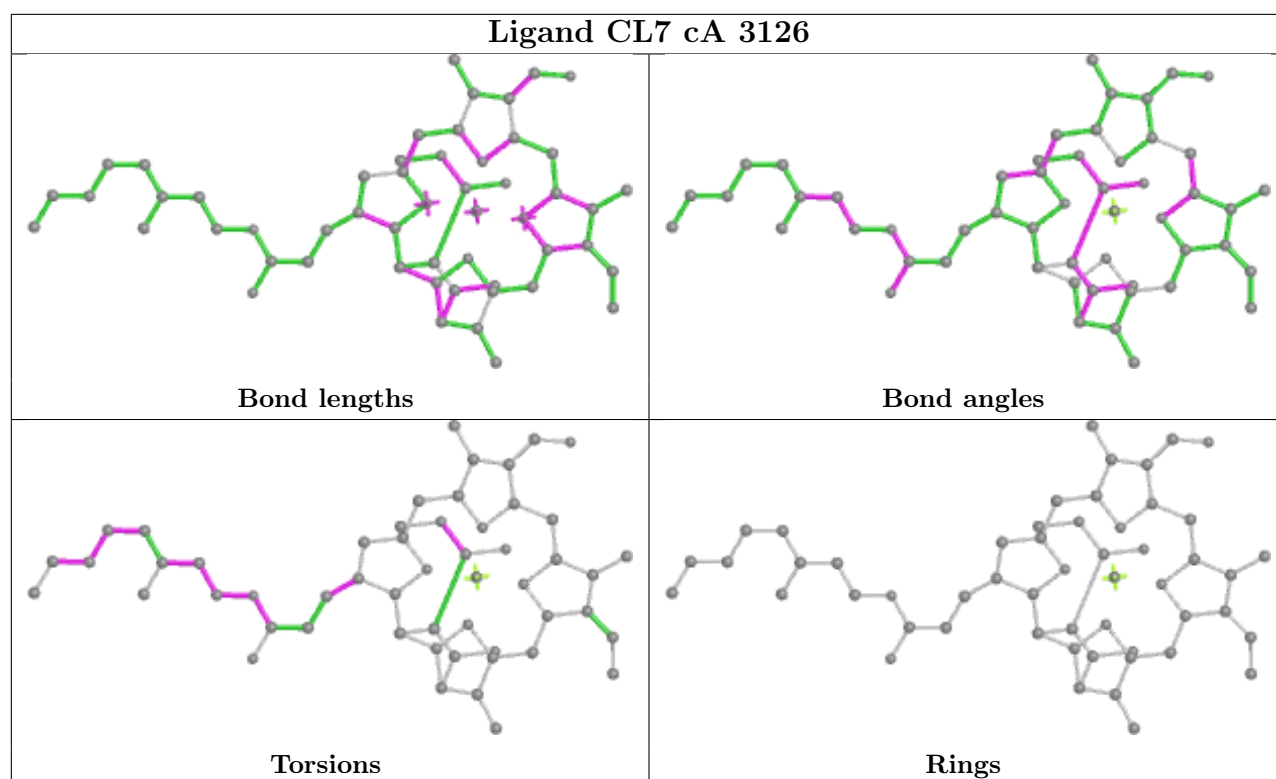
Torsions

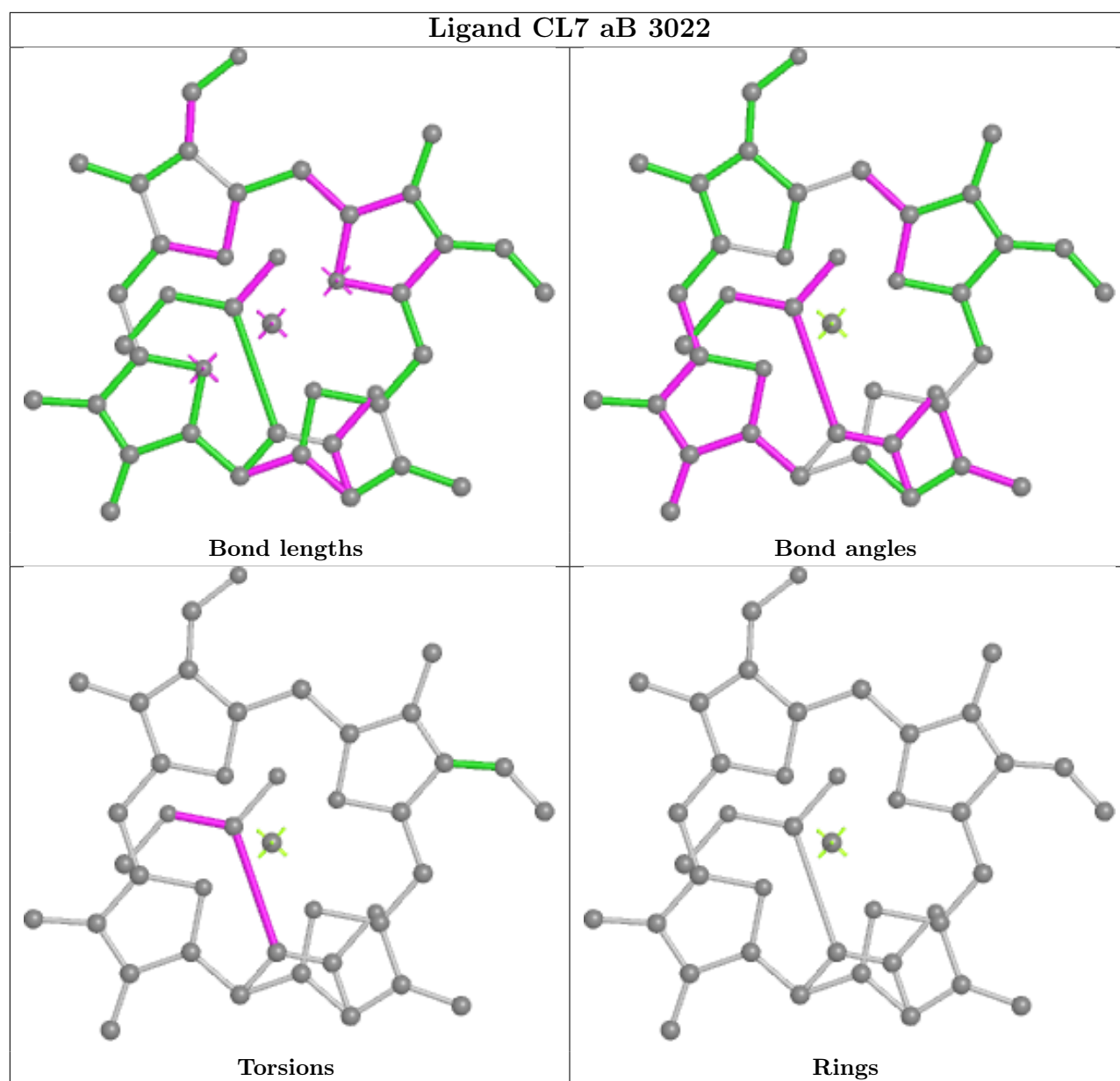


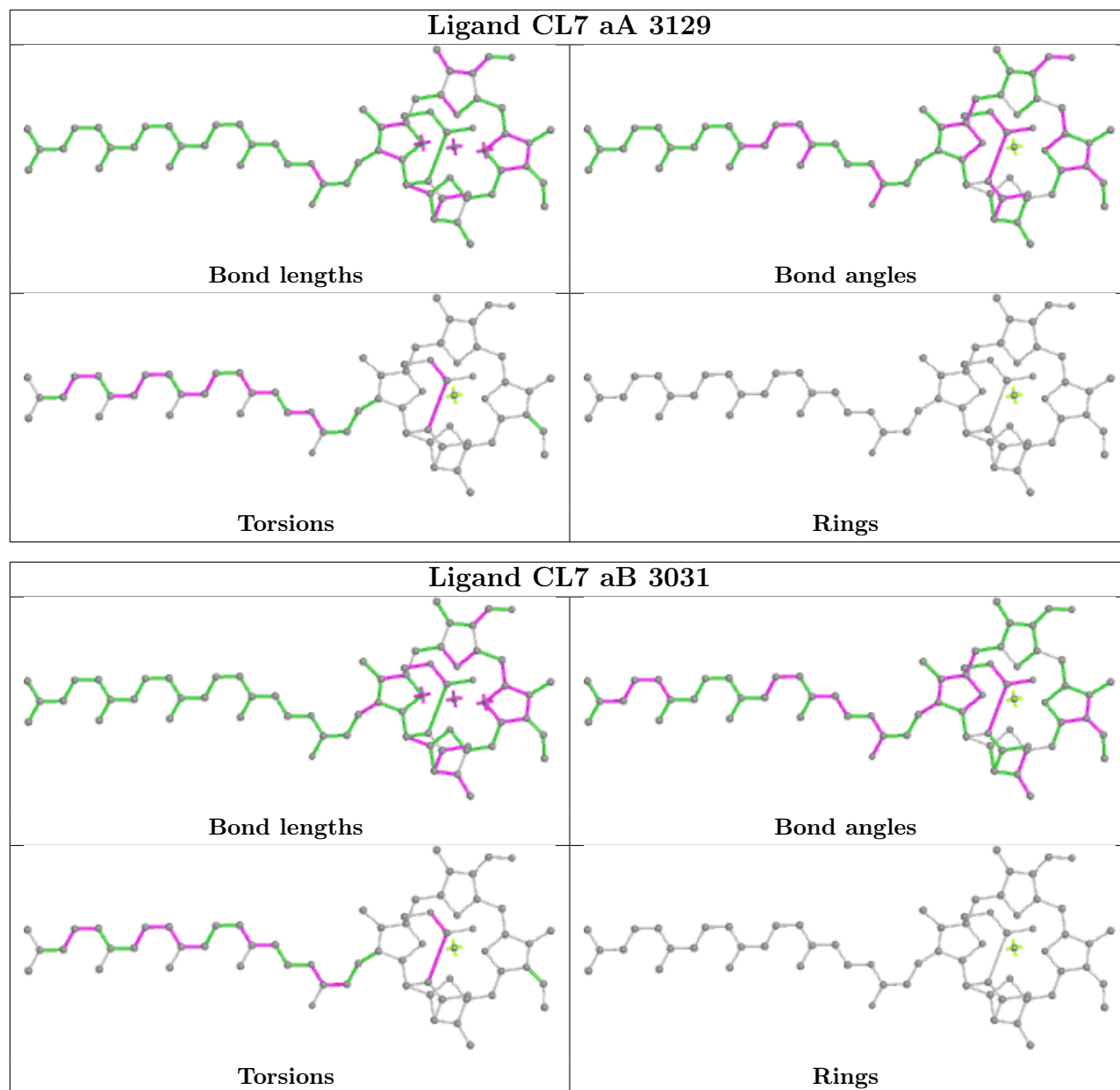
Rings

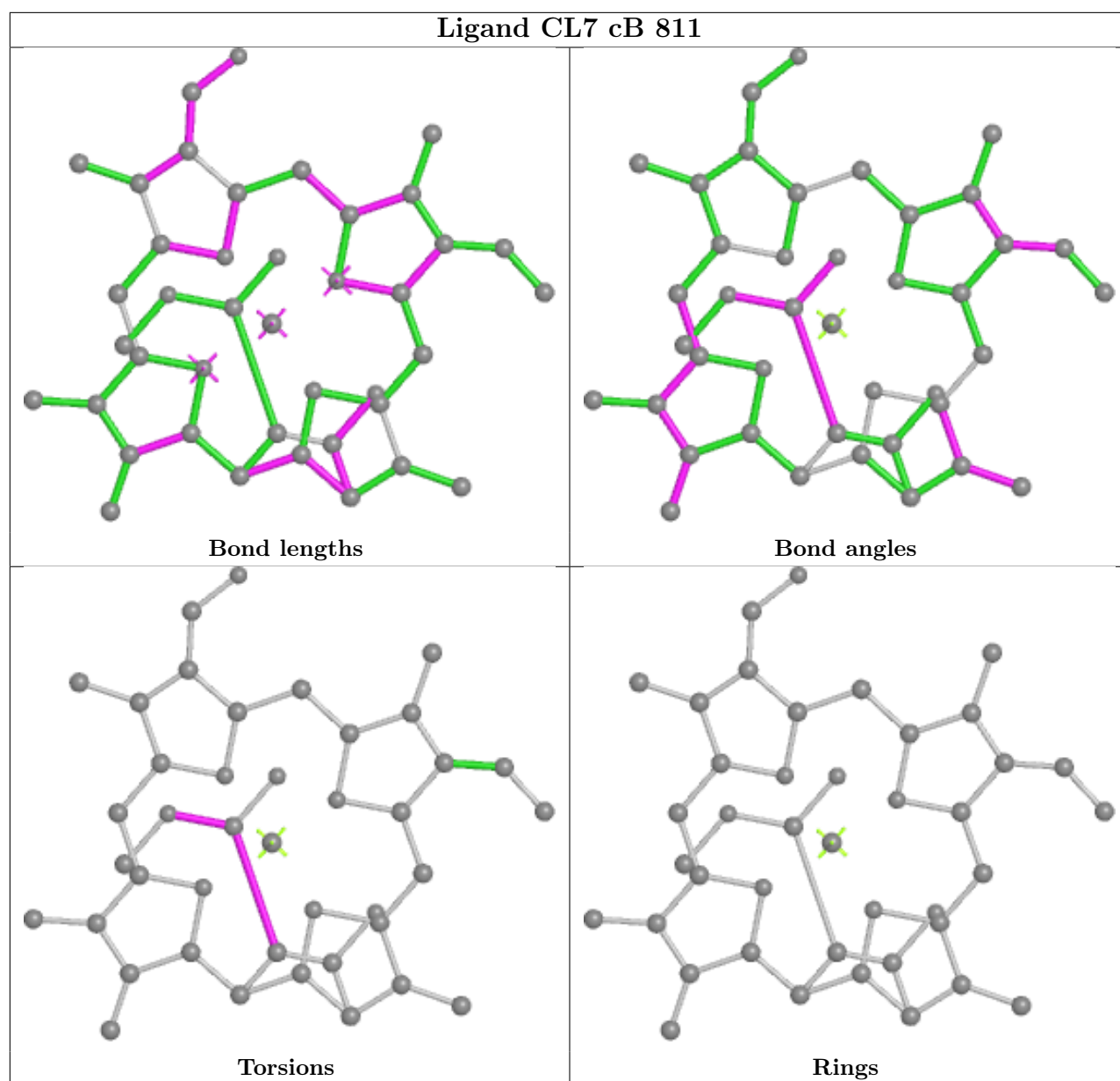




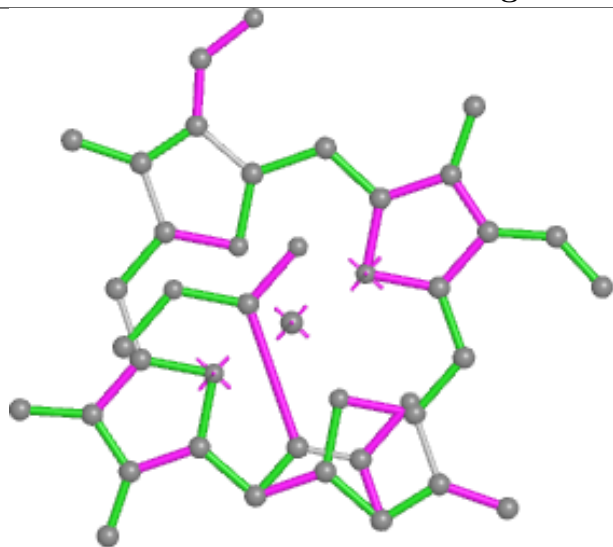




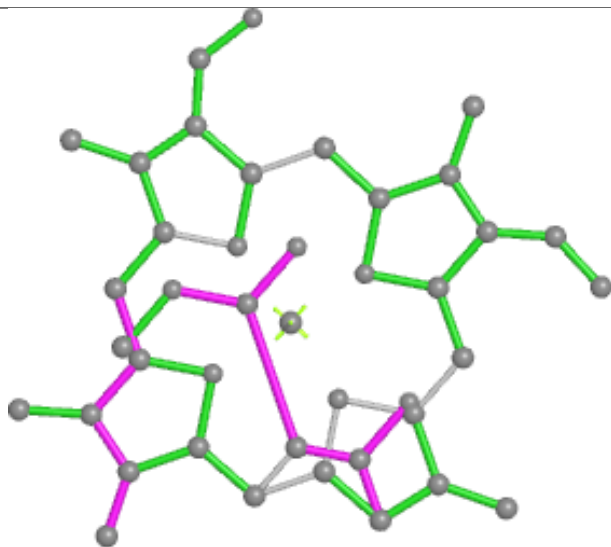




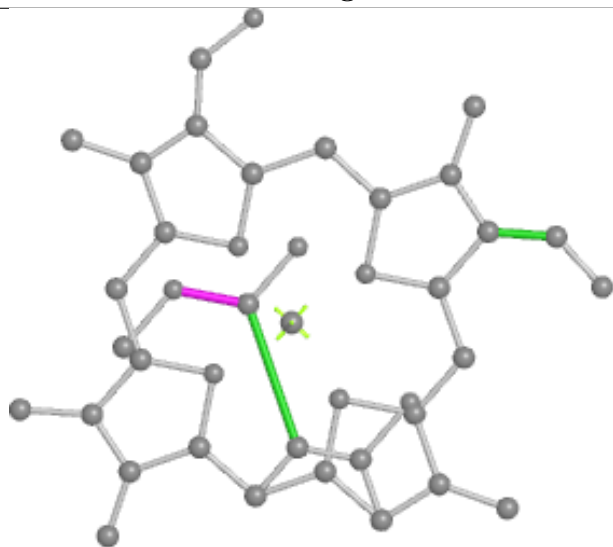
Ligand CL7 aA 3122



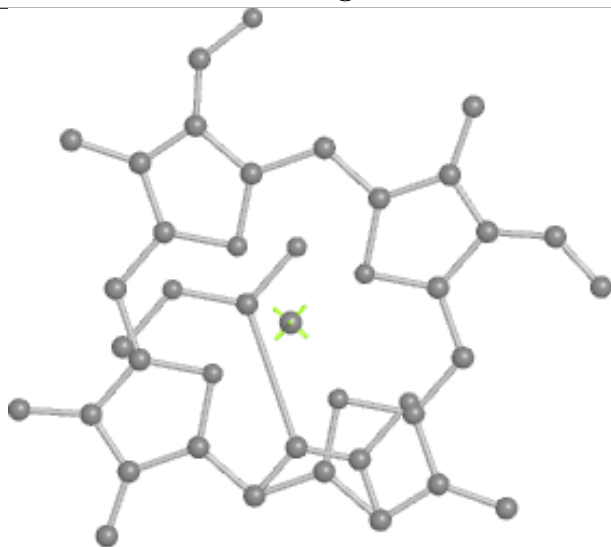
Bond lengths



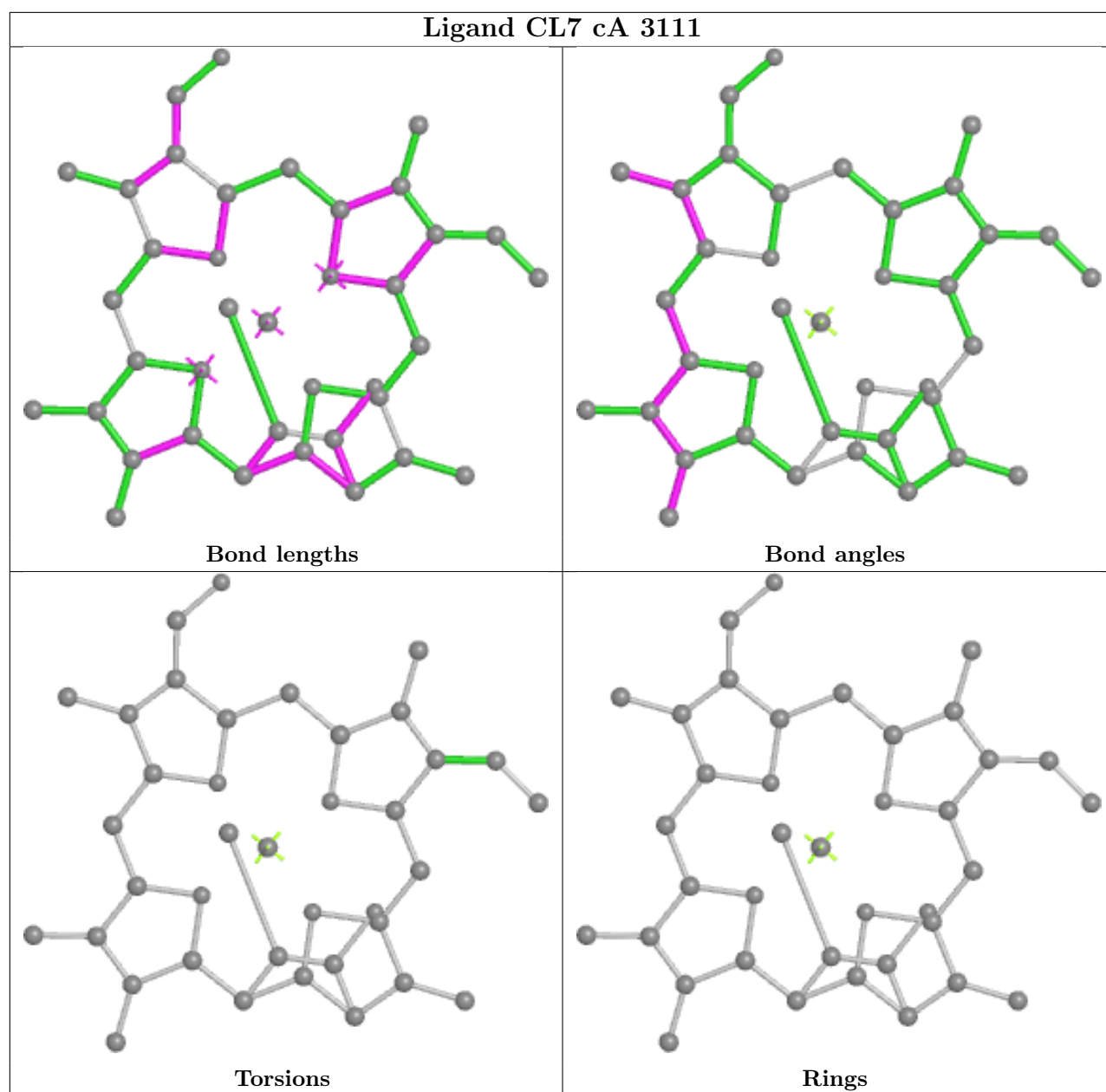
Bond angles

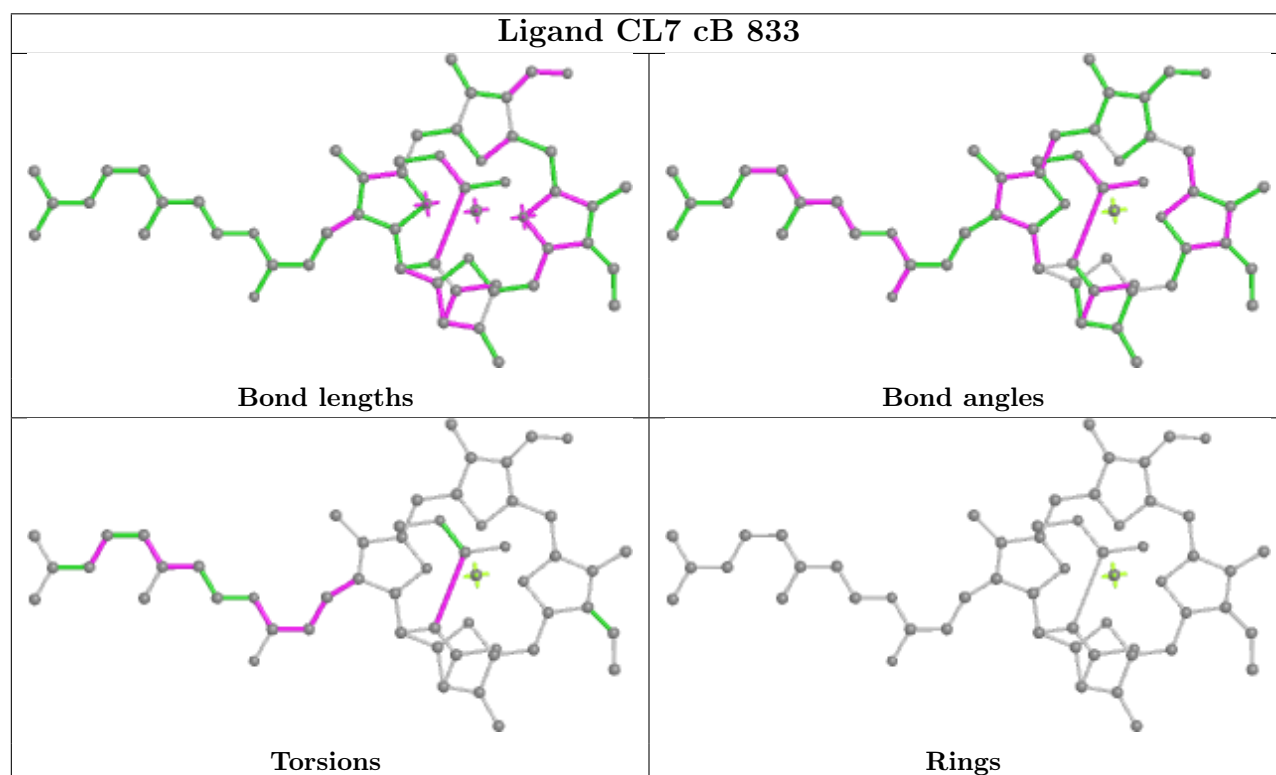
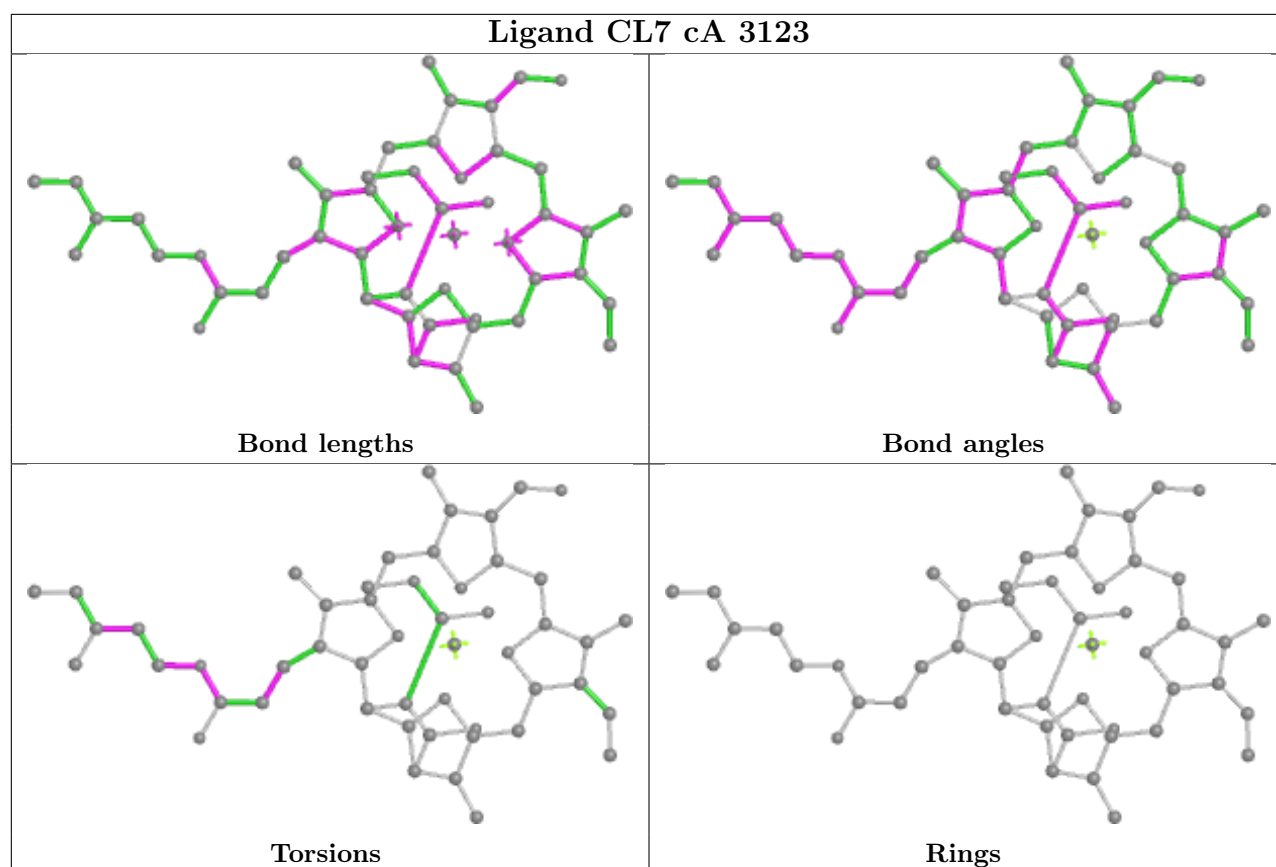


Torsions

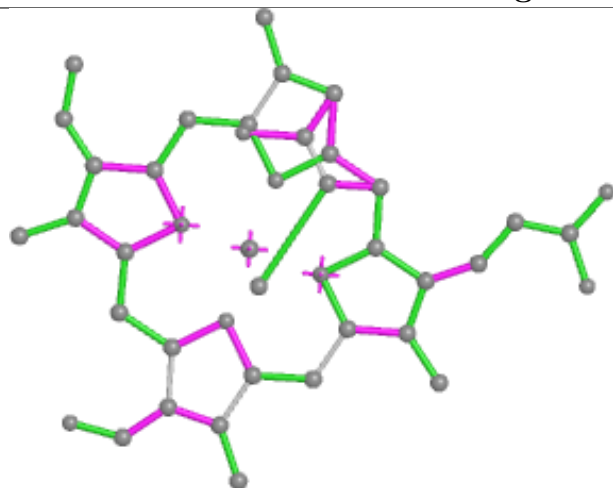


Rings

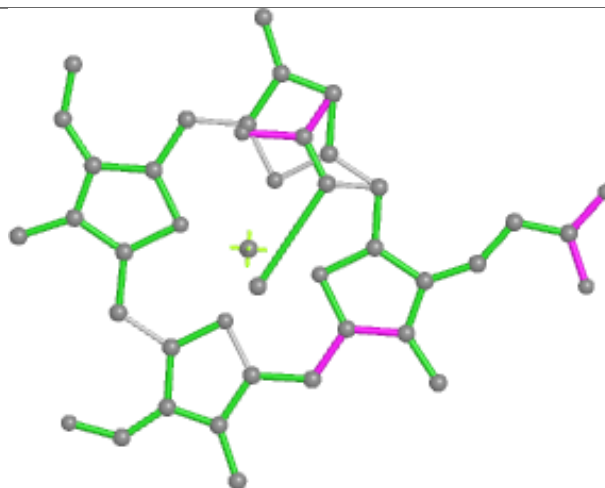




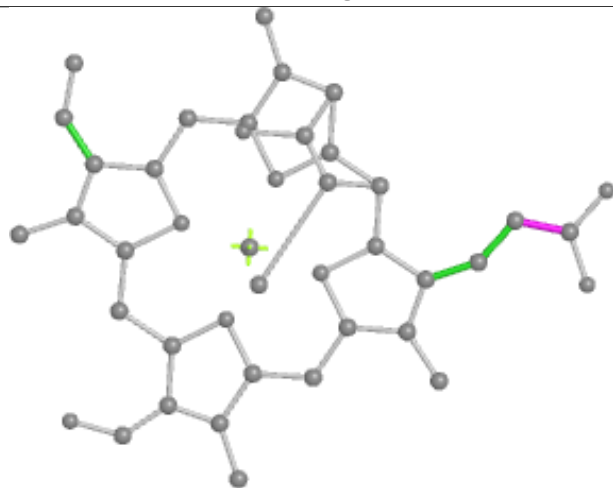
Ligand CL7 cJ 101



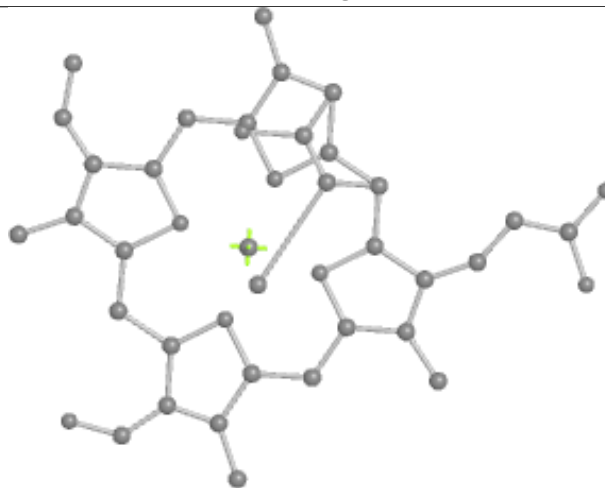
Bond lengths



Bond angles

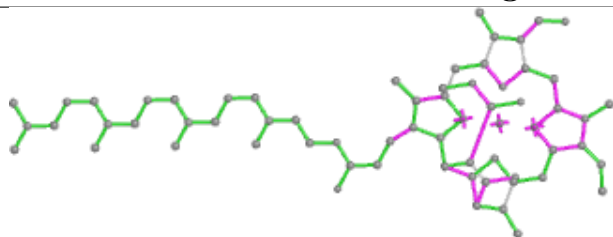


Torsions

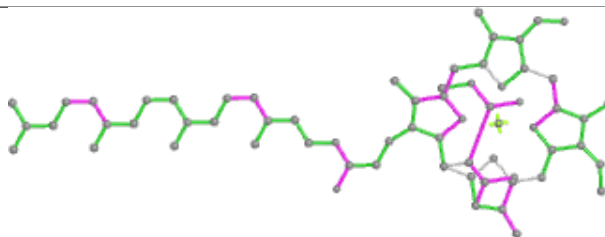


Rings

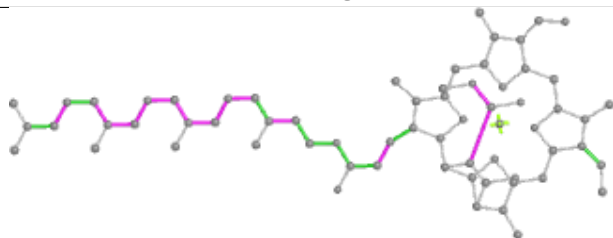
Ligand CL7 aB 3002



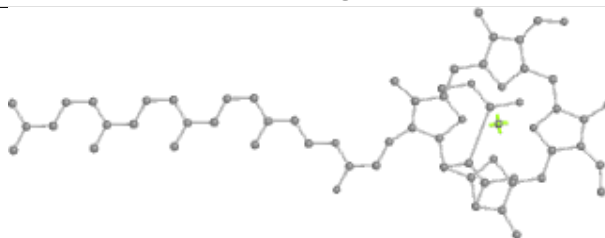
Bond lengths



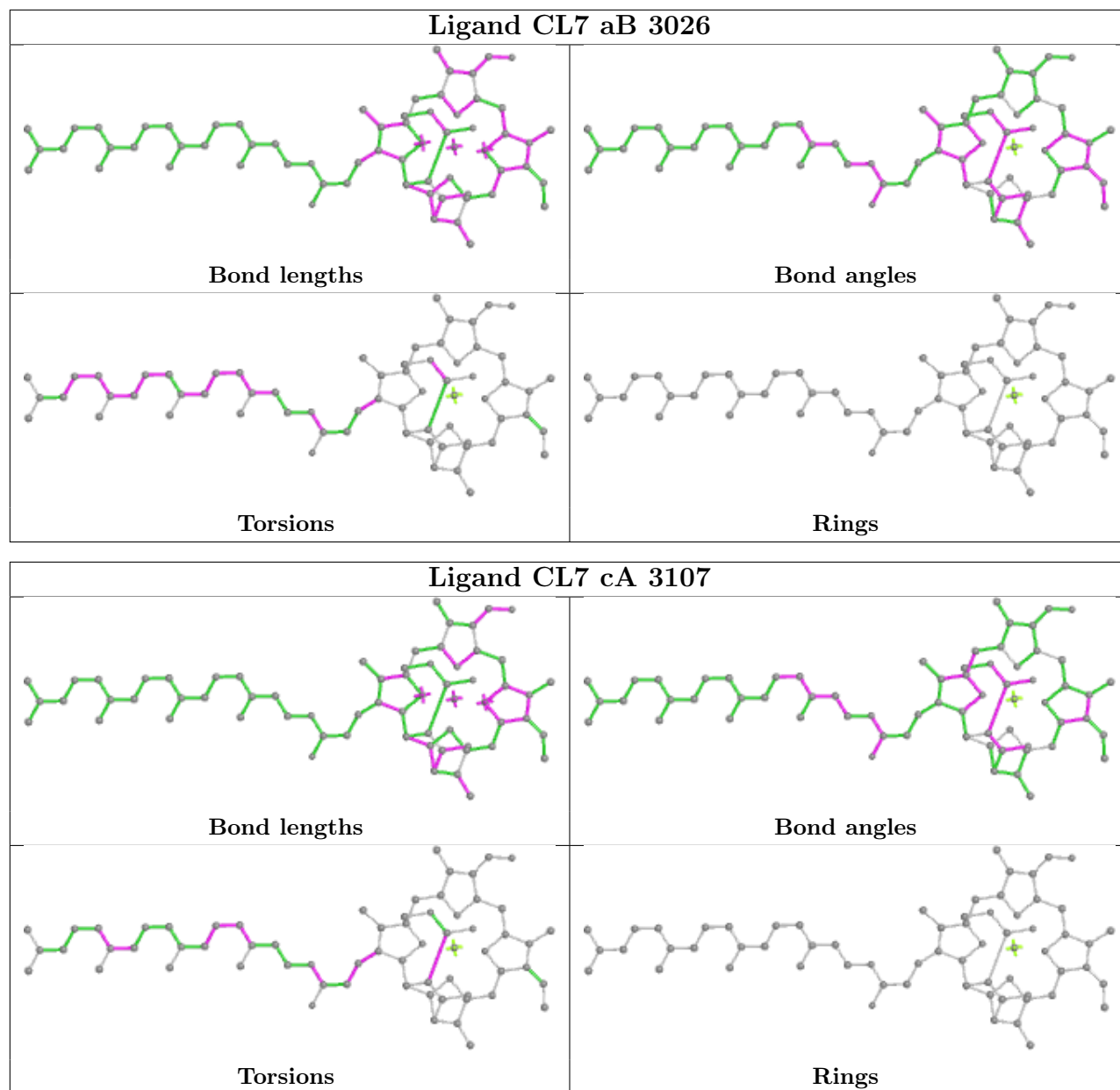
Bond angles

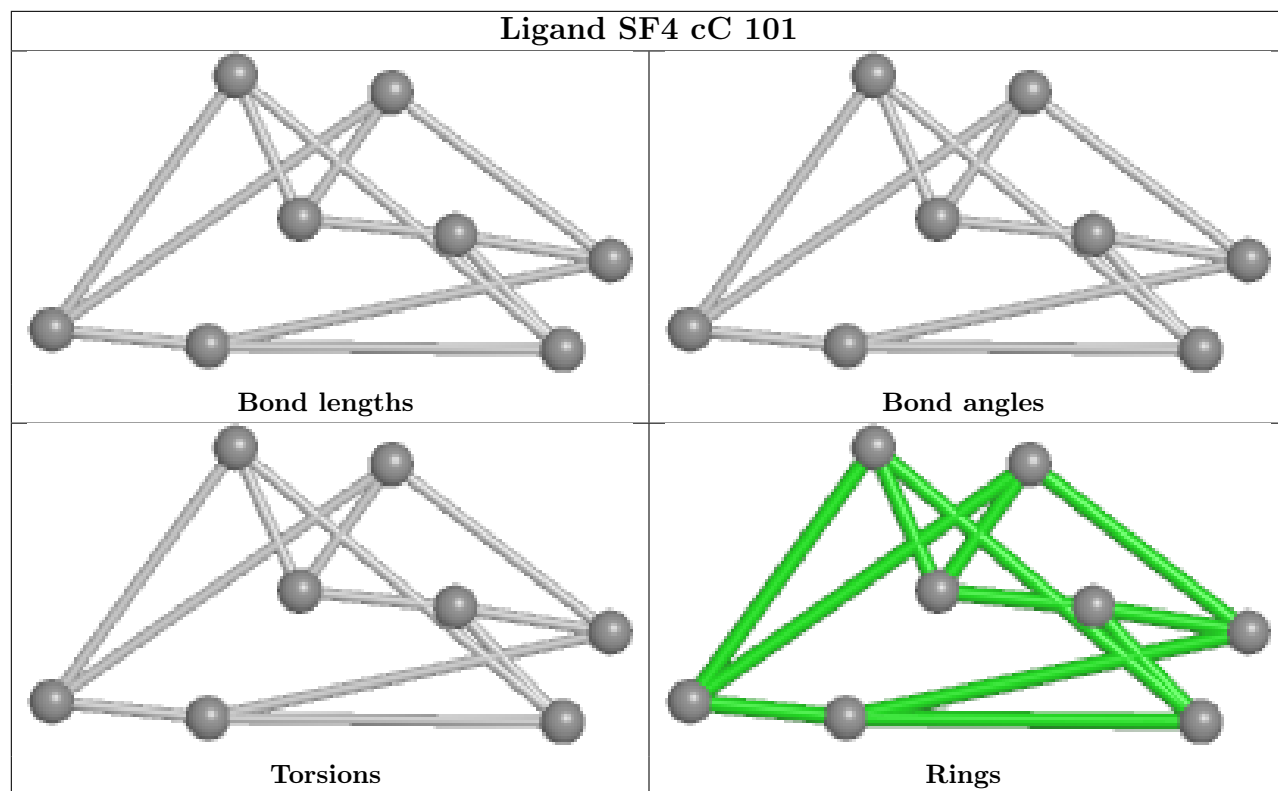


Torsions

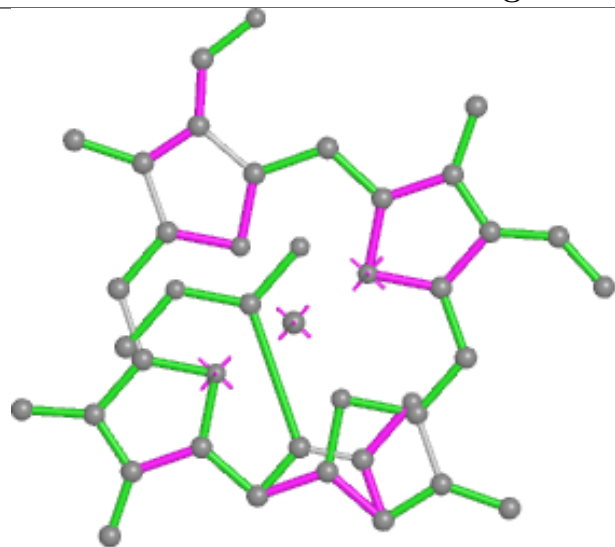


Rings

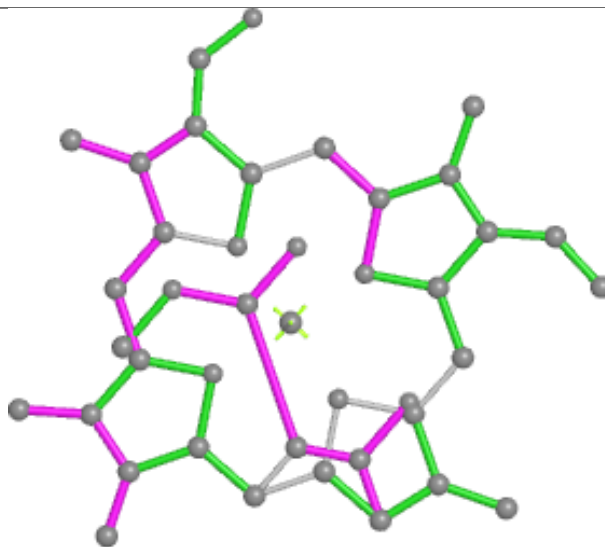




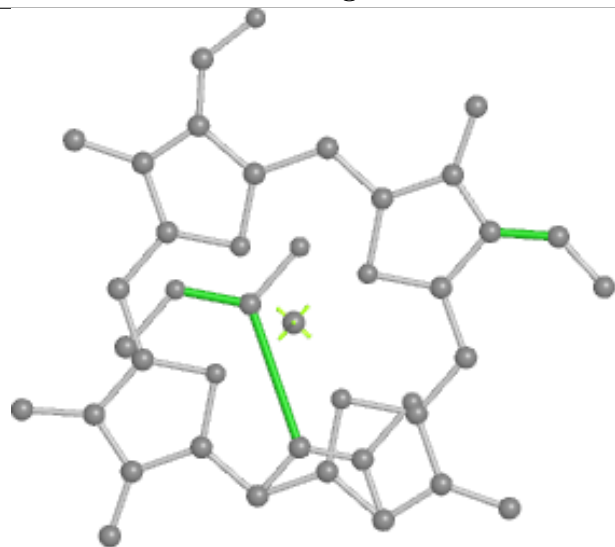
Ligand CL7 cA 3113



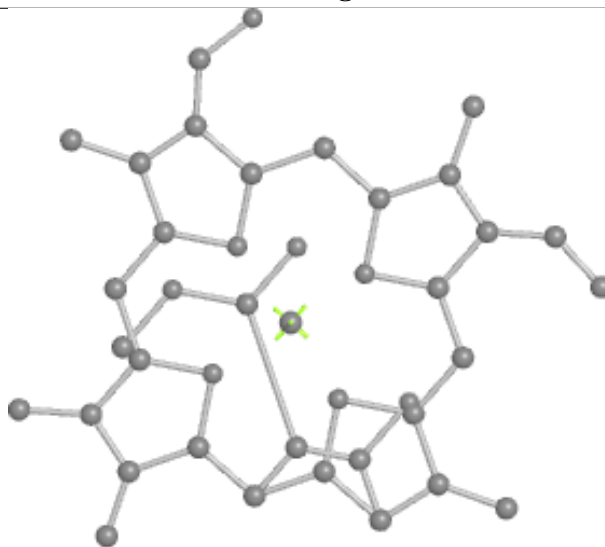
Bond lengths



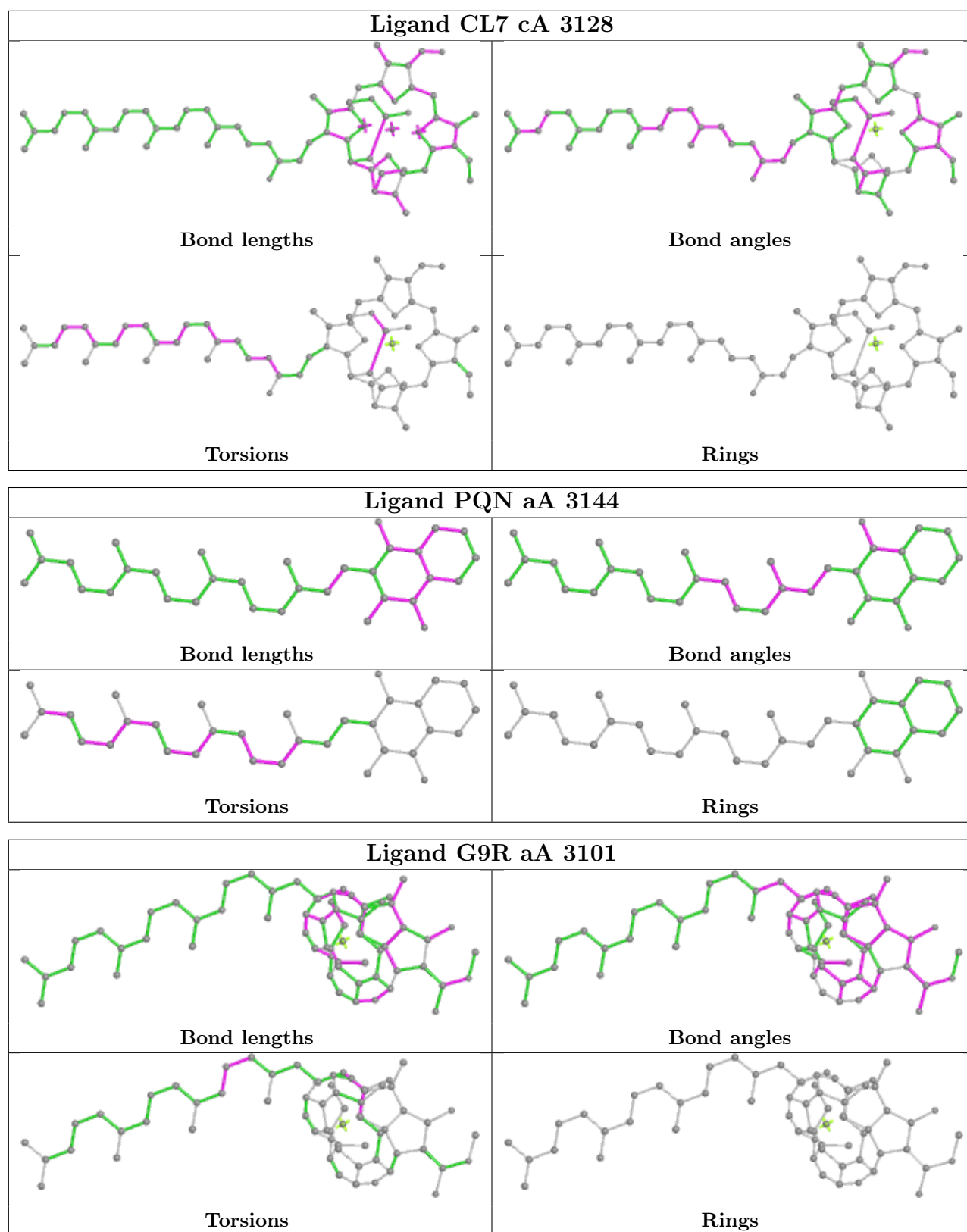
Bond angles



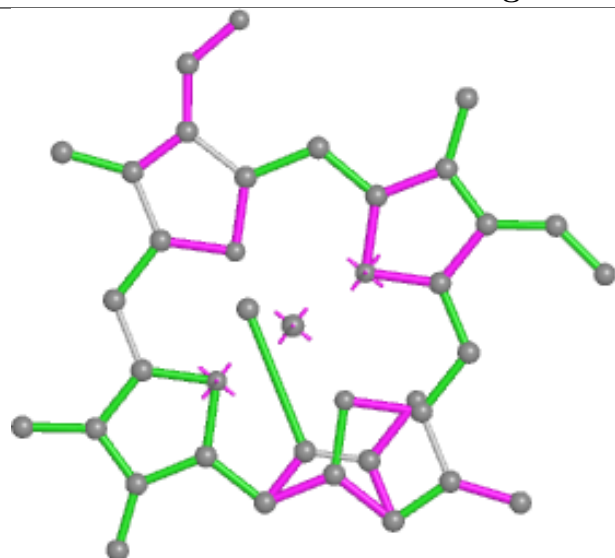
Torsions



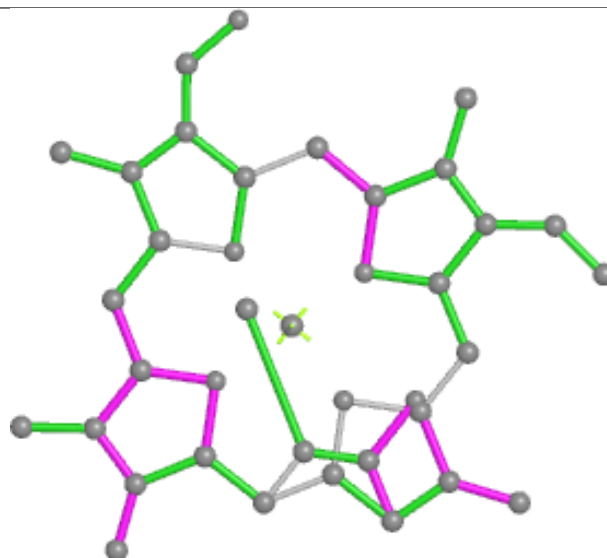
Rings



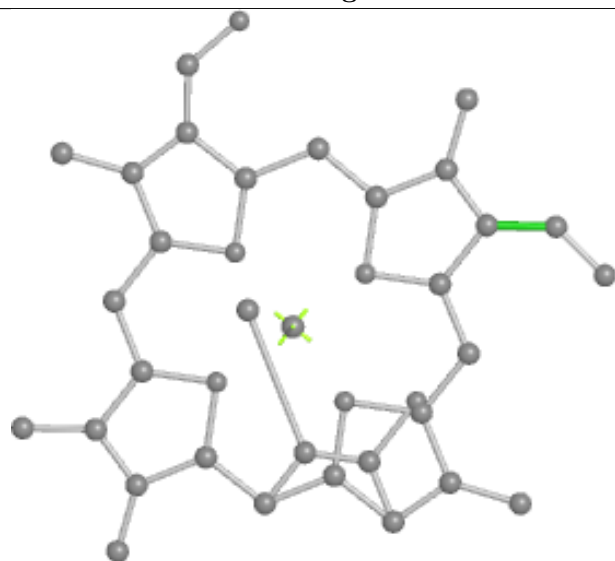
Ligand CL7 aA 3119



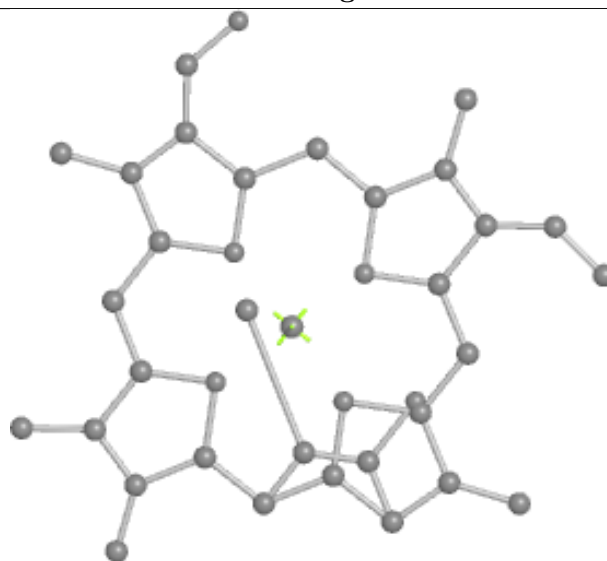
Bond lengths



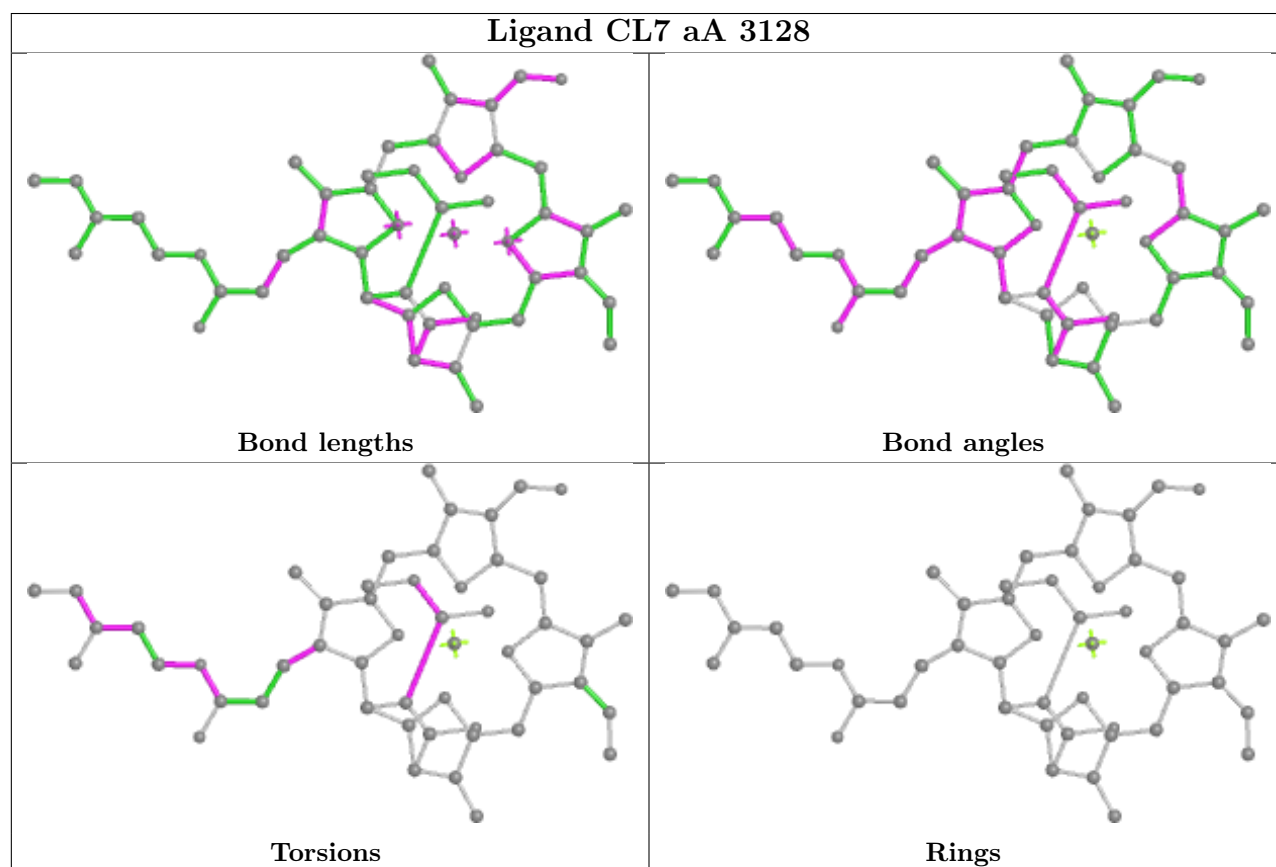
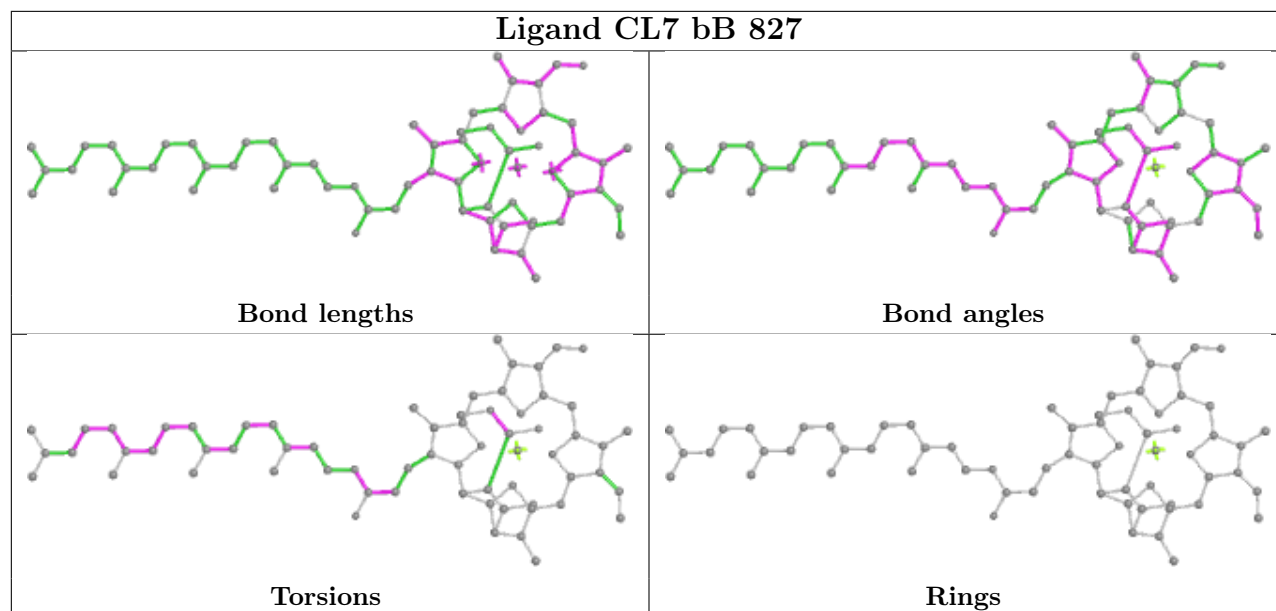
Bond angles

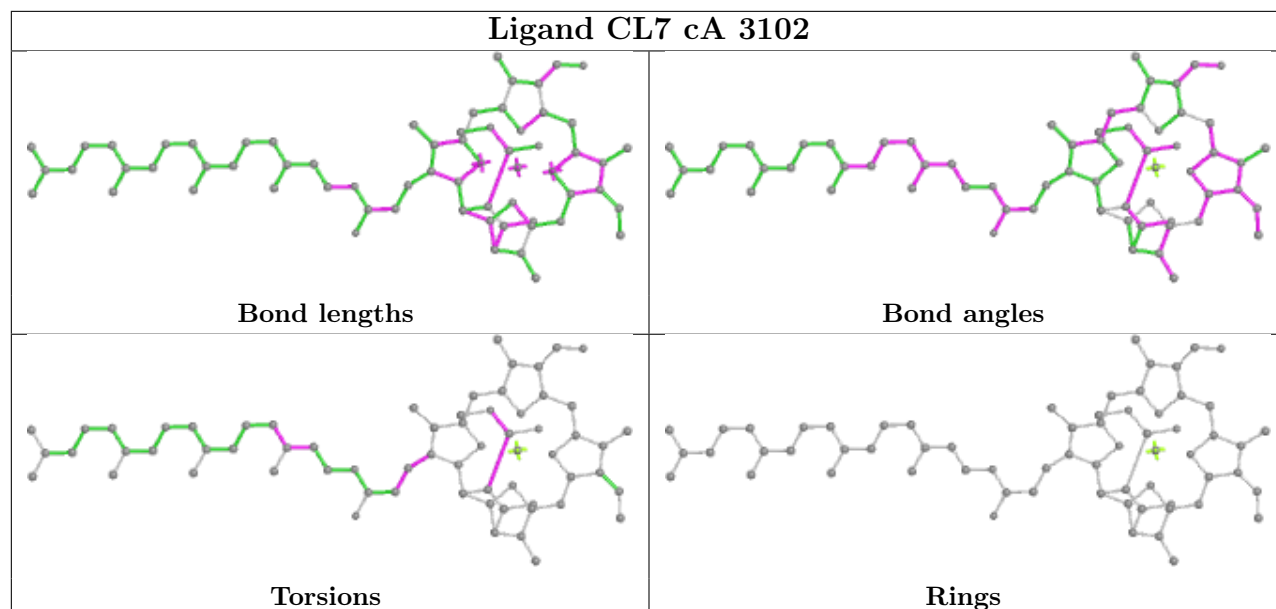
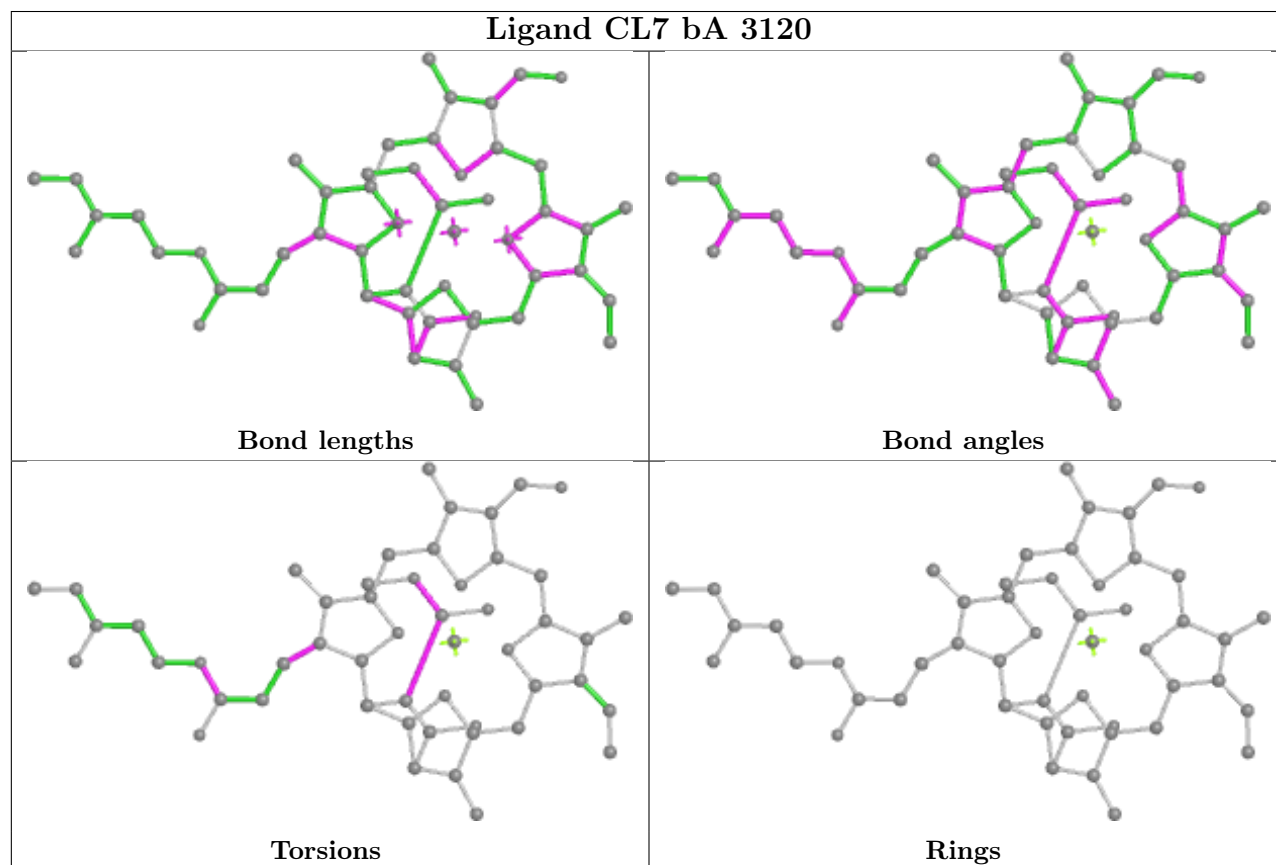


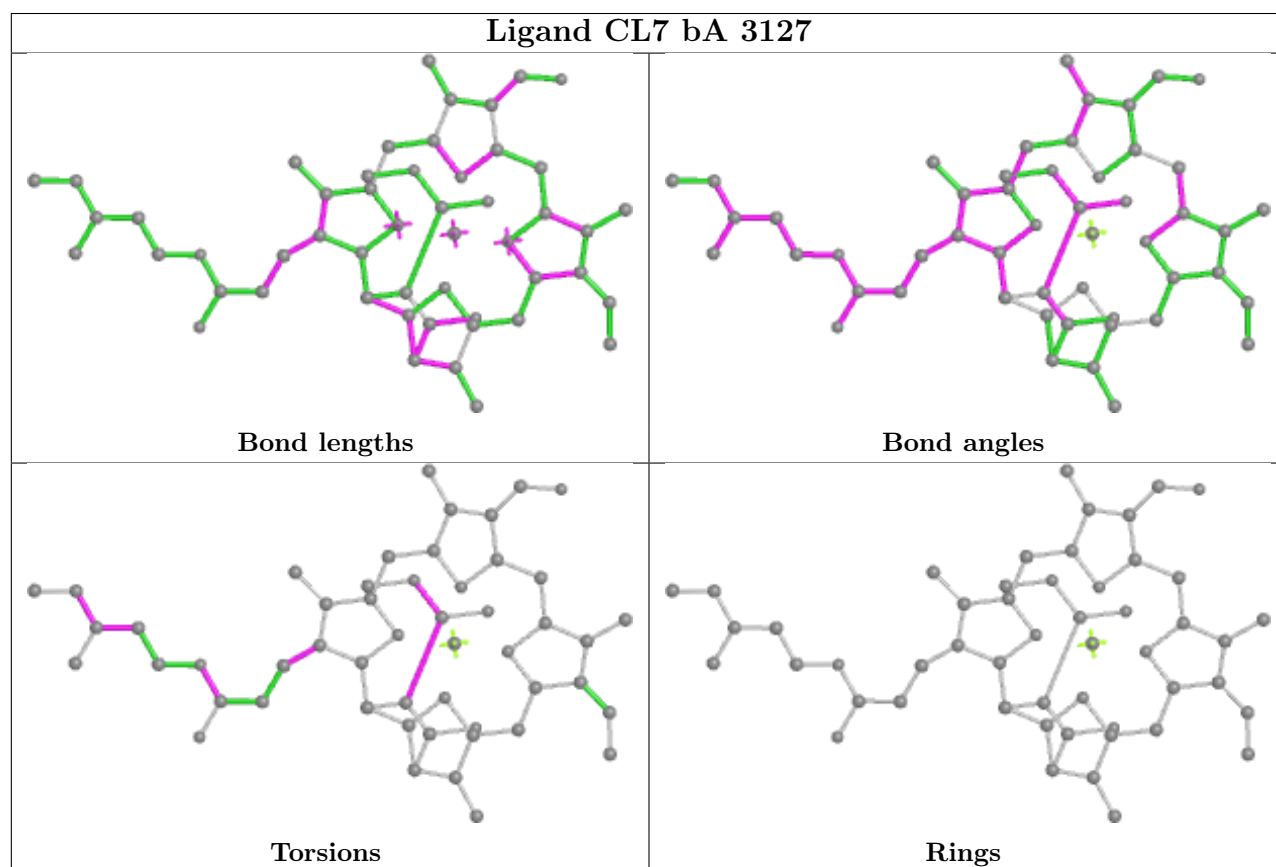
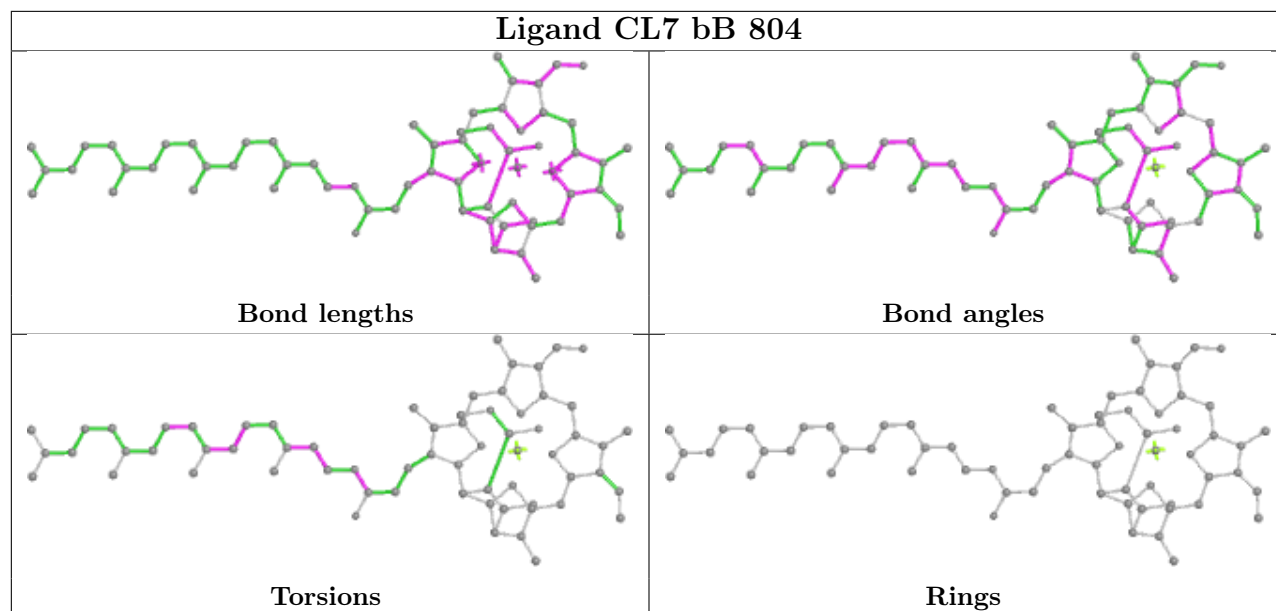
Torsions

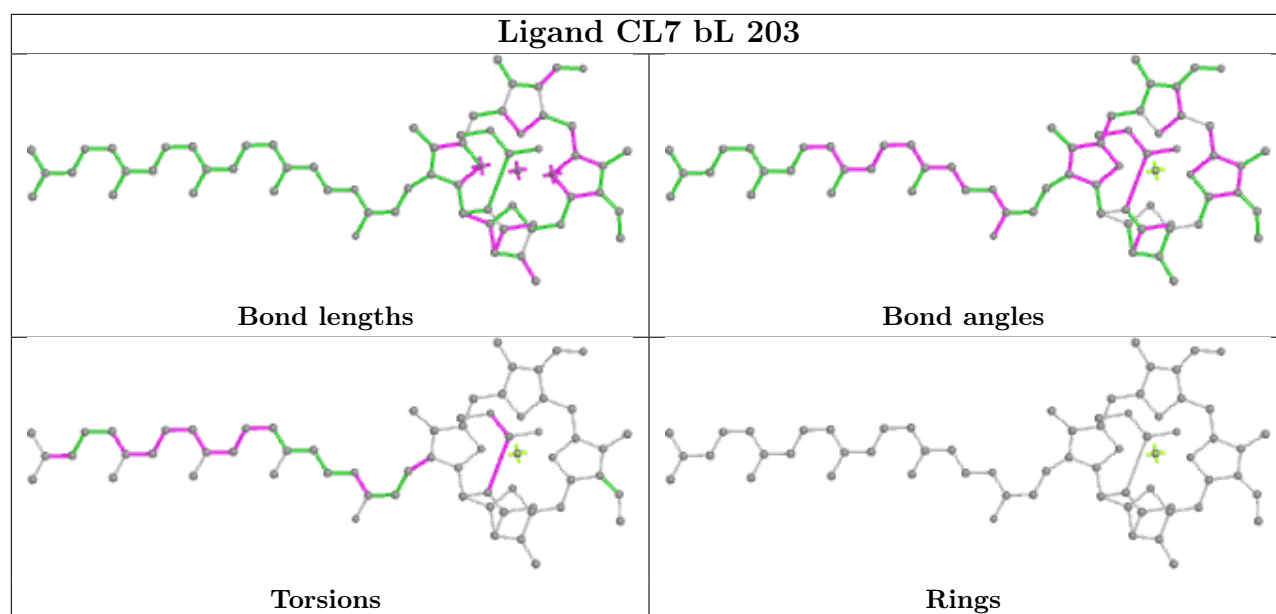


Rings

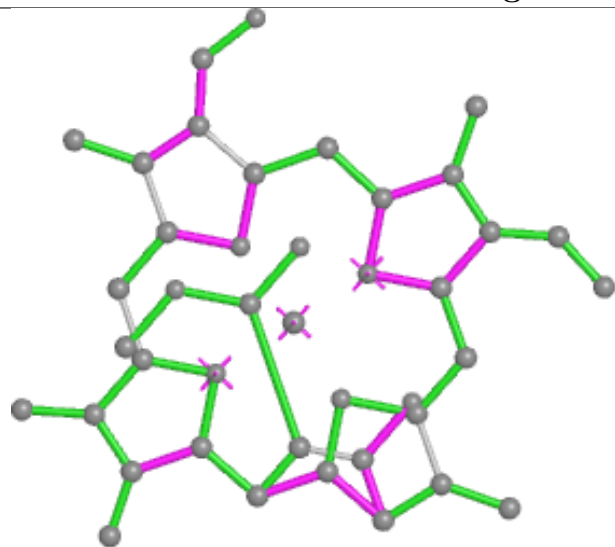


Ligand CL7 cA 3102**Ligand CL7 bA 3120**

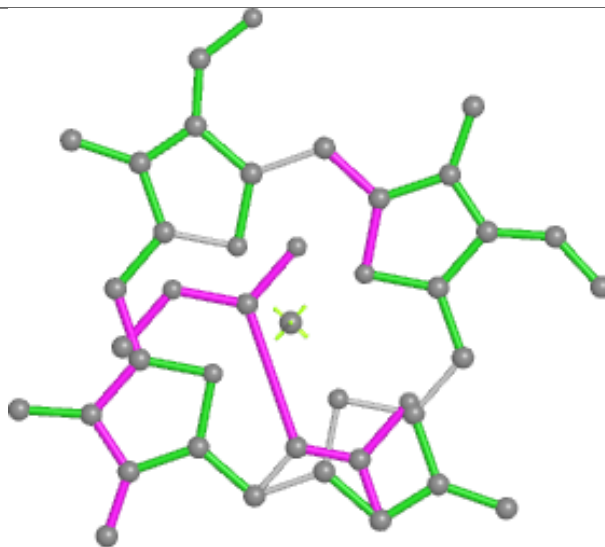




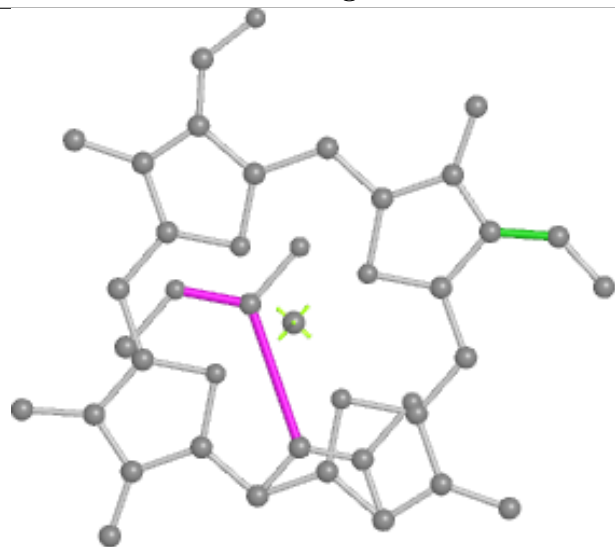
Ligand CL7 aB 3013



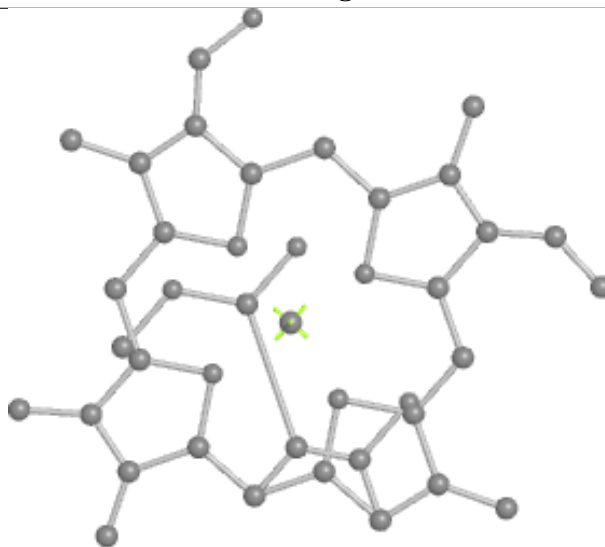
Bond lengths



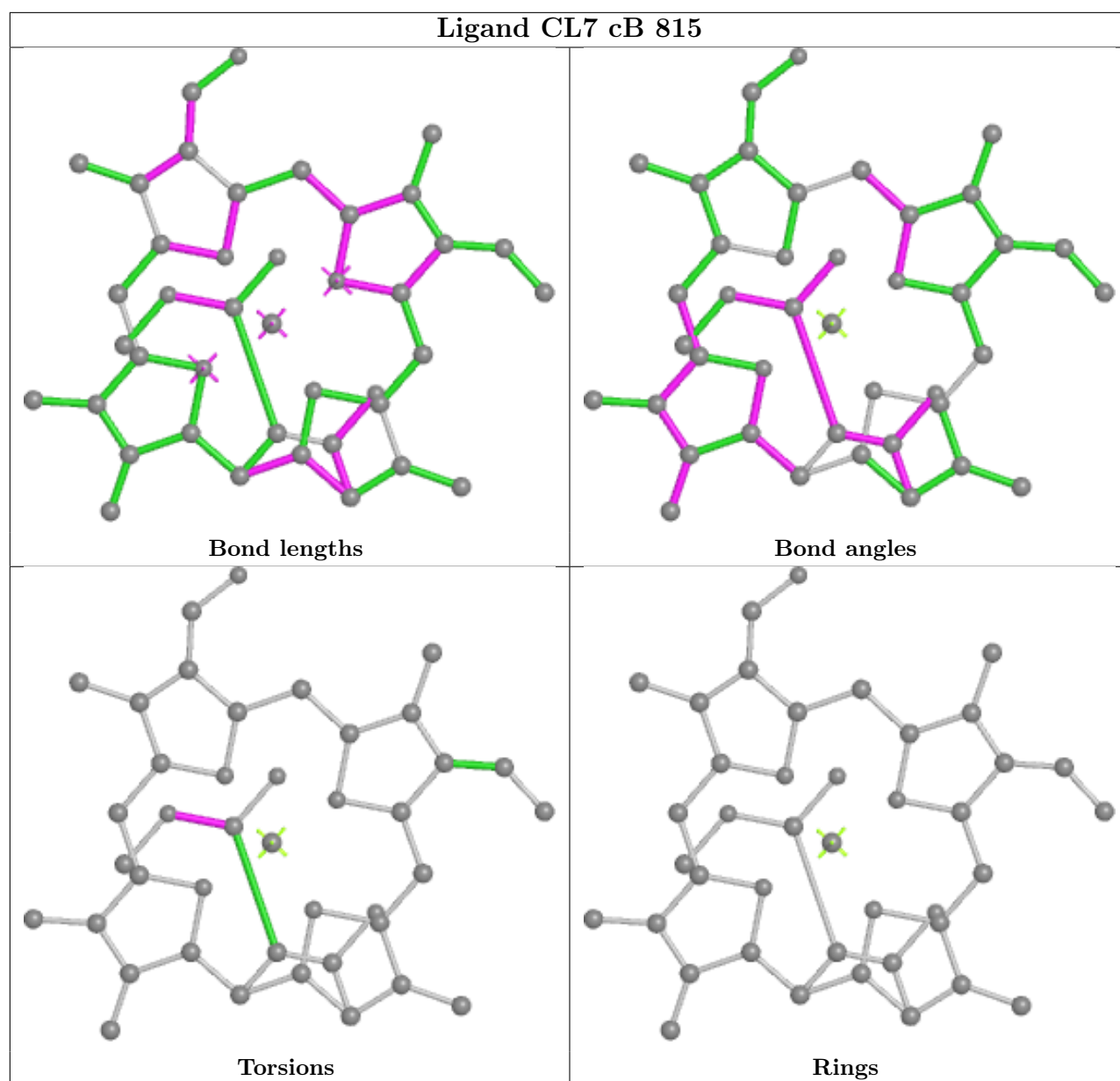
Bond angles

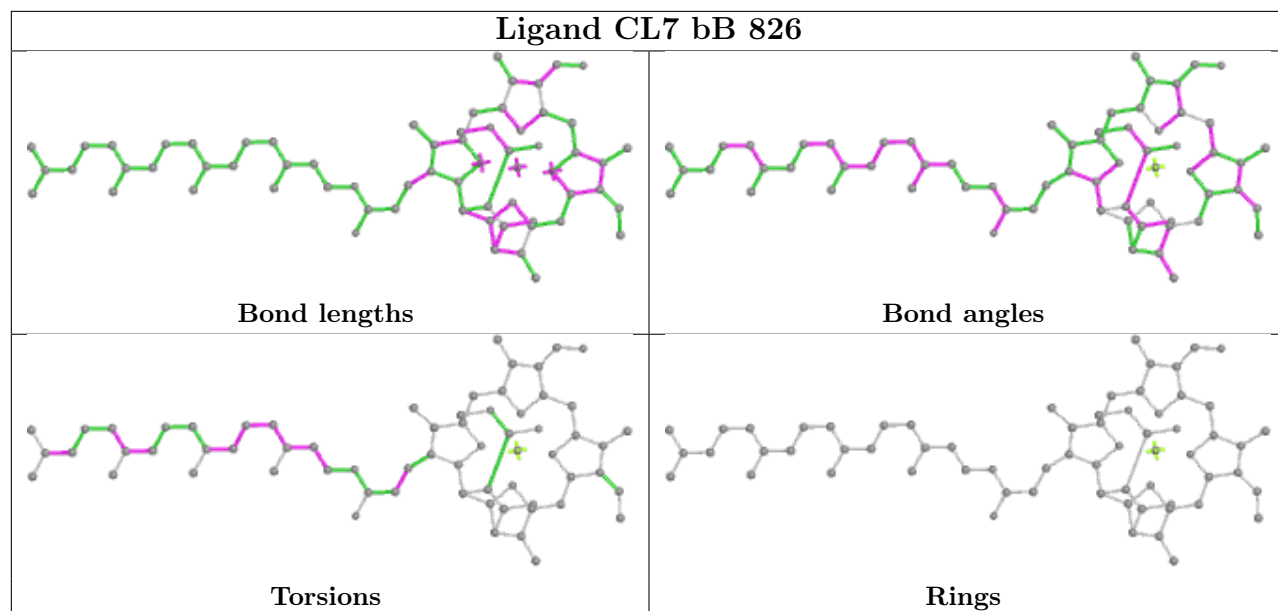


Torsions

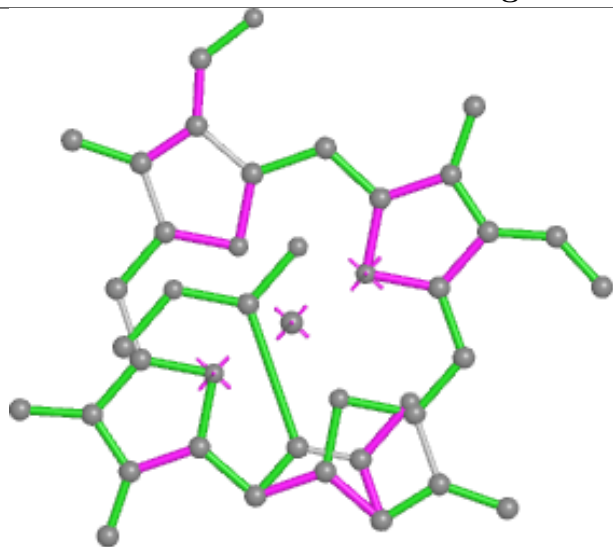


Rings

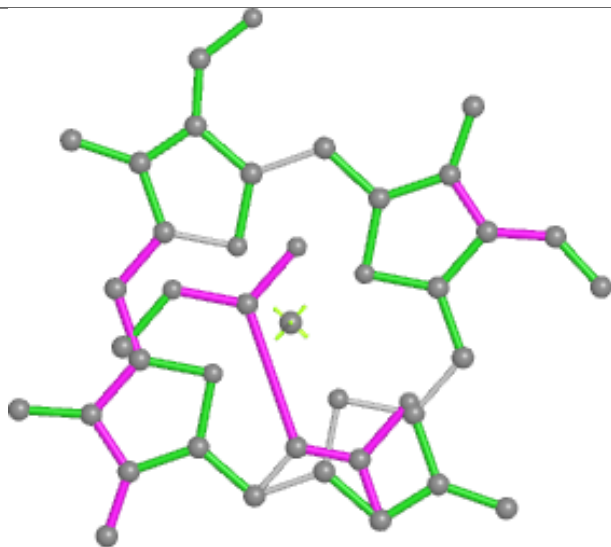




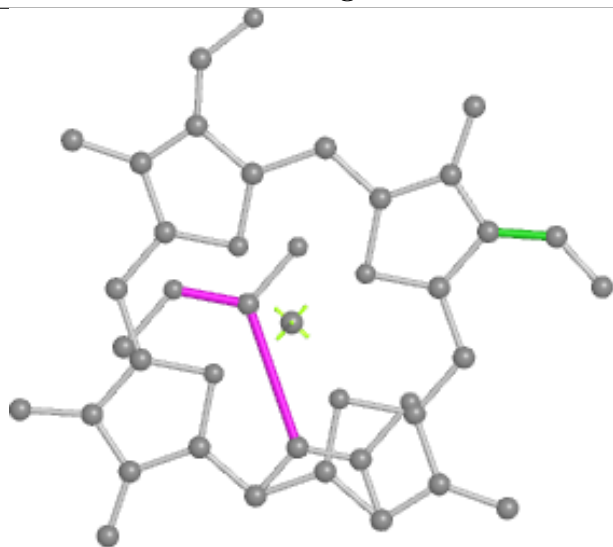
Ligand CL7 cA 3112



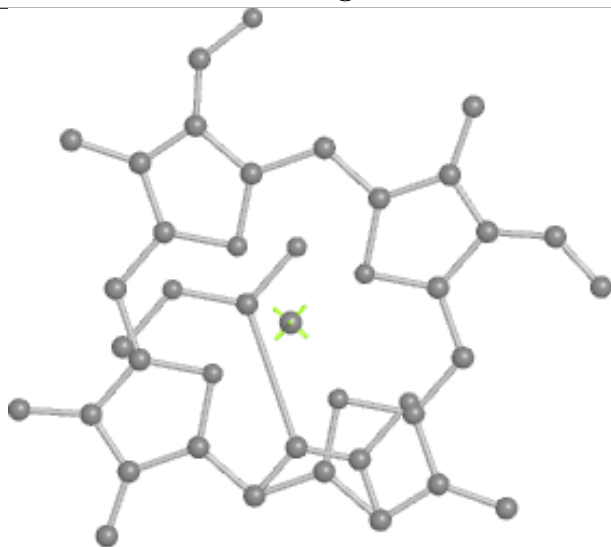
Bond lengths



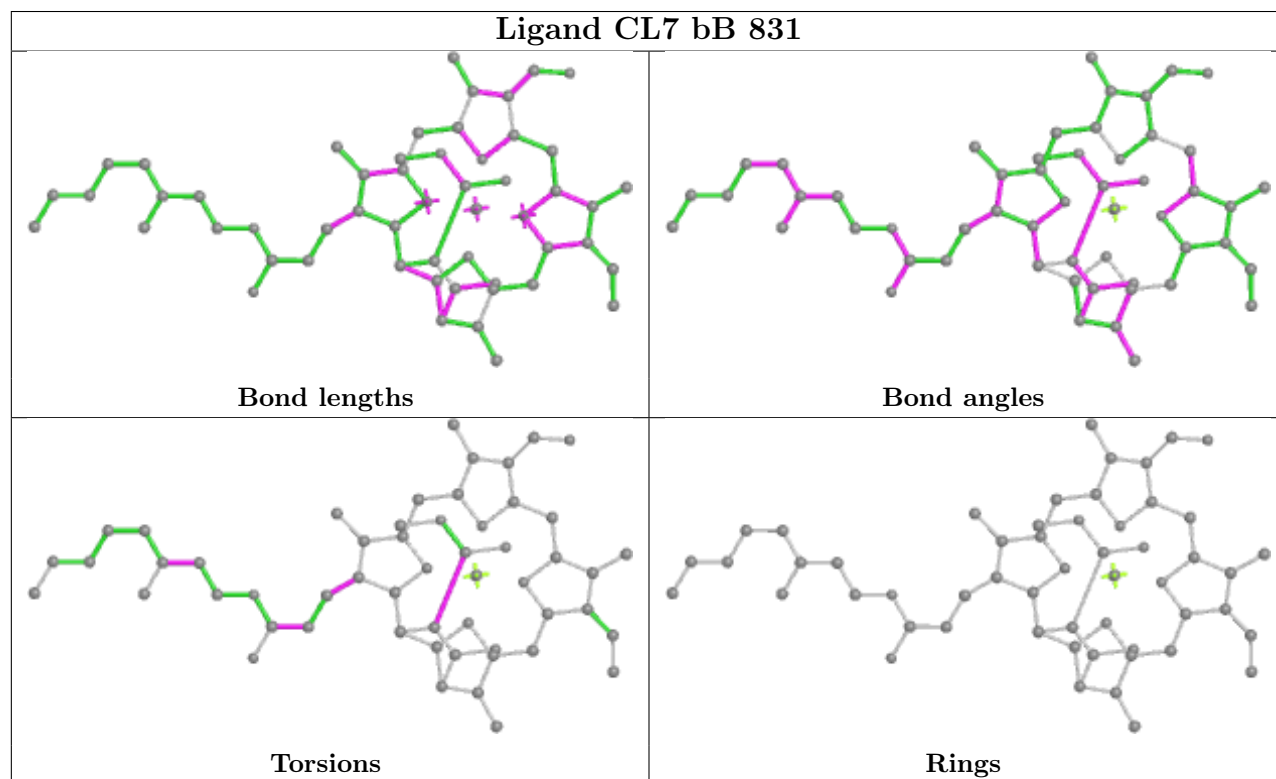
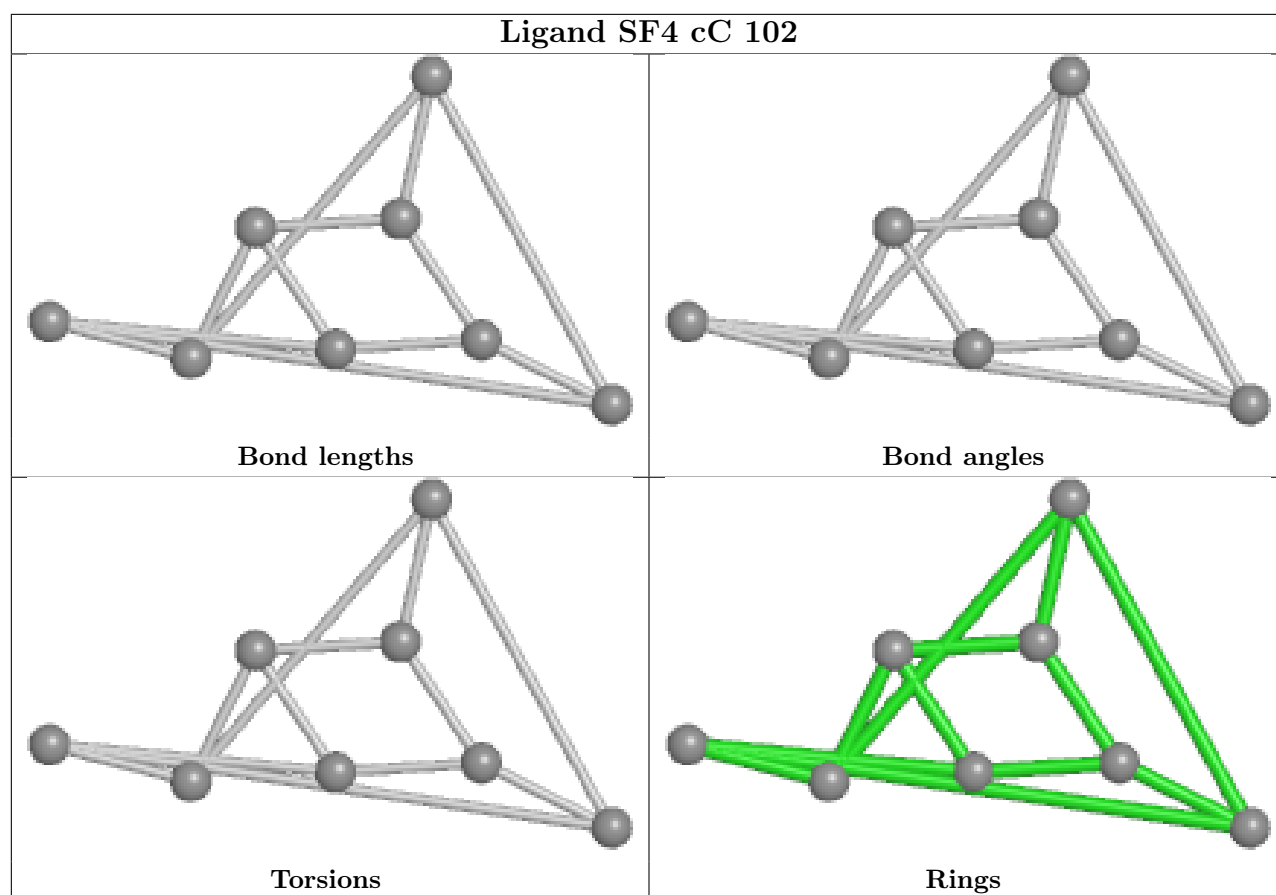
Bond angles

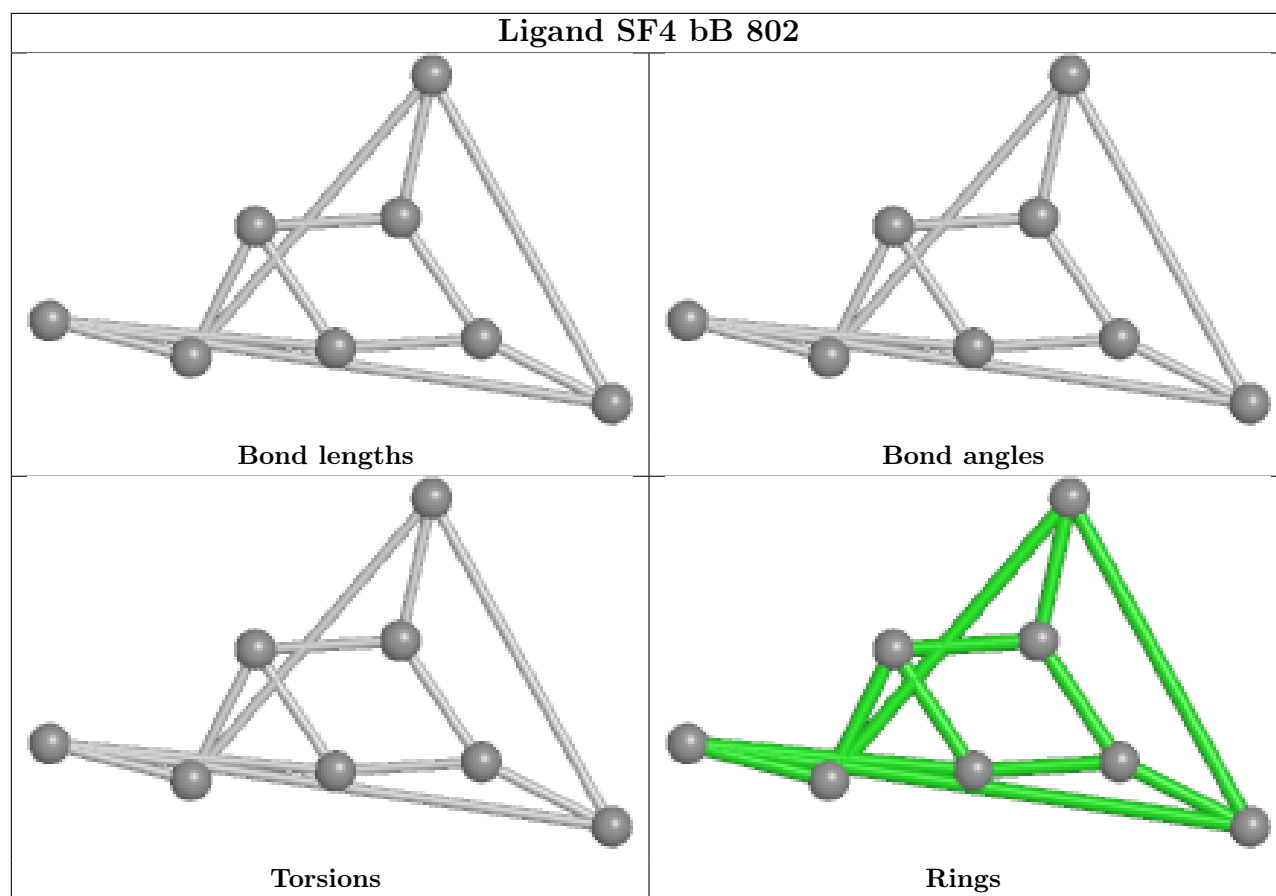
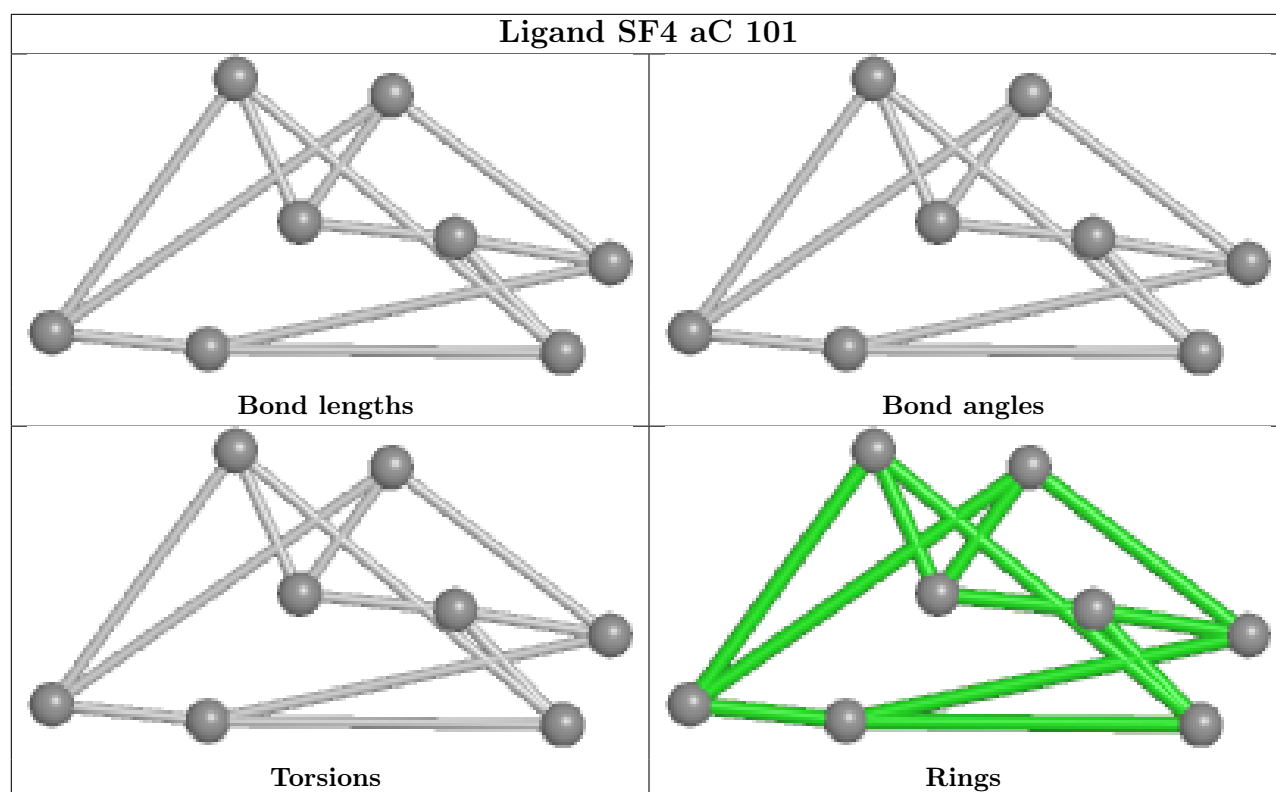


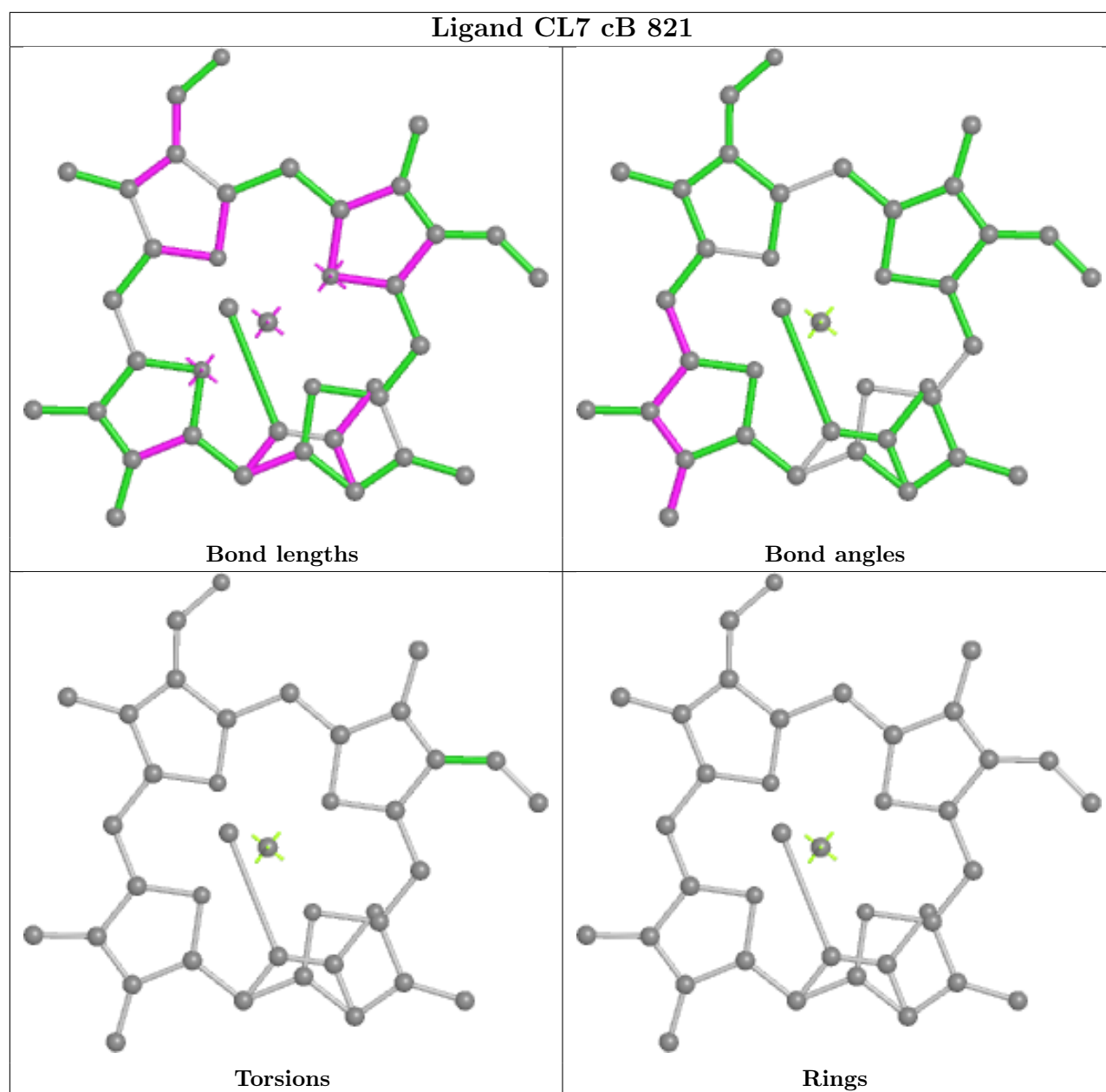
Torsions



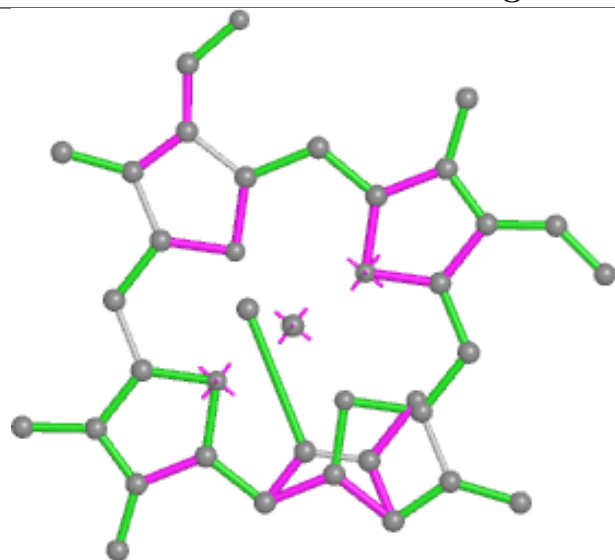
Rings



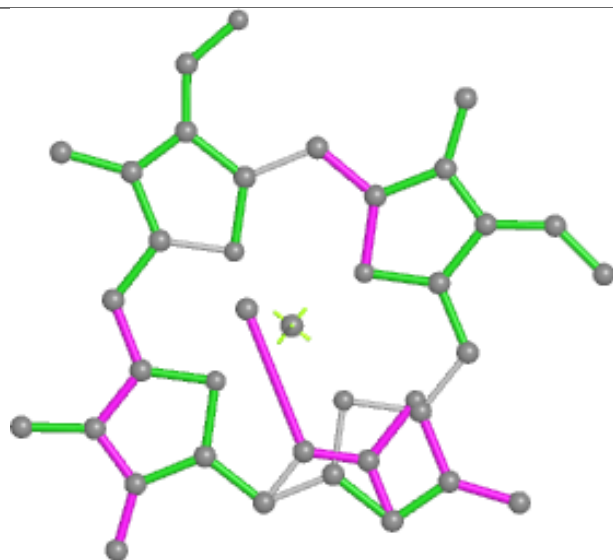




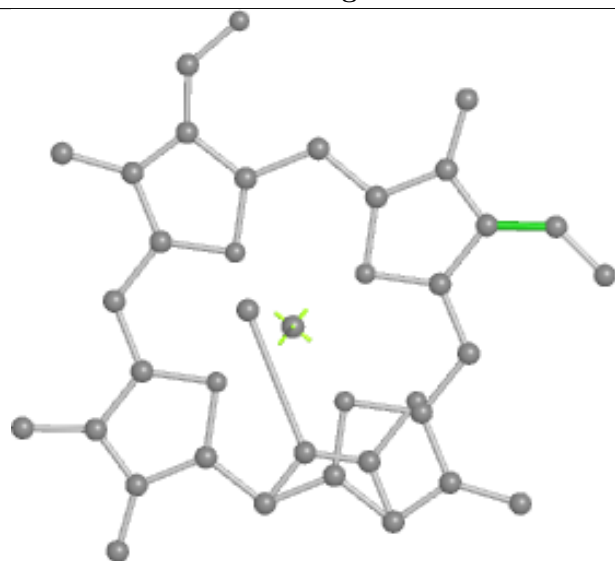
Ligand CL7 cA 3117



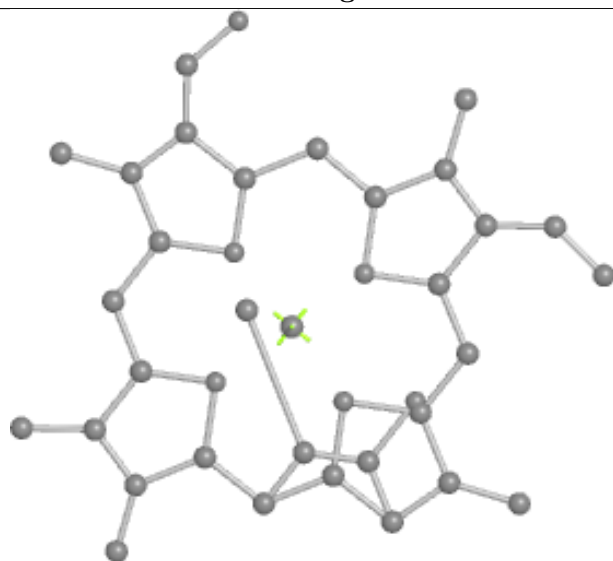
Bond lengths



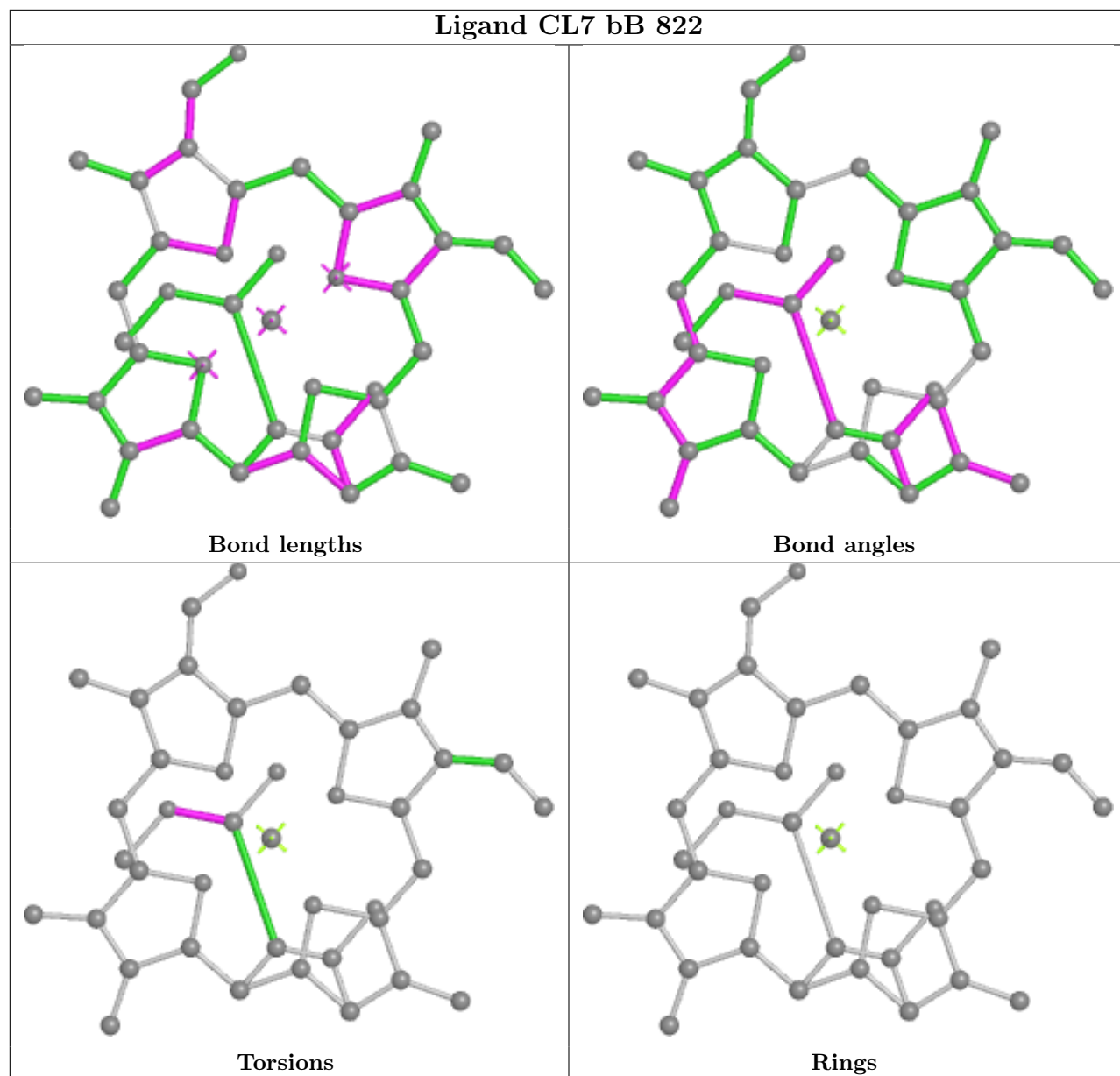
Bond angles



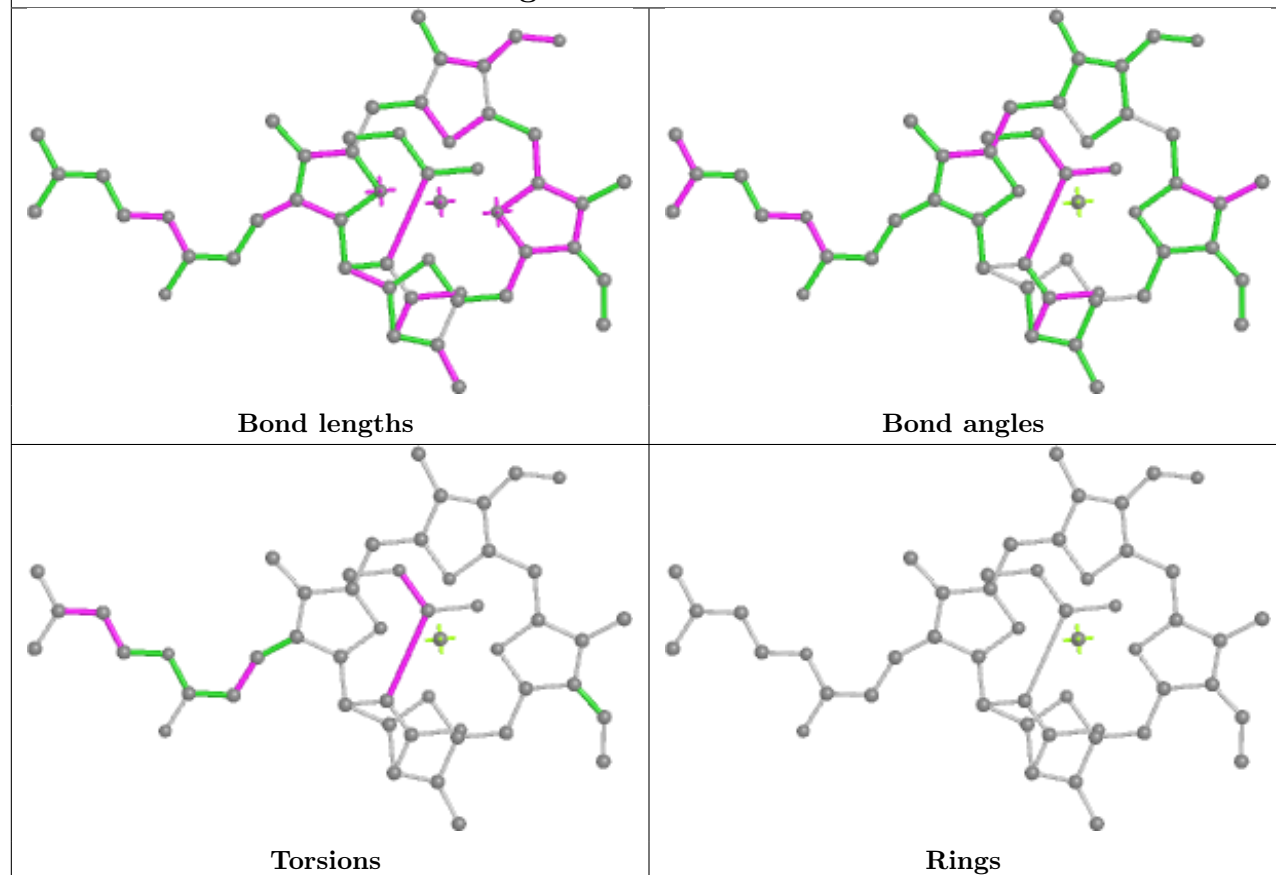
Torsions



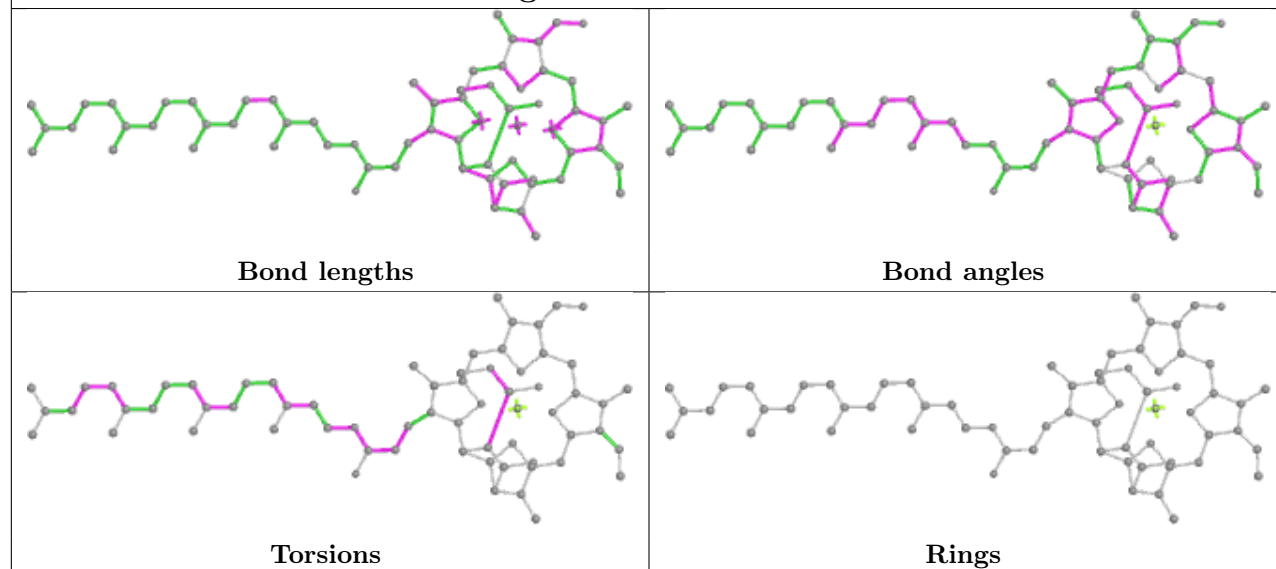
Rings



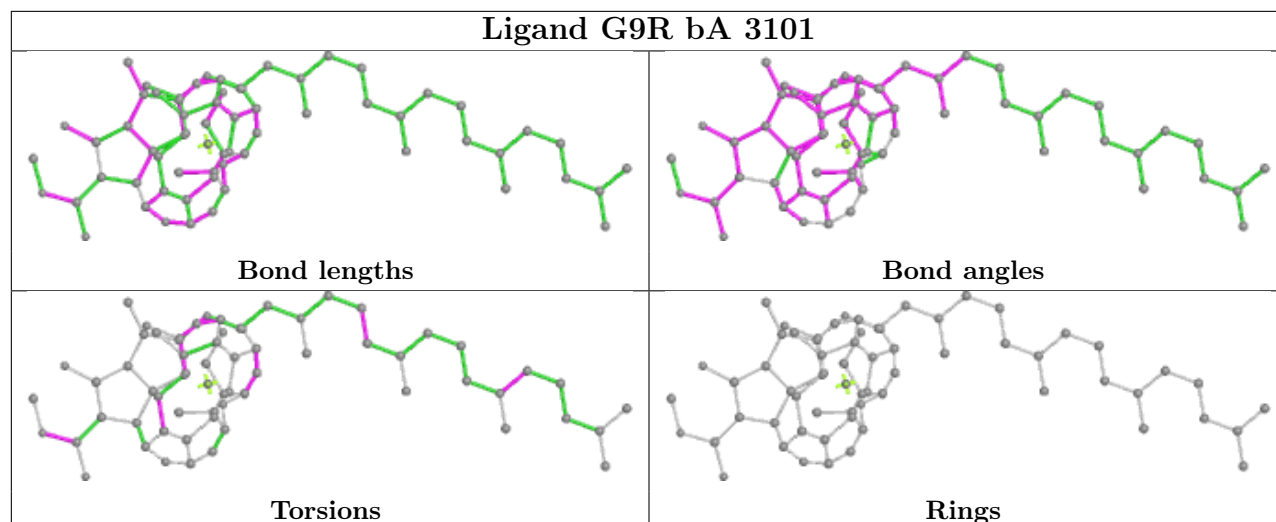
Ligand CL7 aB 3015



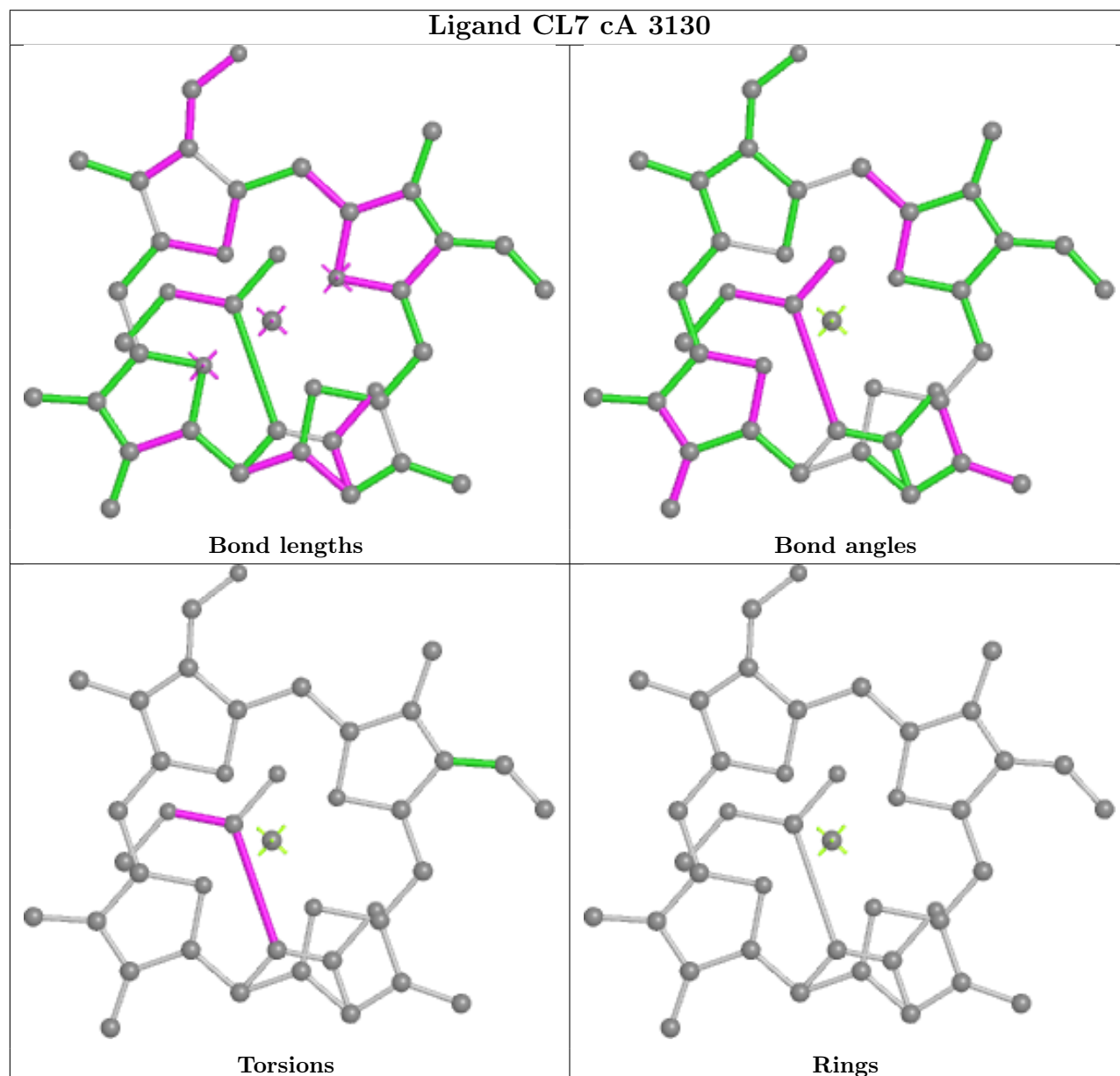
Ligand CL7 aB 3009

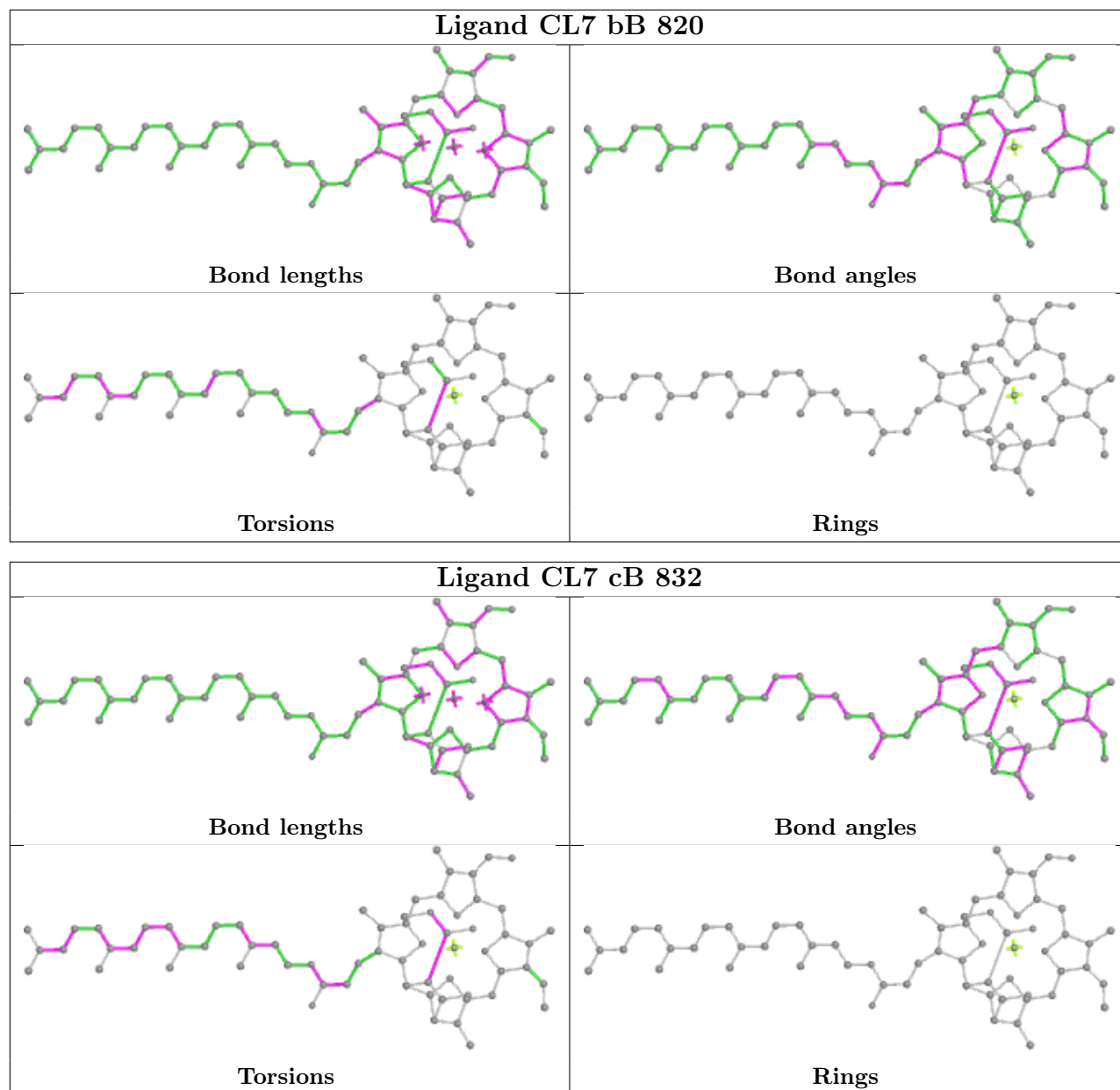


Ligand G9R bA 3101

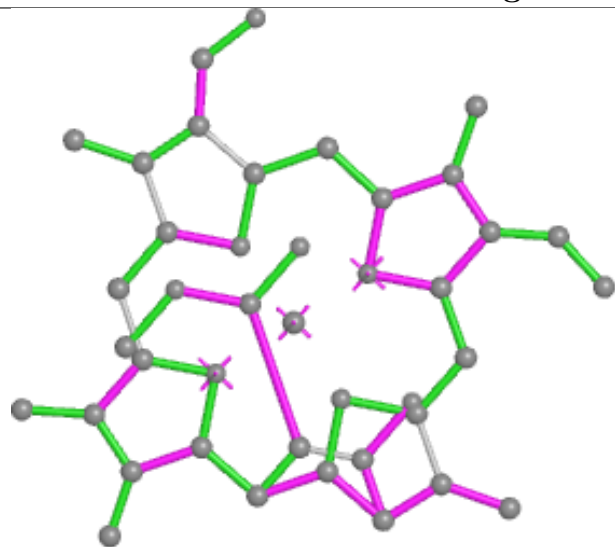


Ligand CL7 cA 3130

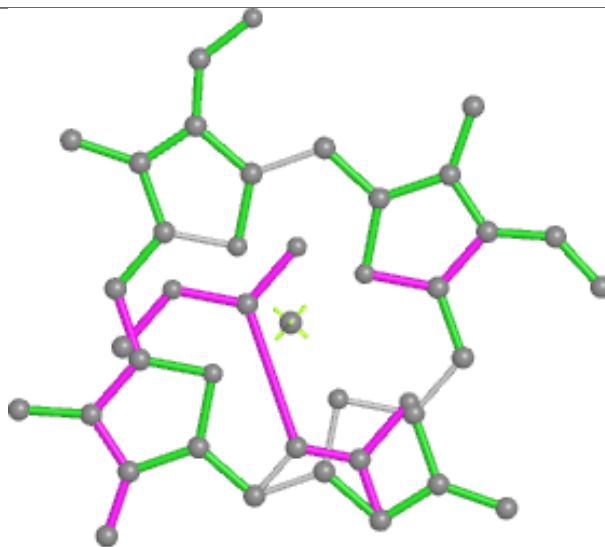




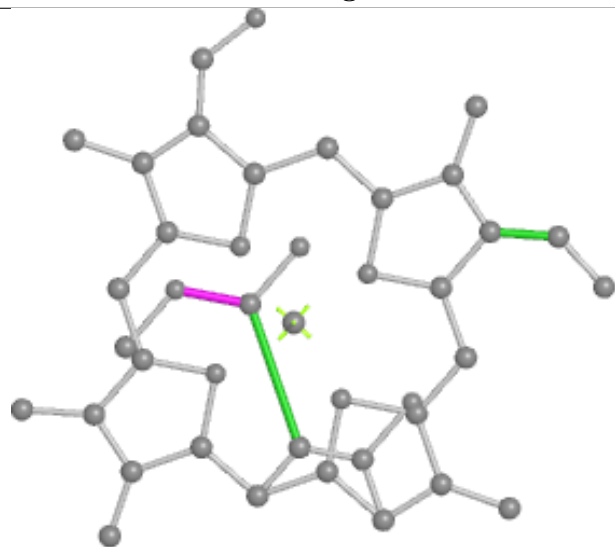
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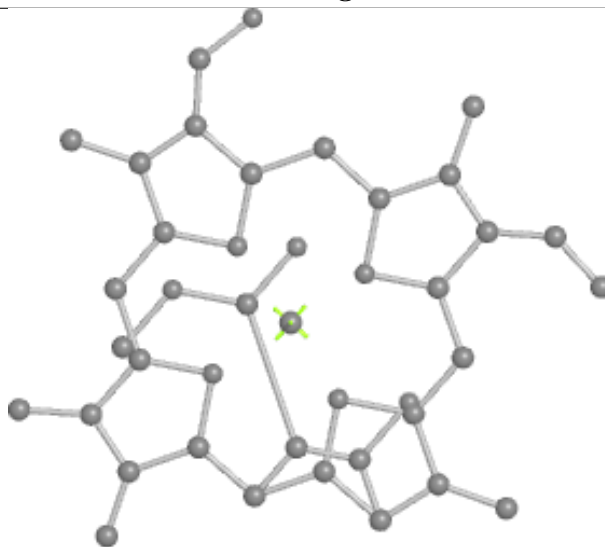
Bond lengths



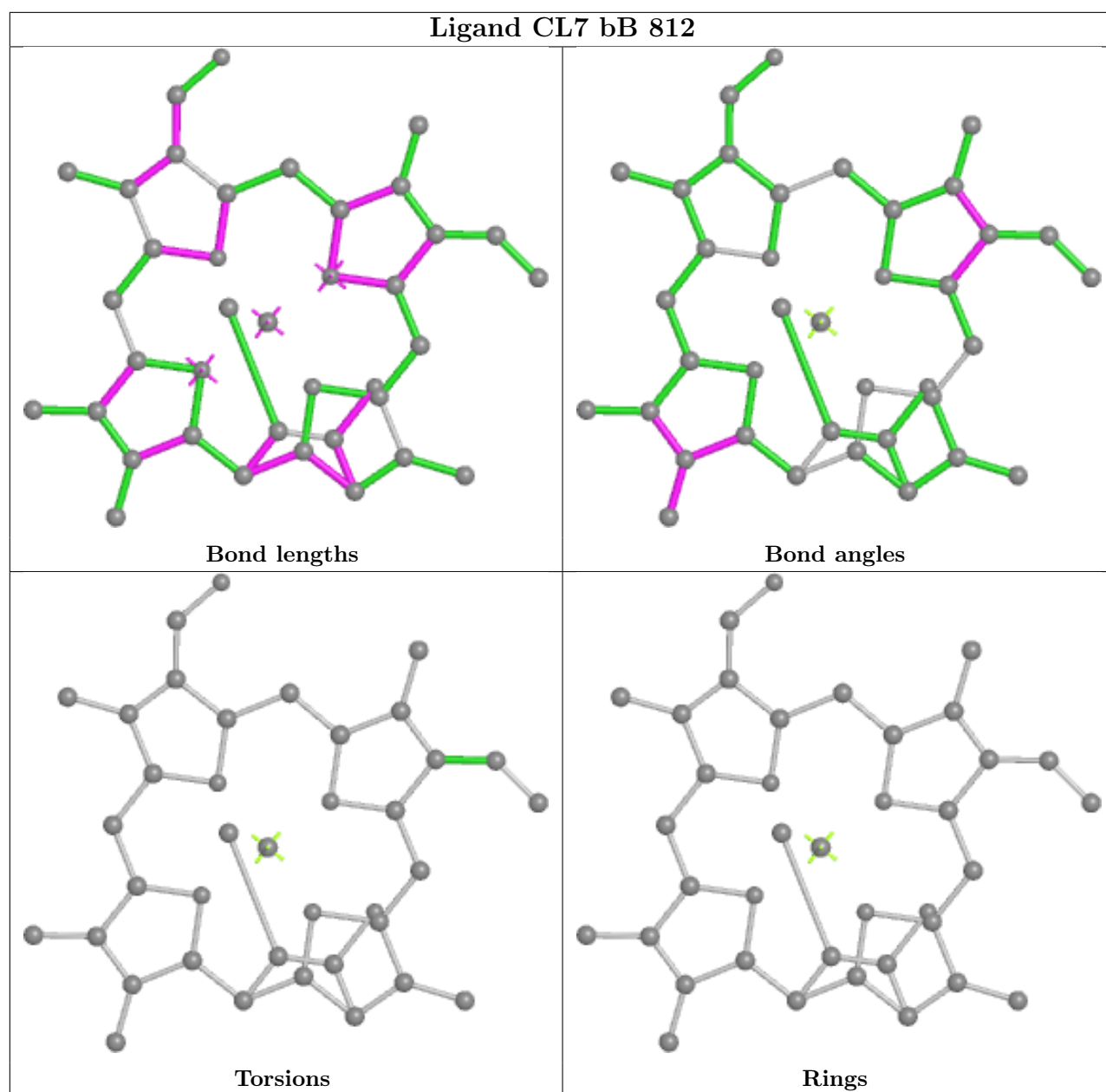
Bond angles



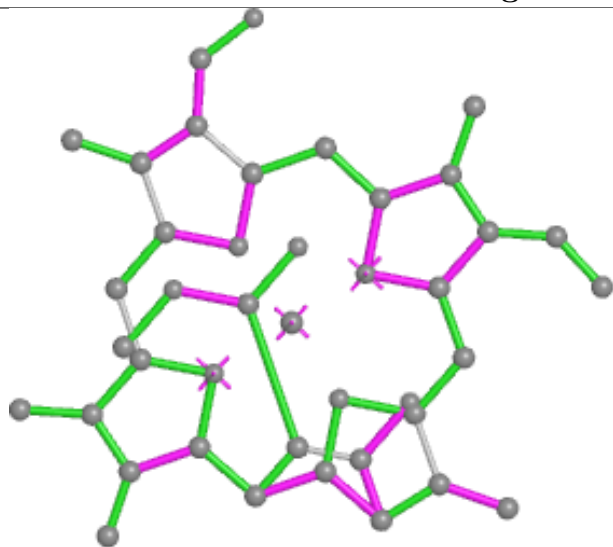
Torsions



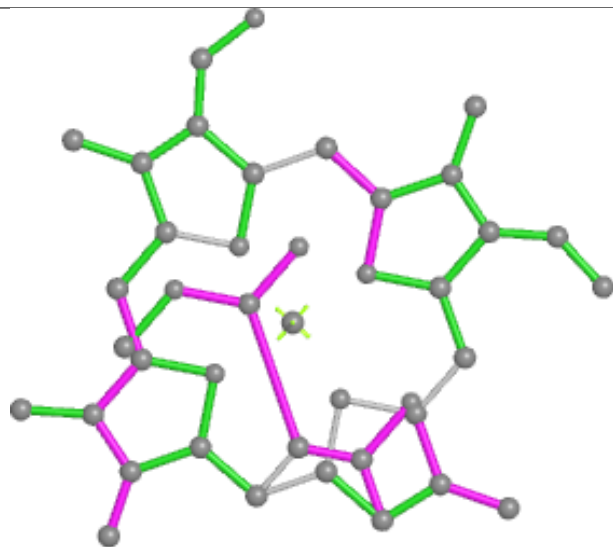
Rings



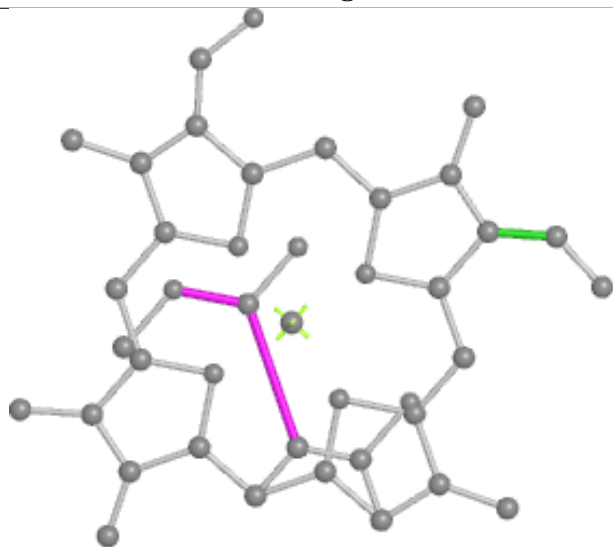
Ligand CL7 aB 3016



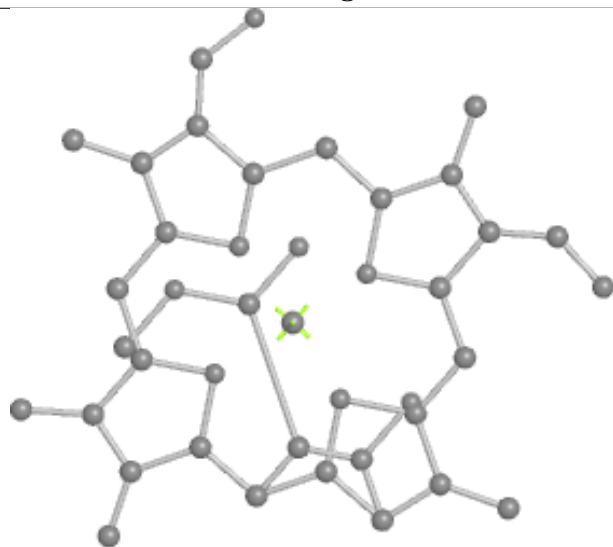
Bond lengths



Bond angles

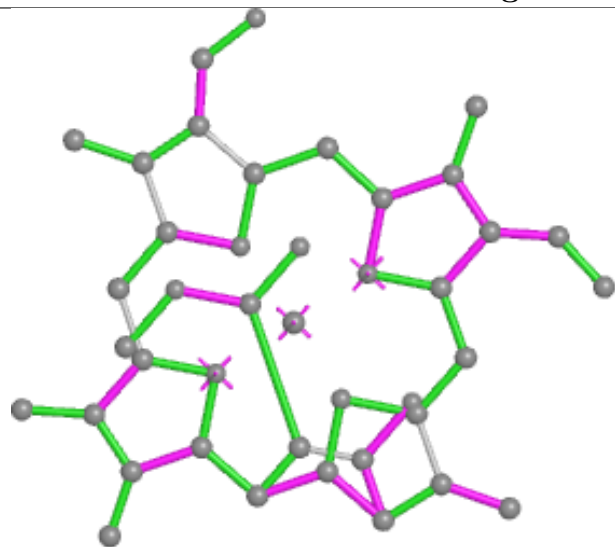


Torsions

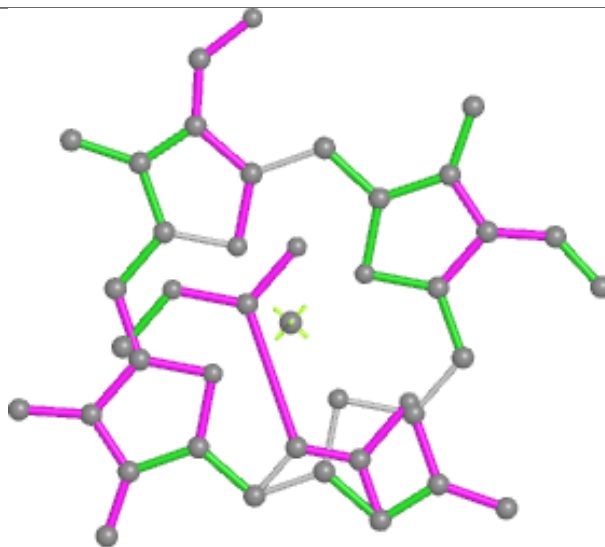


Rings

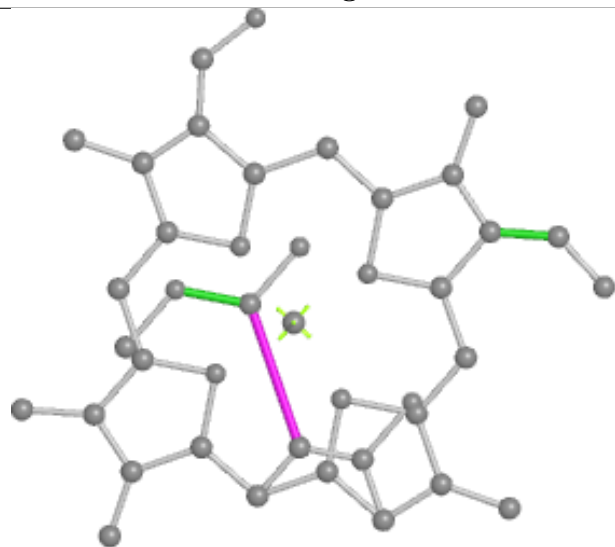
Ligand CL7 bA 3105



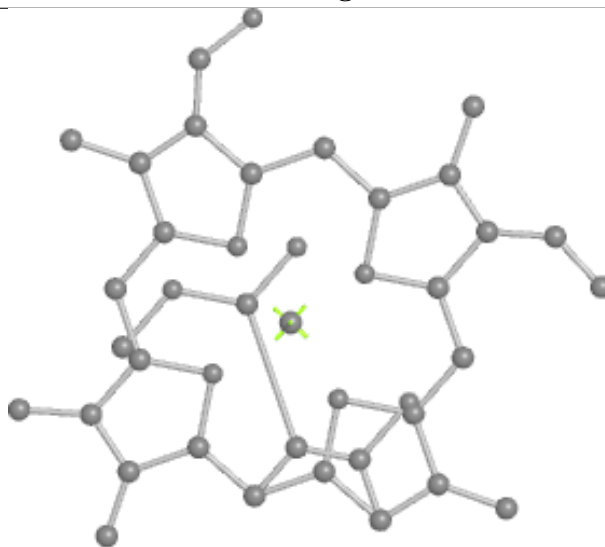
Bond lengths



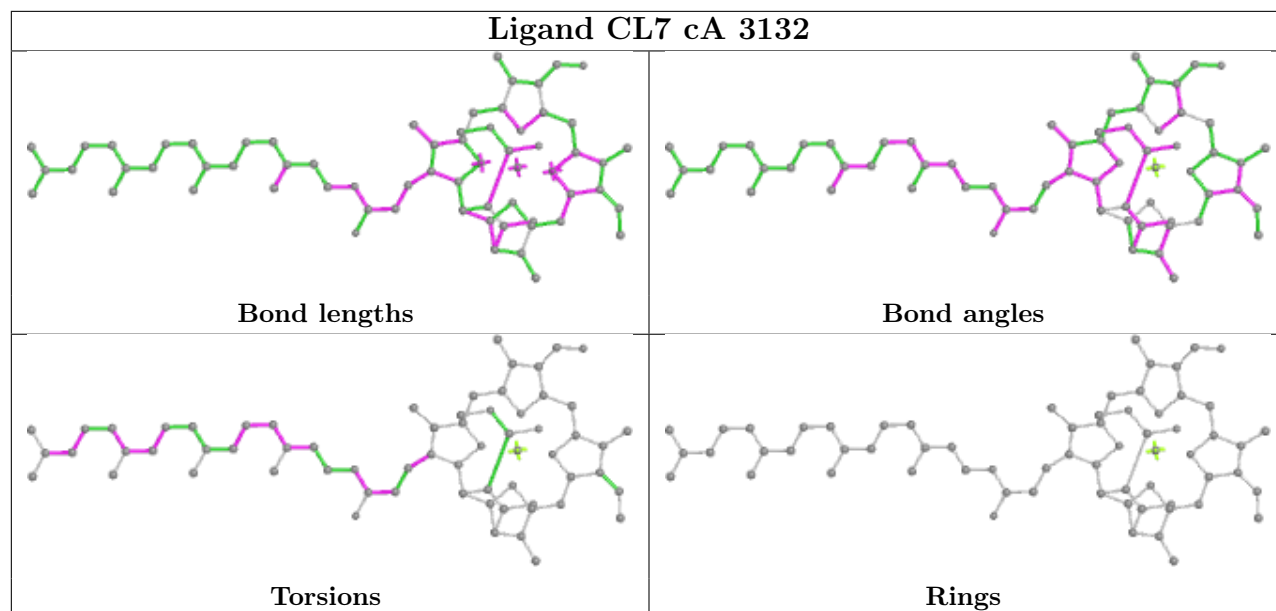
Bond angles

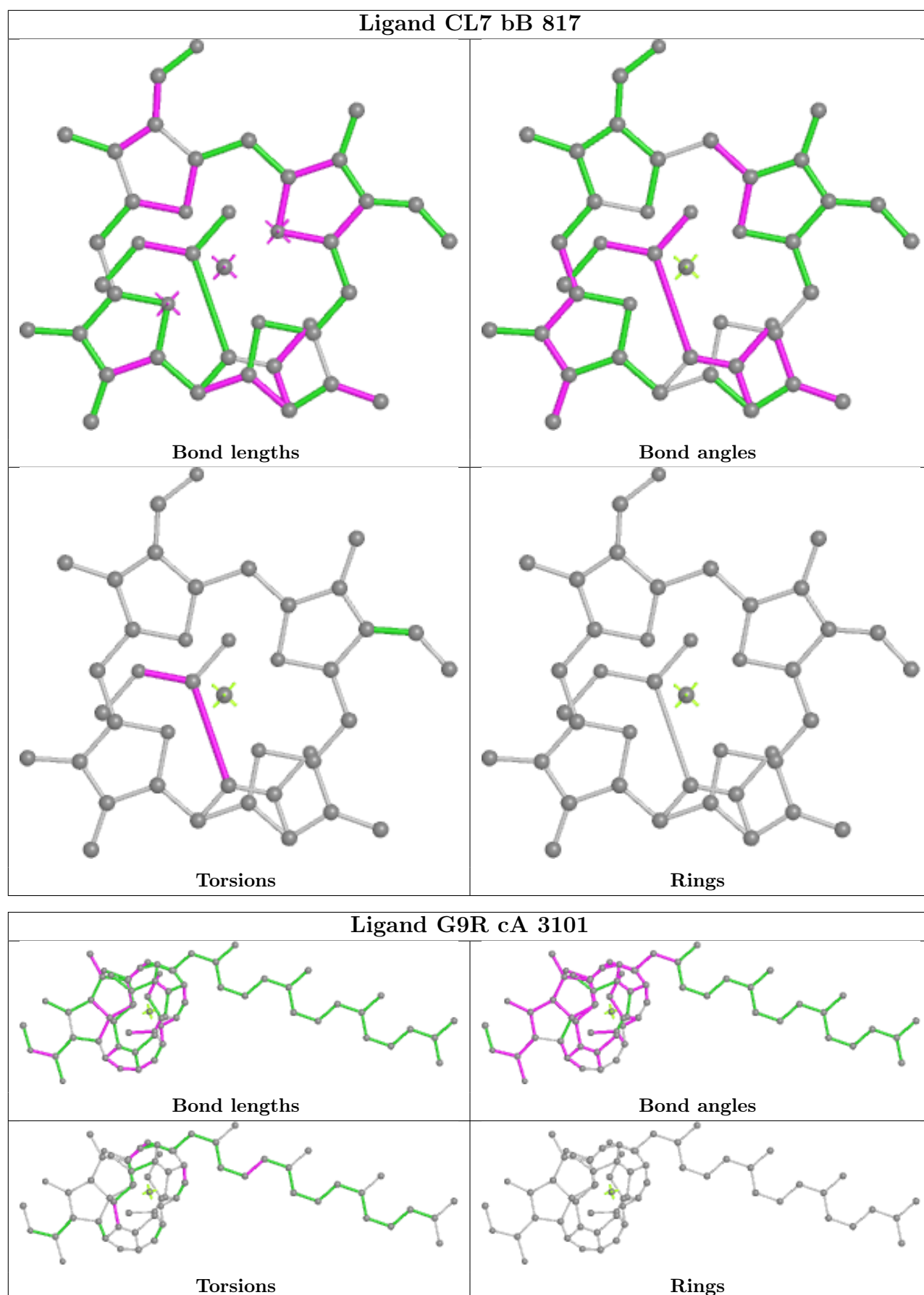


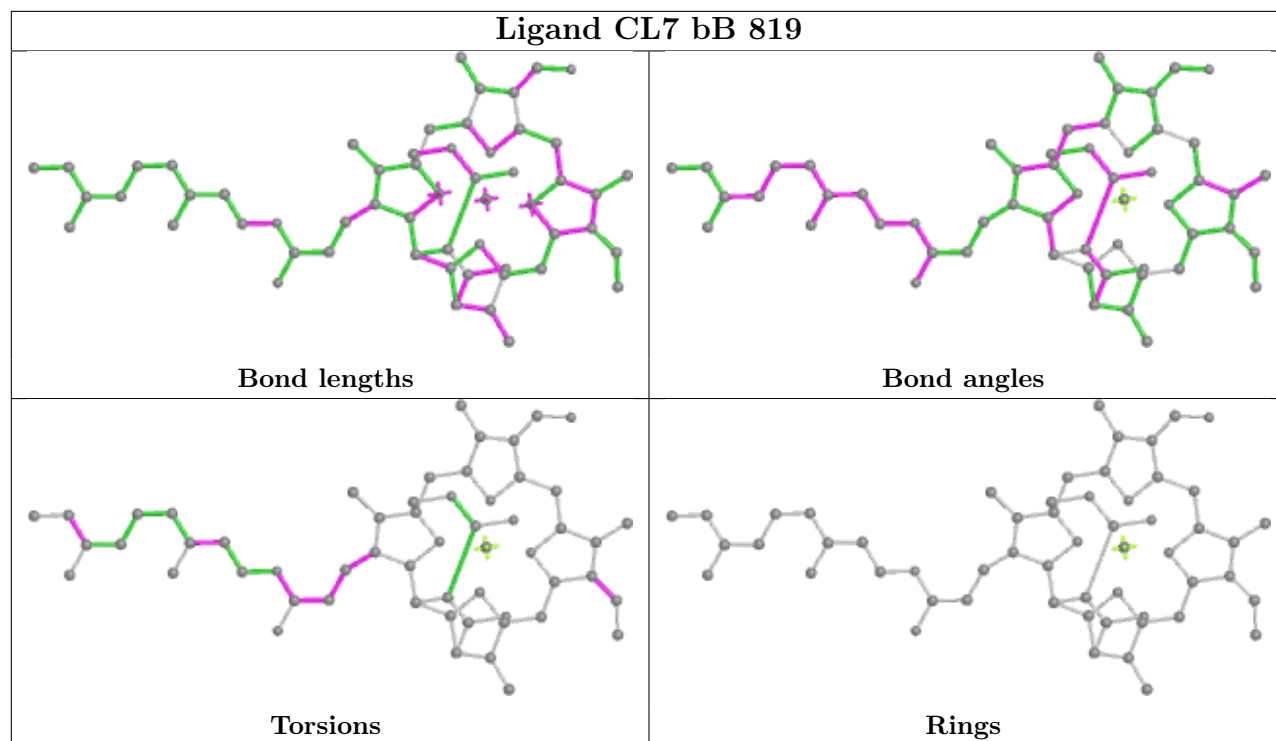
Torsions

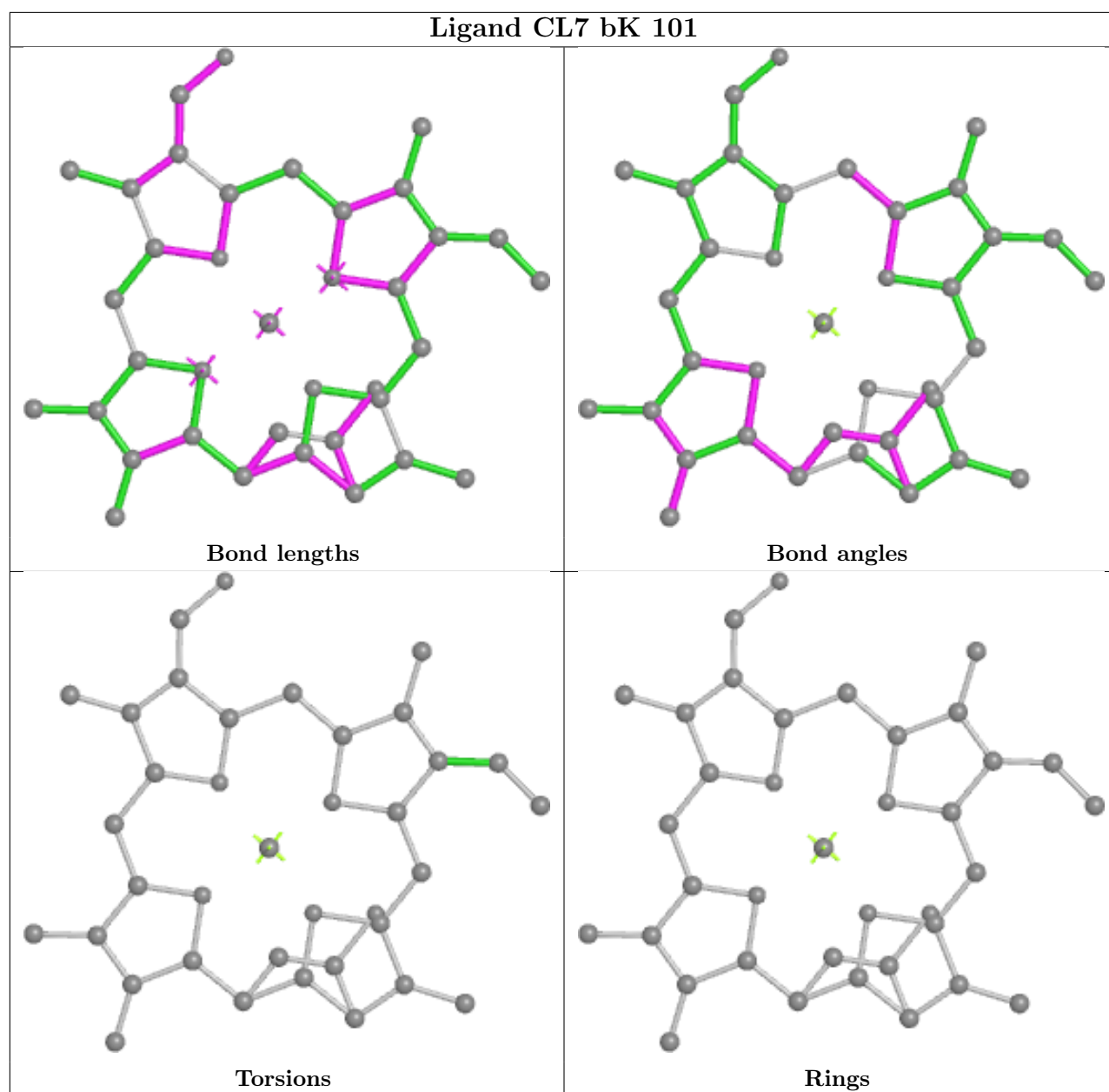


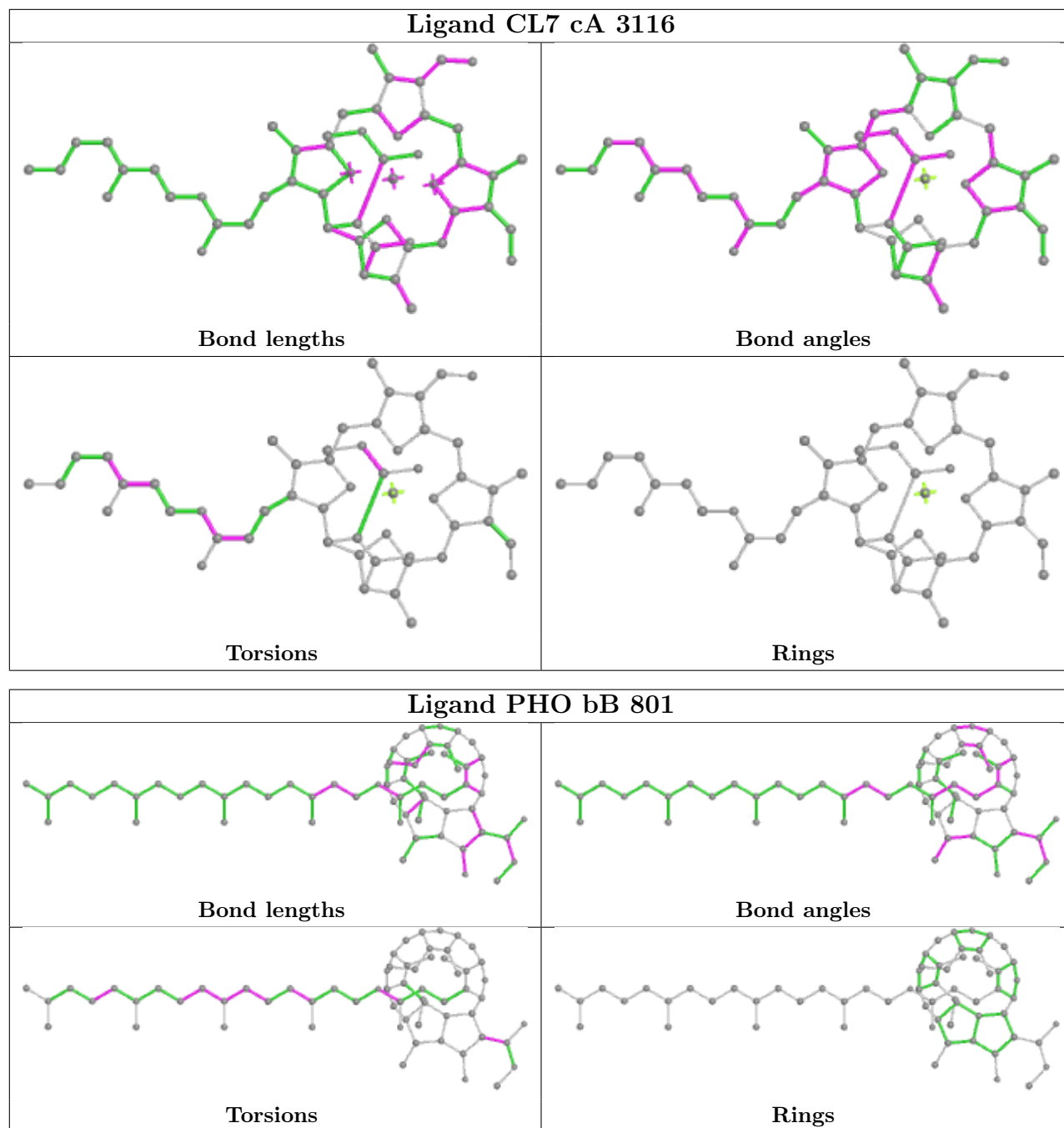
Rings

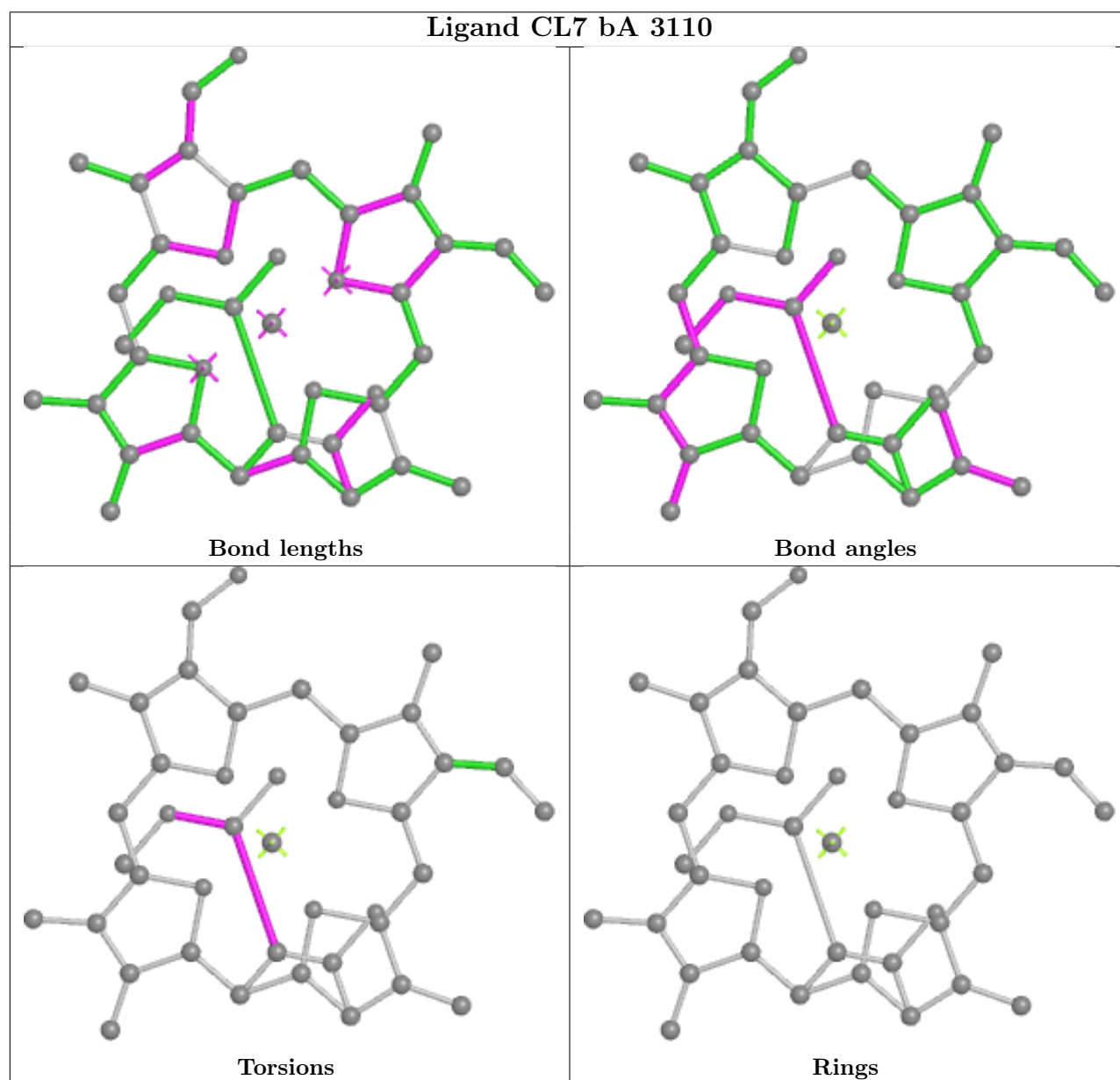
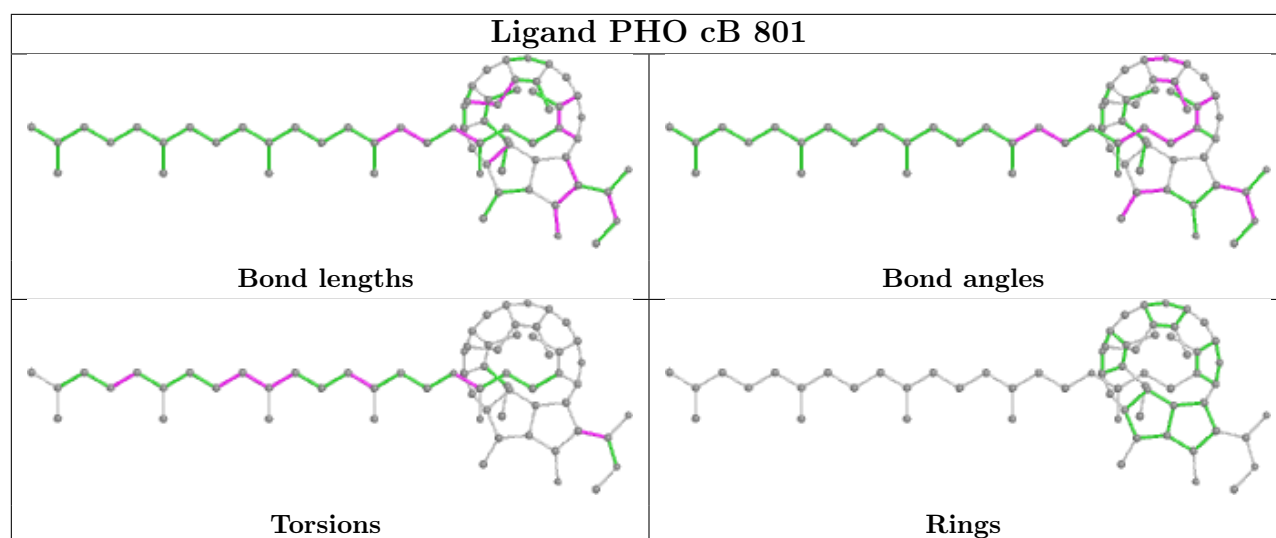


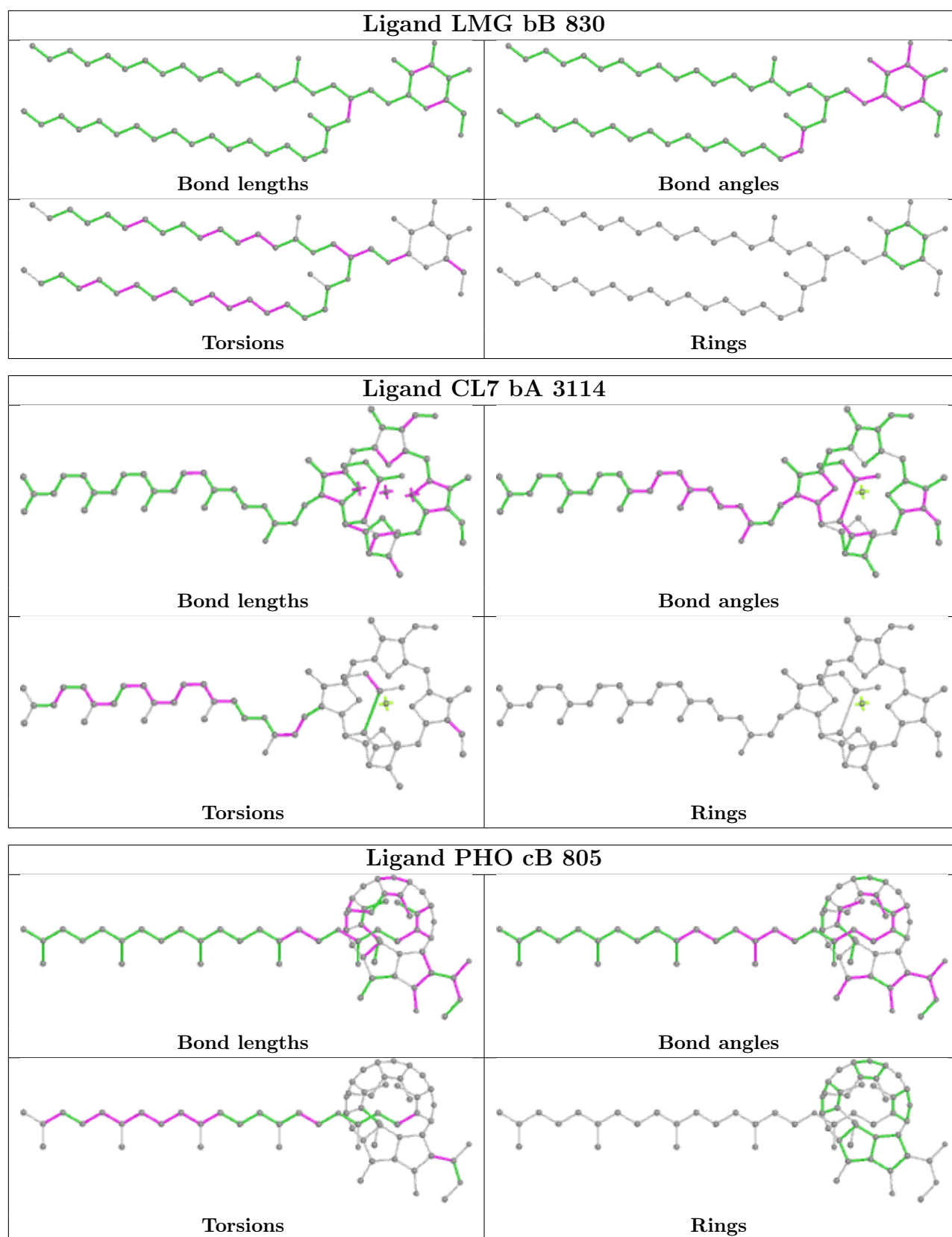


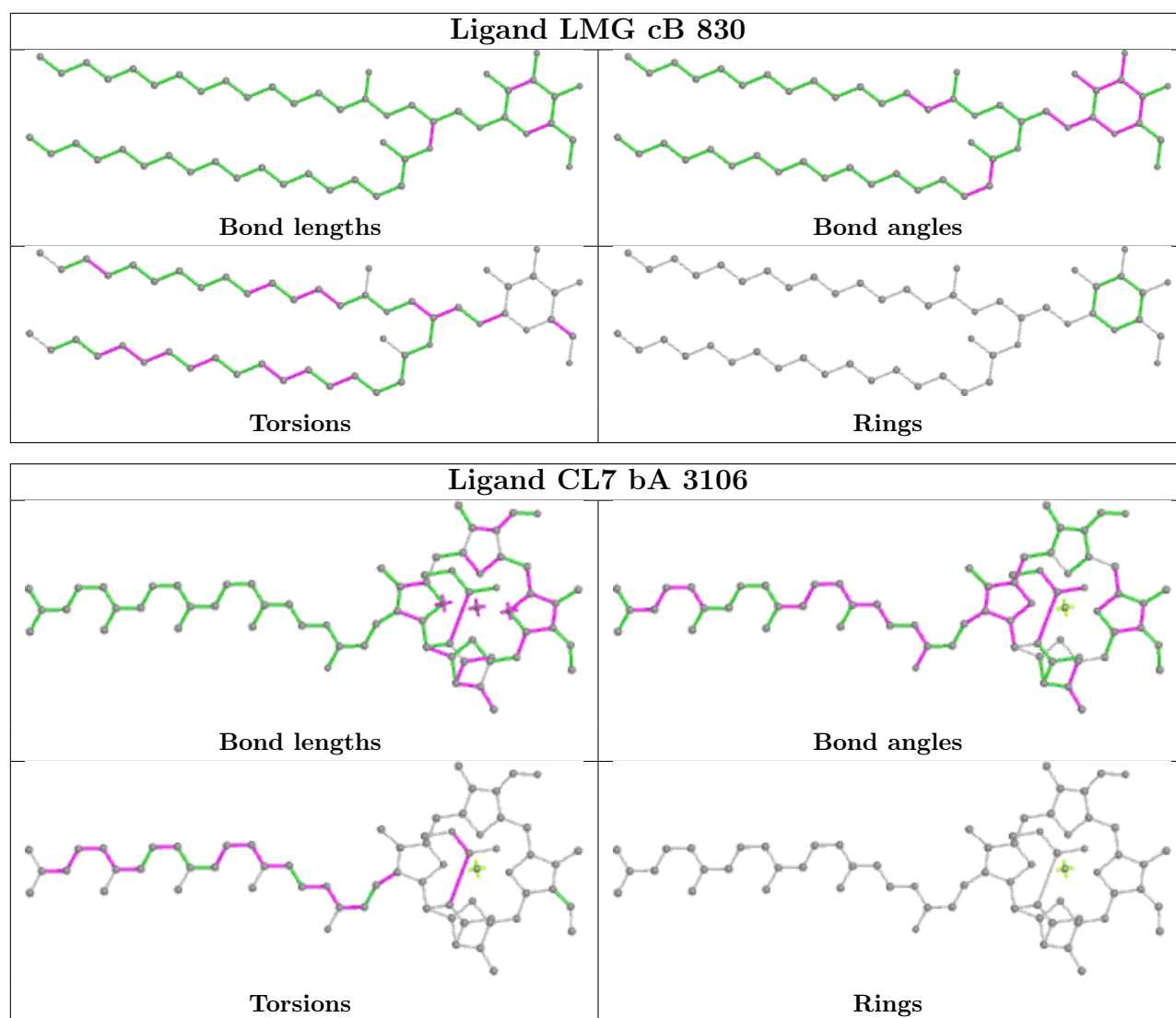


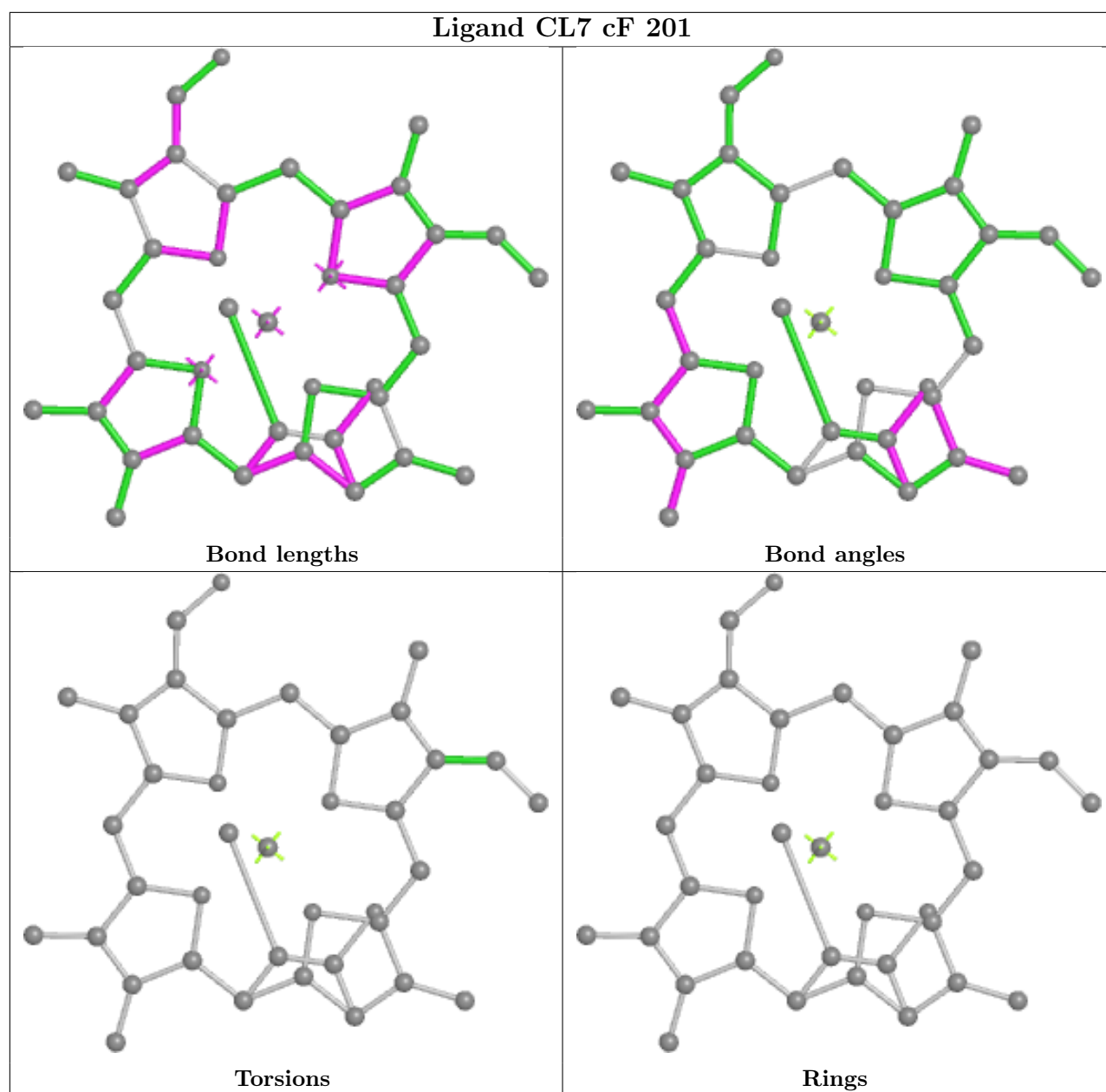


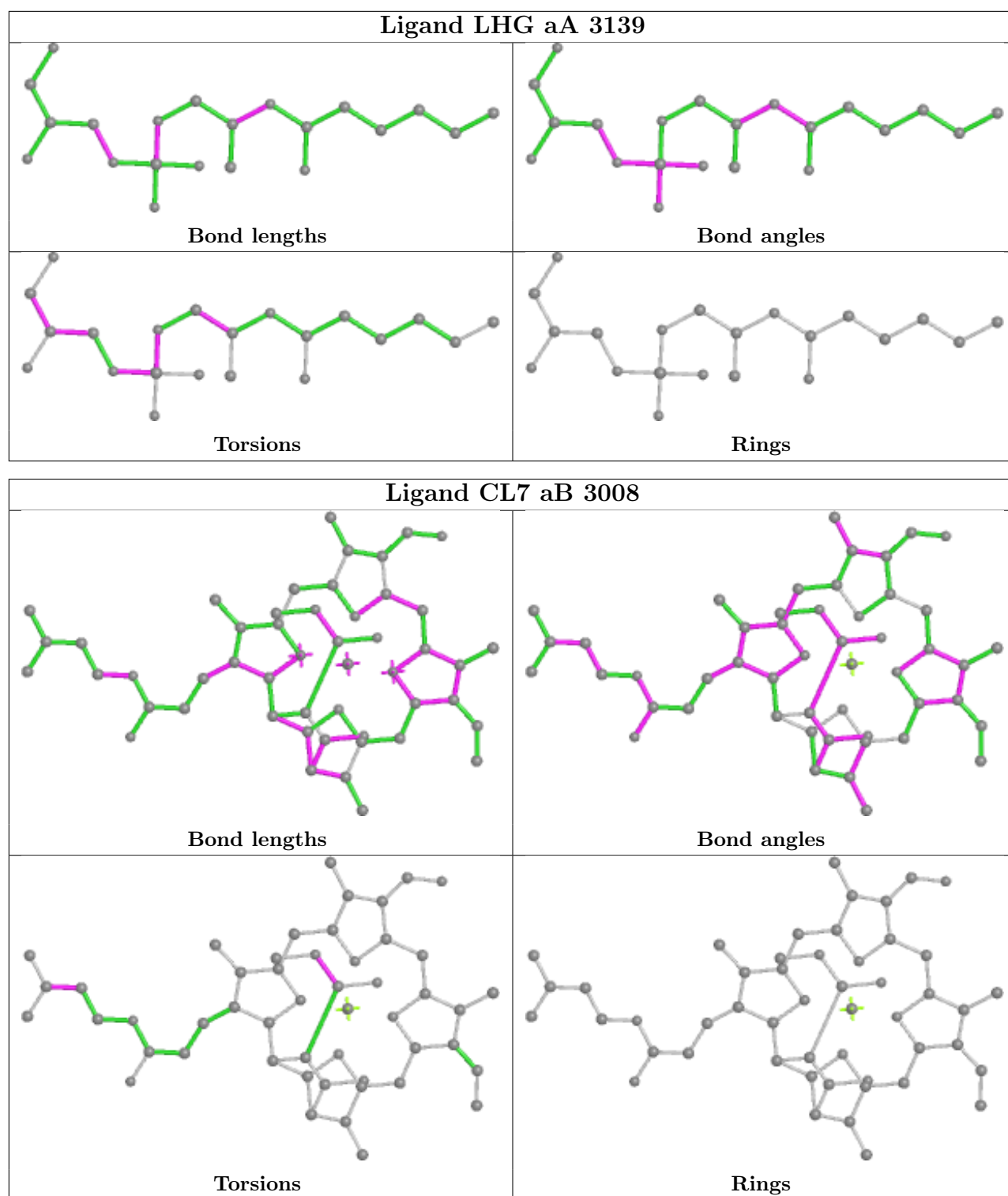




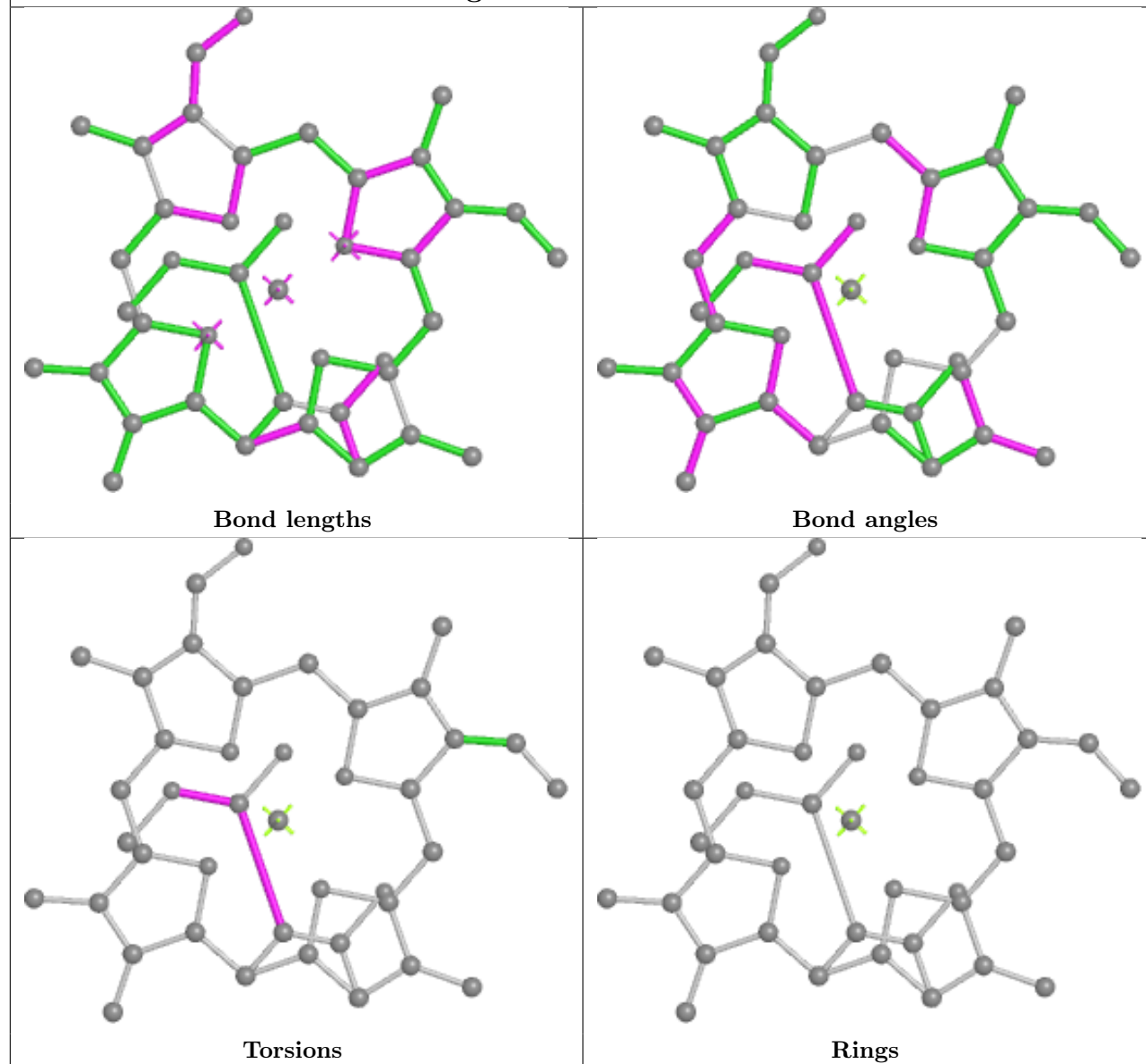




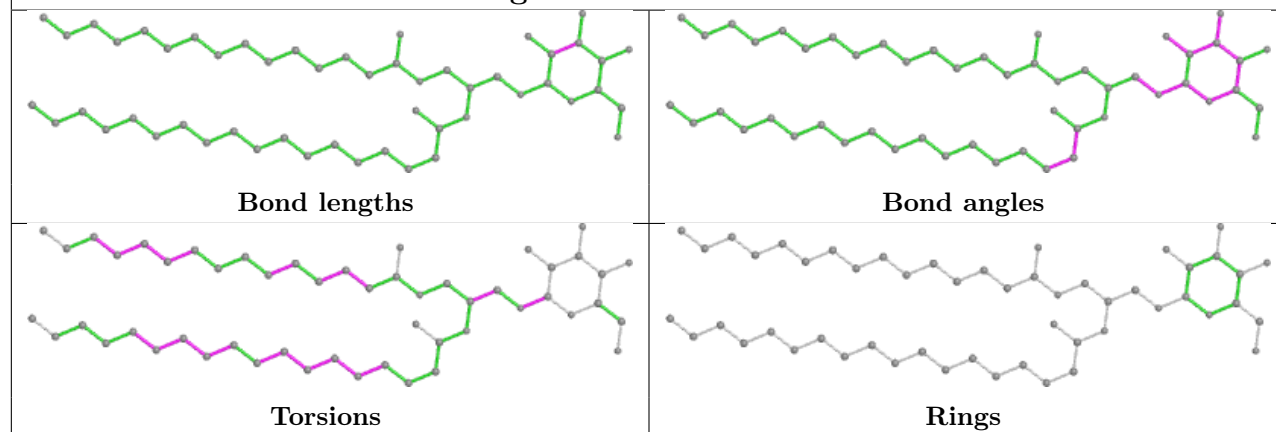




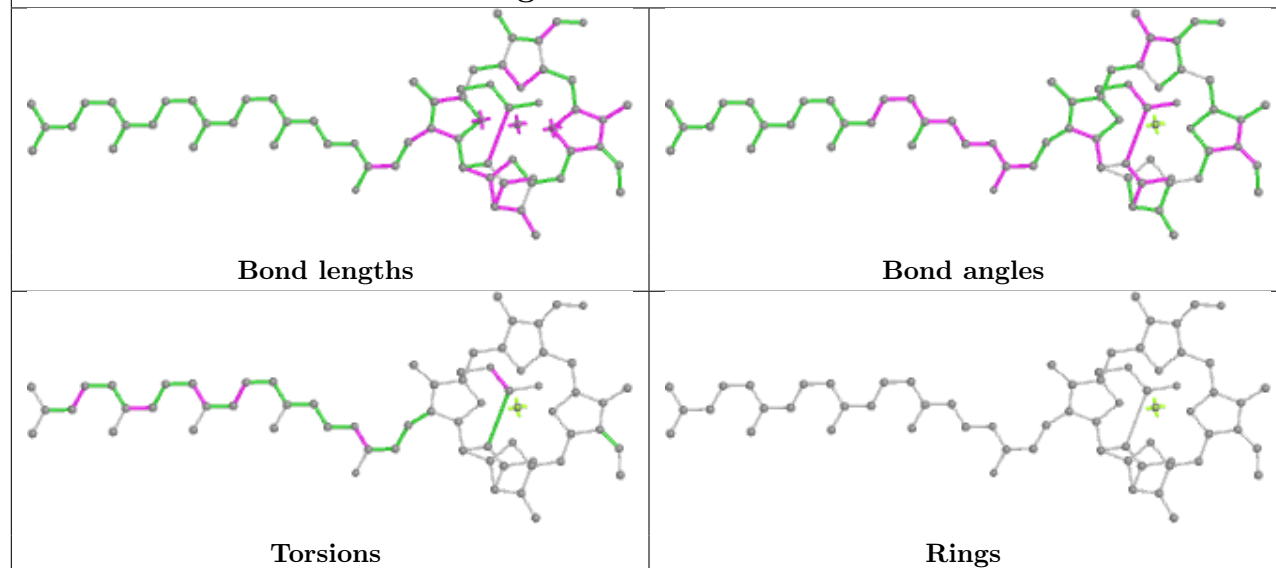
Ligand CL7 aB 3017



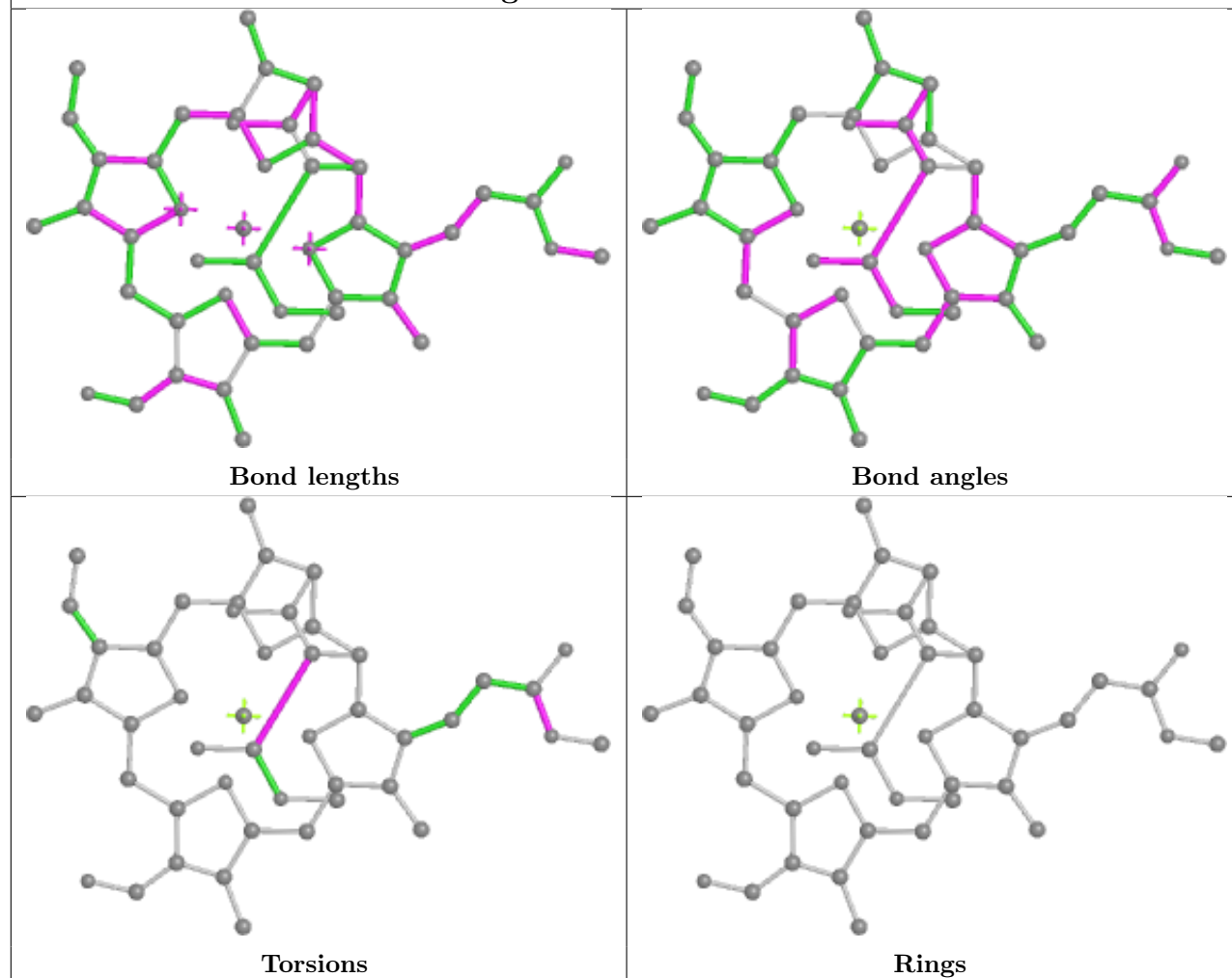
Ligand LMG aB 3029



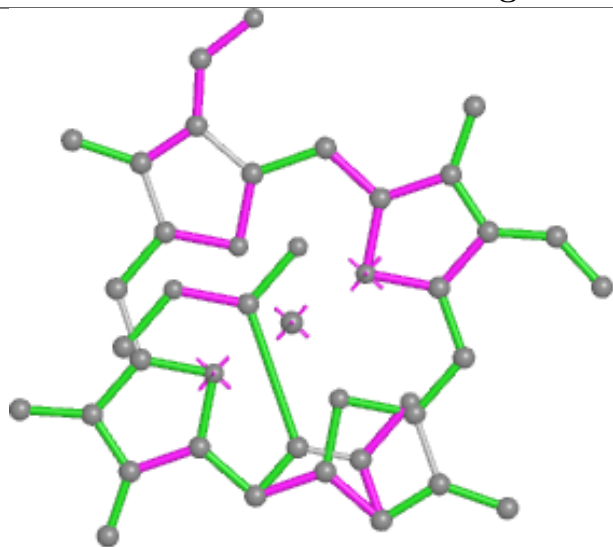
Ligand CL7 bA 3124



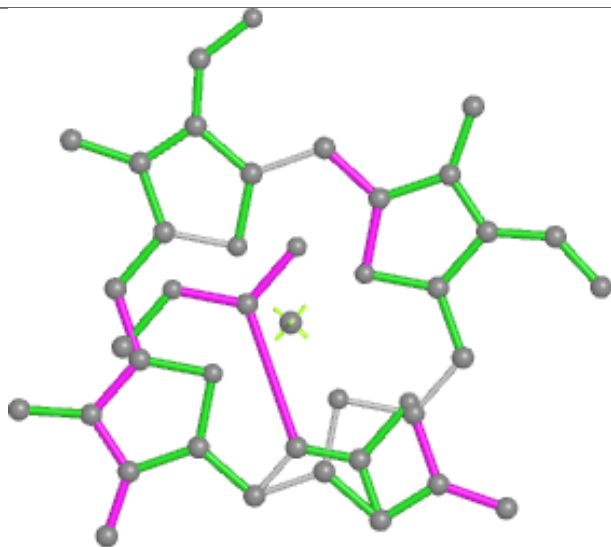
Ligand CL7 cA 3119



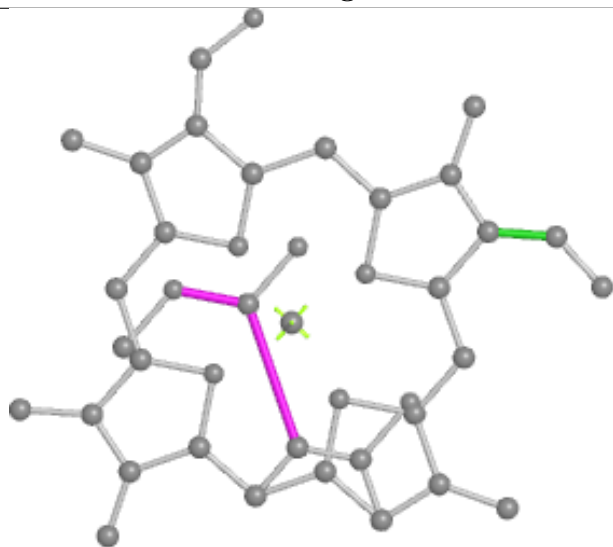
Ligand CL7 bA 3130



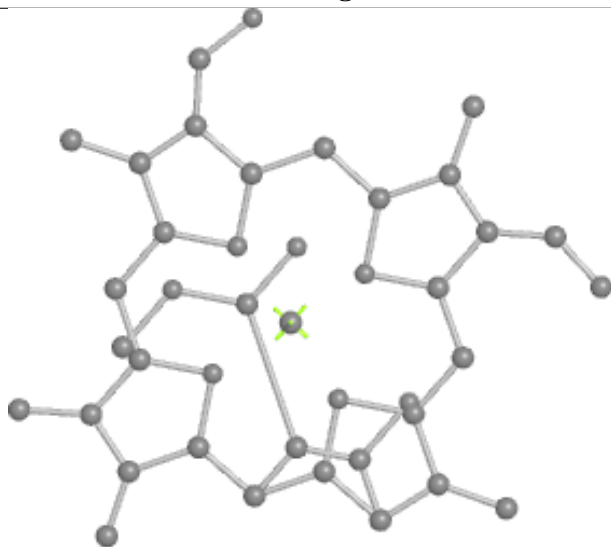
Bond lengths



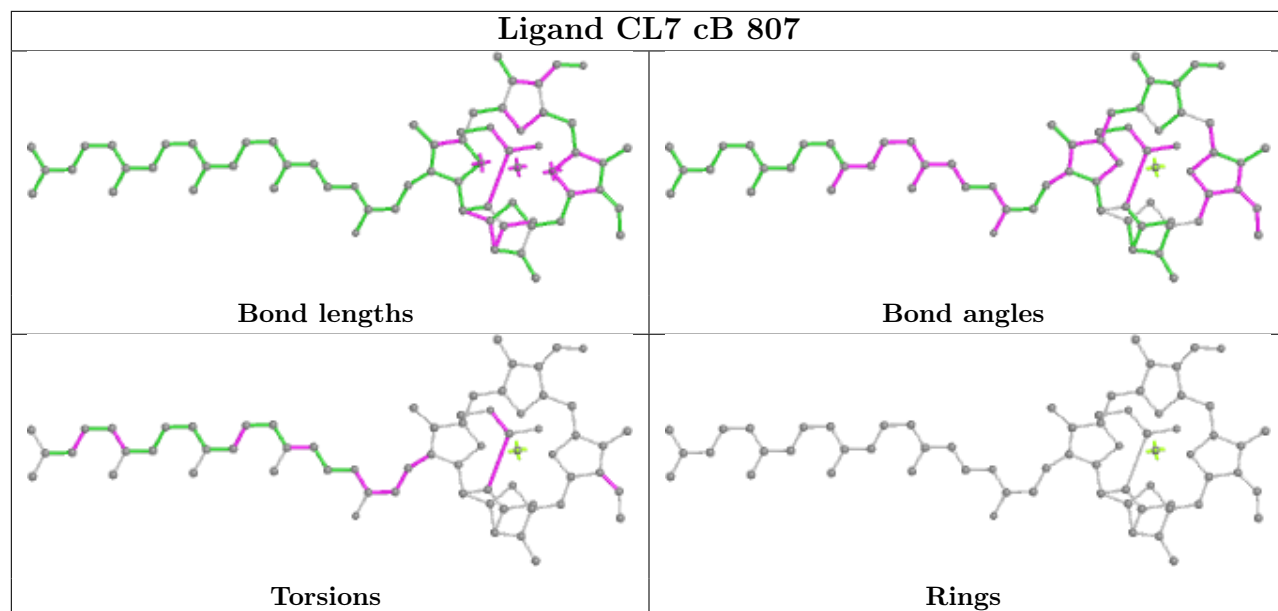
Bond angles



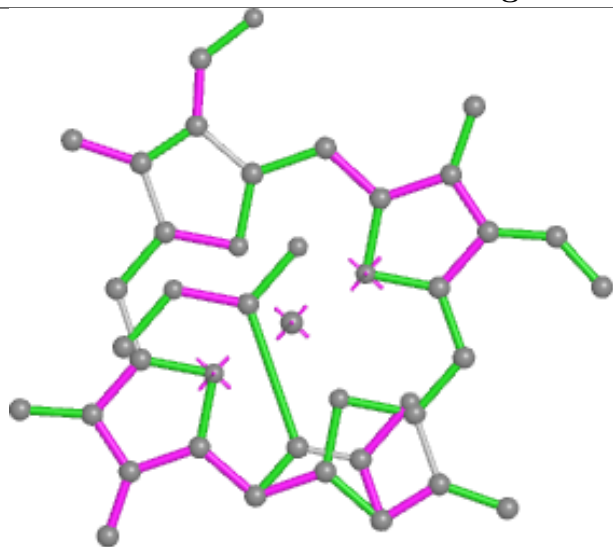
Torsions



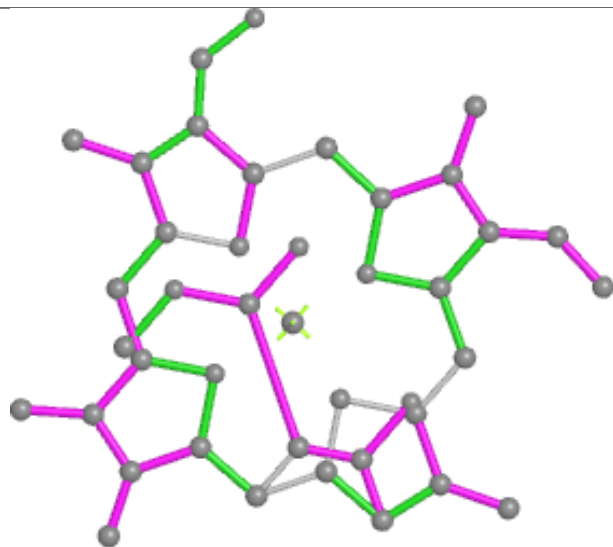
Rings



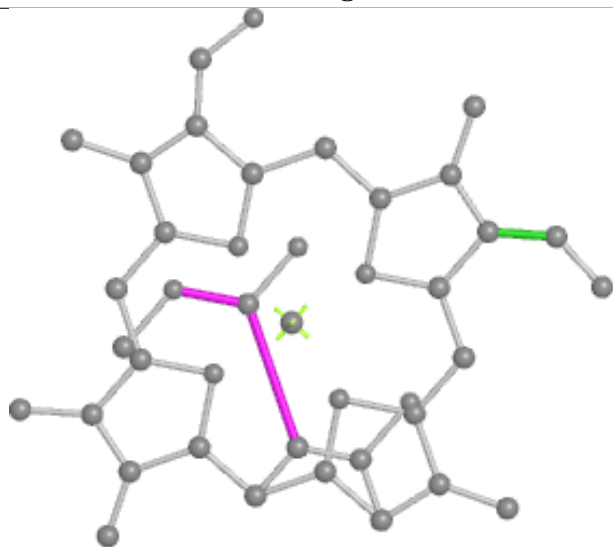
Ligand CL7 cA 3129



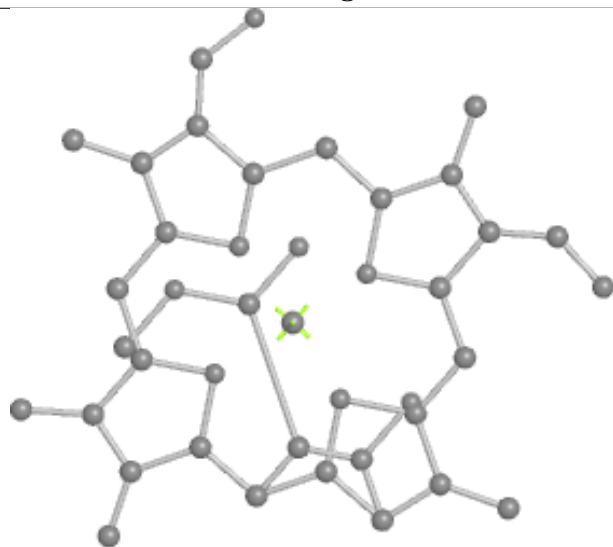
Bond lengths



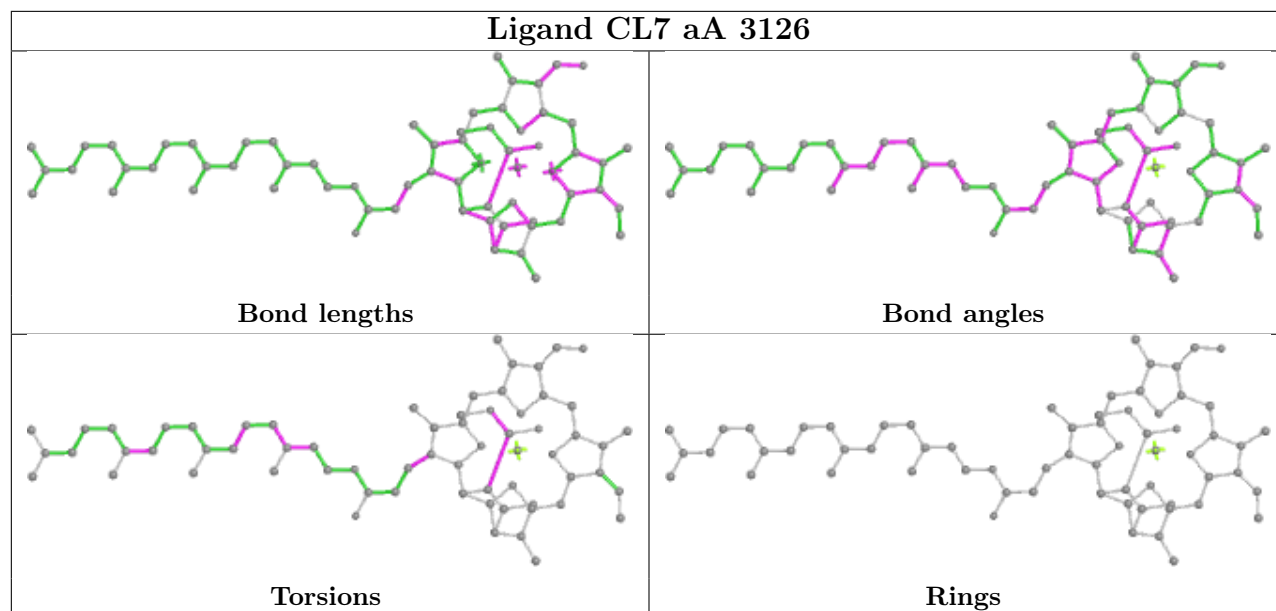
Bond angles



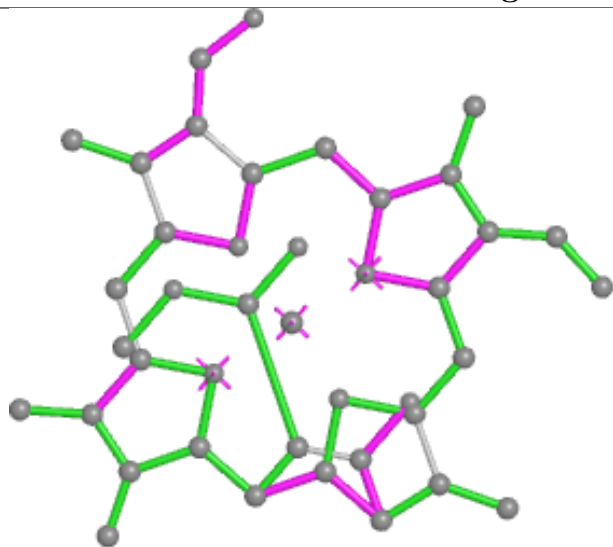
Torsions



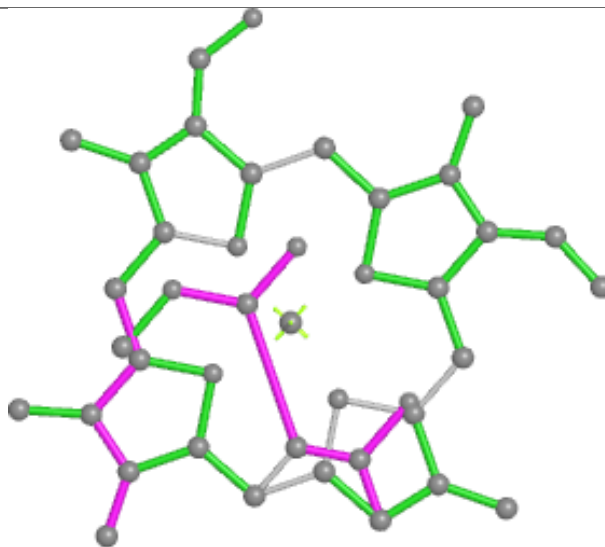
Rings



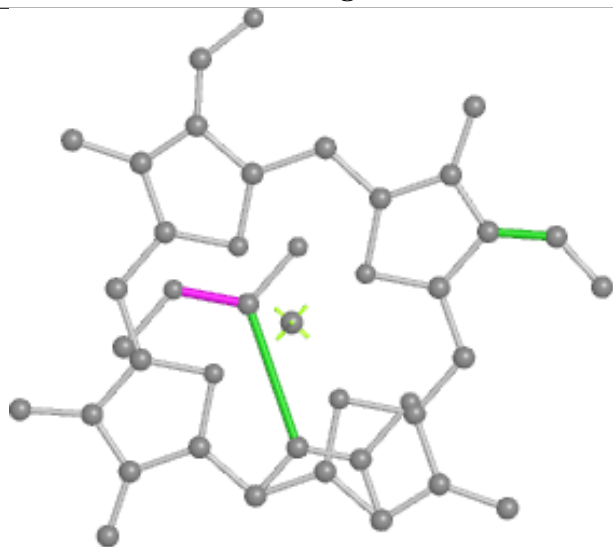
Ligand CL7 aB 3014



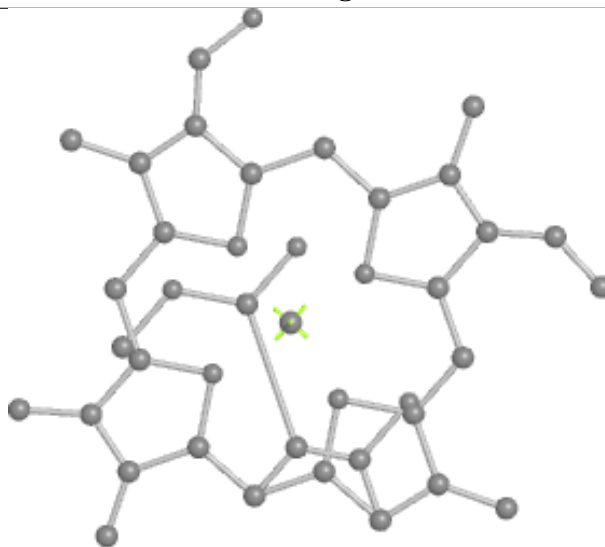
Bond lengths



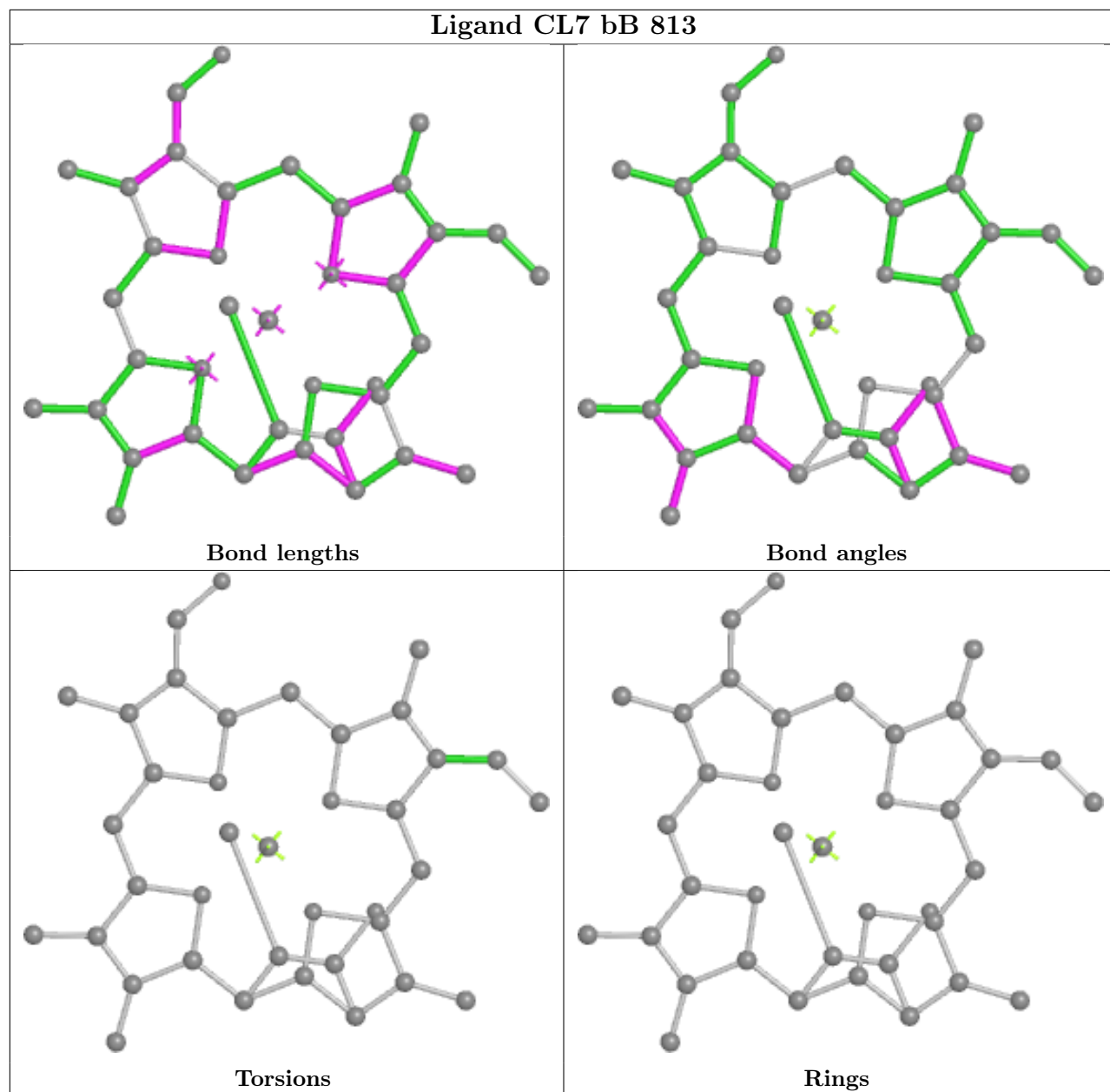
Bond angles

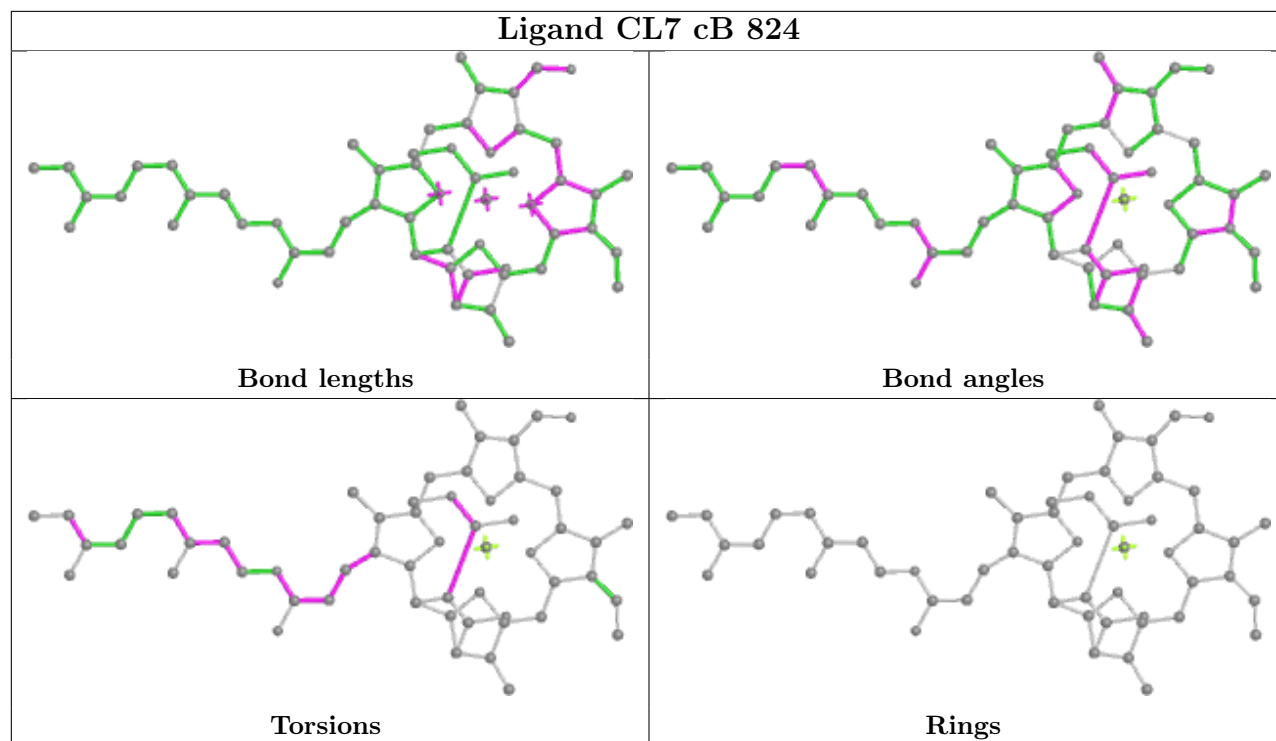


Torsions

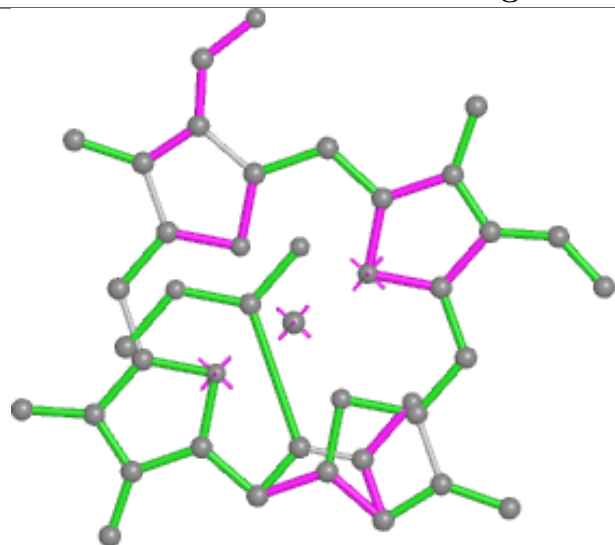


Rings

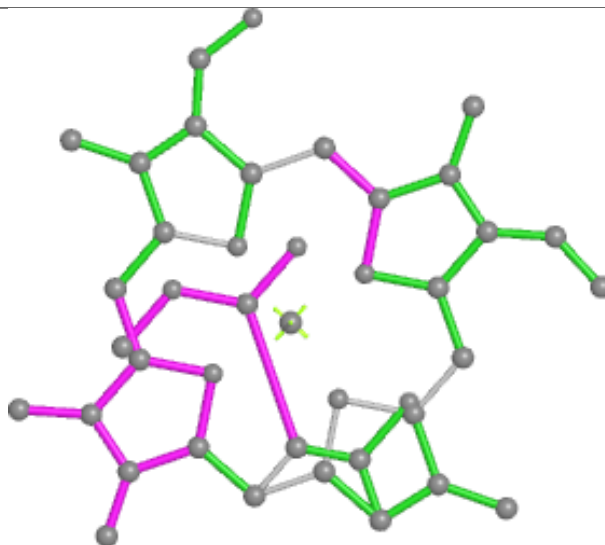




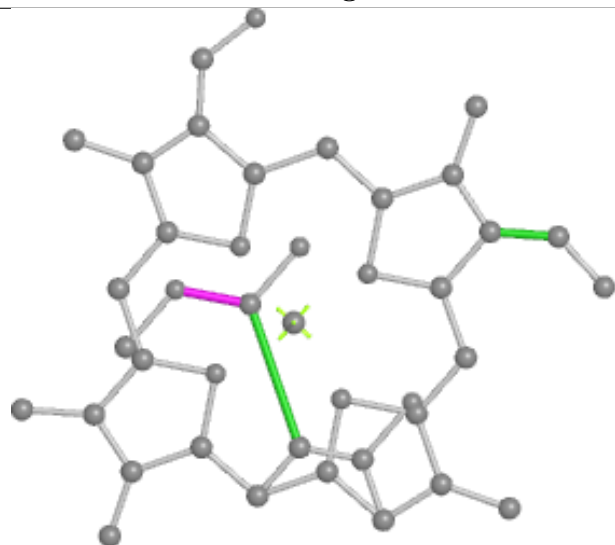
Ligand CL7 bA 3109



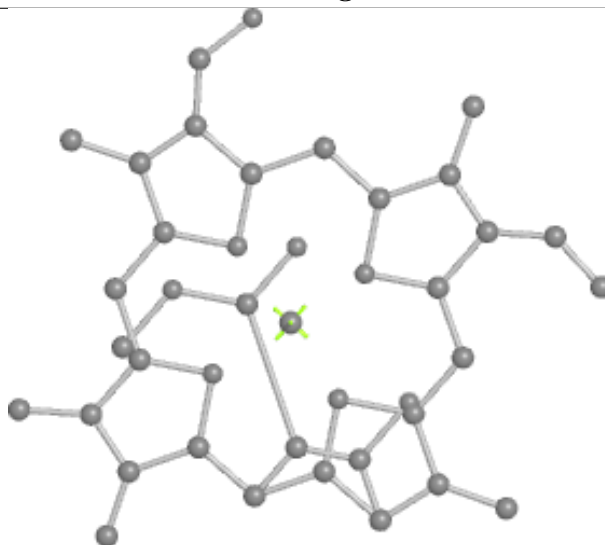
Bond lengths



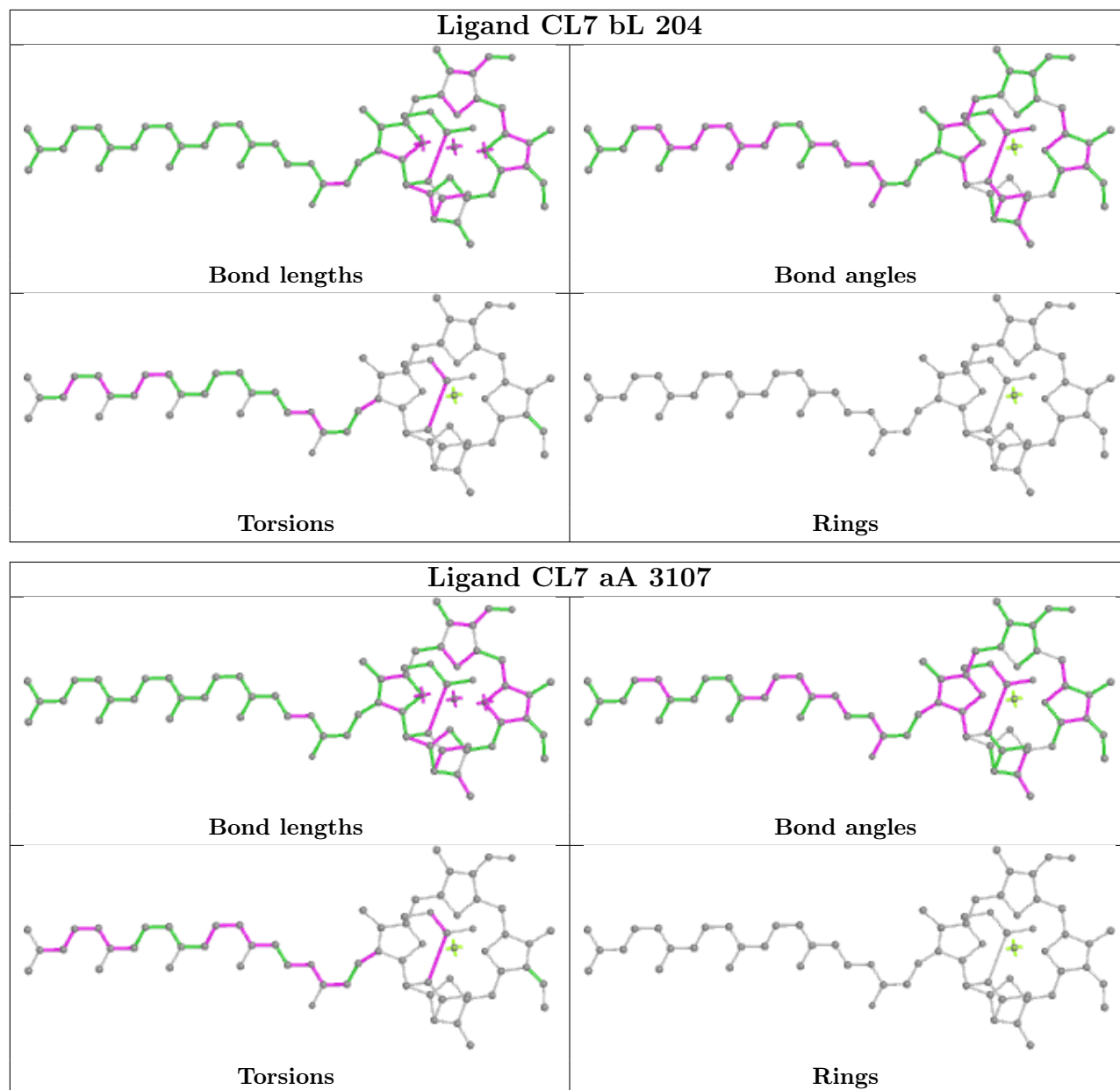
Bond angles

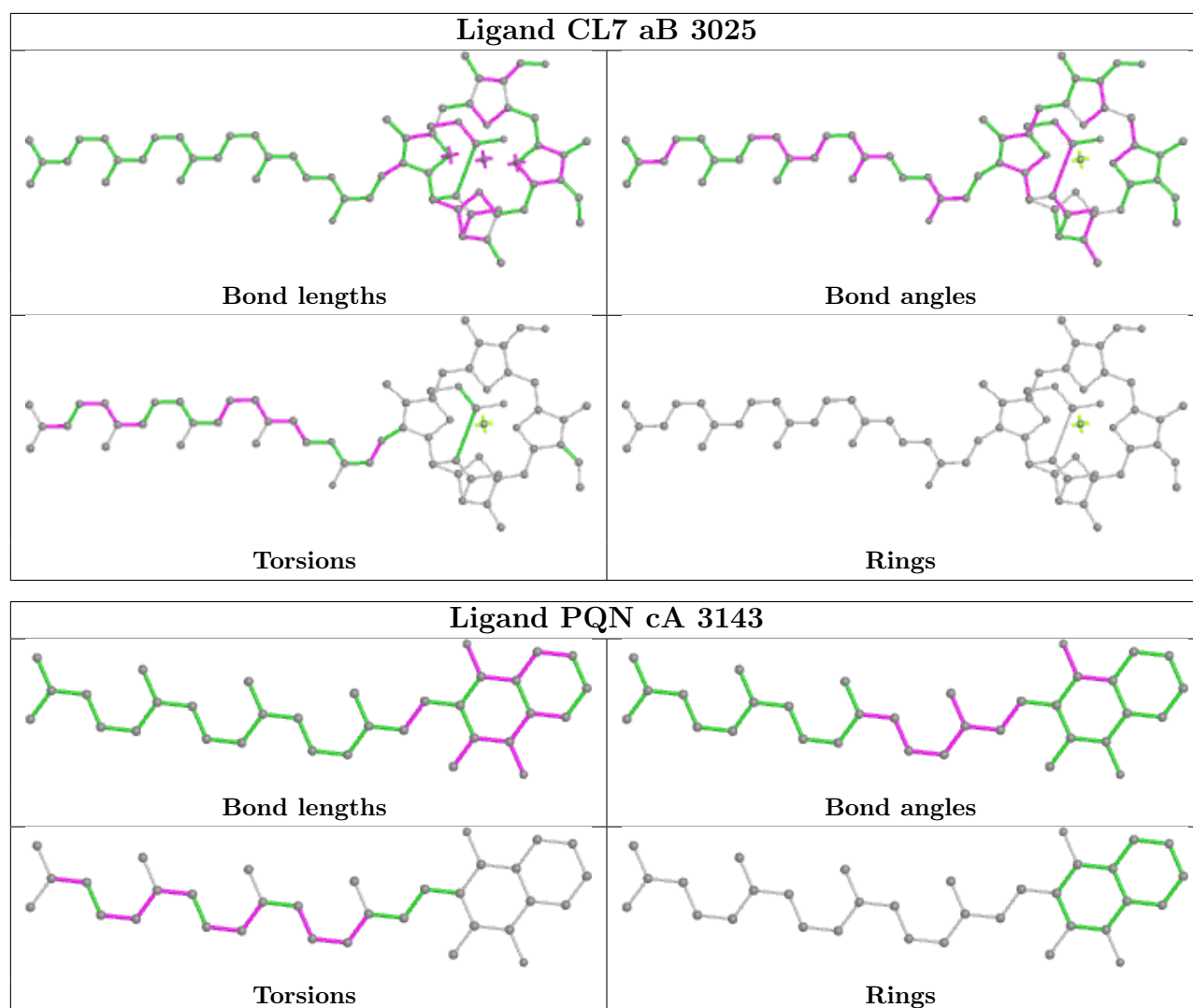


Torsions

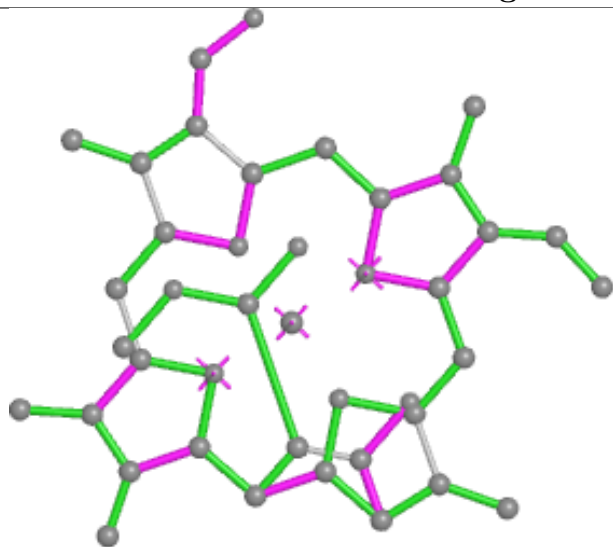


Rings

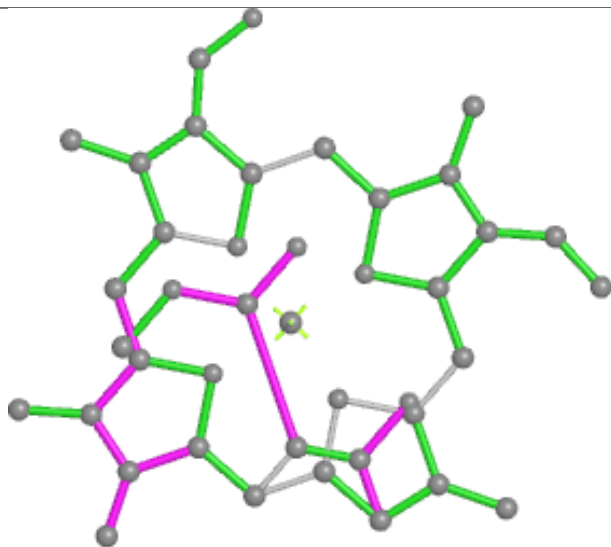




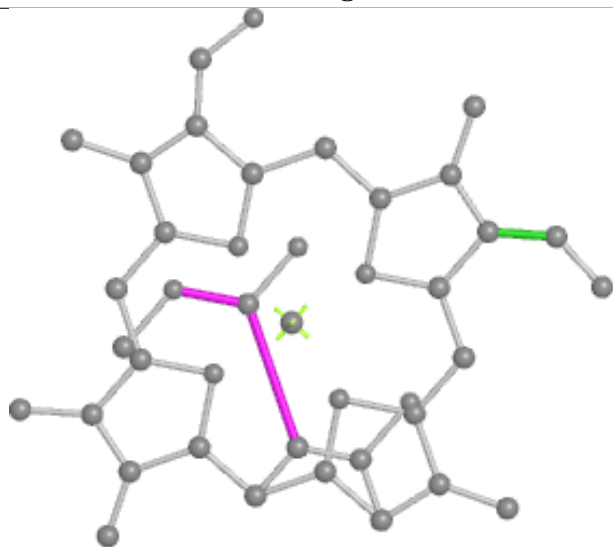
Ligand CL7 bA 3133



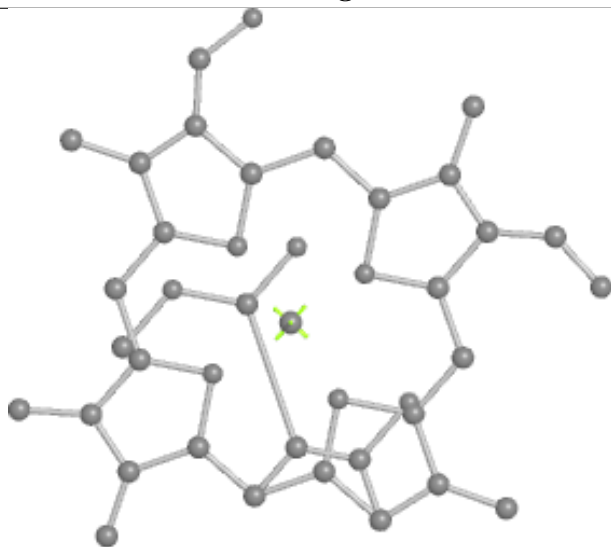
Bond lengths



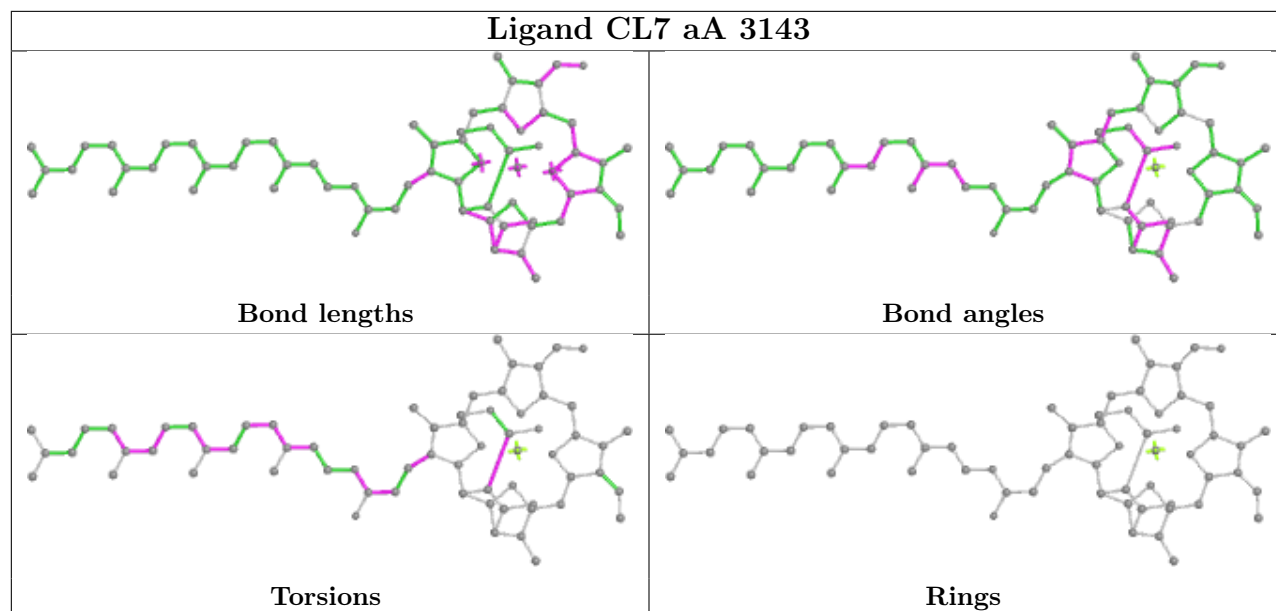
Bond angles

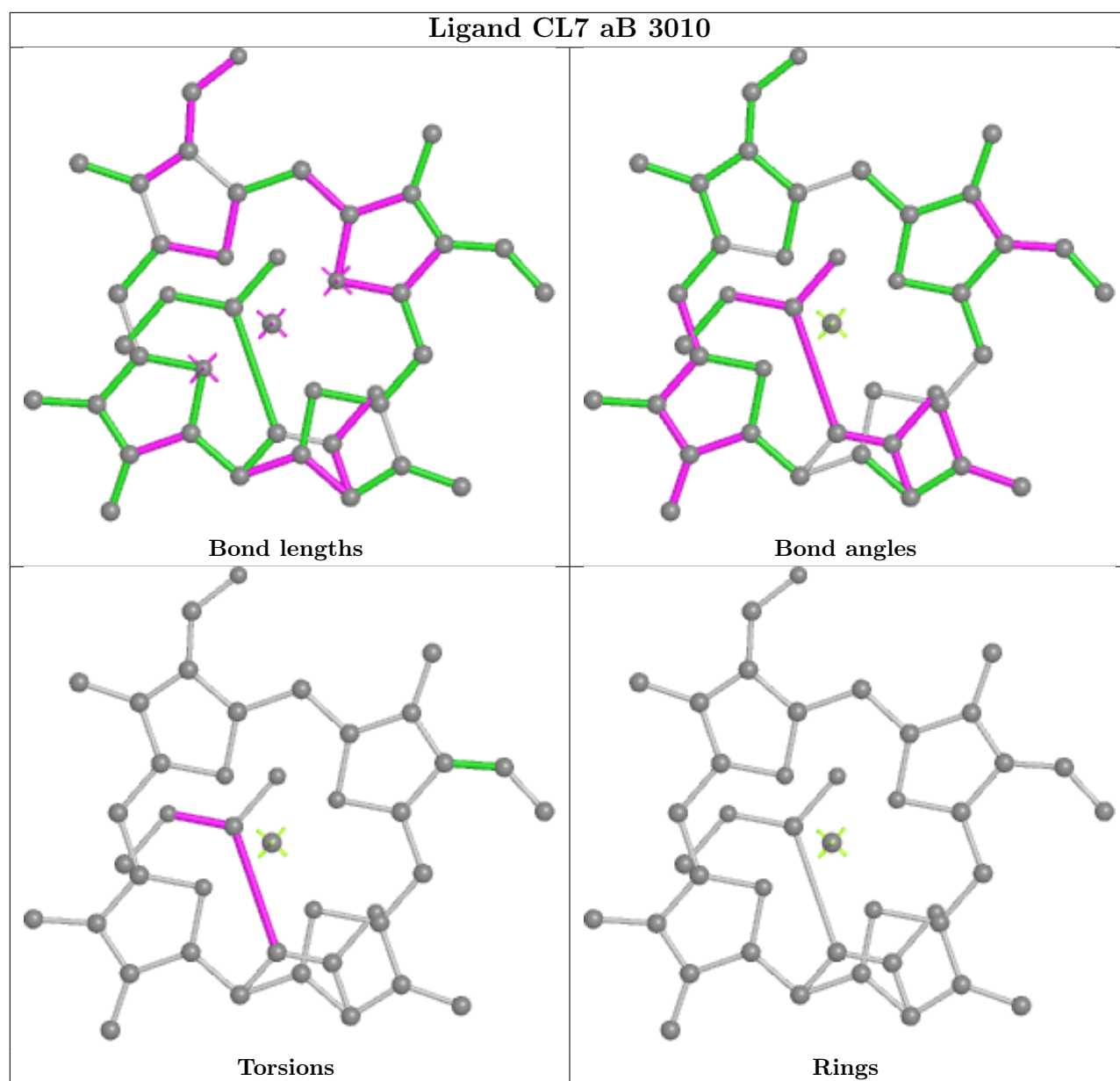


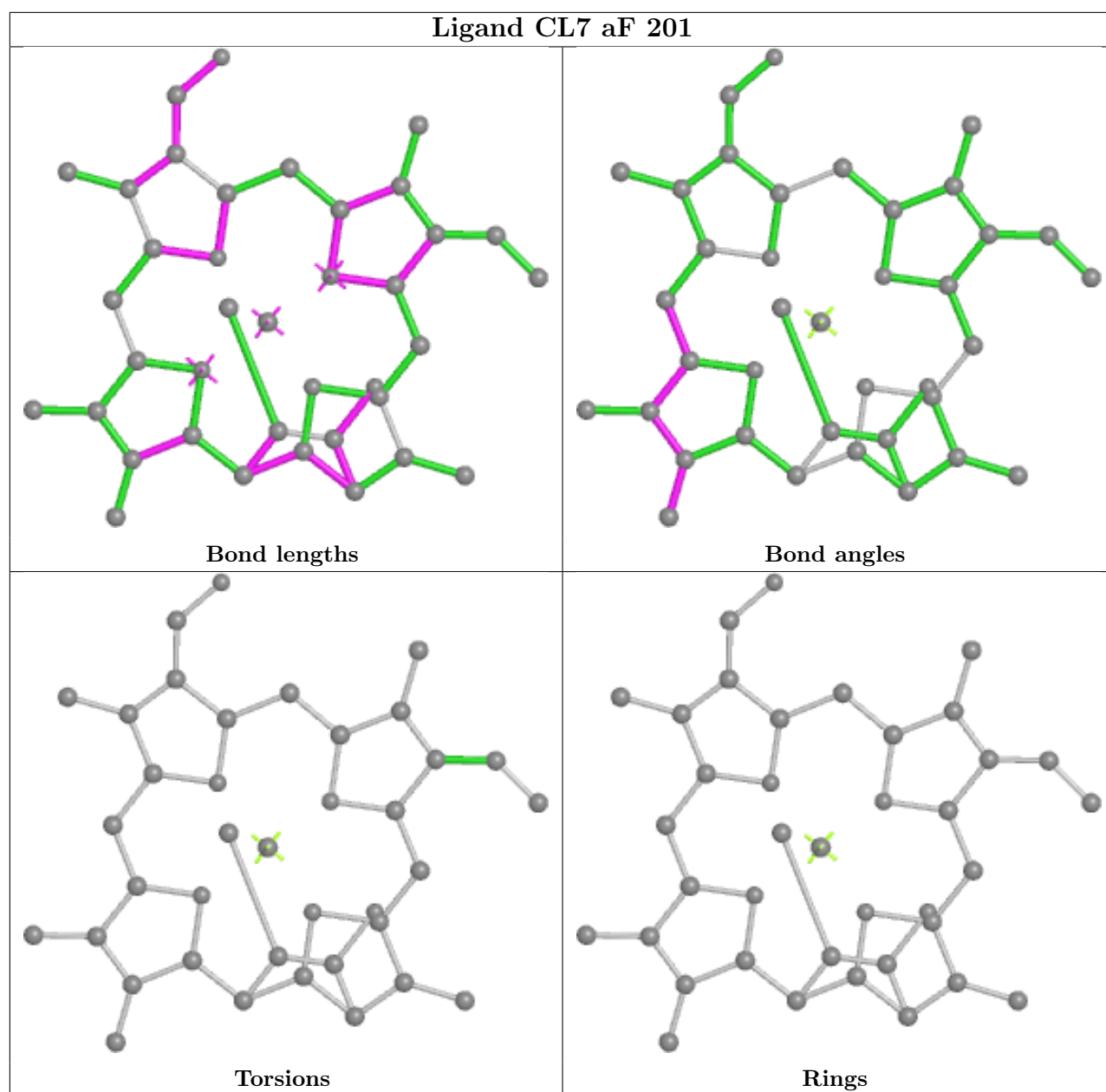
Torsions

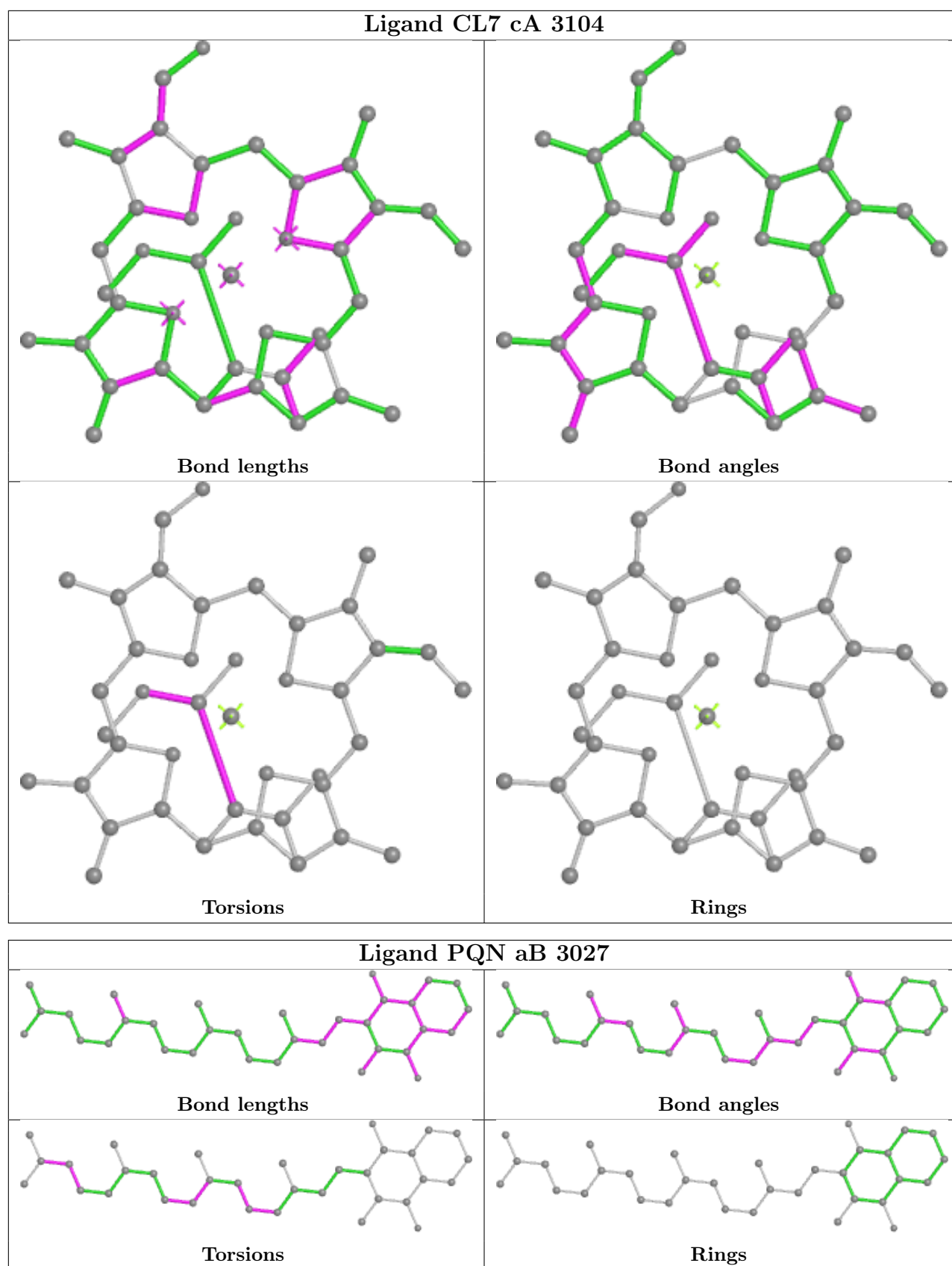


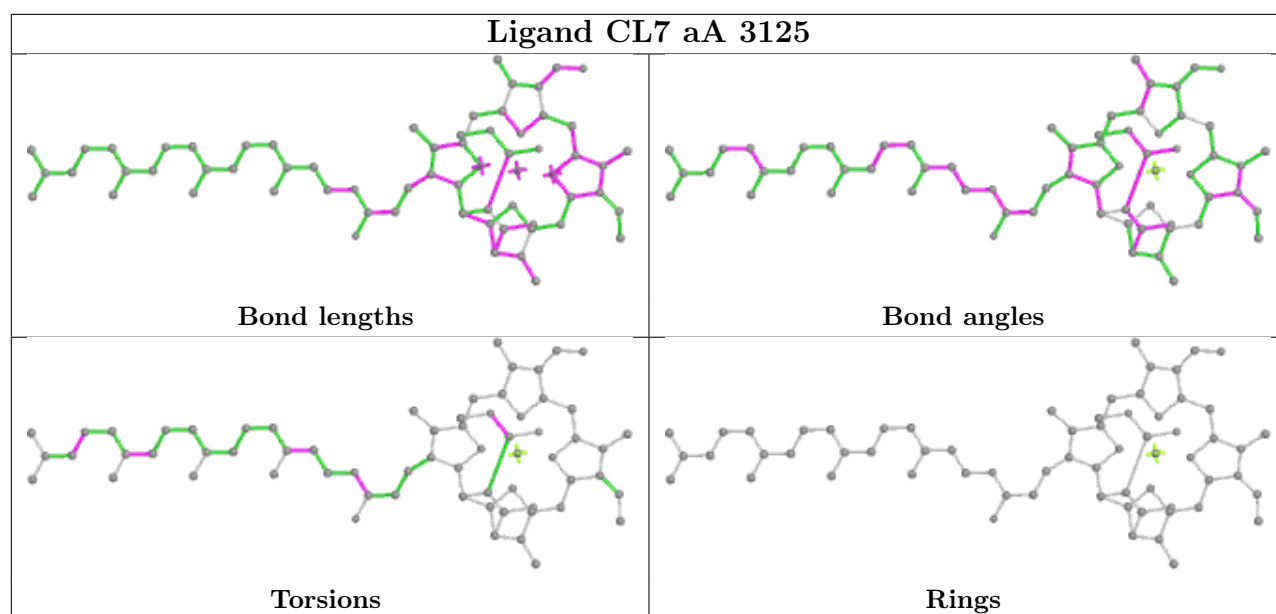
Rings



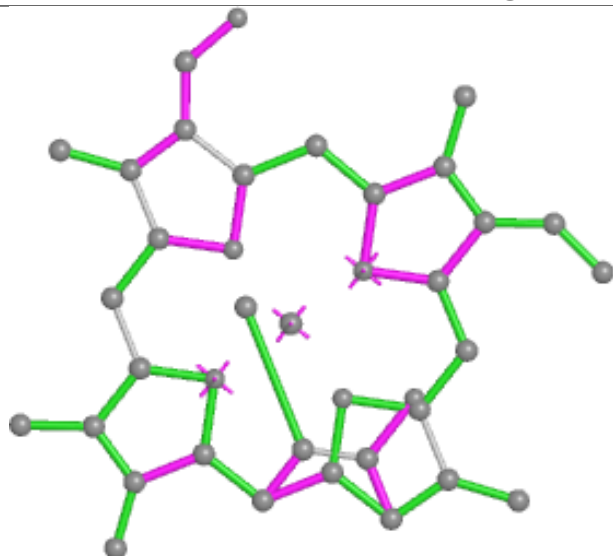




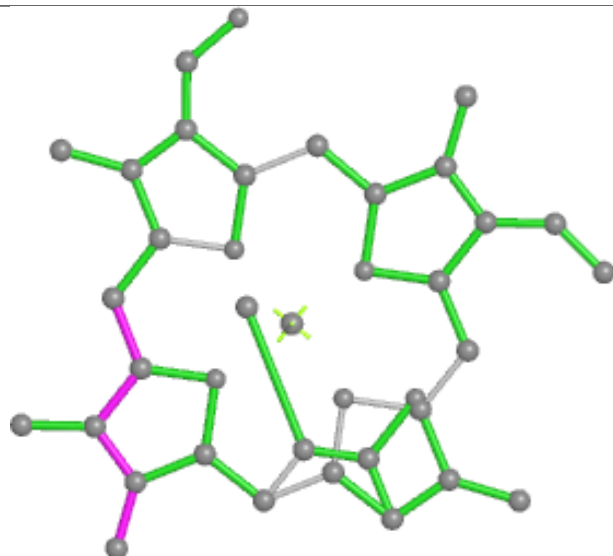




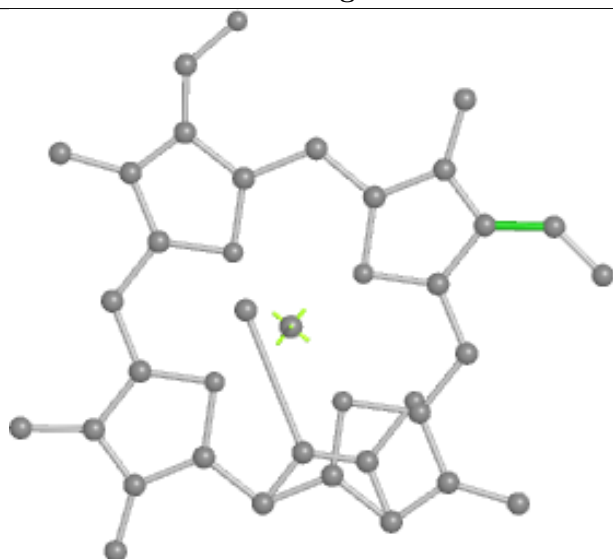
Ligand CL7 aB 3020



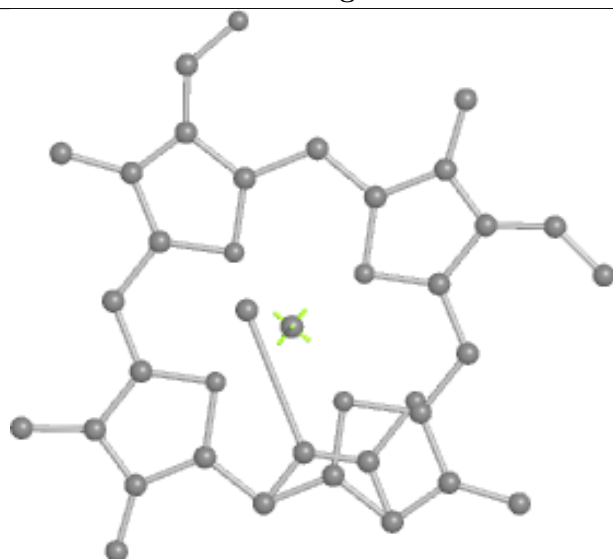
Bond lengths



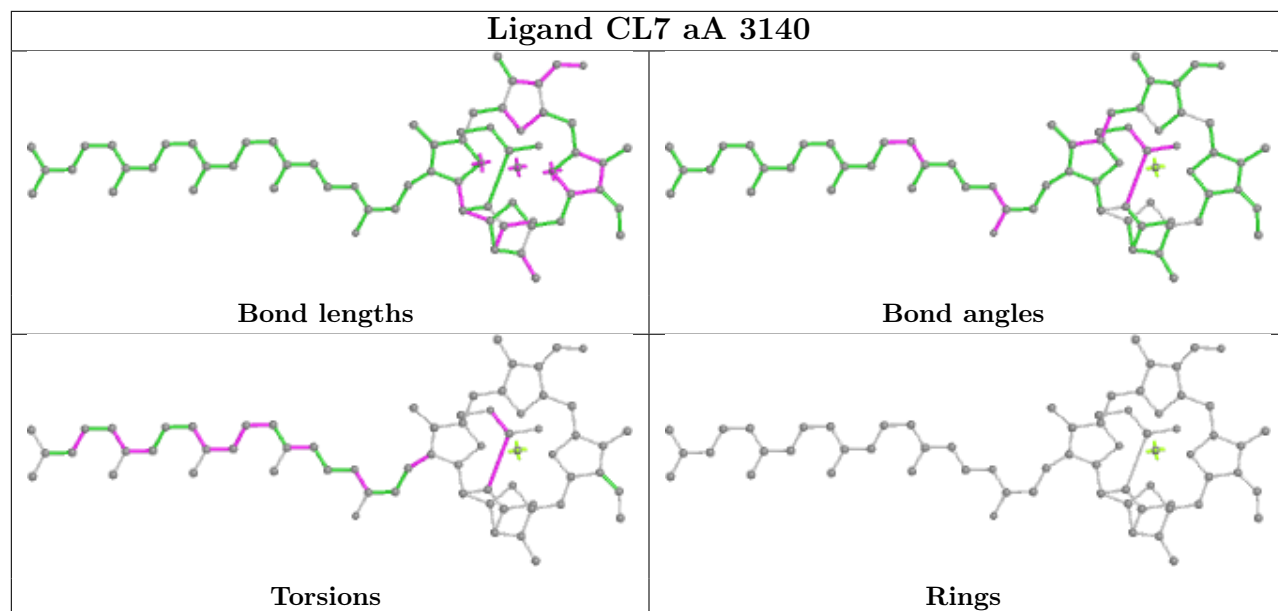
Bond angles

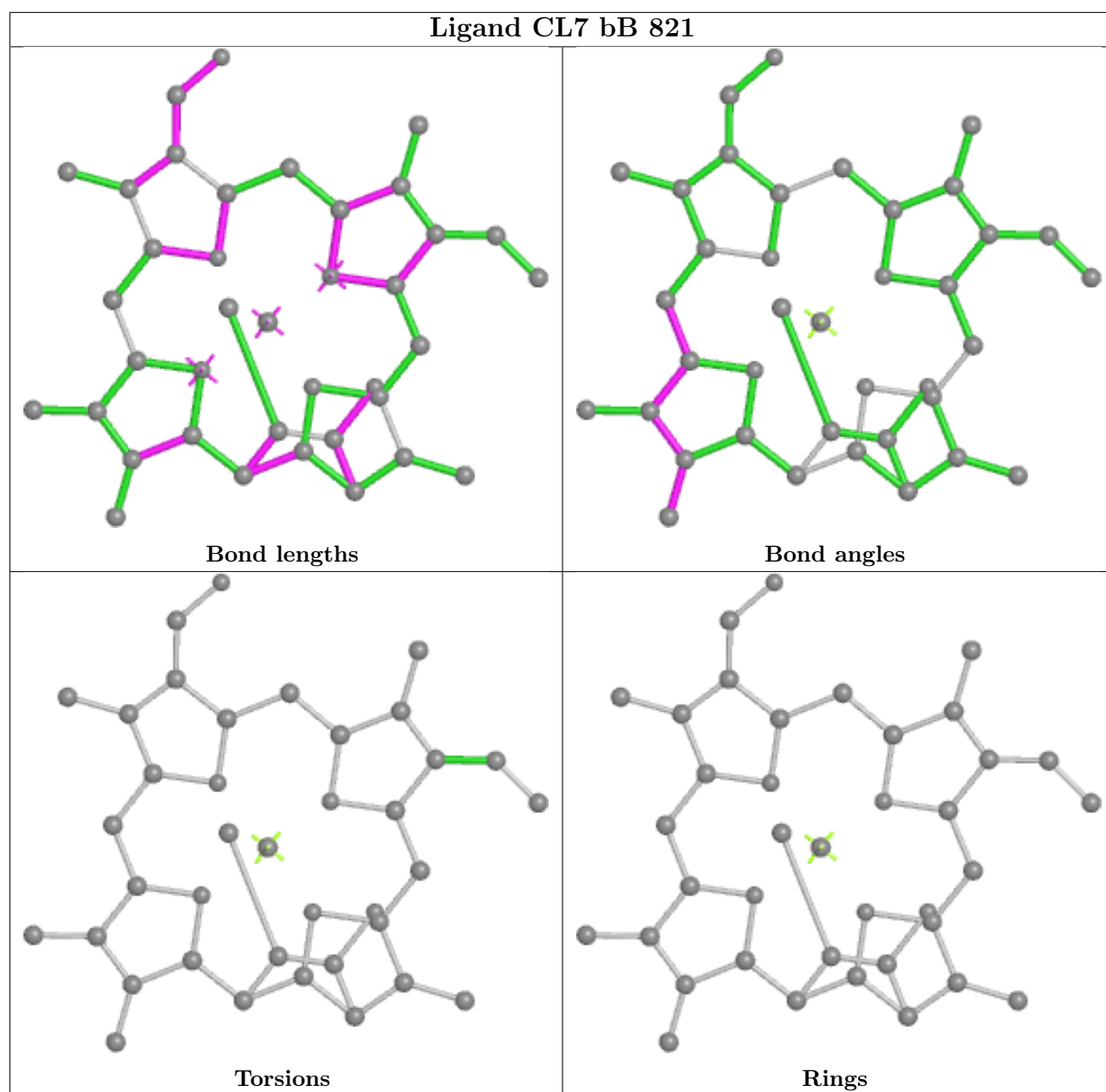


Torsions

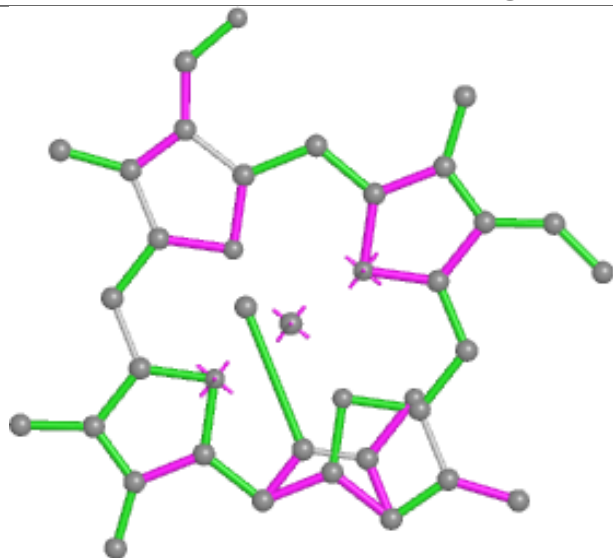


Rings

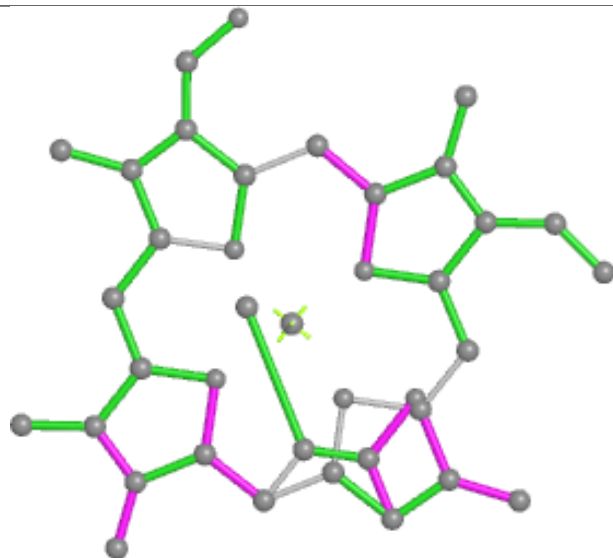




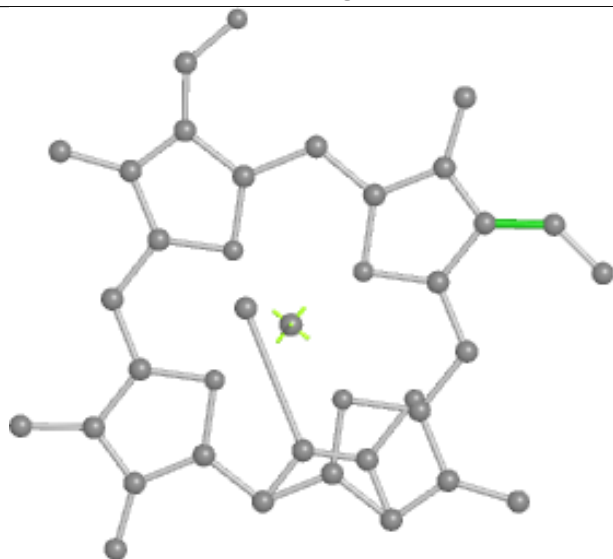
Ligand CL7 aB 3012



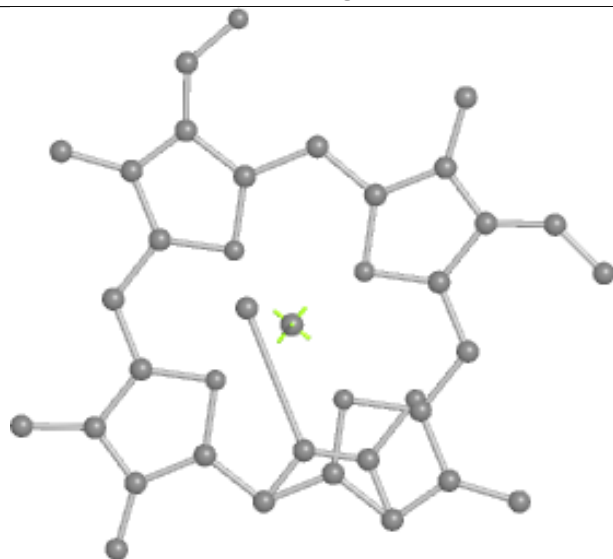
Bond lengths



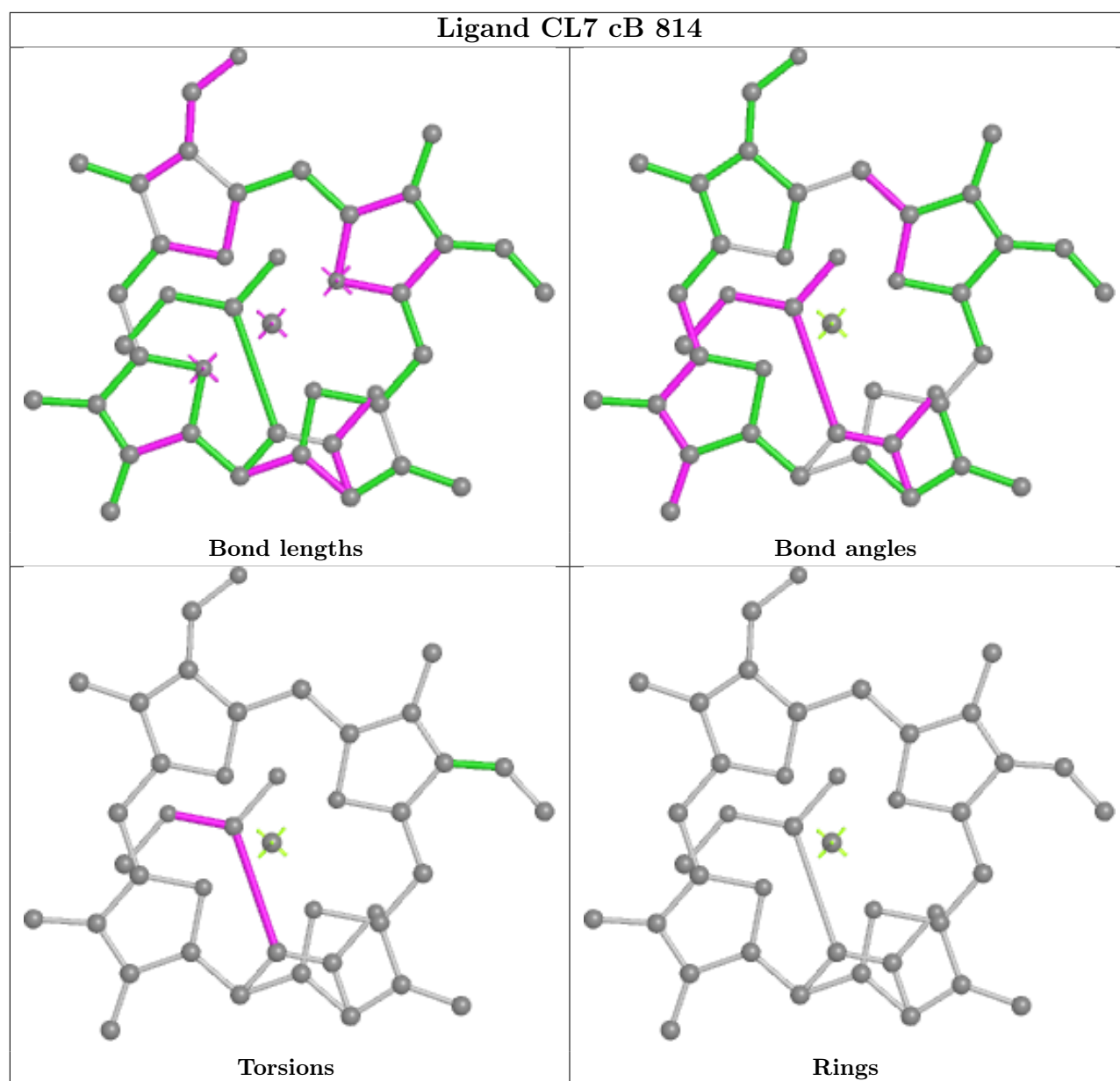
Bond angles



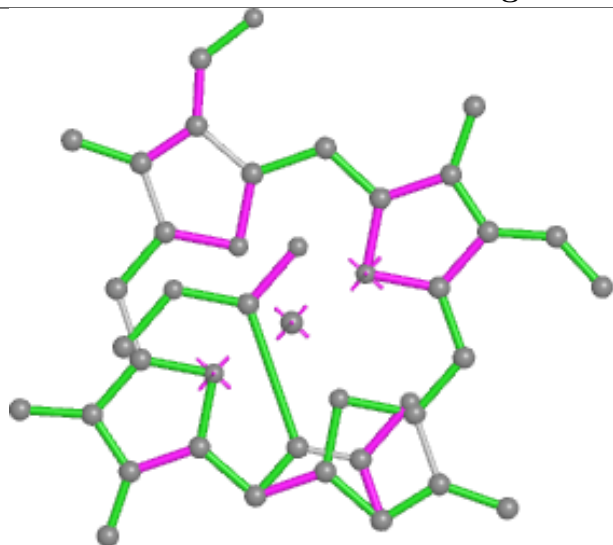
Torsions



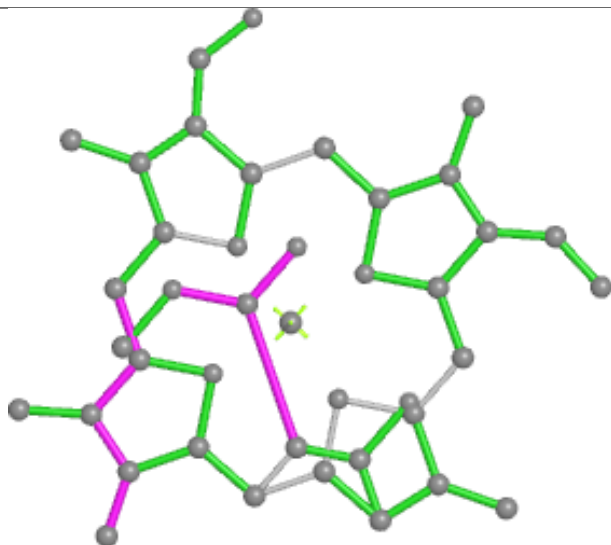
Rings



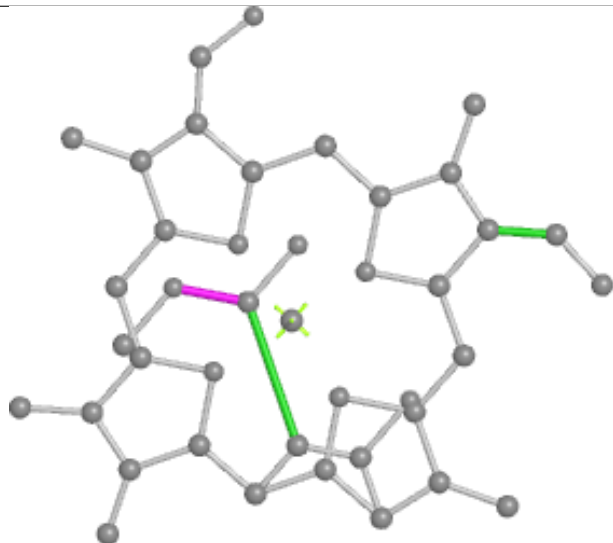
Ligand CL7 cA 3110



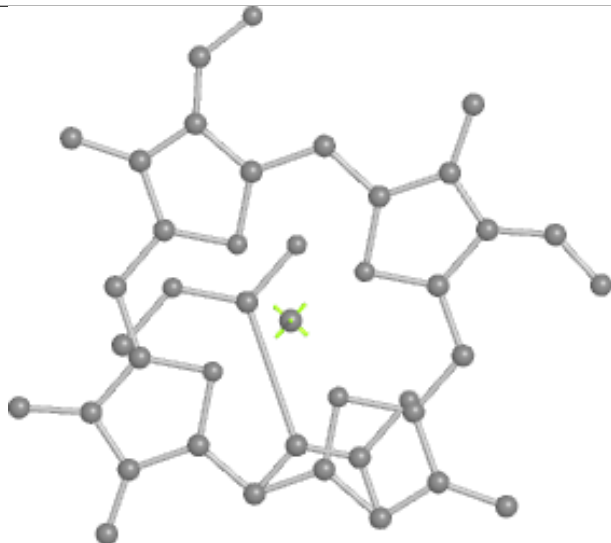
Bond lengths



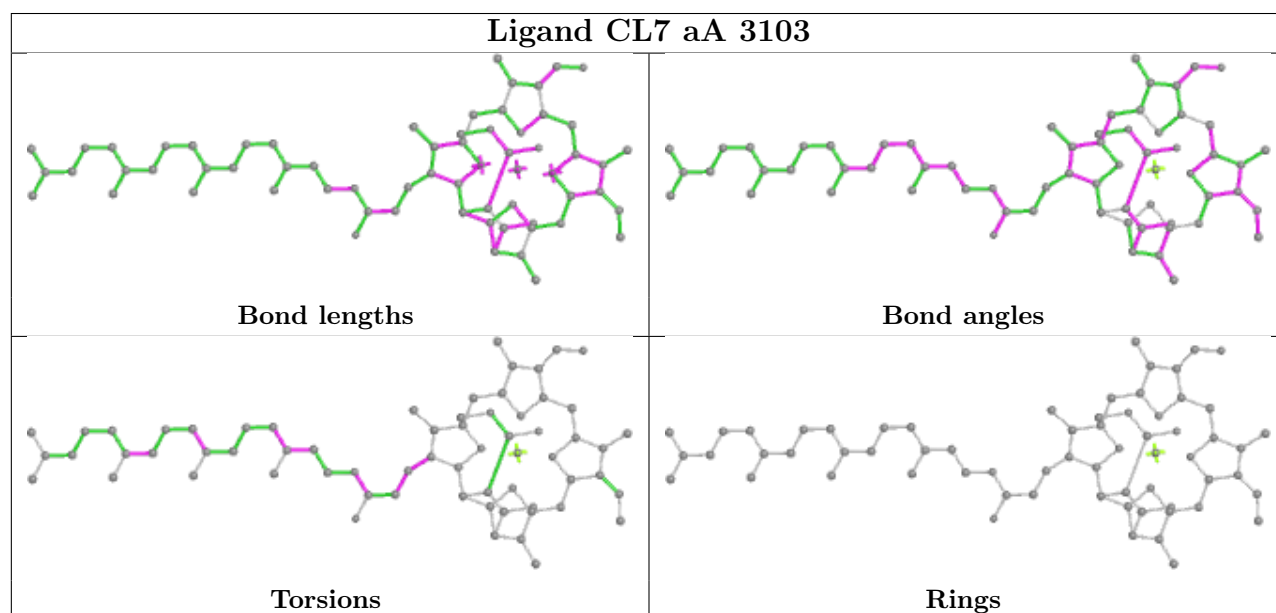
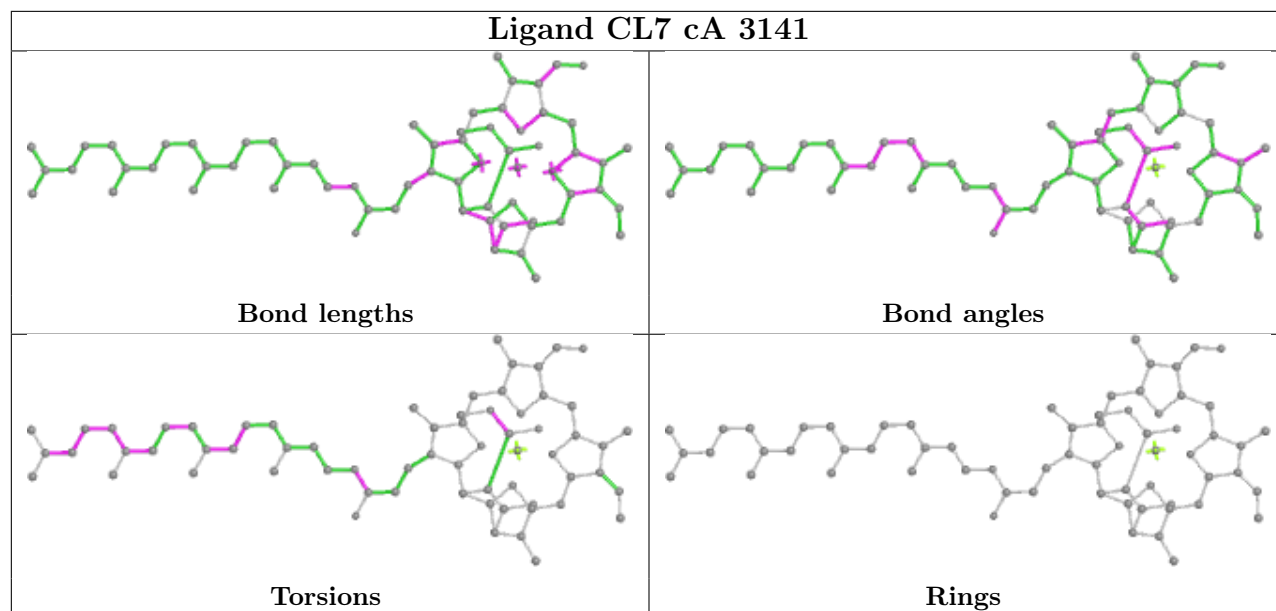
Bond angles

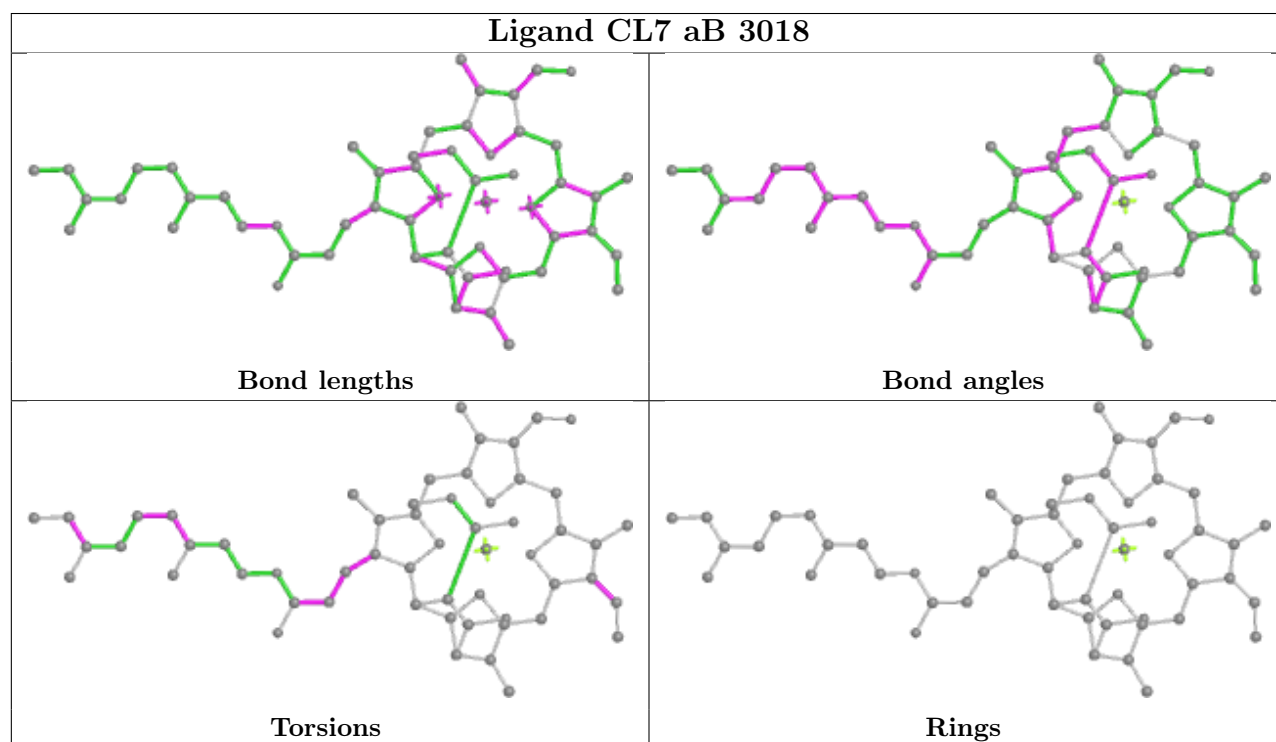
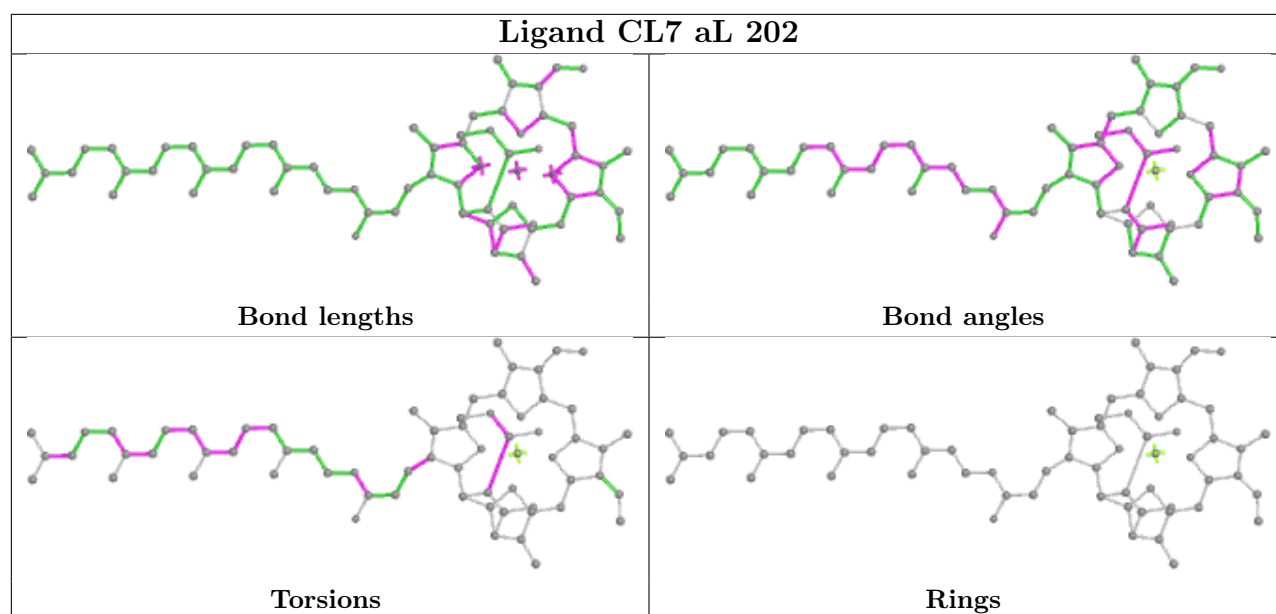


Torsions

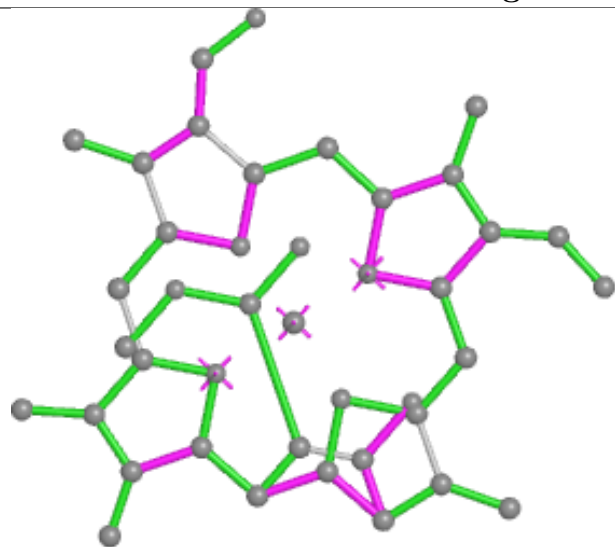


Rings

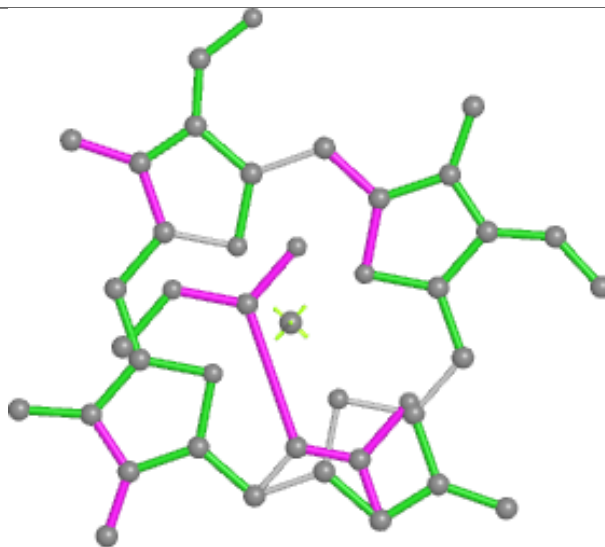




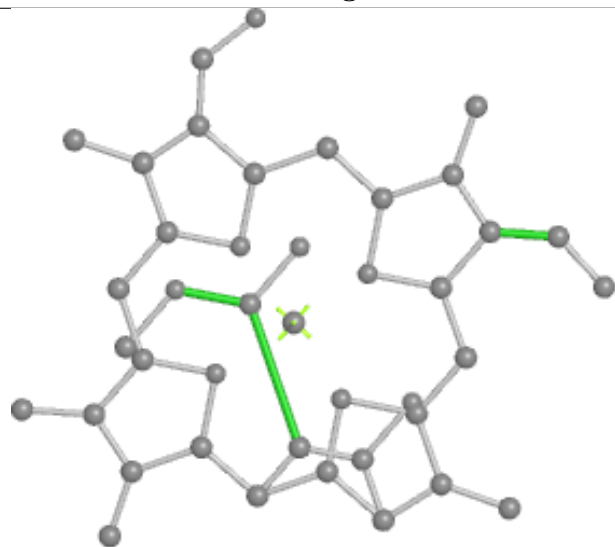
Ligand CL7 aA 3114



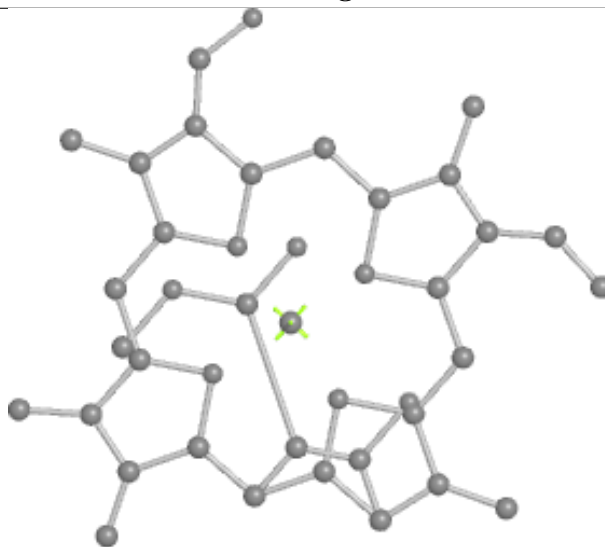
Bond lengths



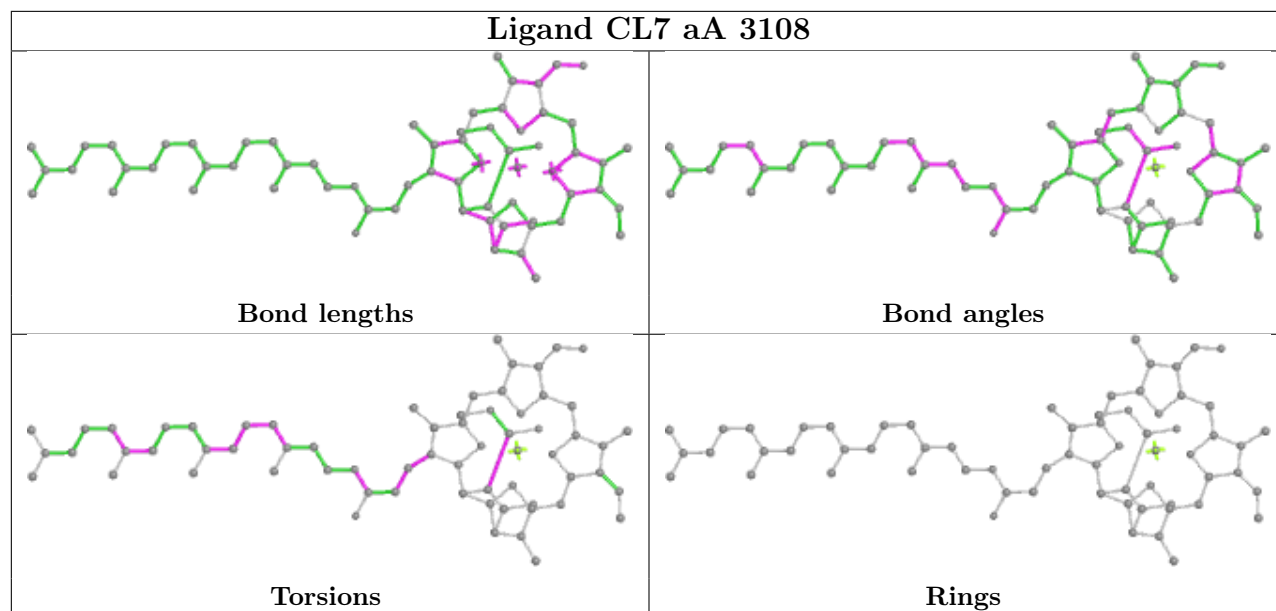
Bond angles

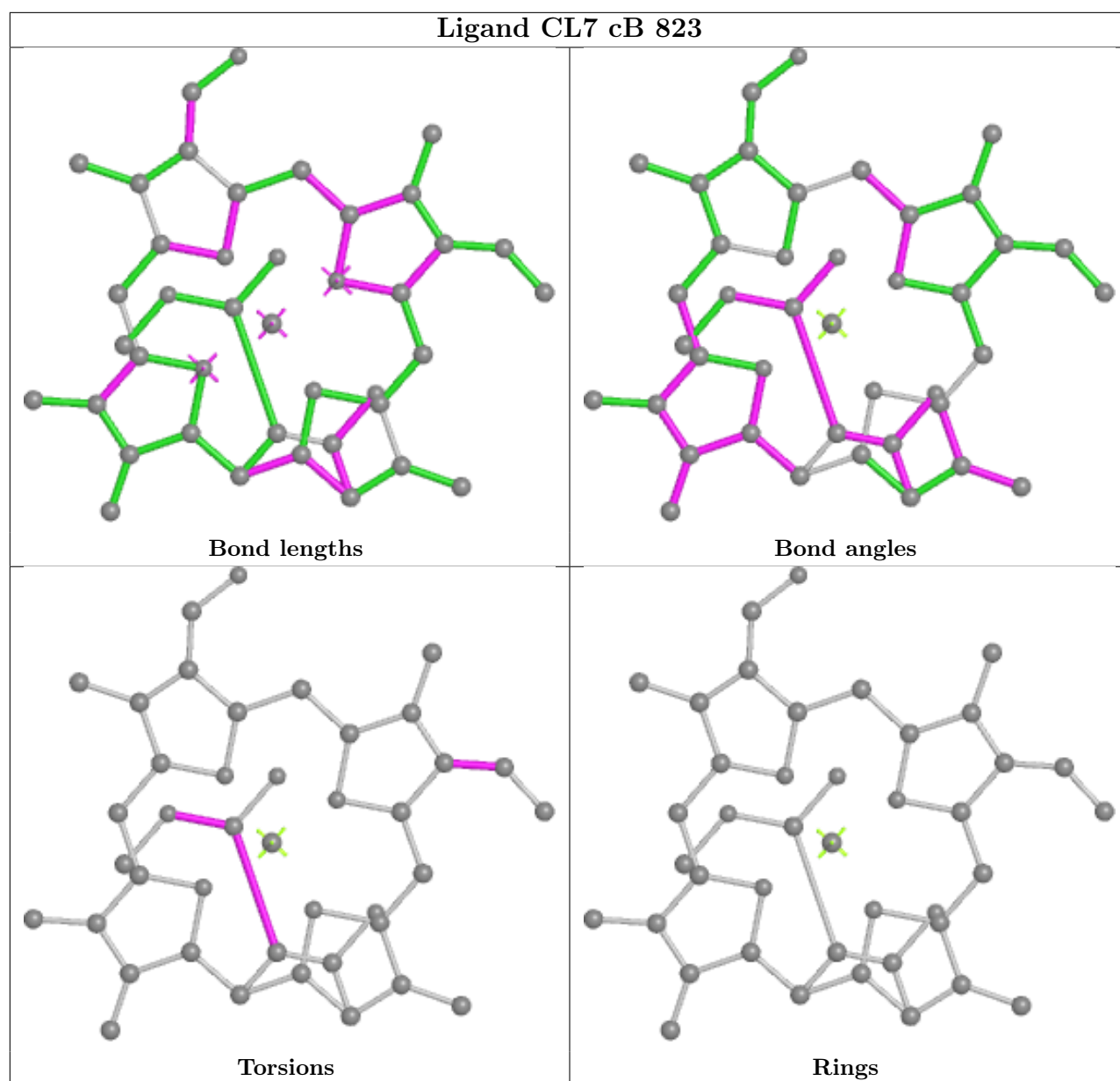


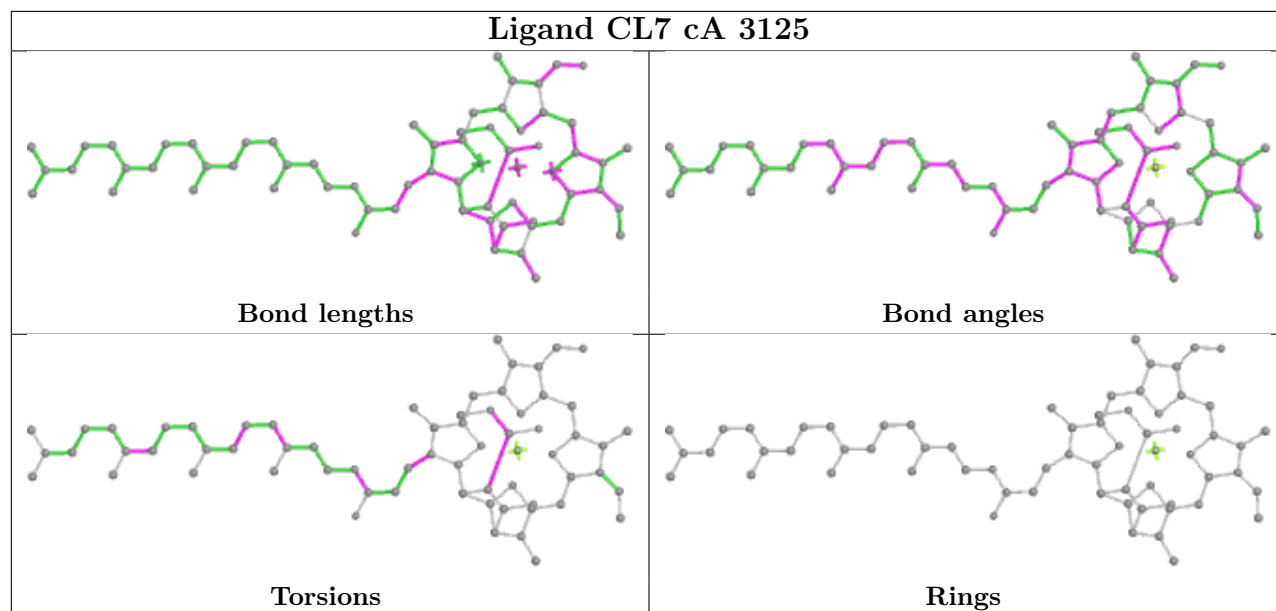
Torsions

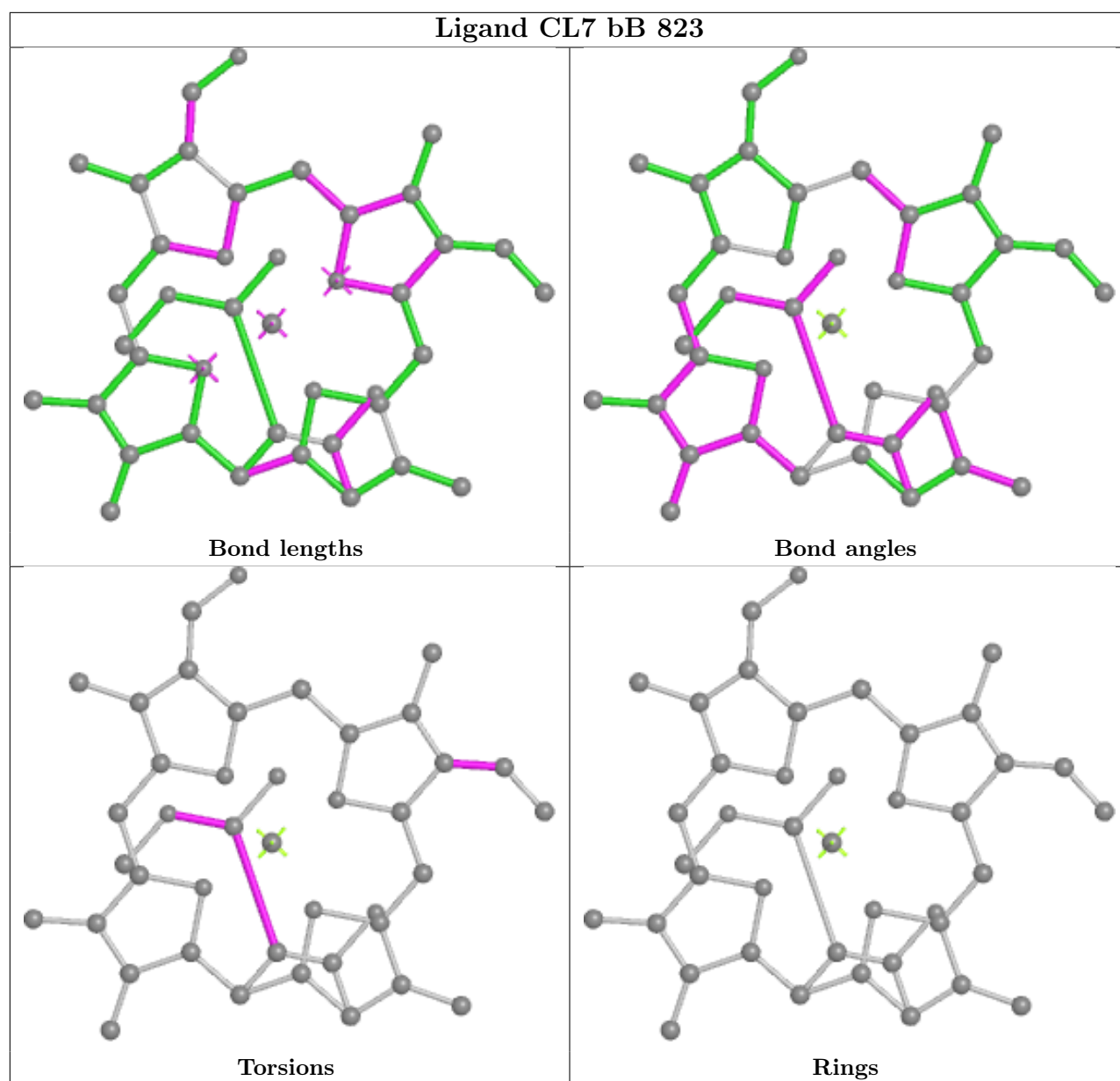


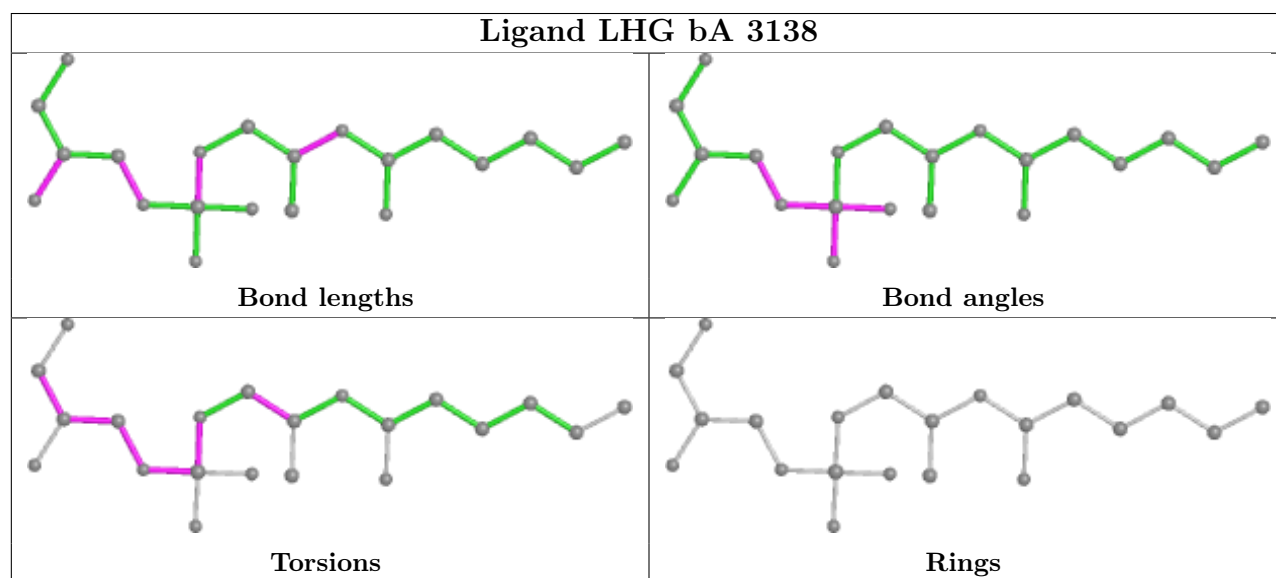
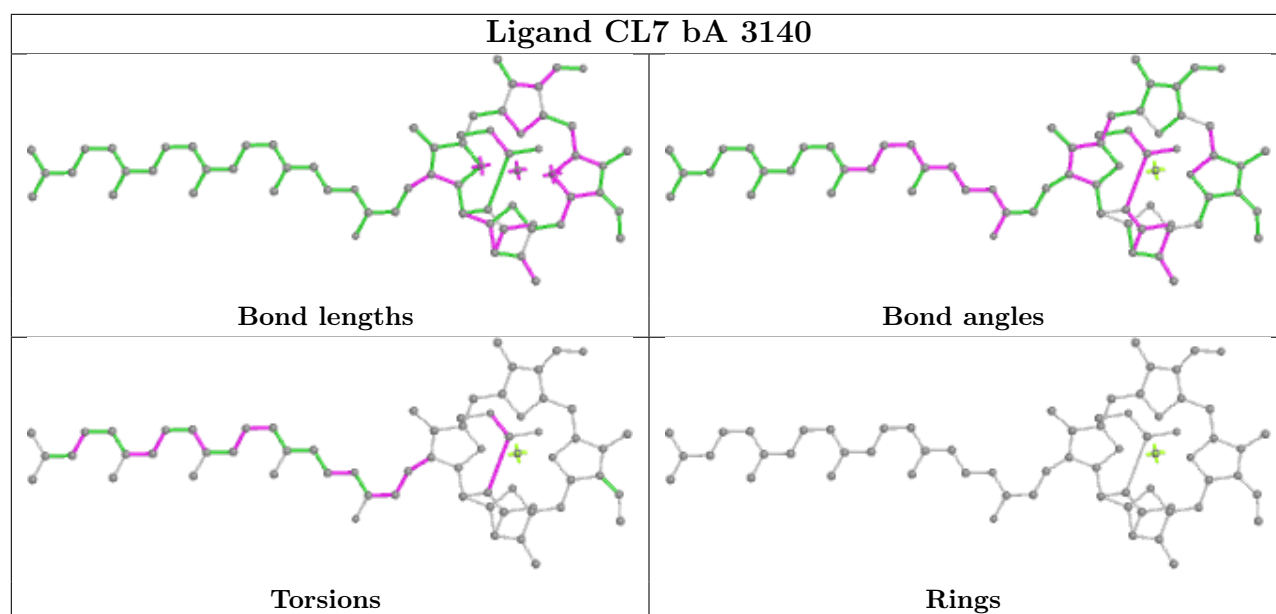
Rings

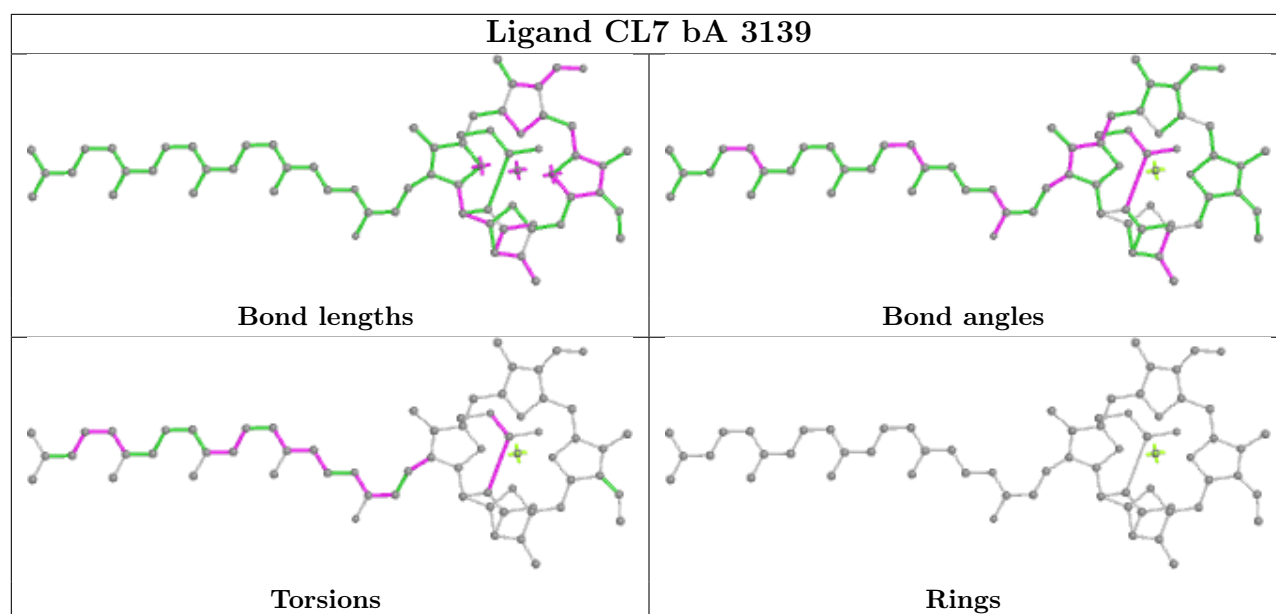




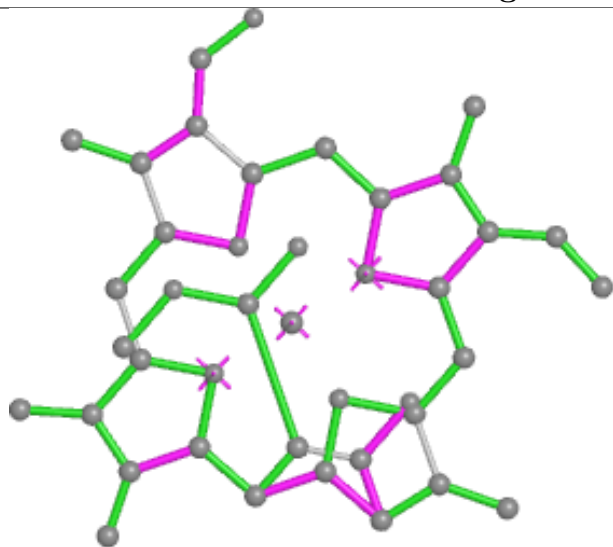




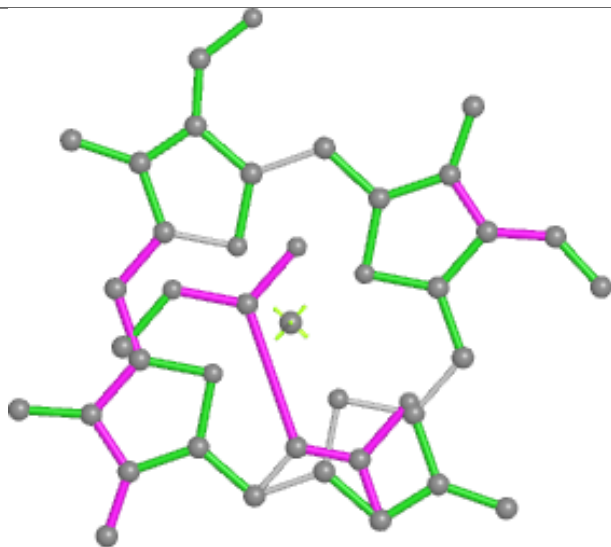




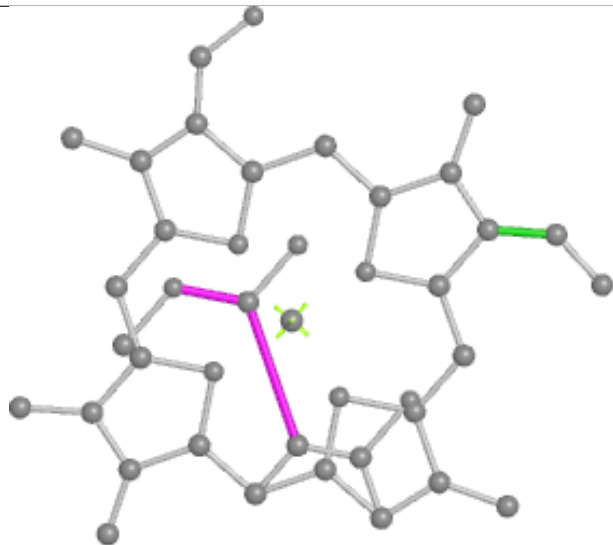
Ligand CL7 bA 3112



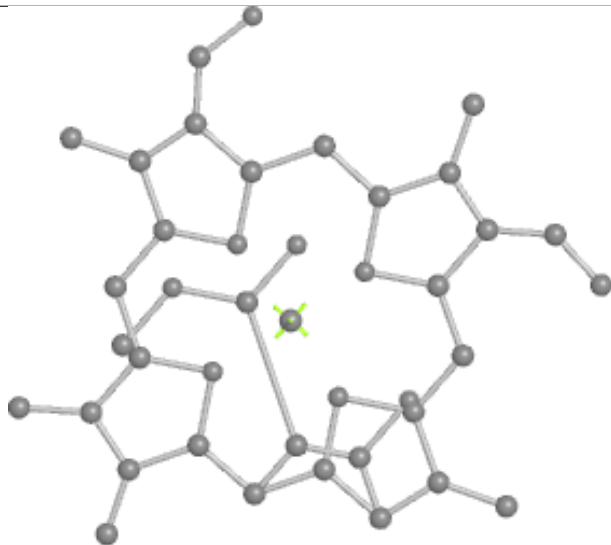
Bond lengths



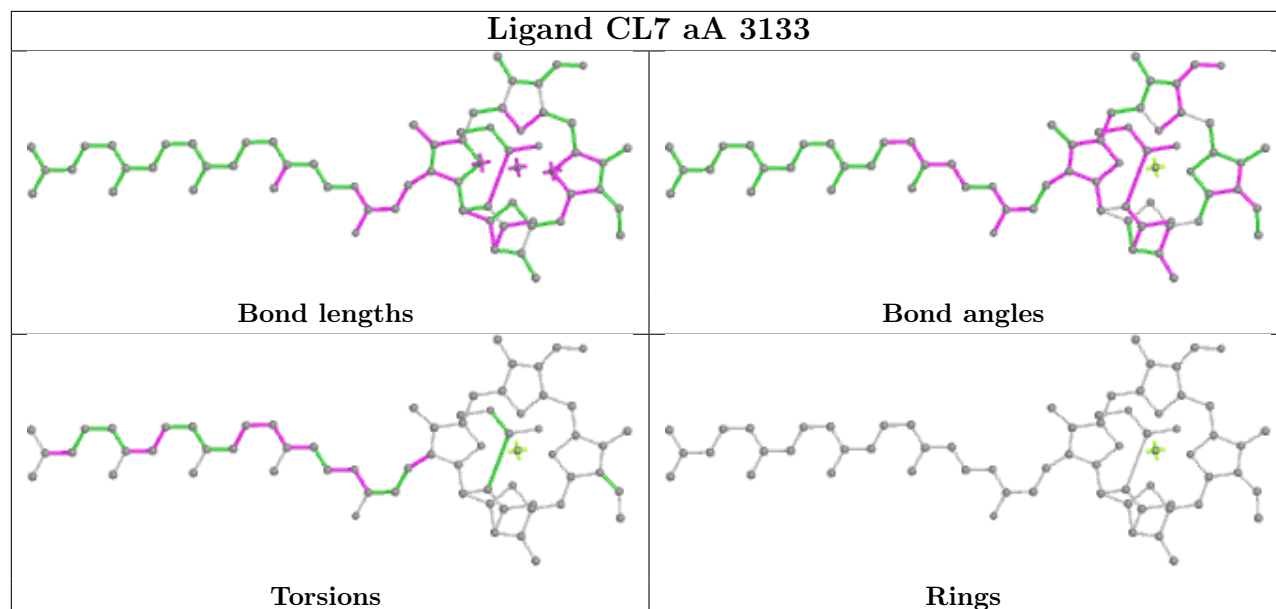
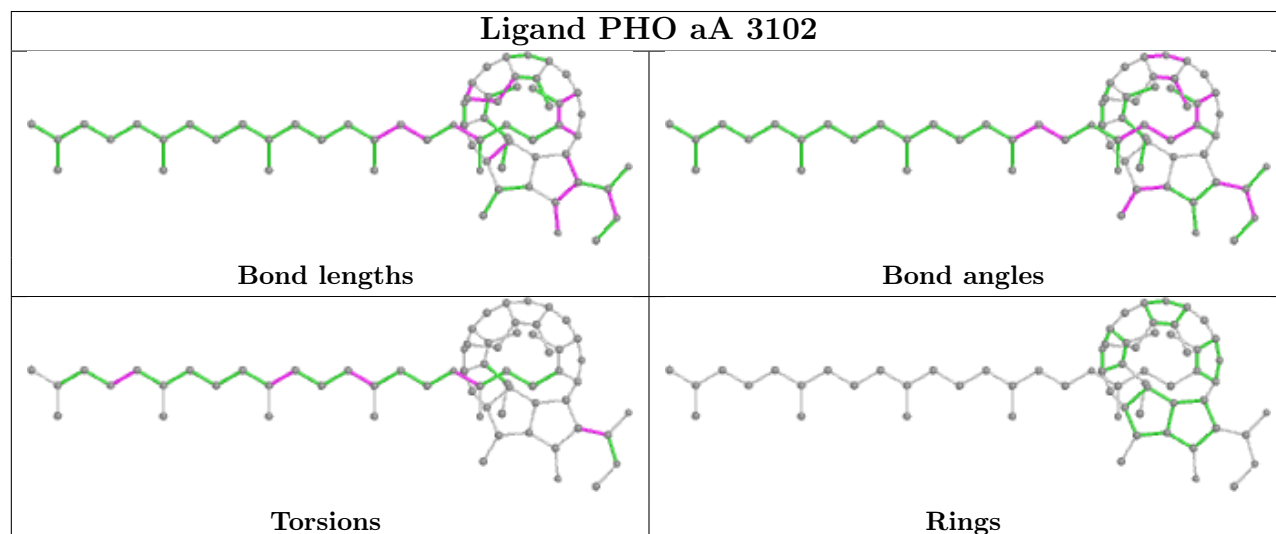
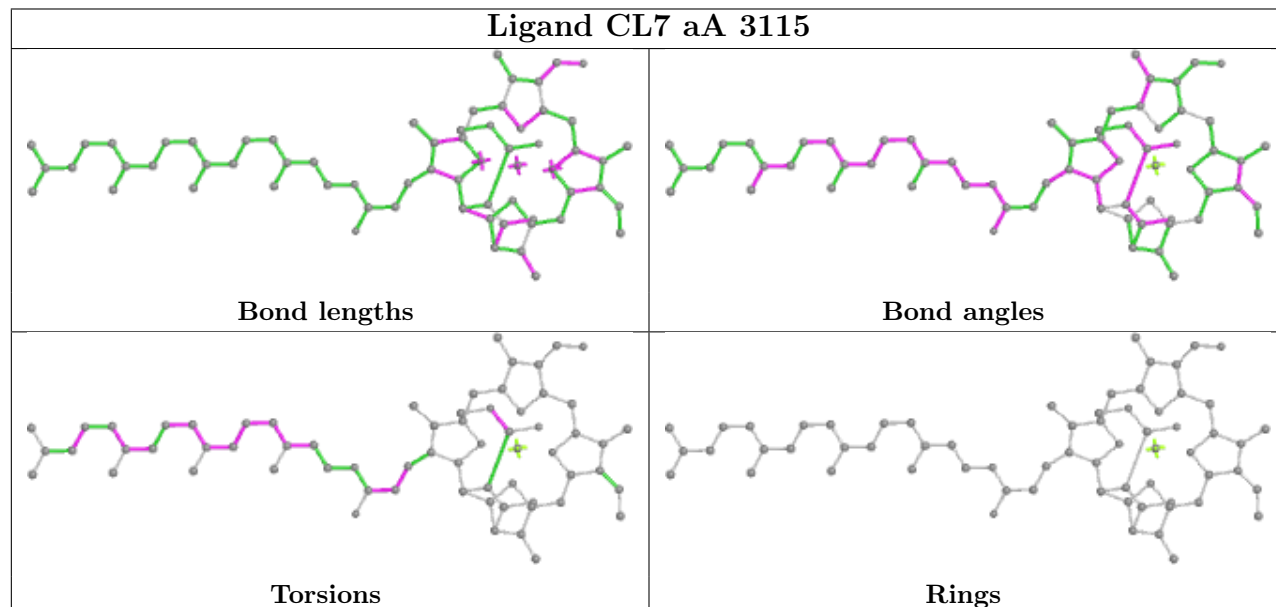
Bond angles



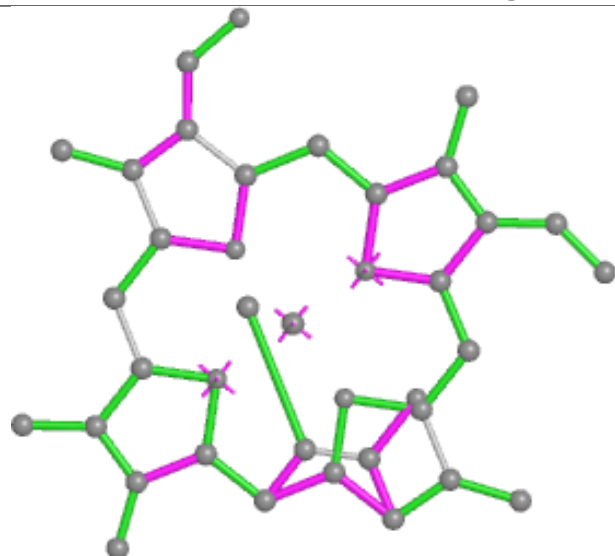
Torsions



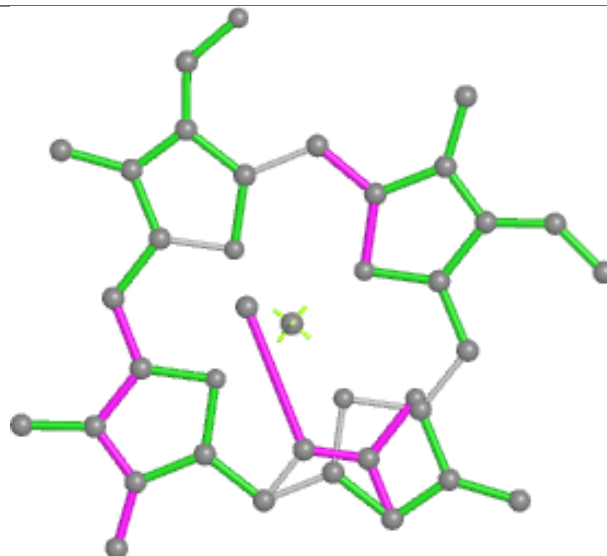
Rings

Ligand CL7 aA 3133**Ligand PHO aA 3102****Ligand CL7 aA 3115**

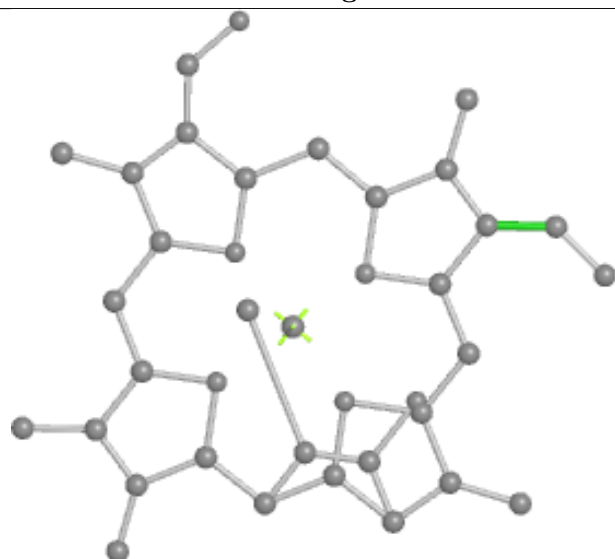
Ligand CL7 aA 3118



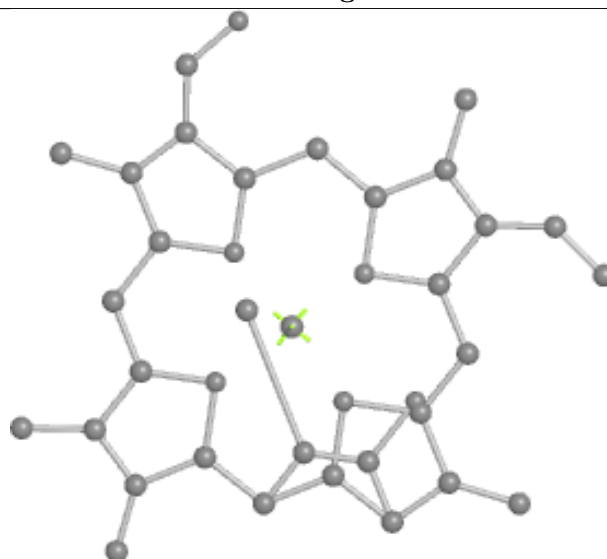
Bond lengths



Bond angles

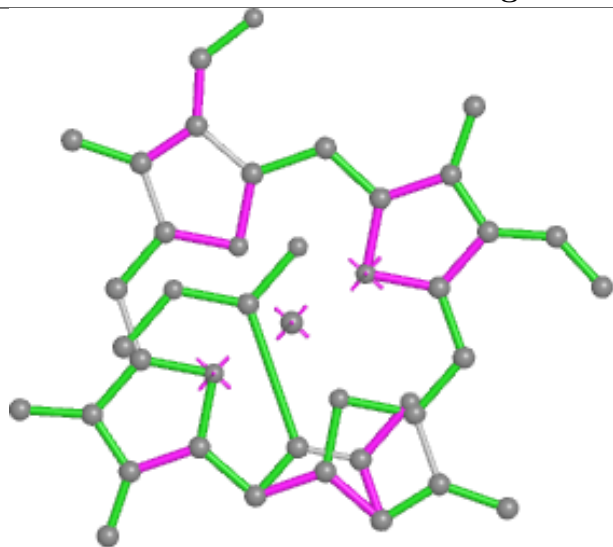


Torsions

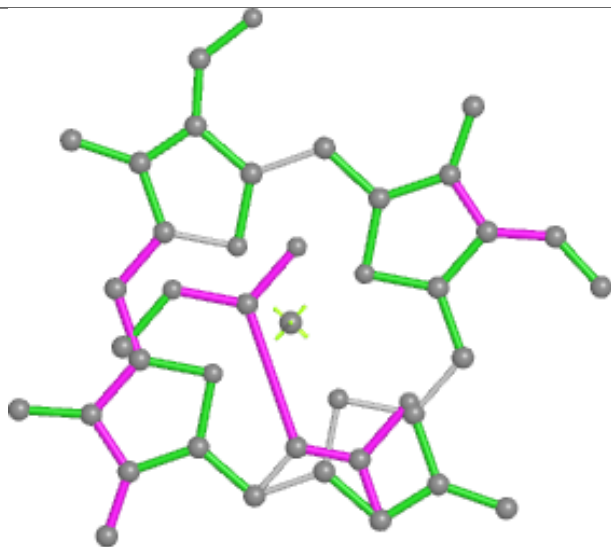


Rings

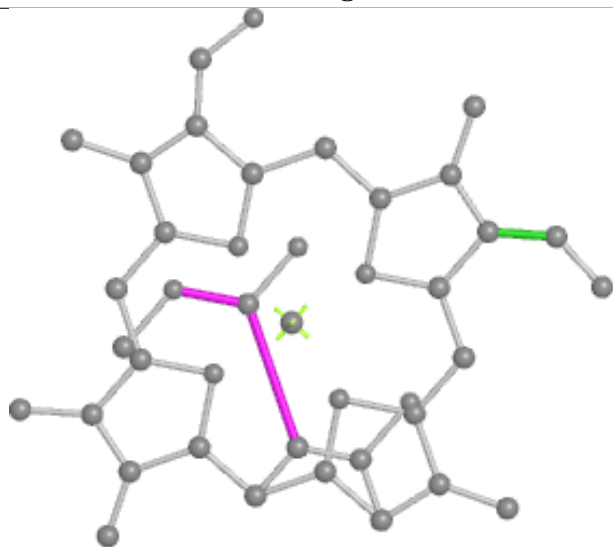
Ligand CL7 aA 3113



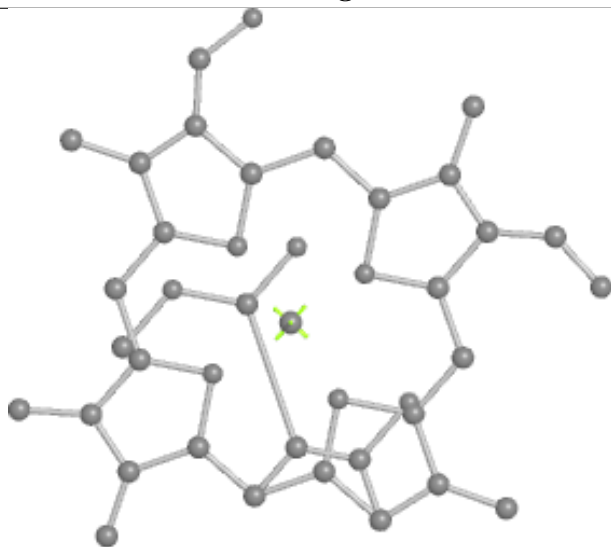
Bond lengths



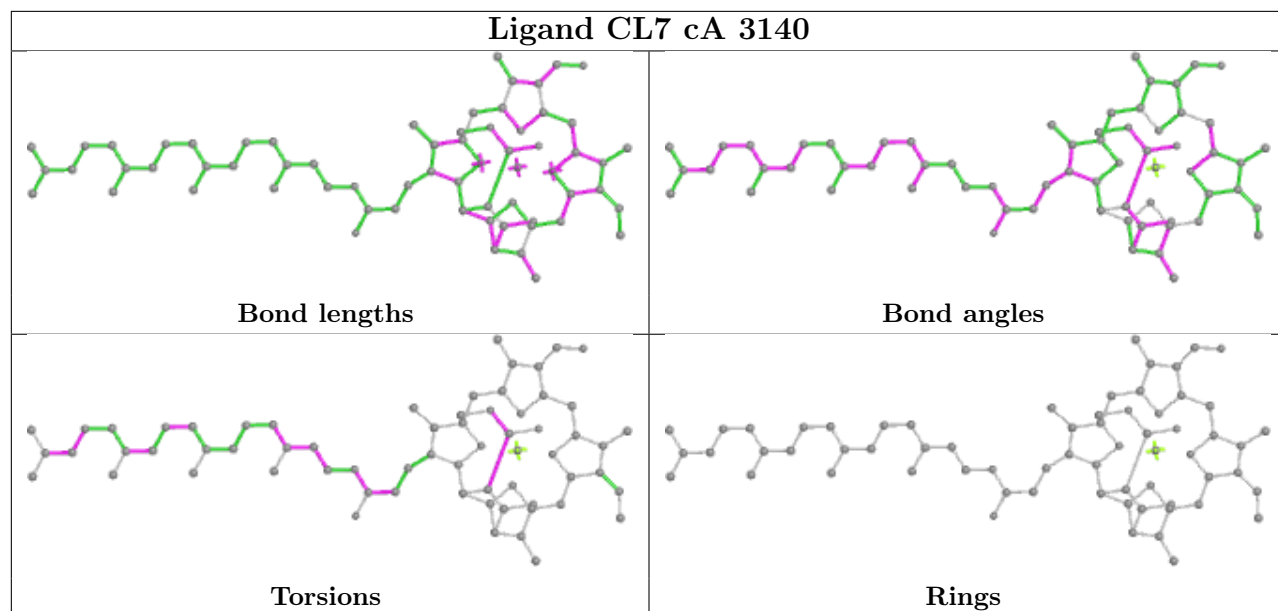
Bond angles

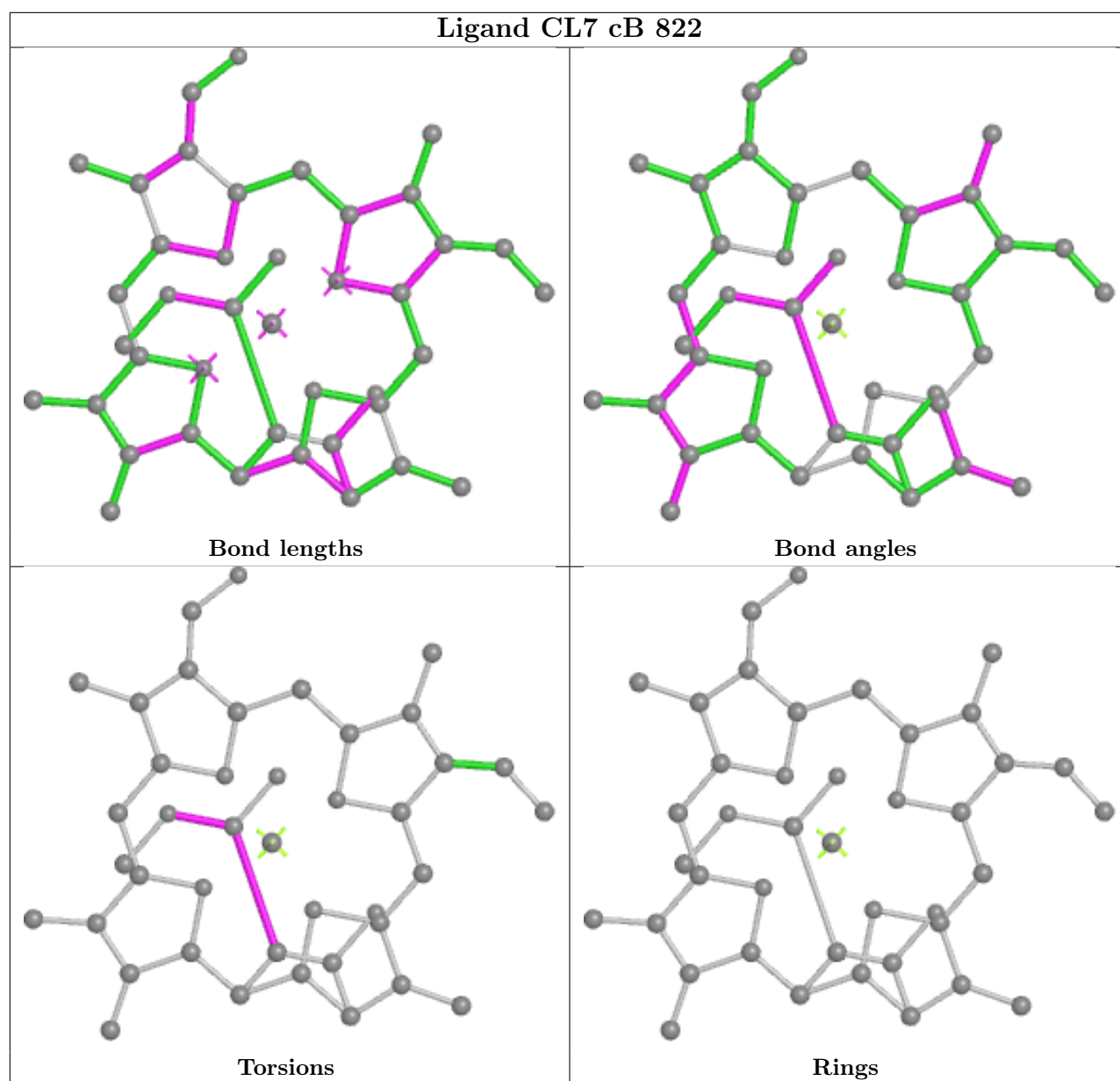


Torsions

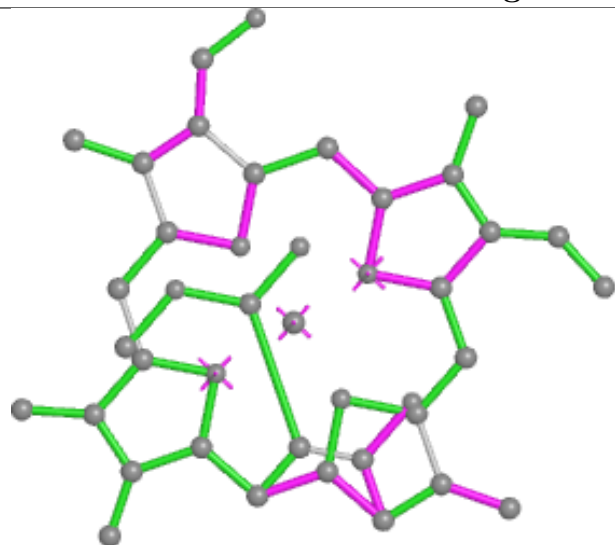


Rings

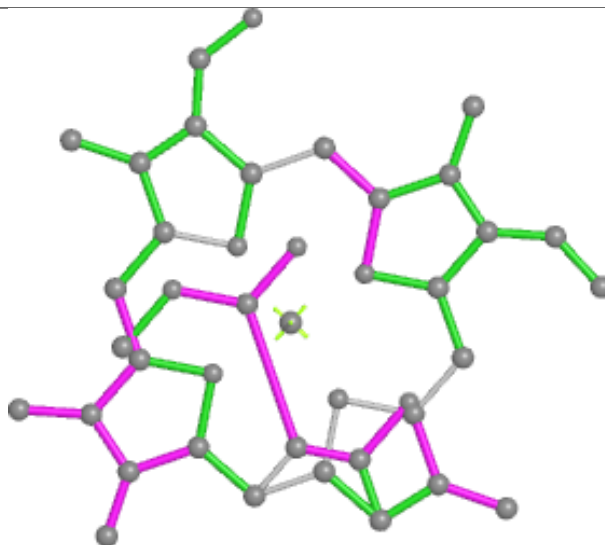




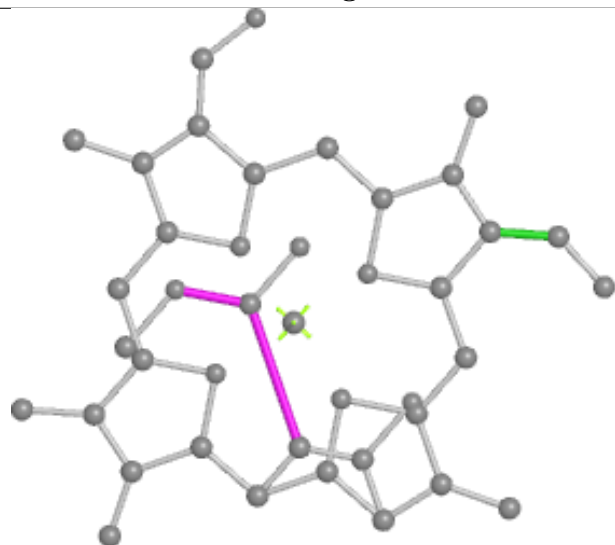
Ligand CL7 cA 3131



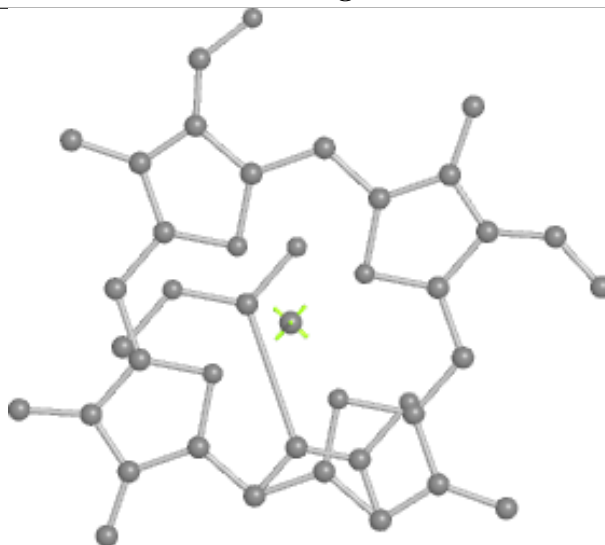
Bond lengths



Bond angles

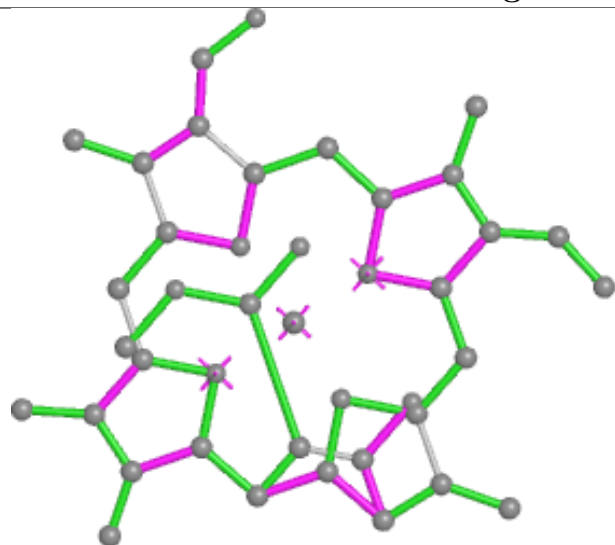


Torsions

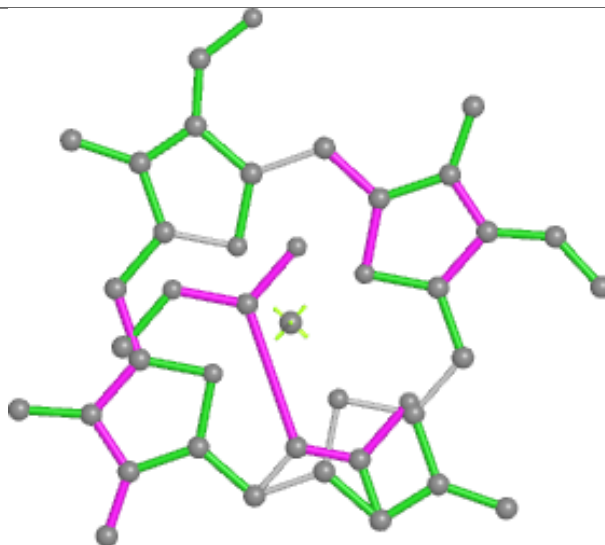


Rings

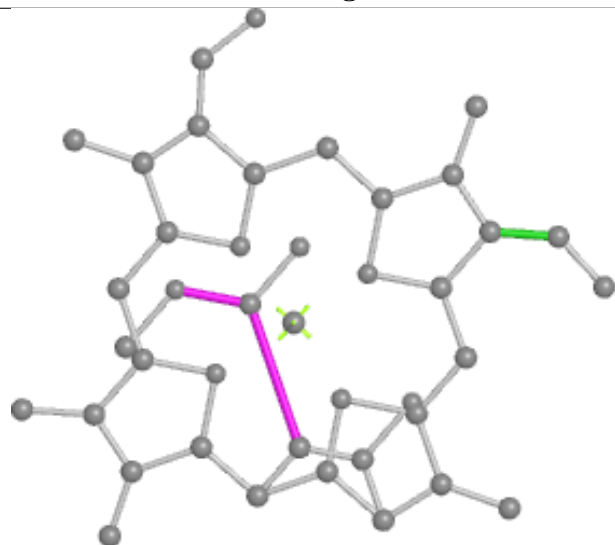
Ligand CL7 cA 3103



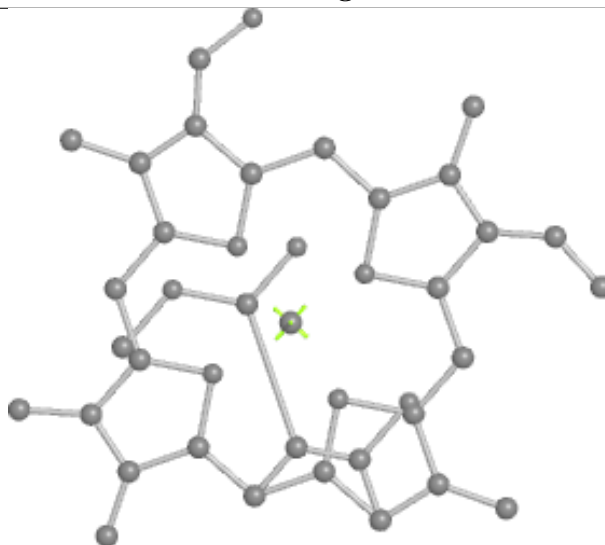
Bond lengths



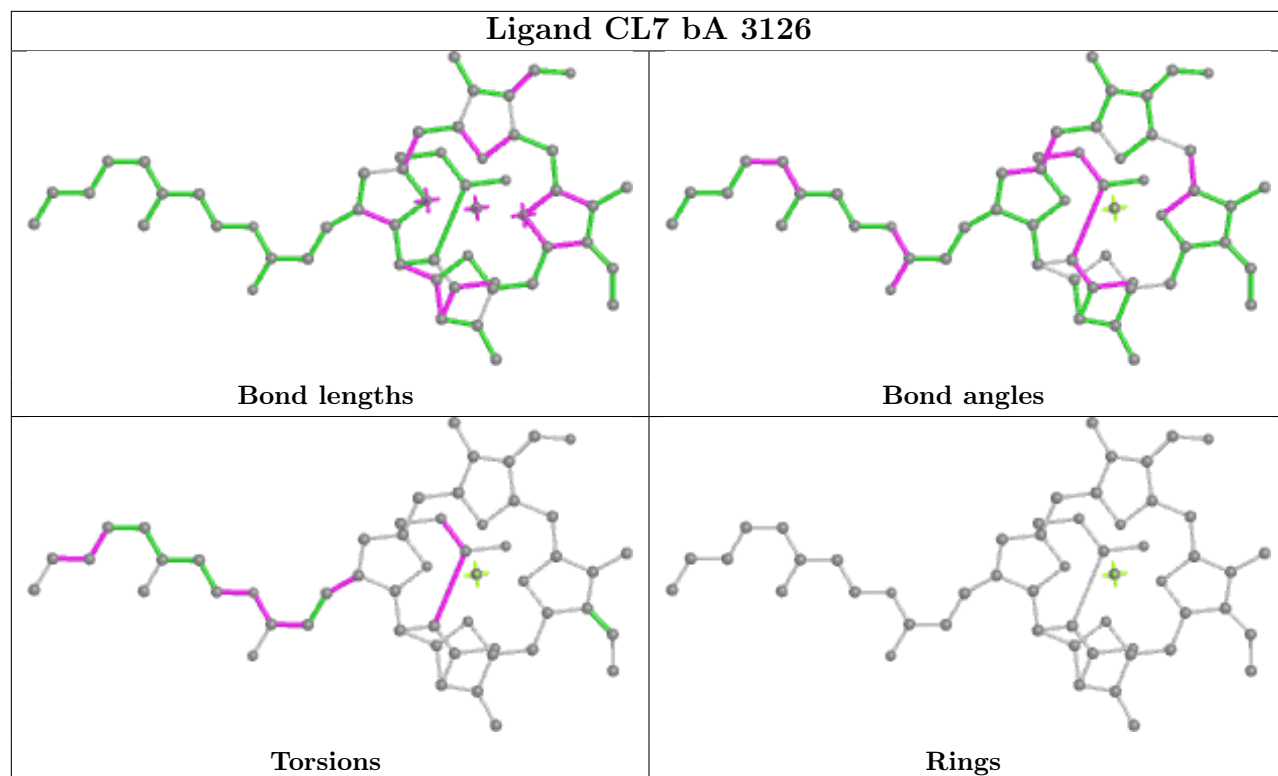
Bond angles

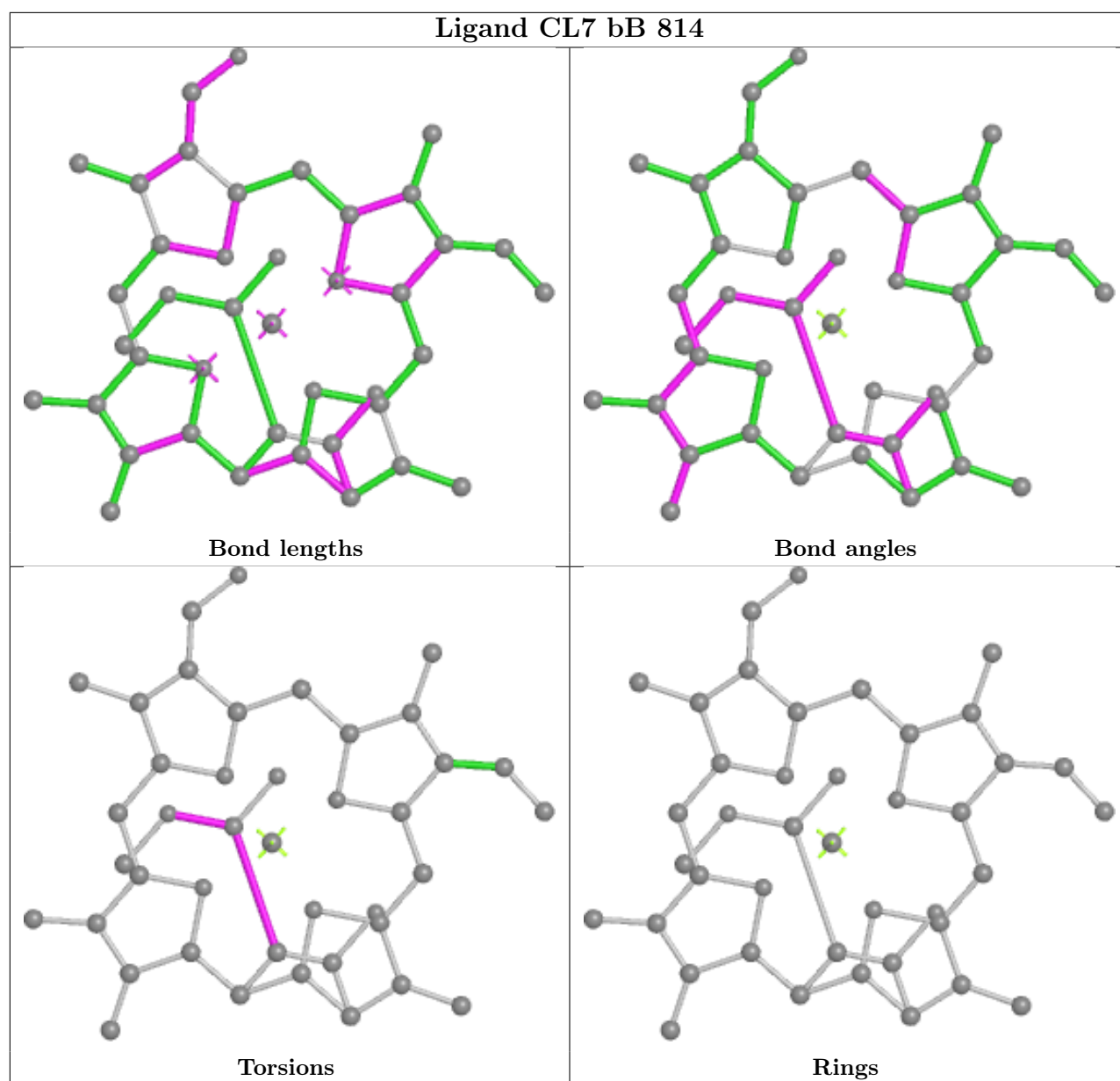


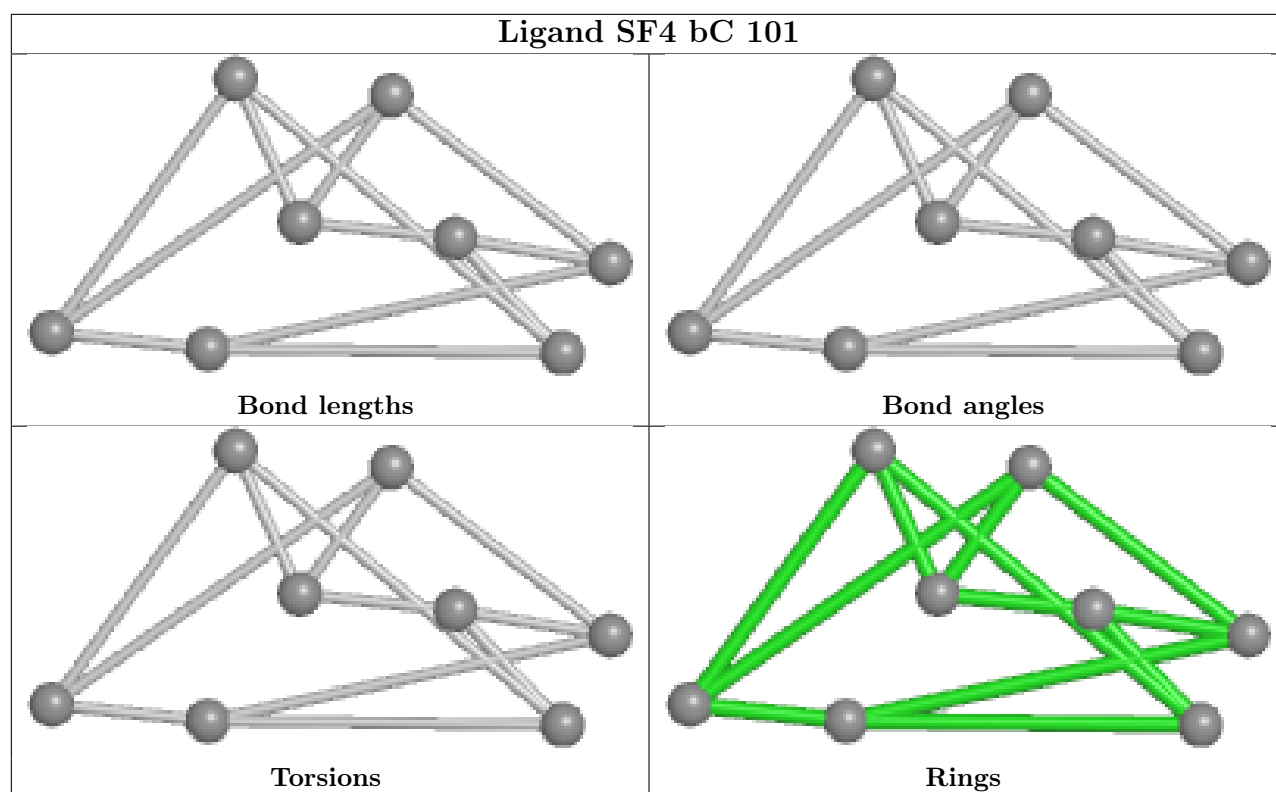
Torsions

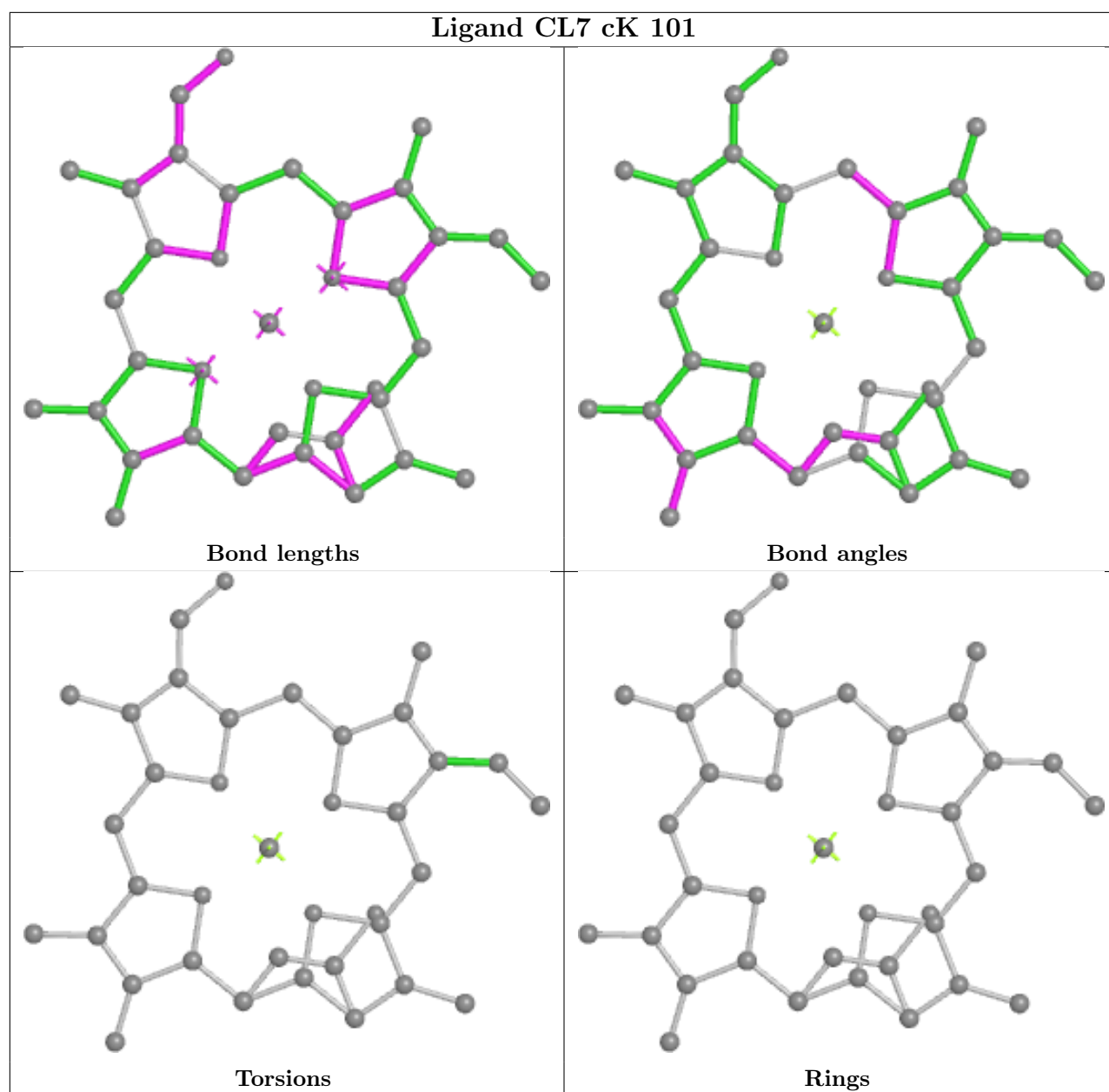


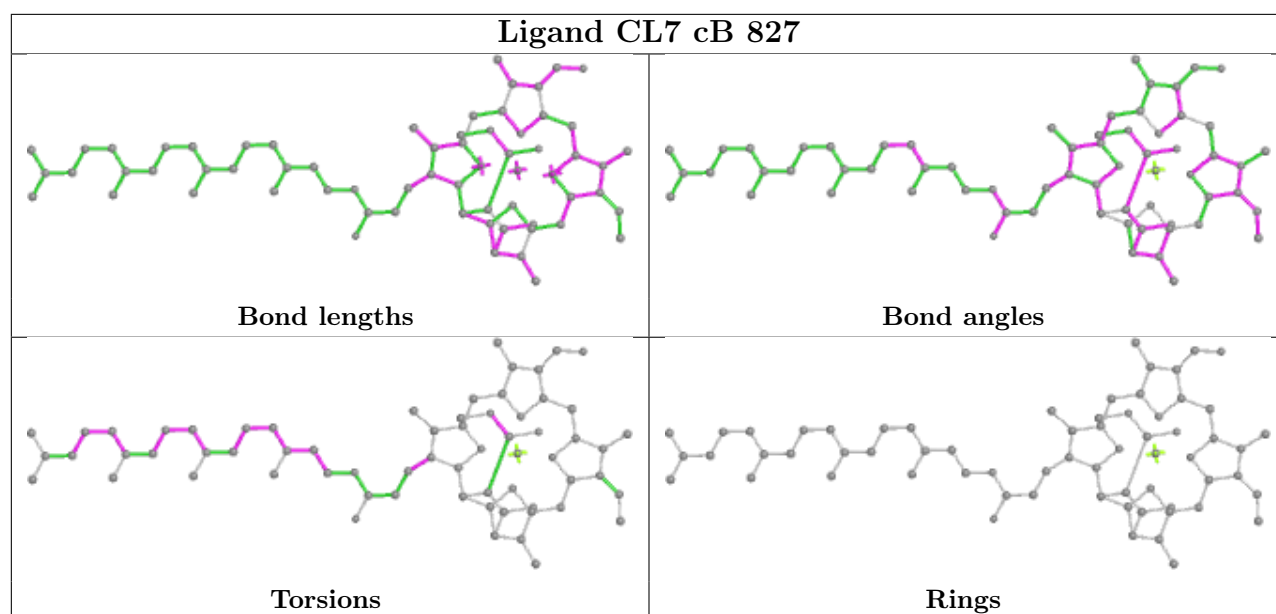
Rings



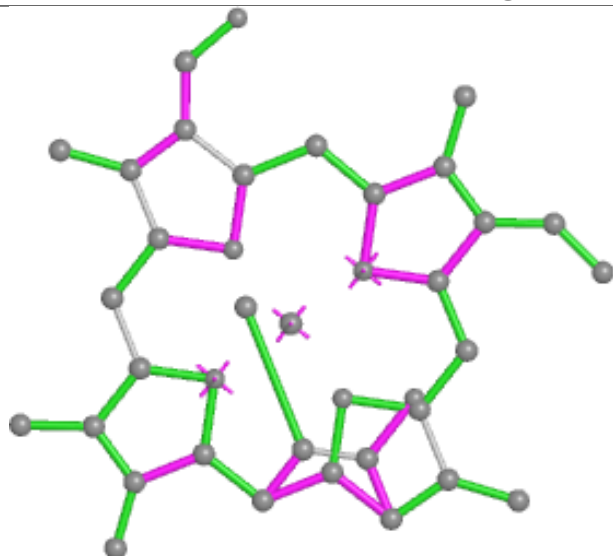




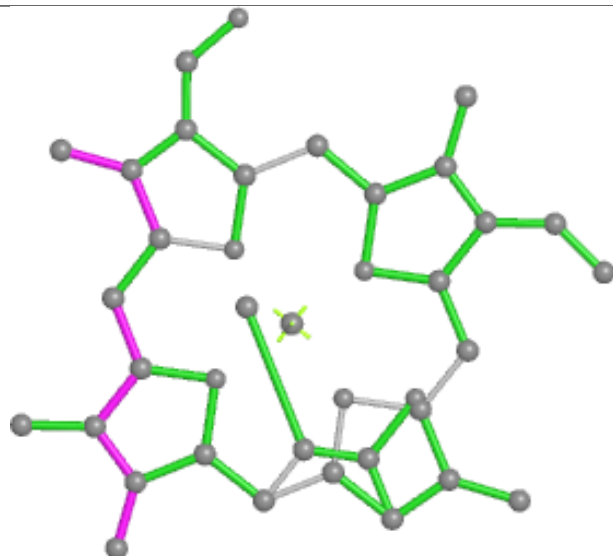




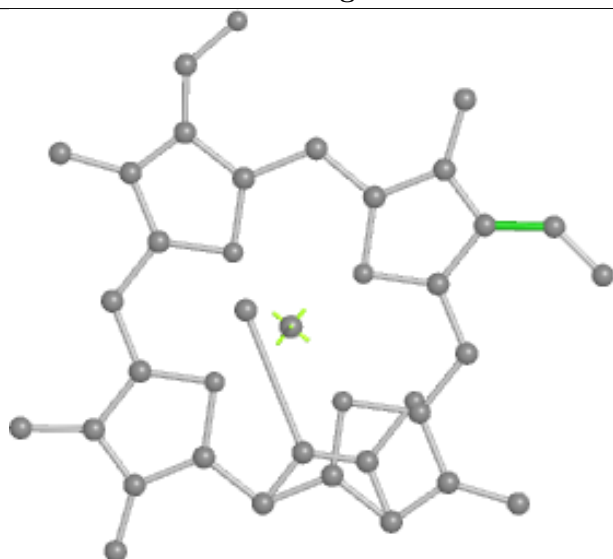
Ligand CL7 bA 3111



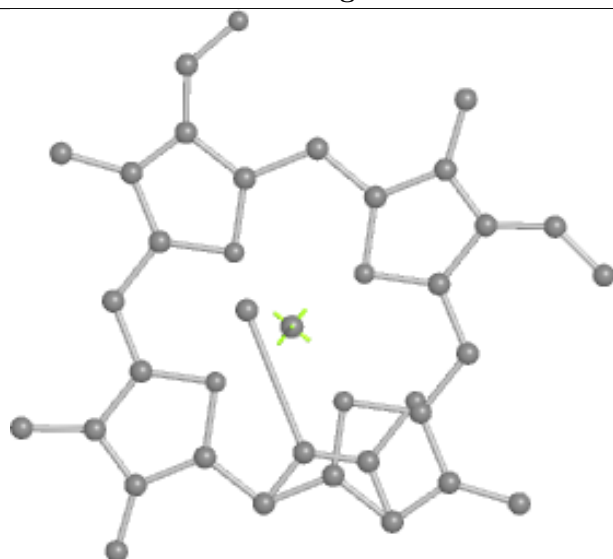
Bond lengths



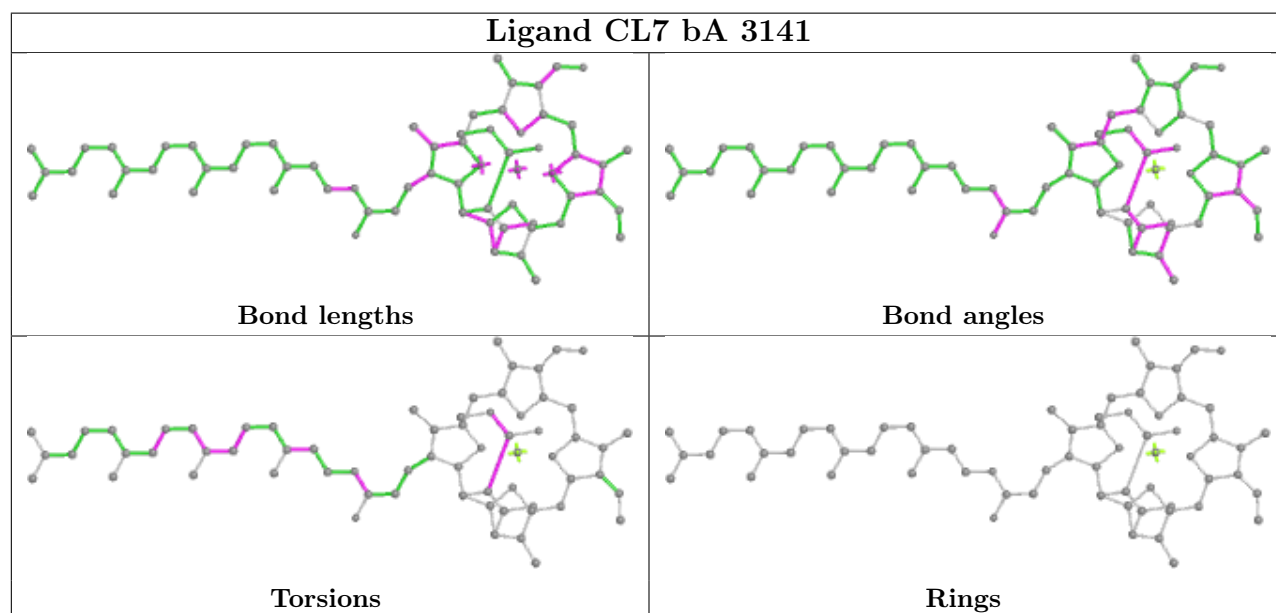
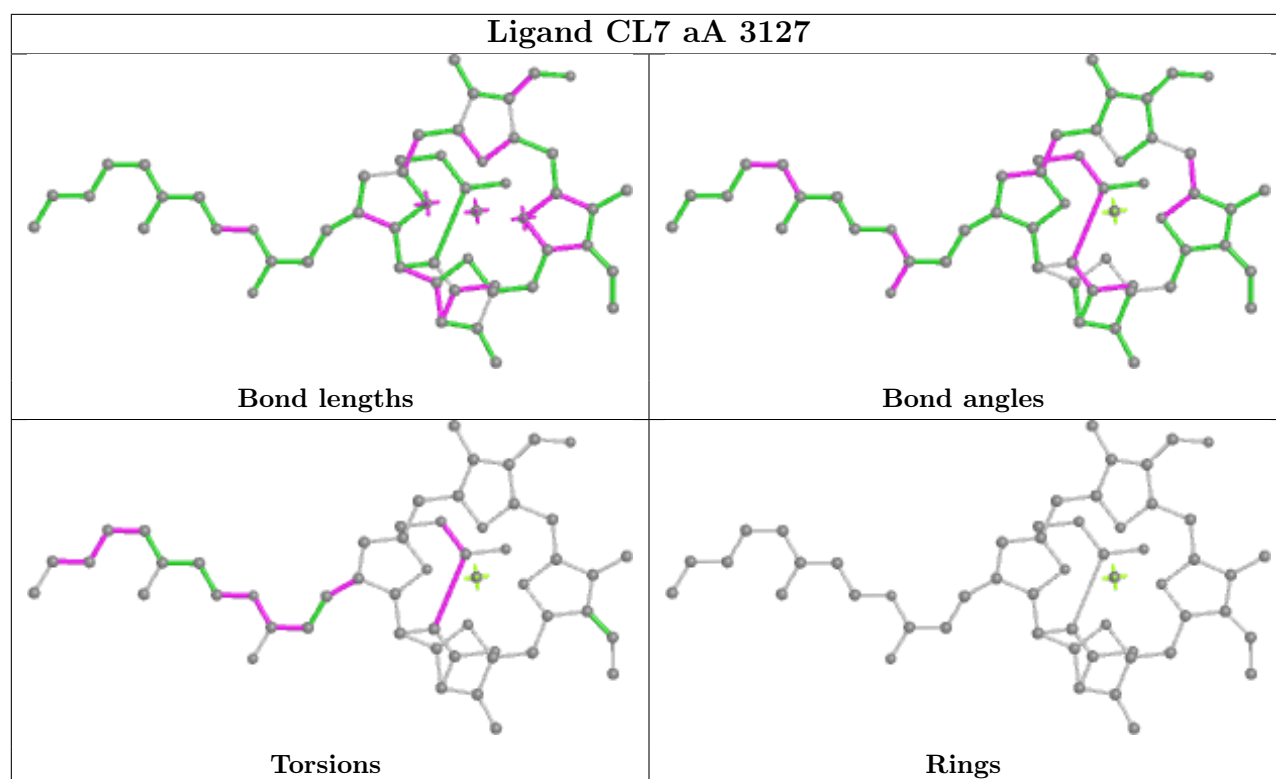
Bond angles

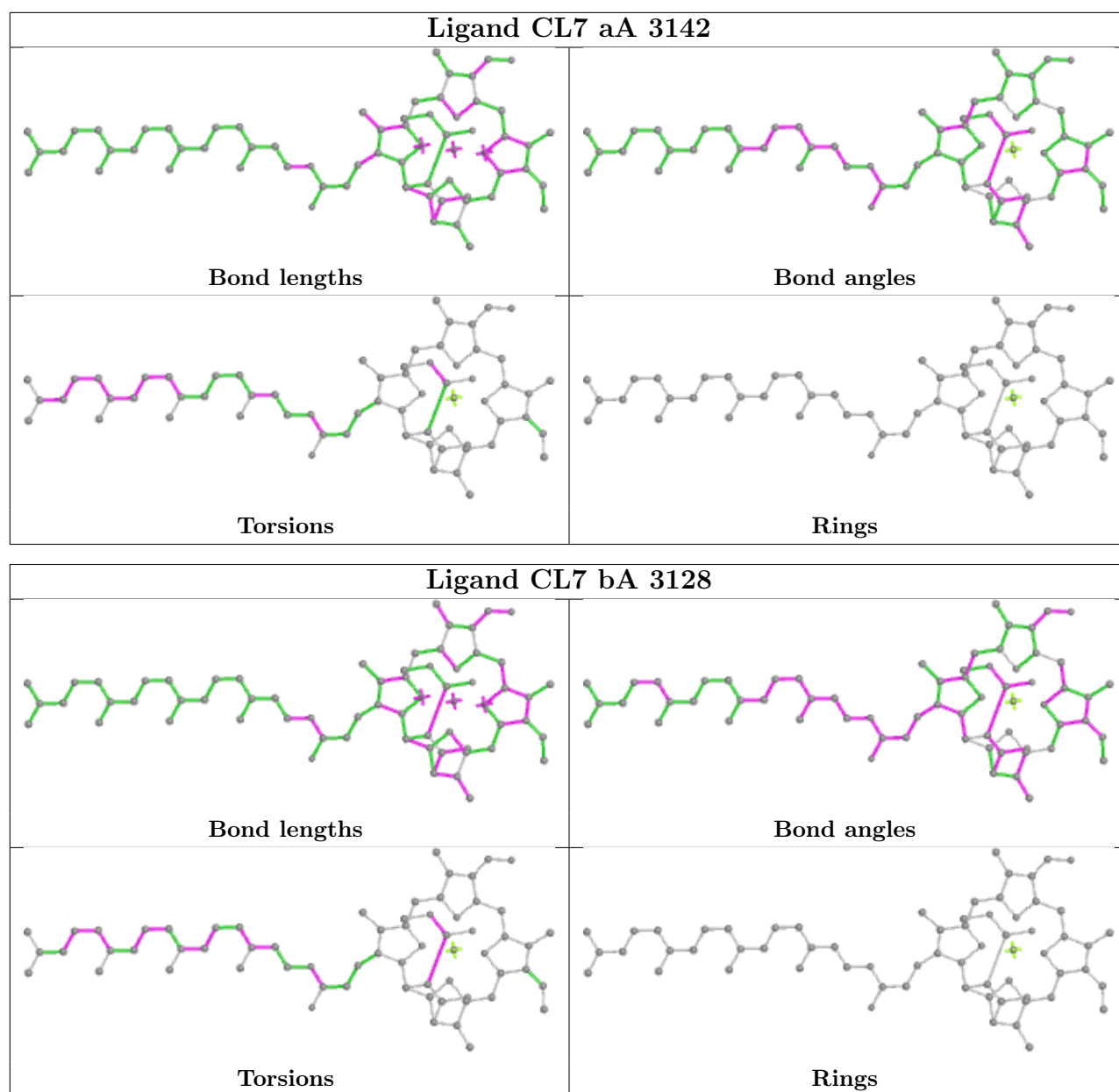


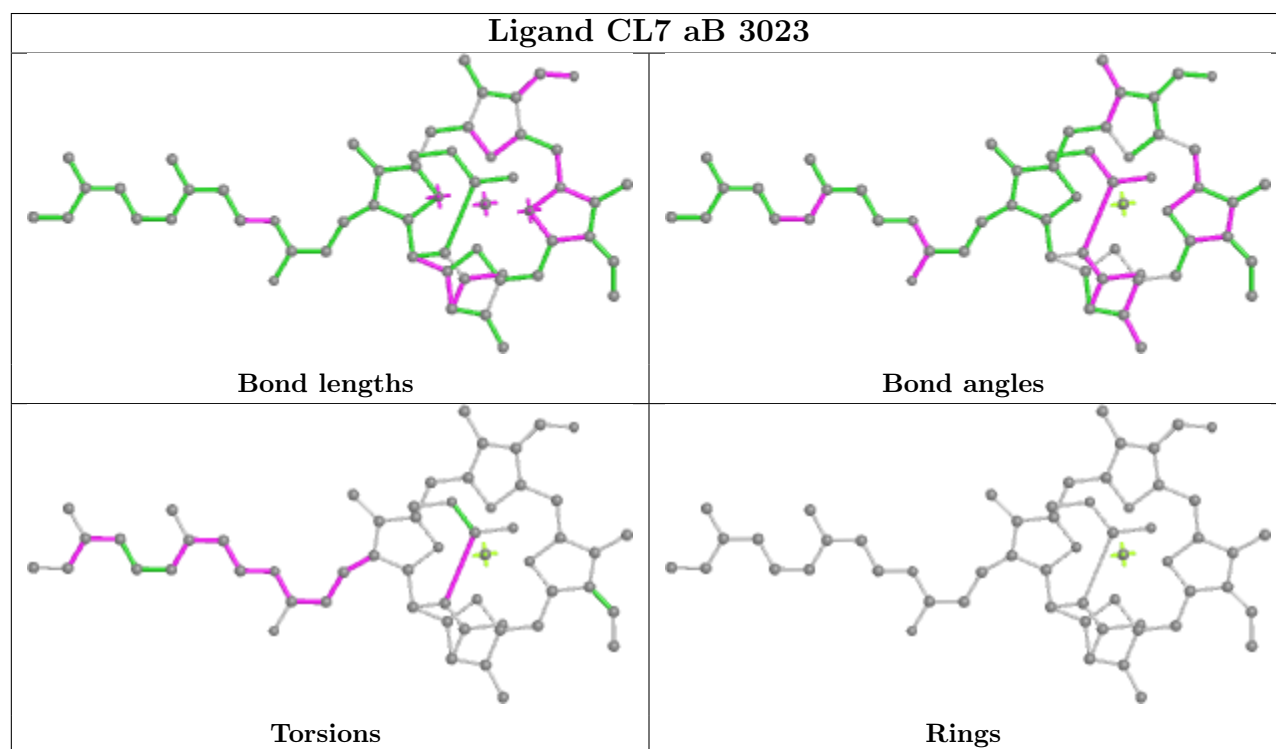
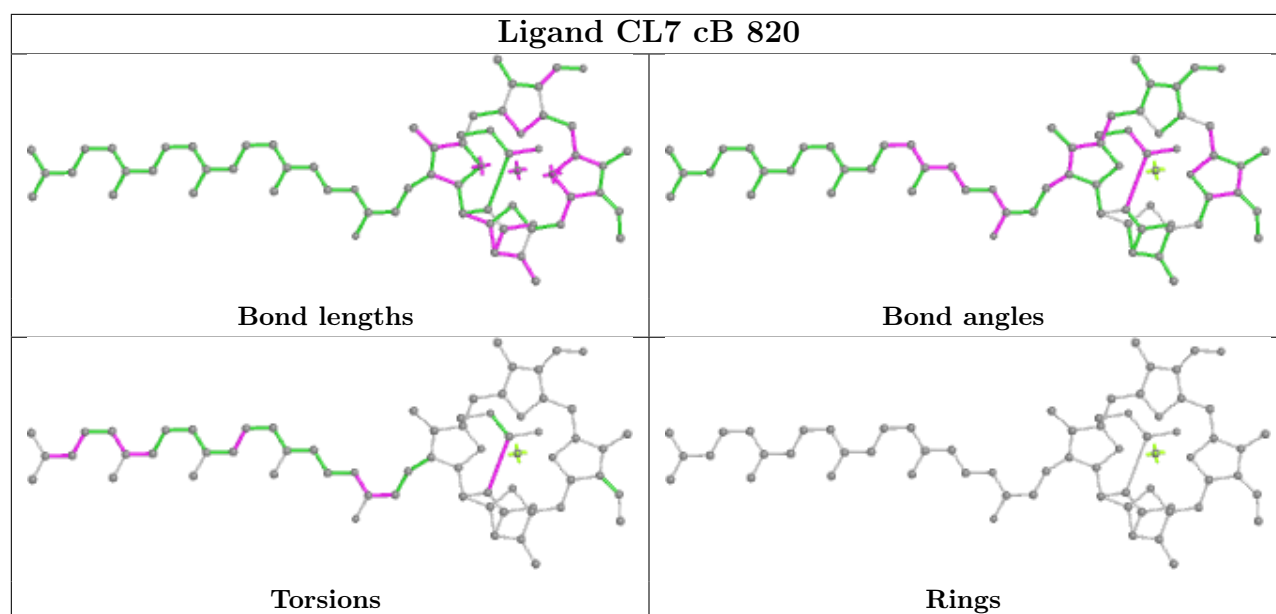
Torsions



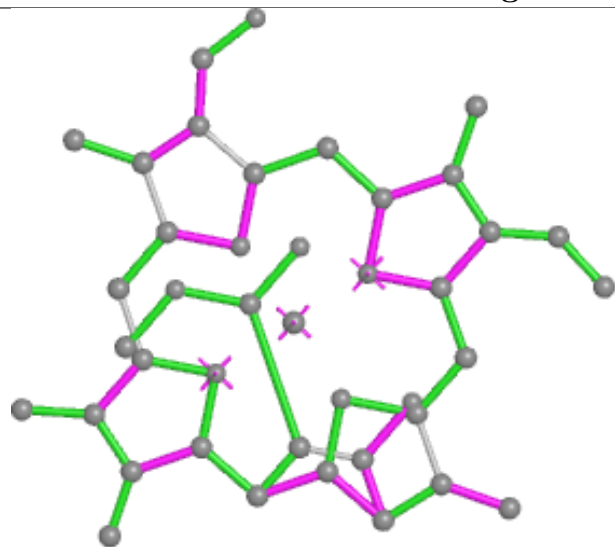
Rings



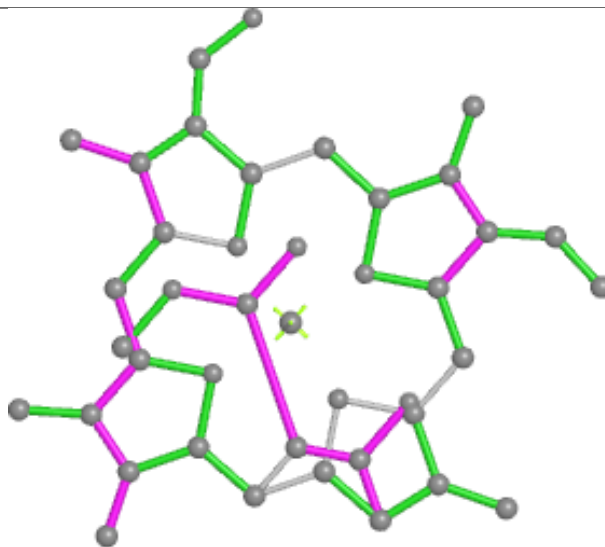




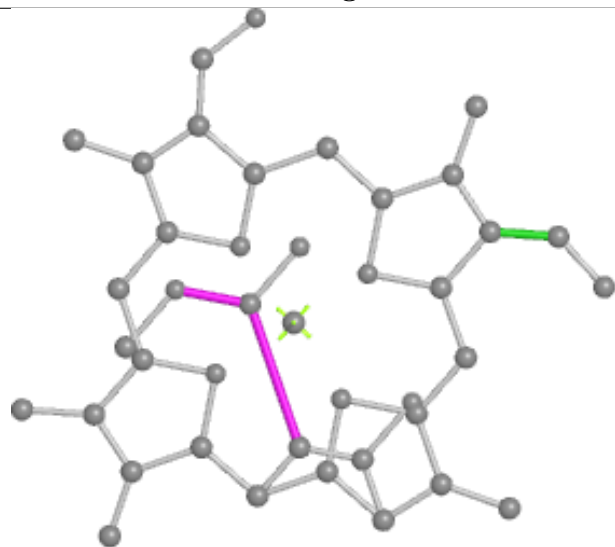
Ligand CL7 bA 3103



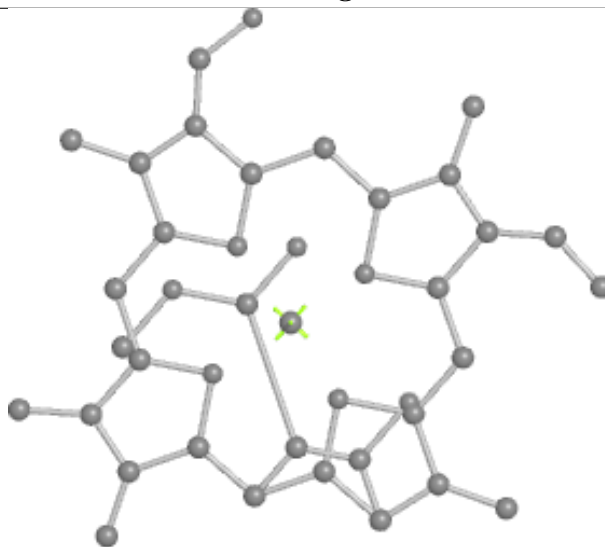
Bond lengths



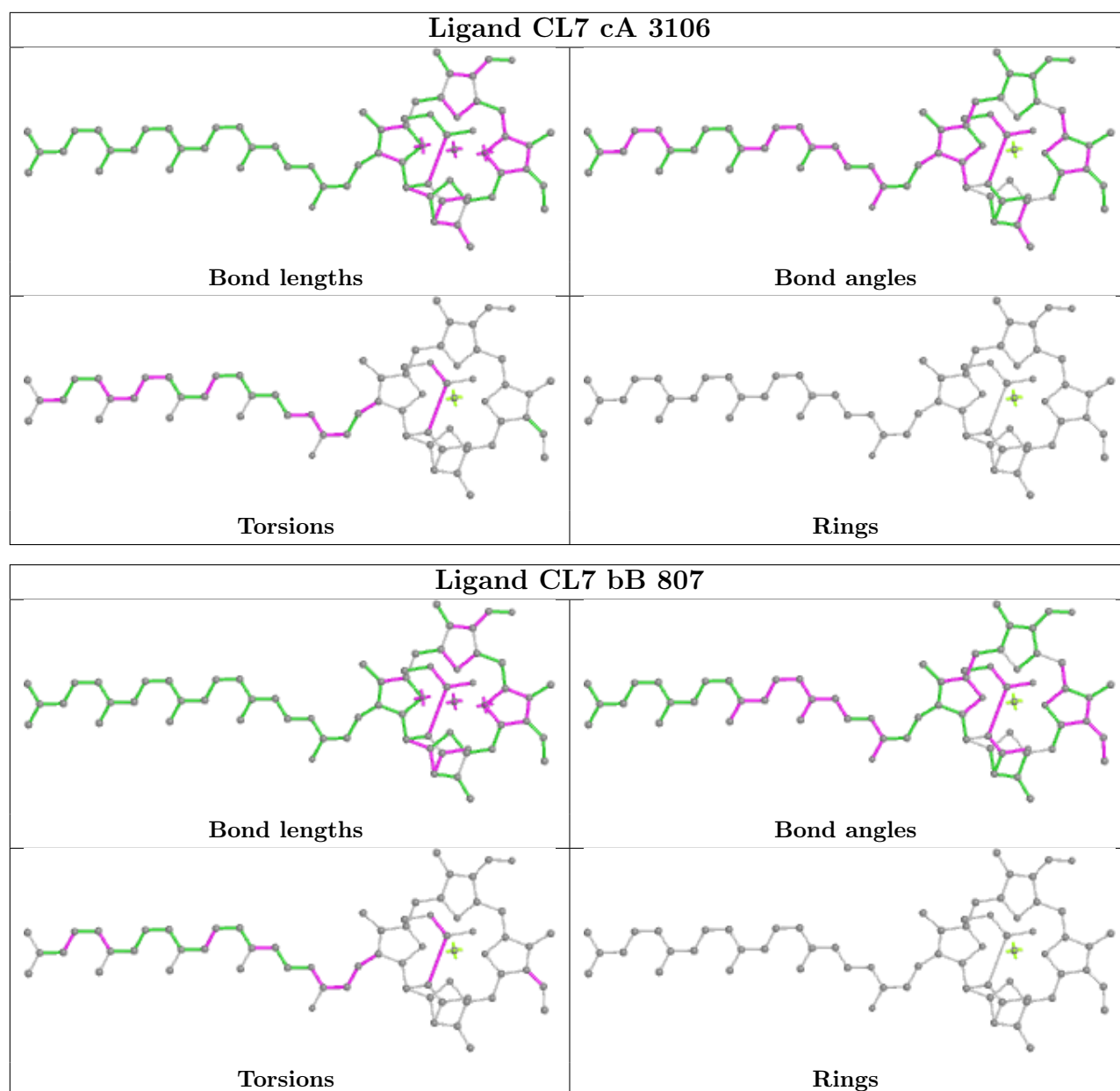
Bond angles

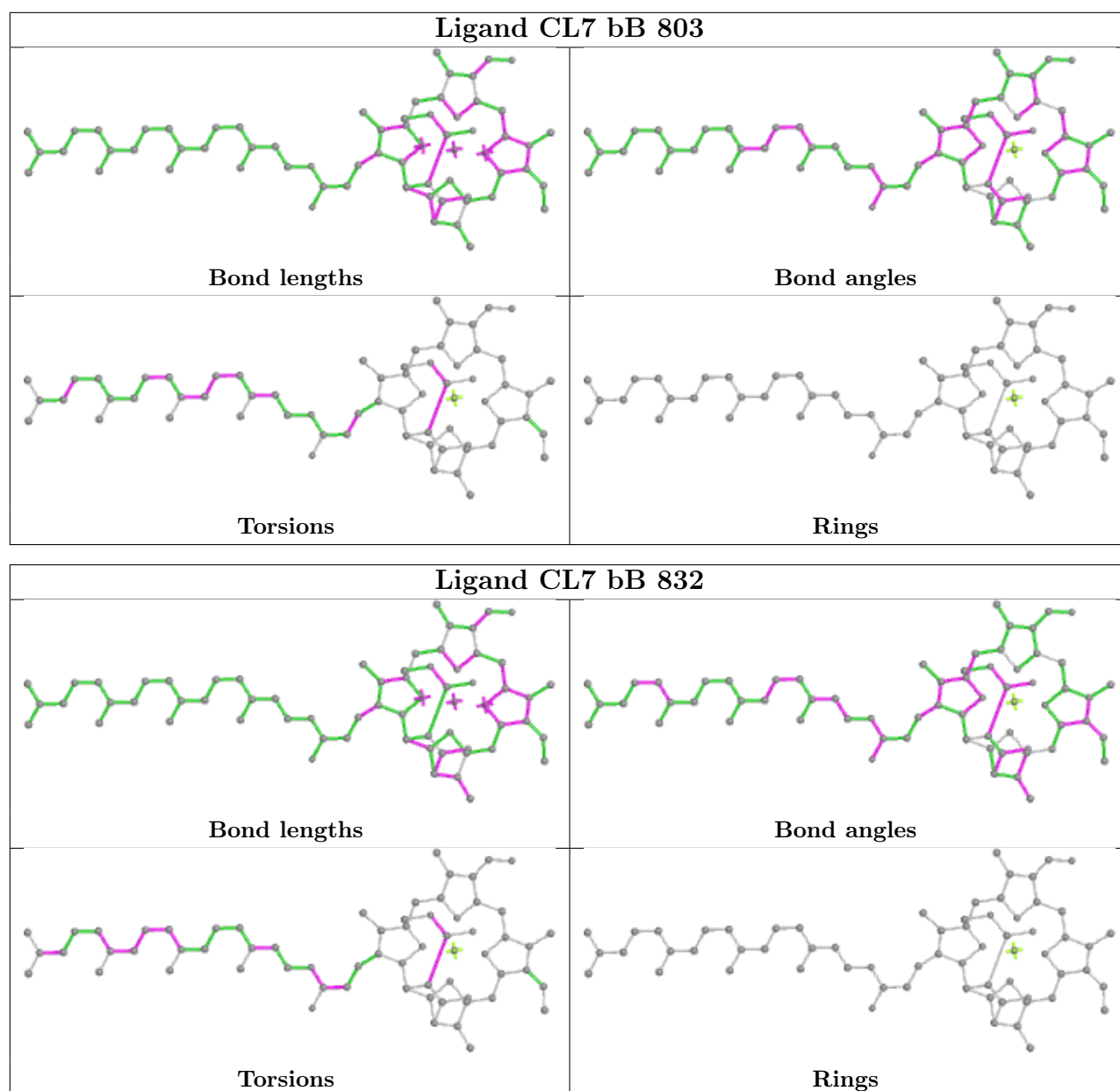


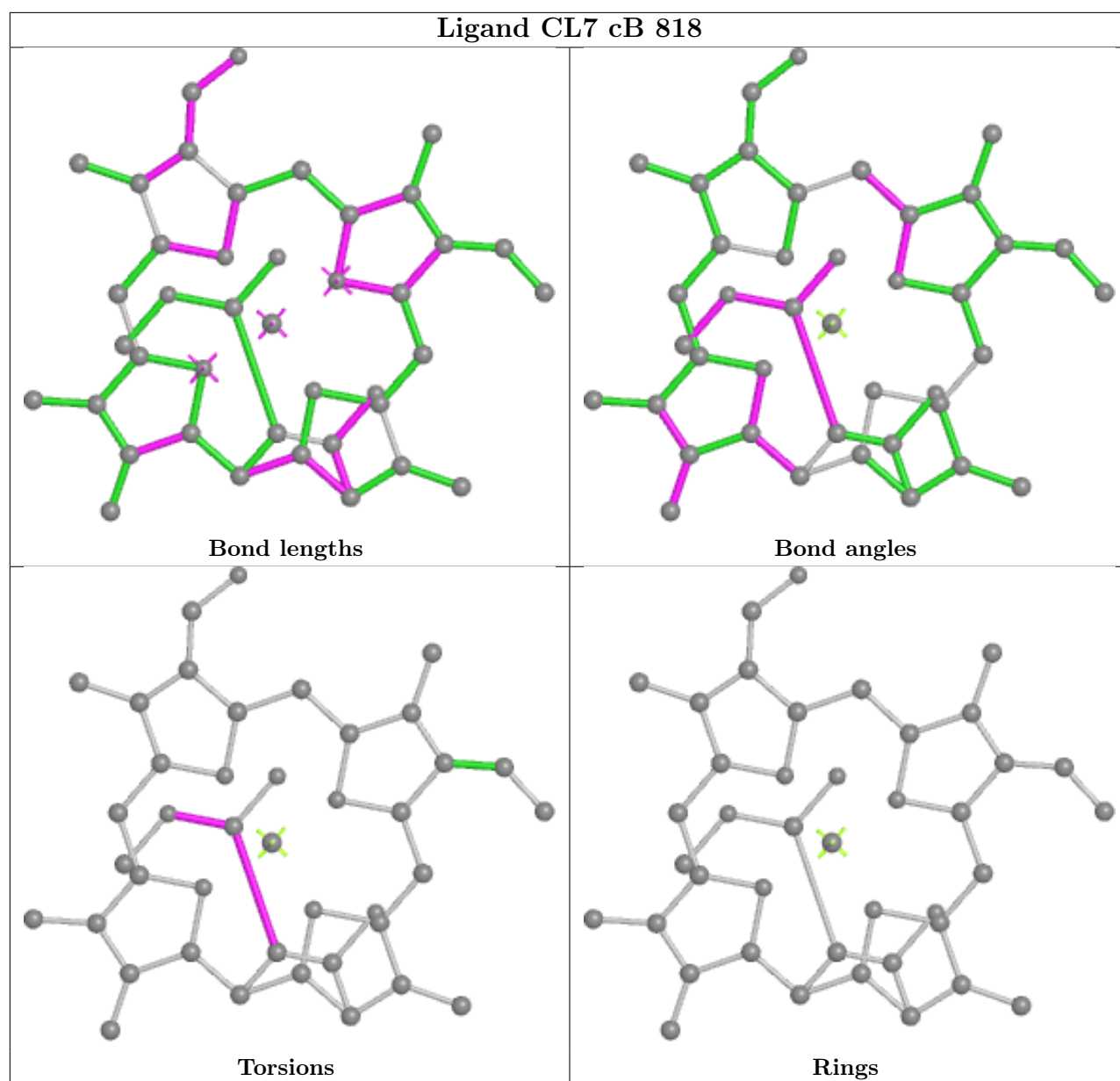
Torsions

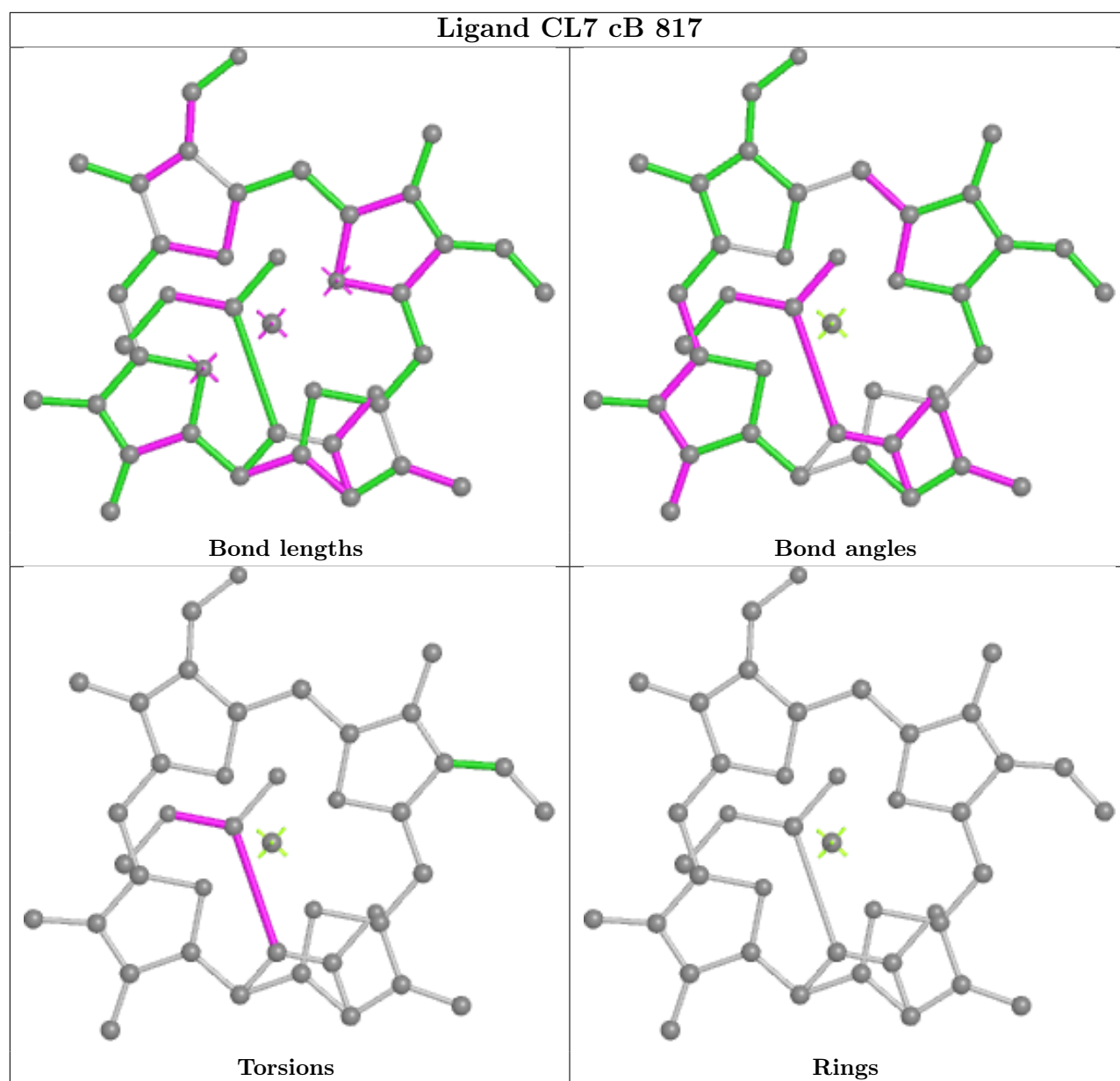


Rings

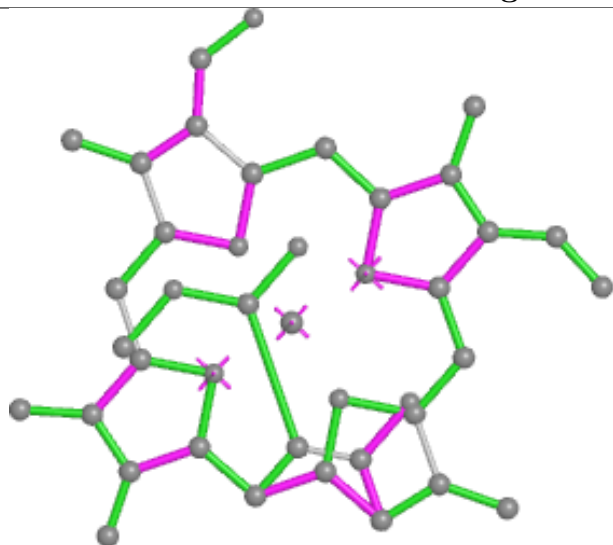




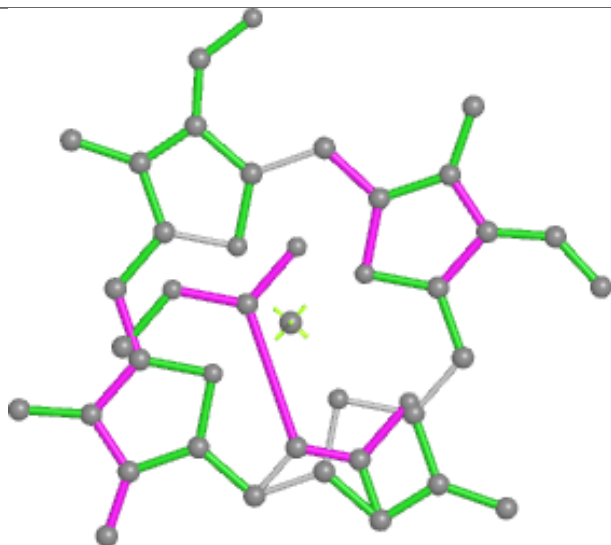




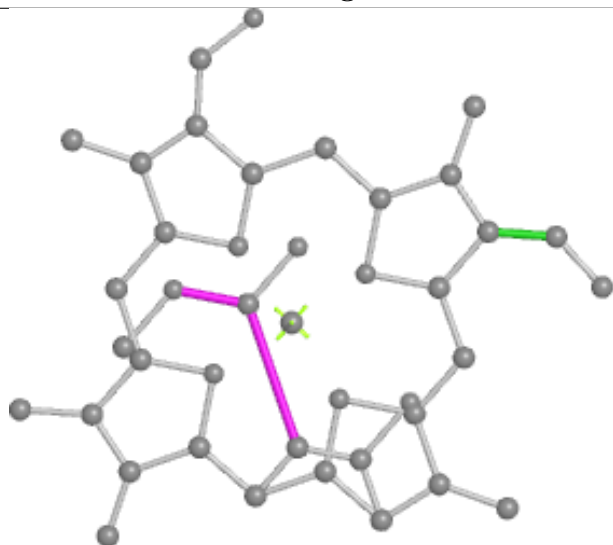
Ligand CL7 aA 3104



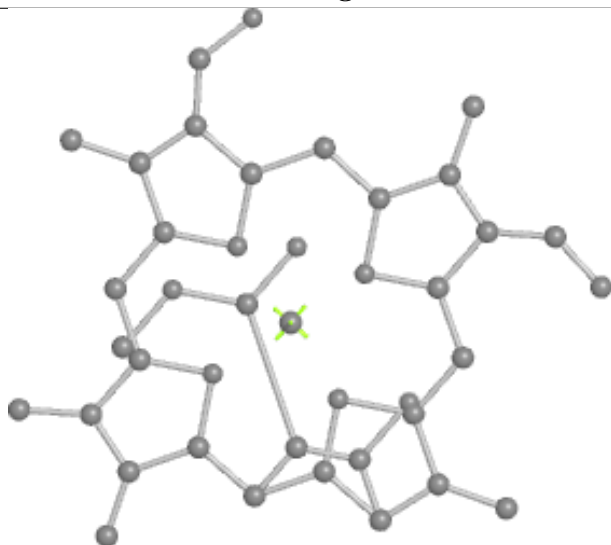
Bond lengths



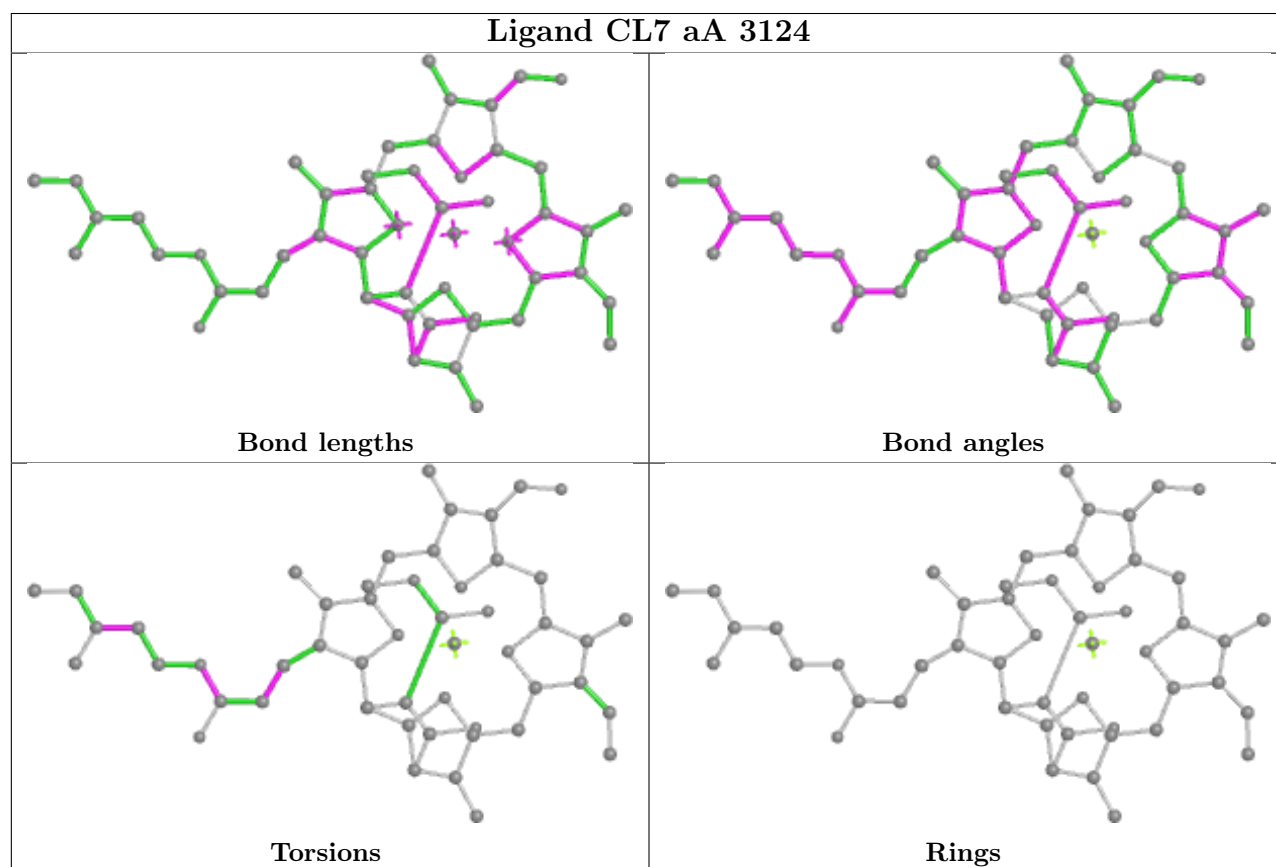
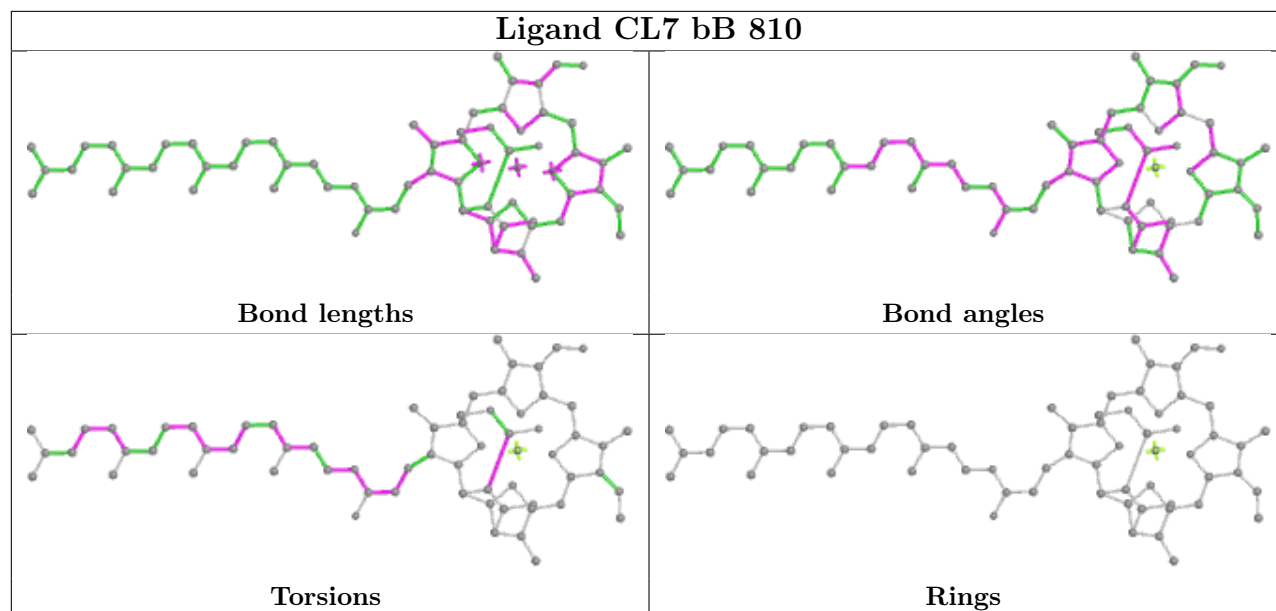
Bond angles

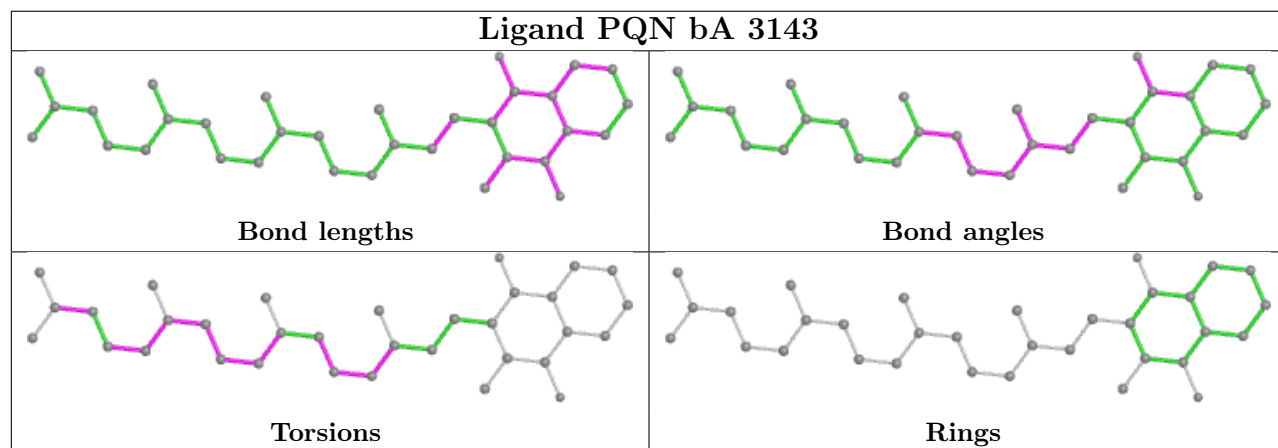
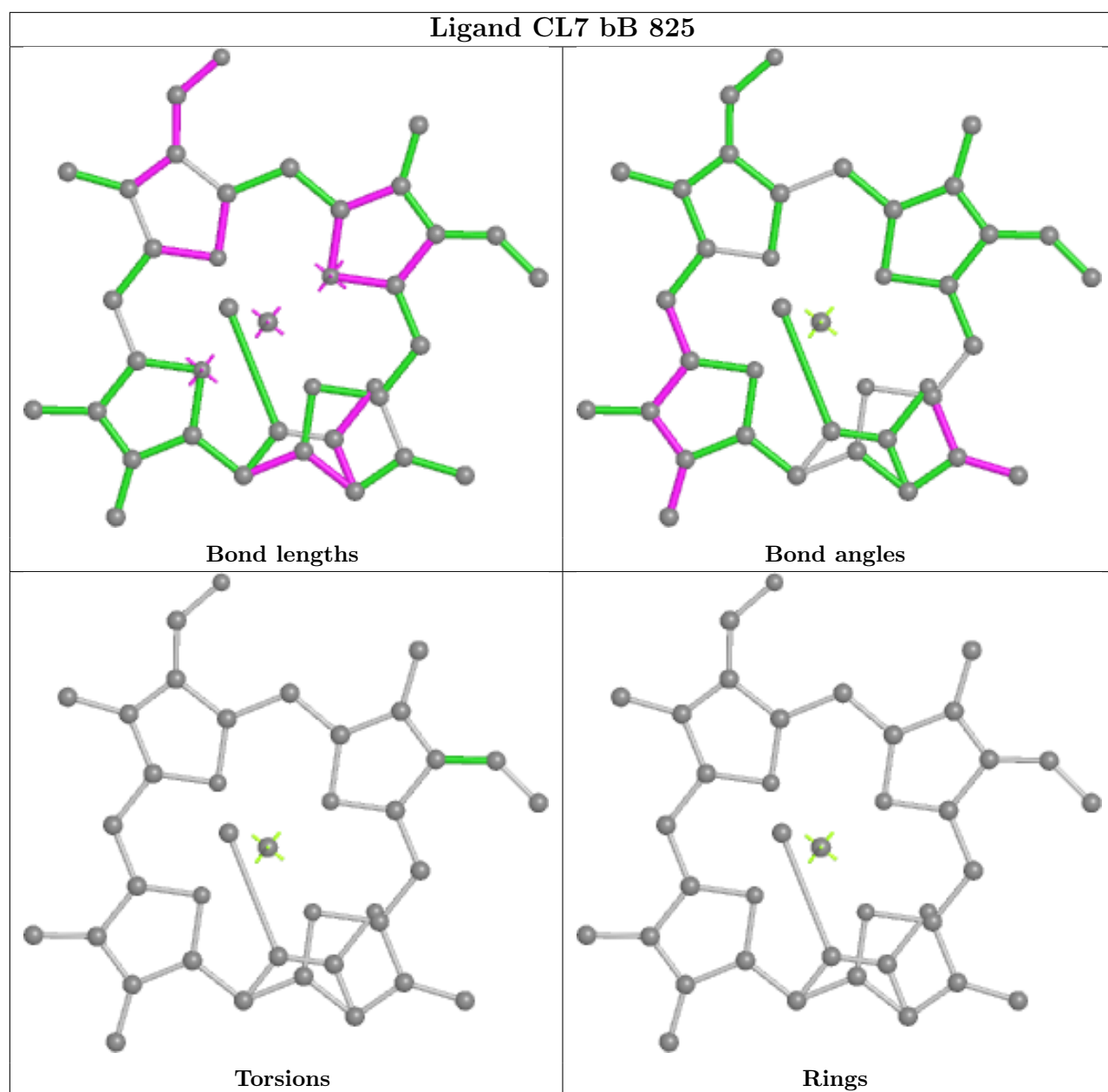


Torsions

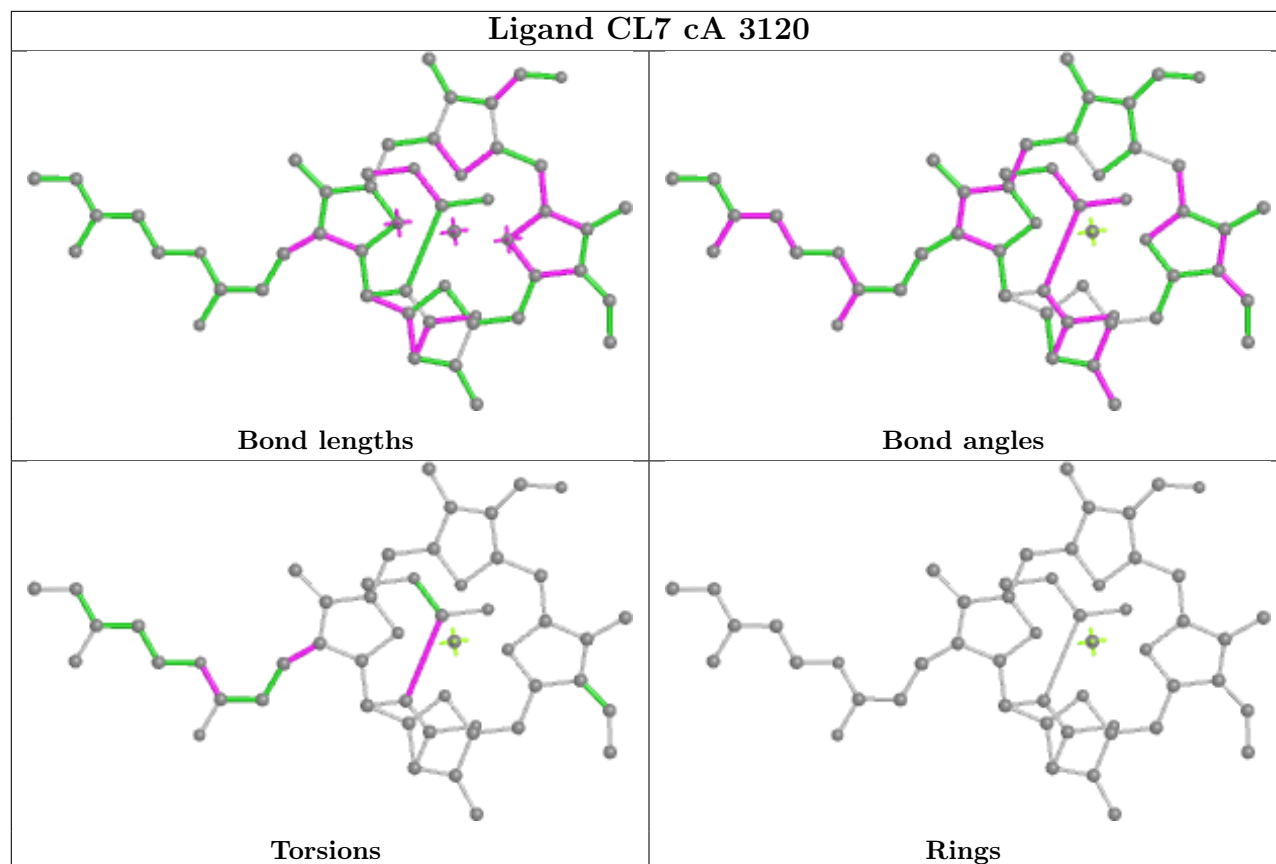


Rings

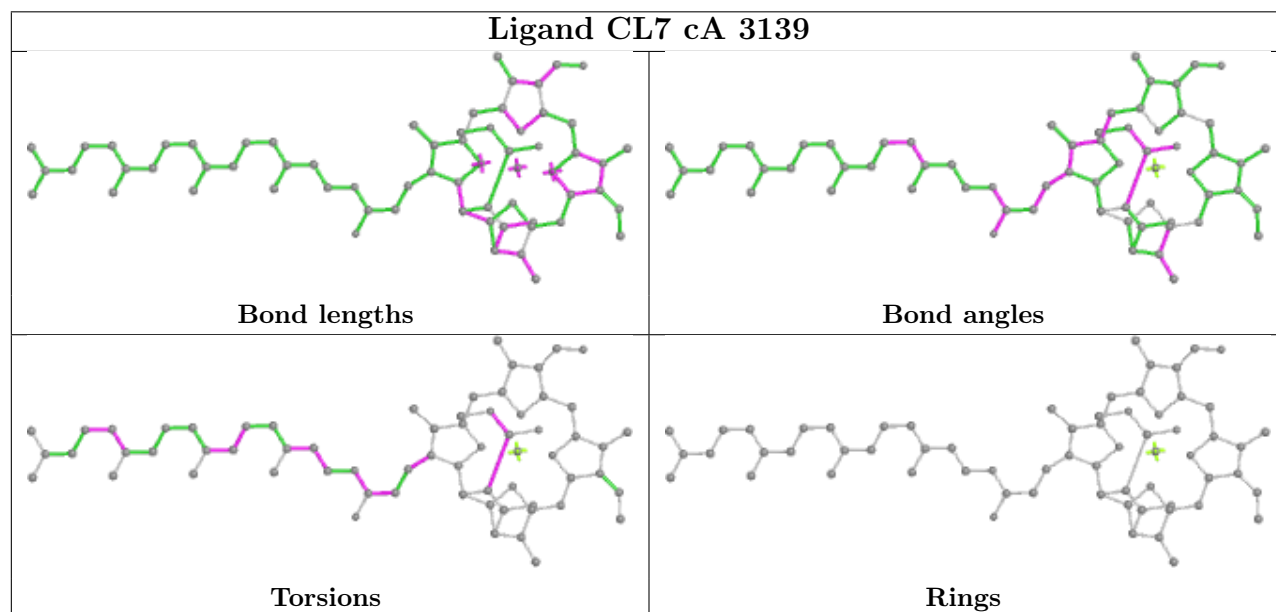


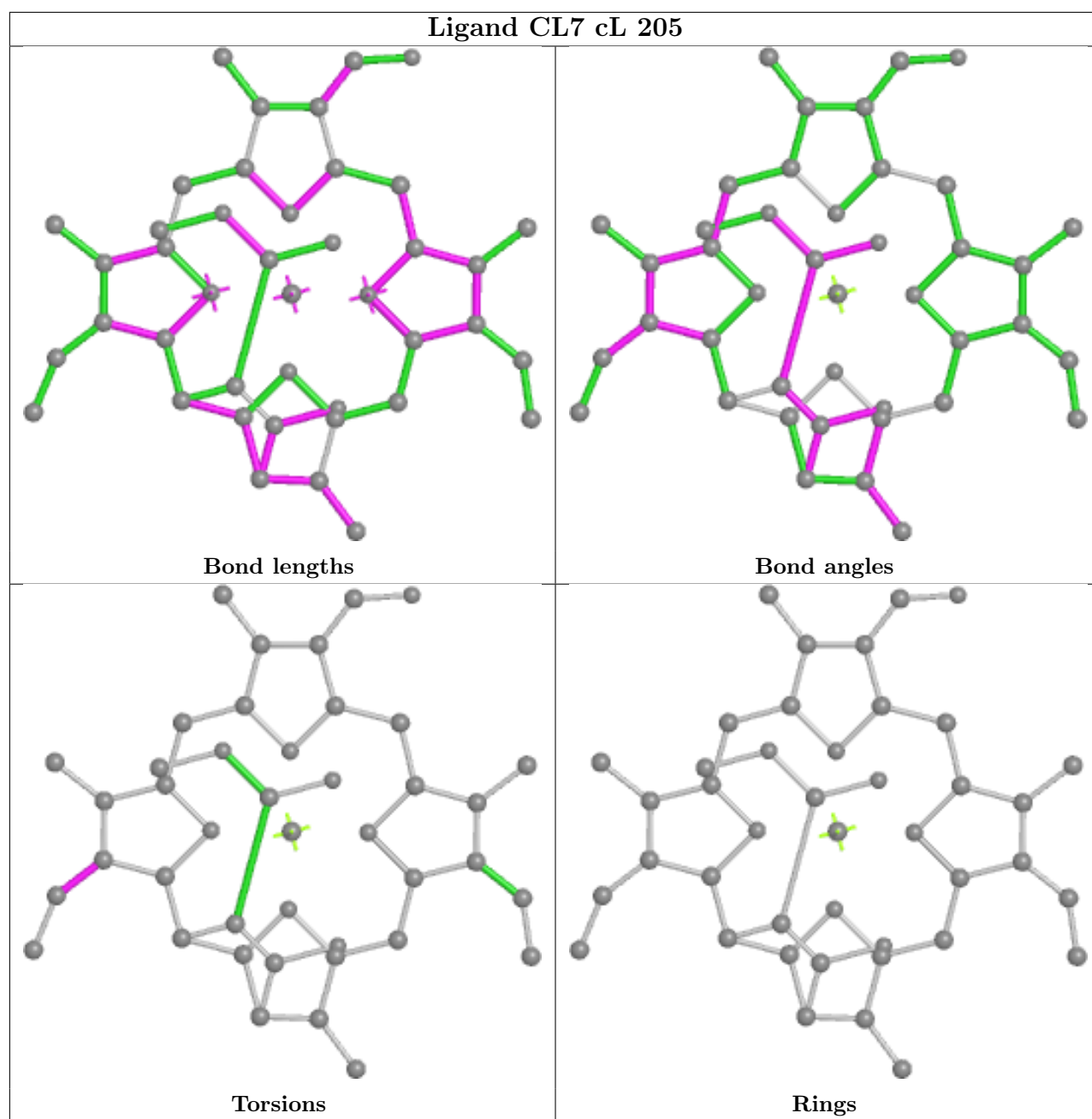


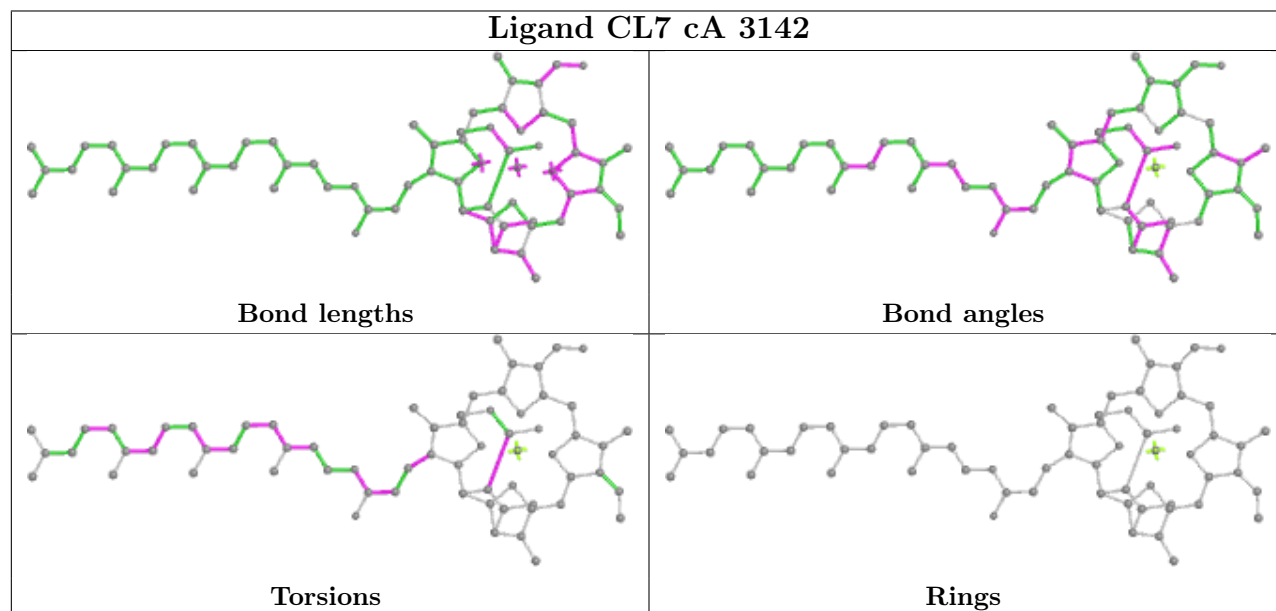
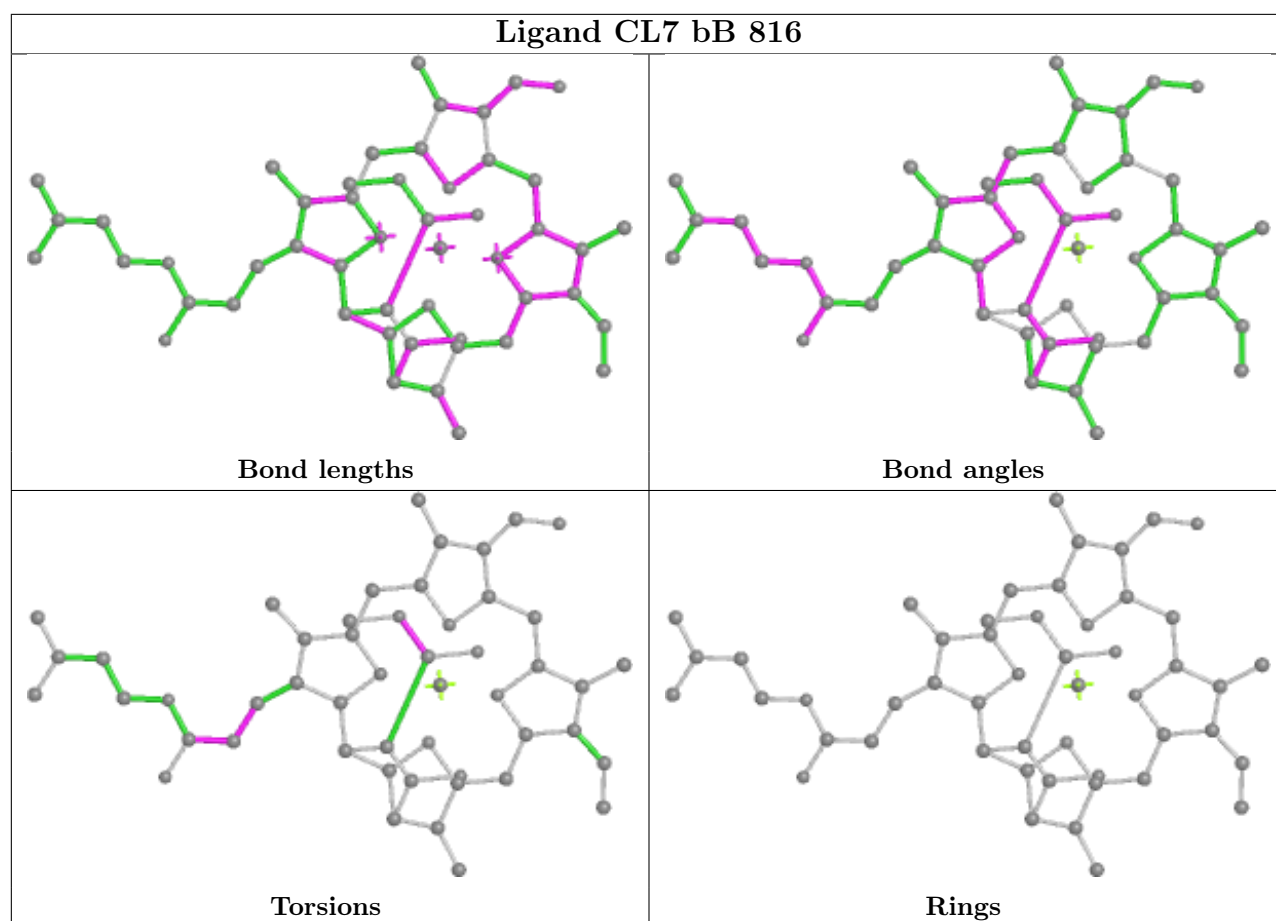
Ligand CL7 cA 3120

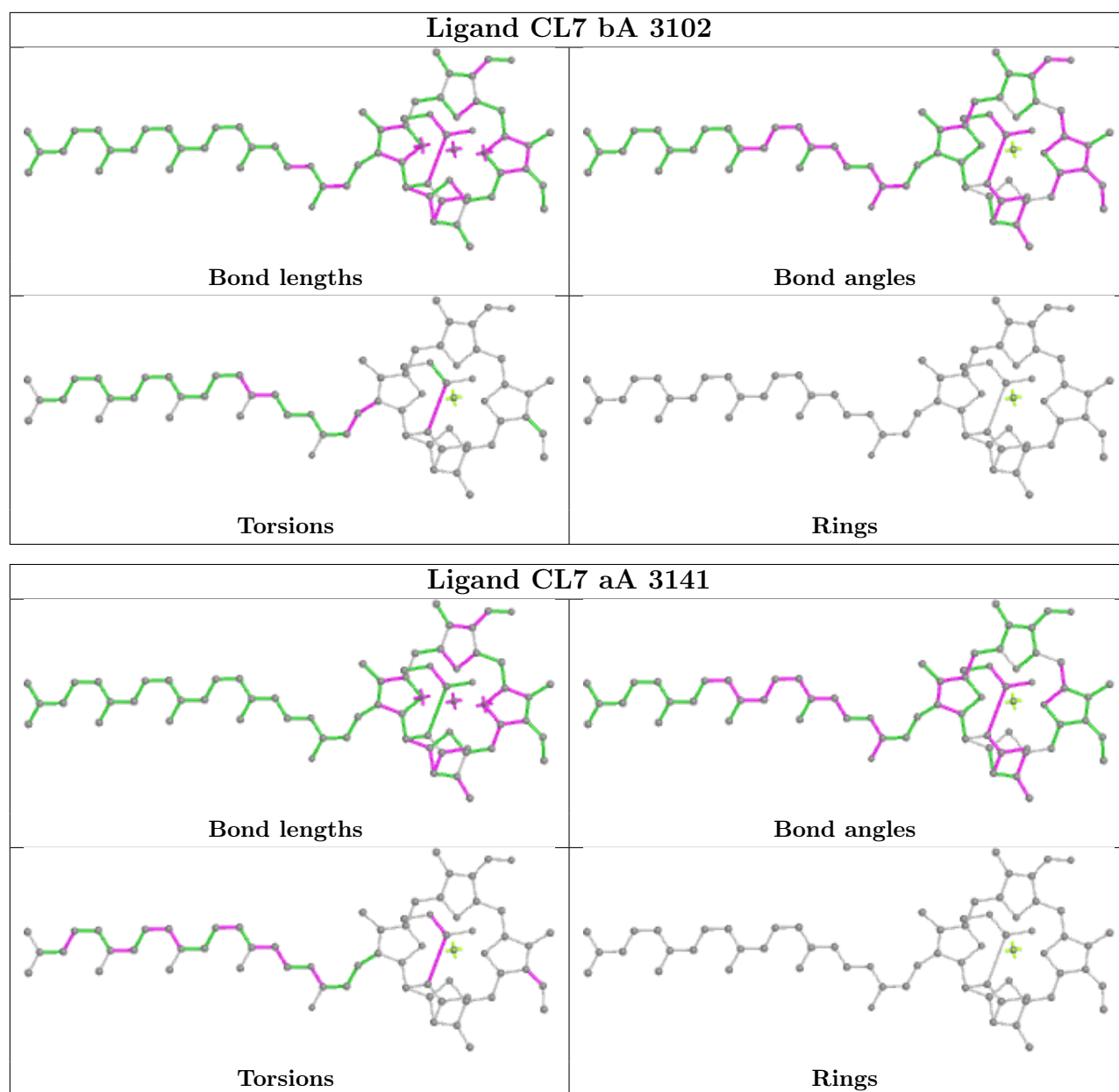


Ligand CL7 cA 3139

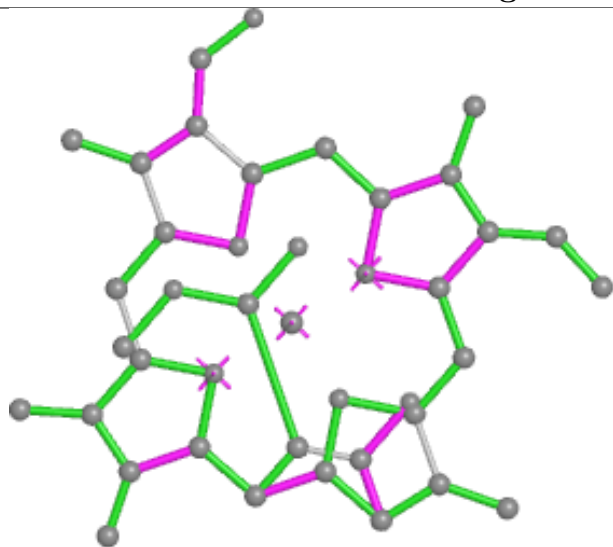




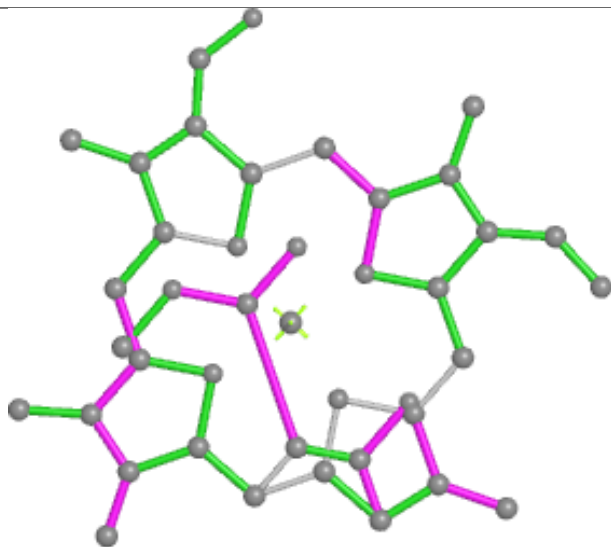




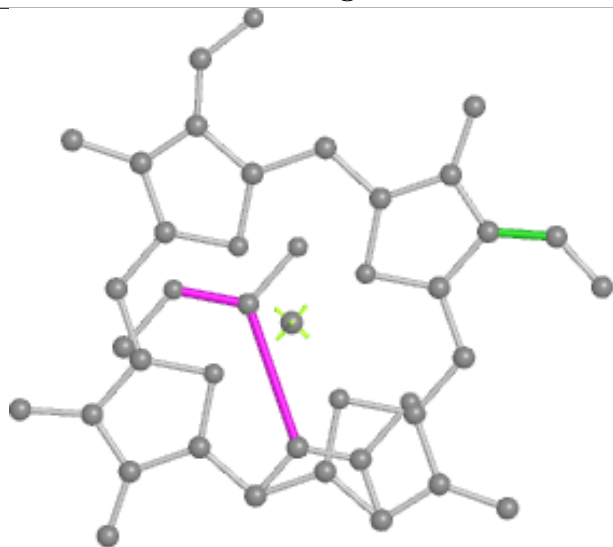
Ligand CL7 bA 3104



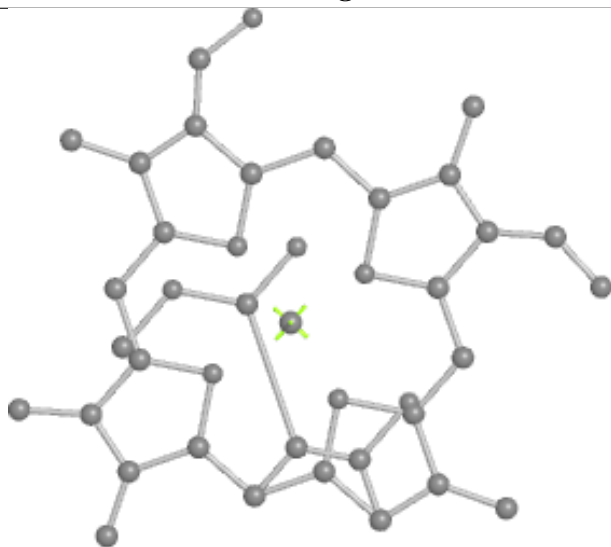
Bond lengths



Bond angles

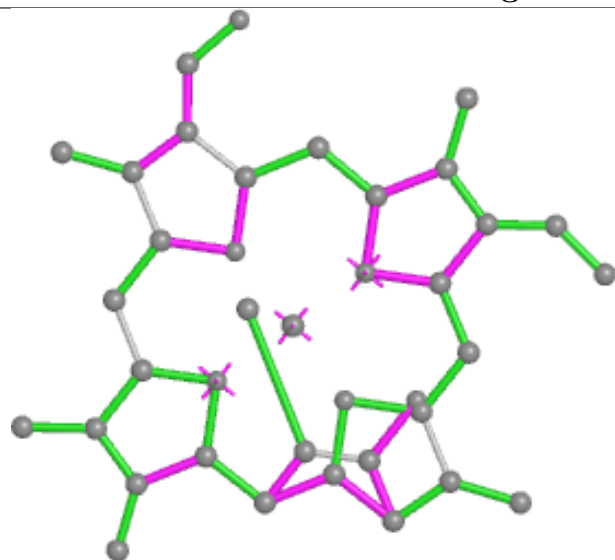


Torsions

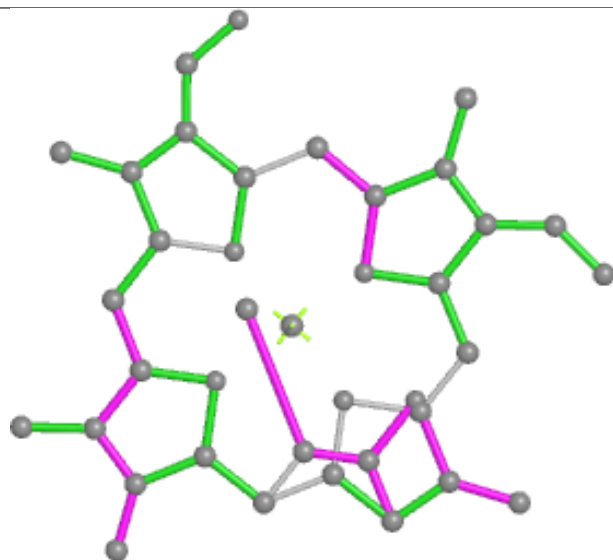


Rings

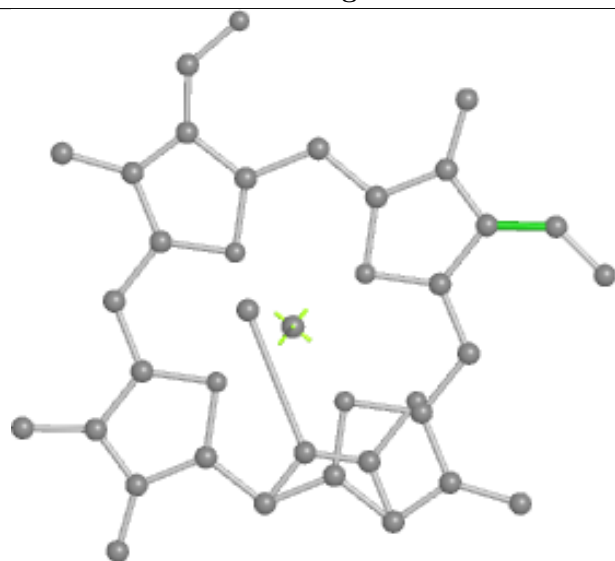
Ligand CL7 bA 3117



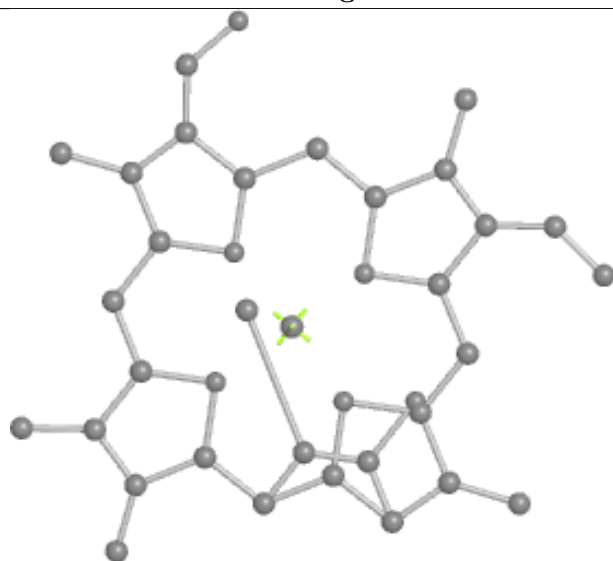
Bond lengths



Bond angles

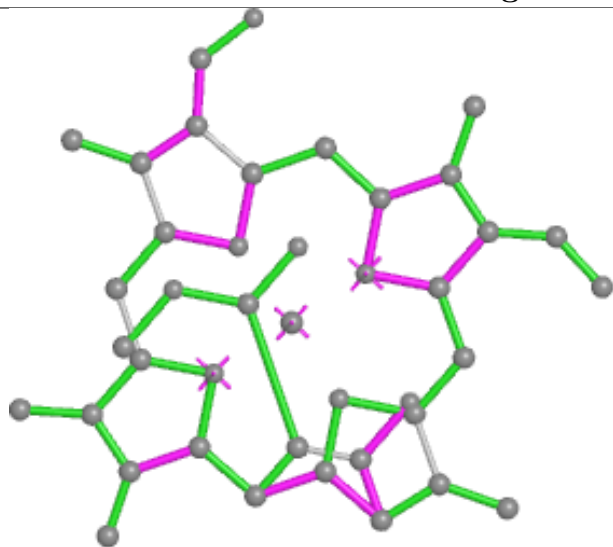


Torsions

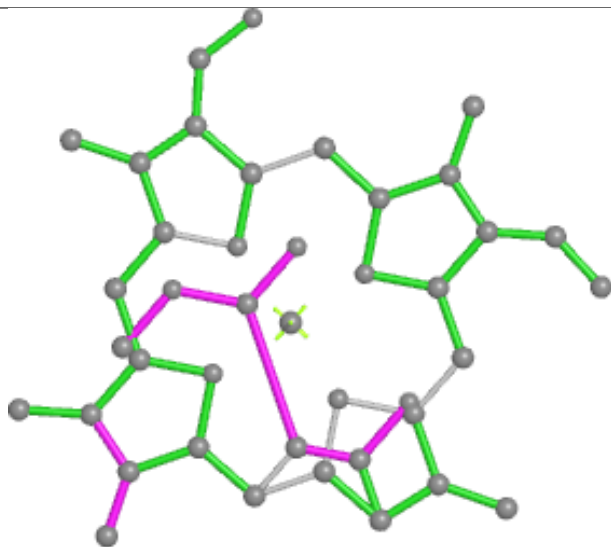


Rings

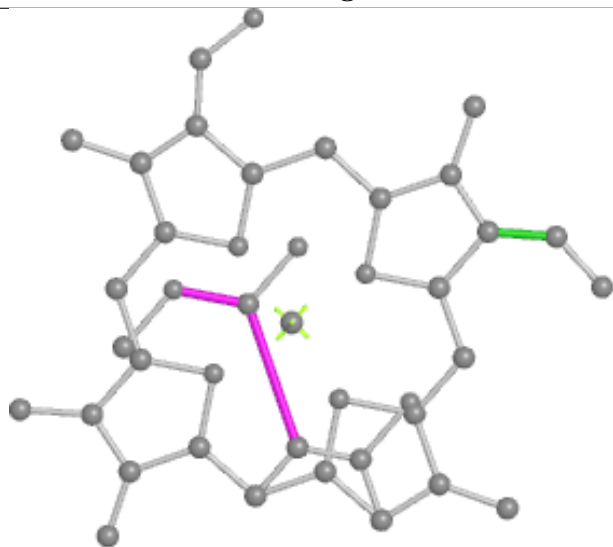
Ligand CL7 cA 3144



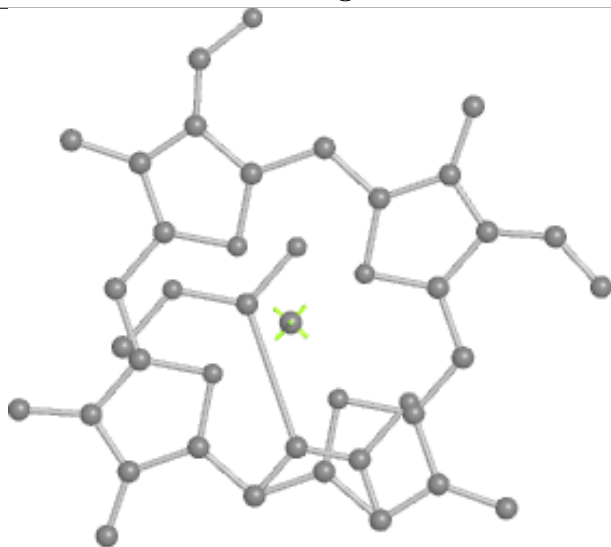
Bond lengths



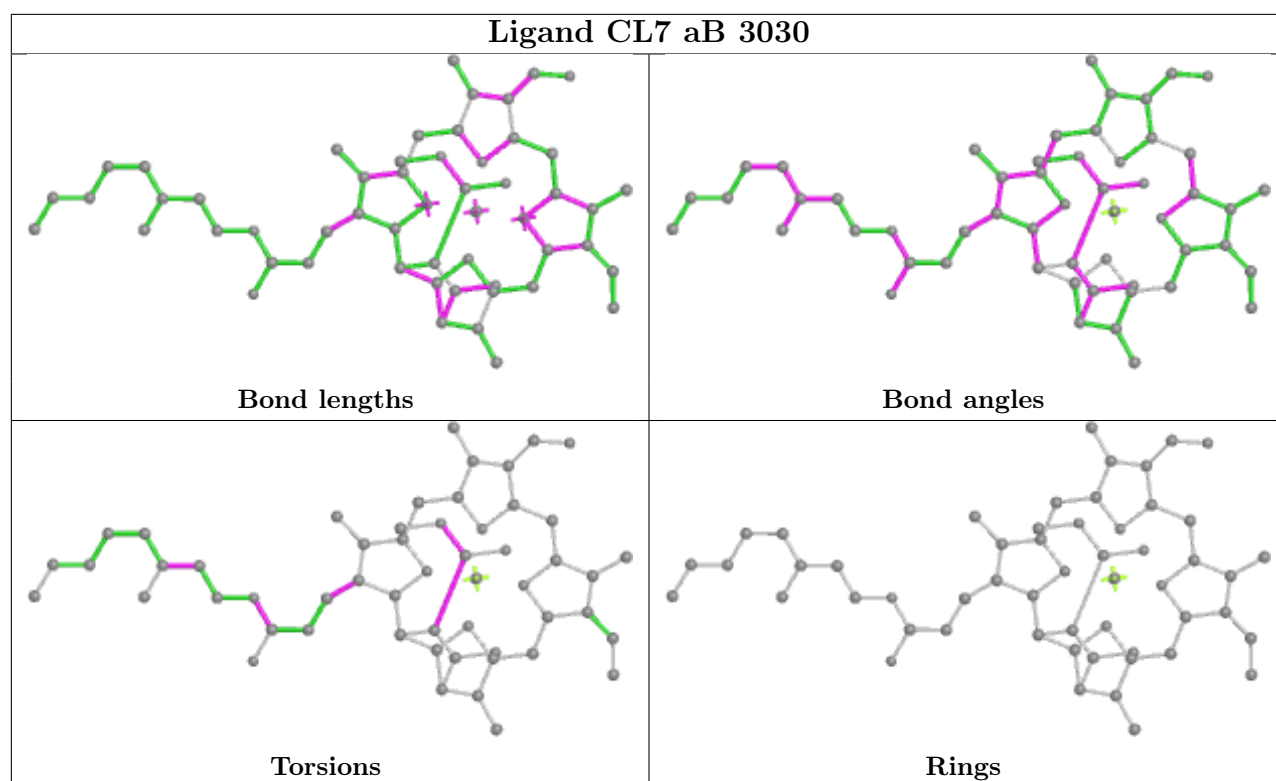
Bond angles

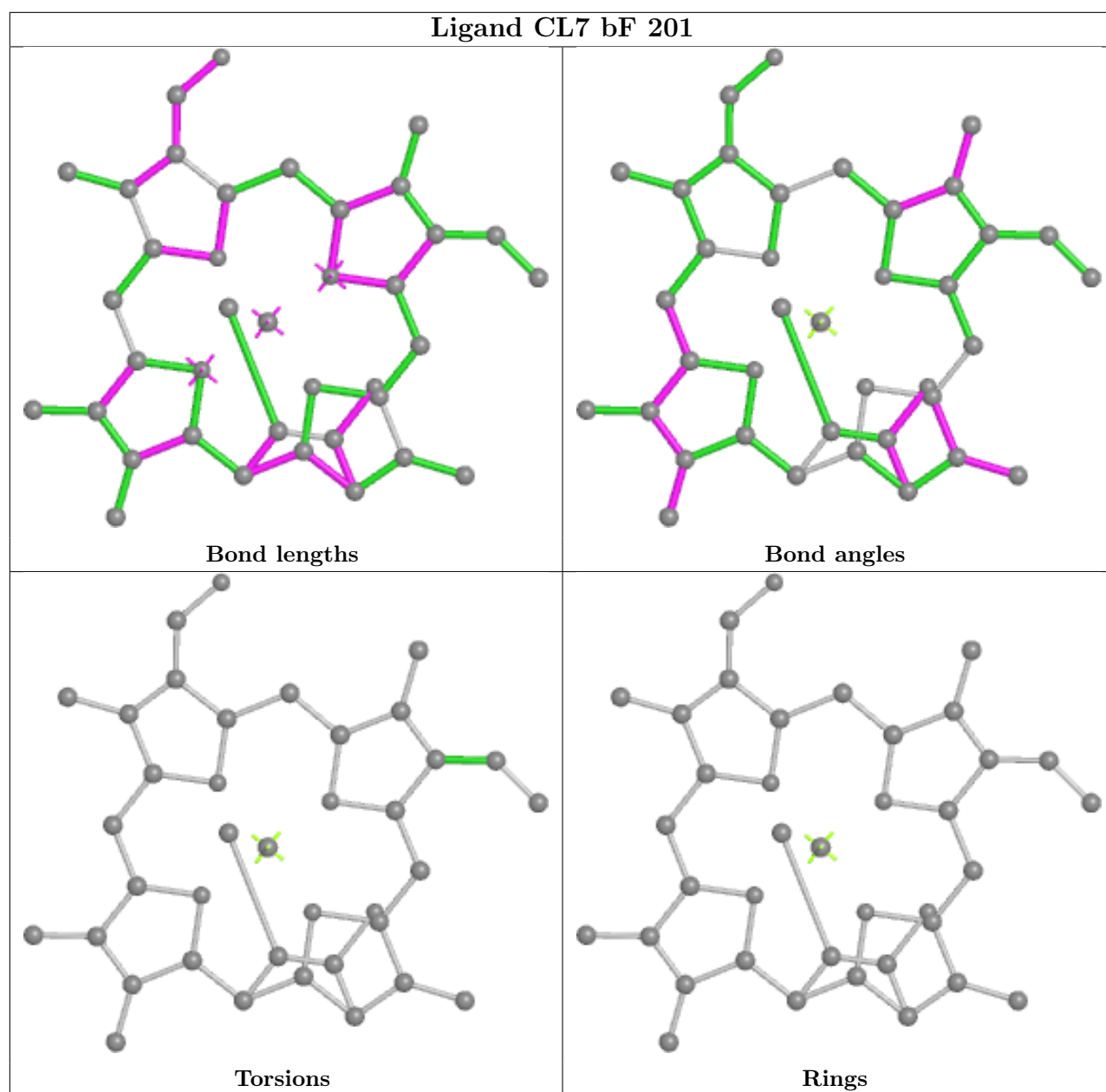


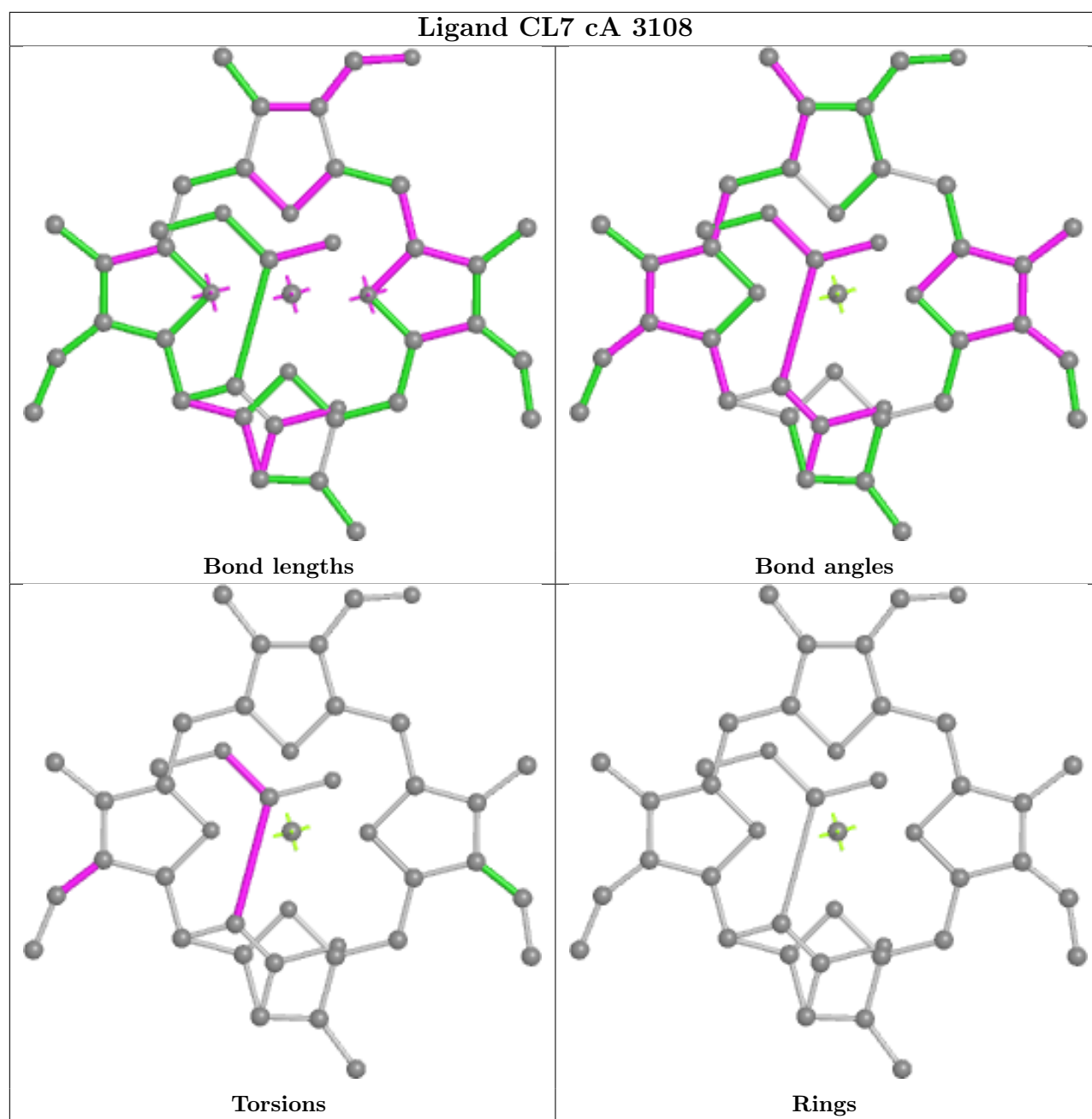
Torsions



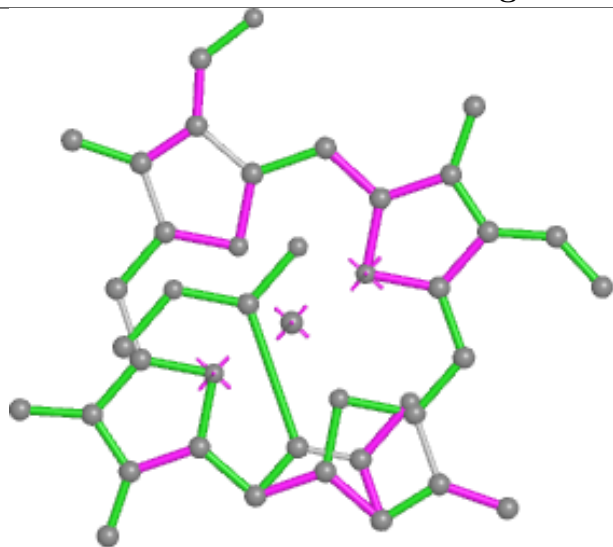
Rings



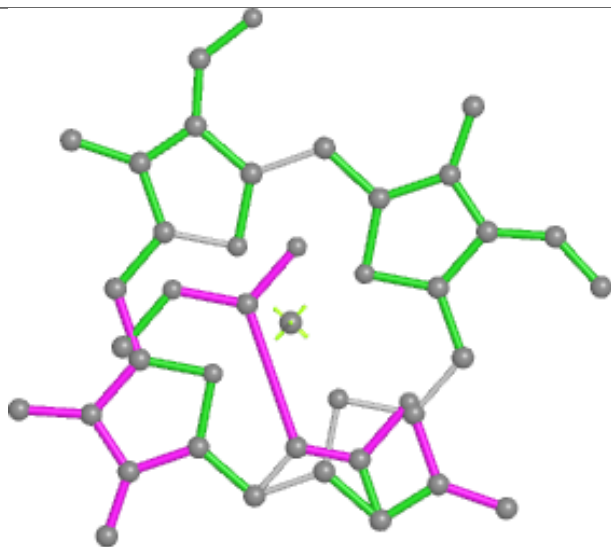




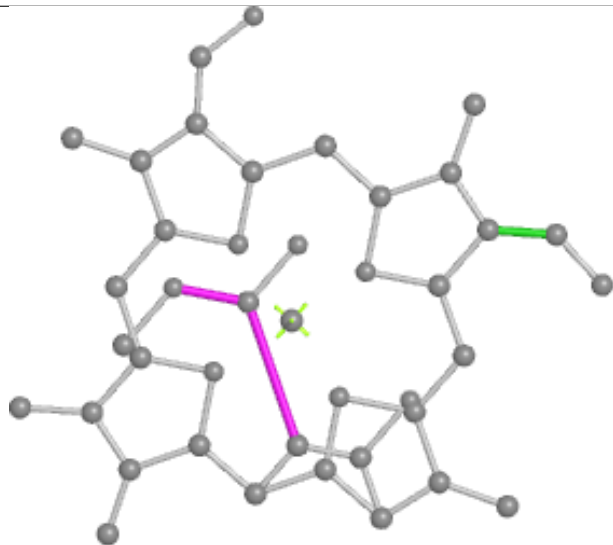
Ligand CL7 bA 3131



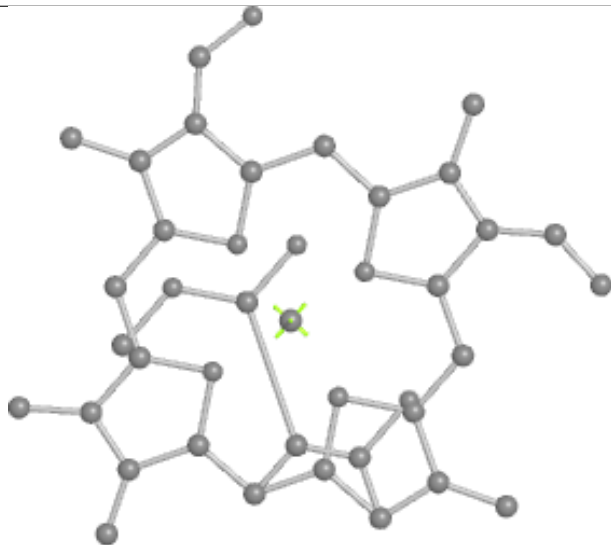
Bond lengths



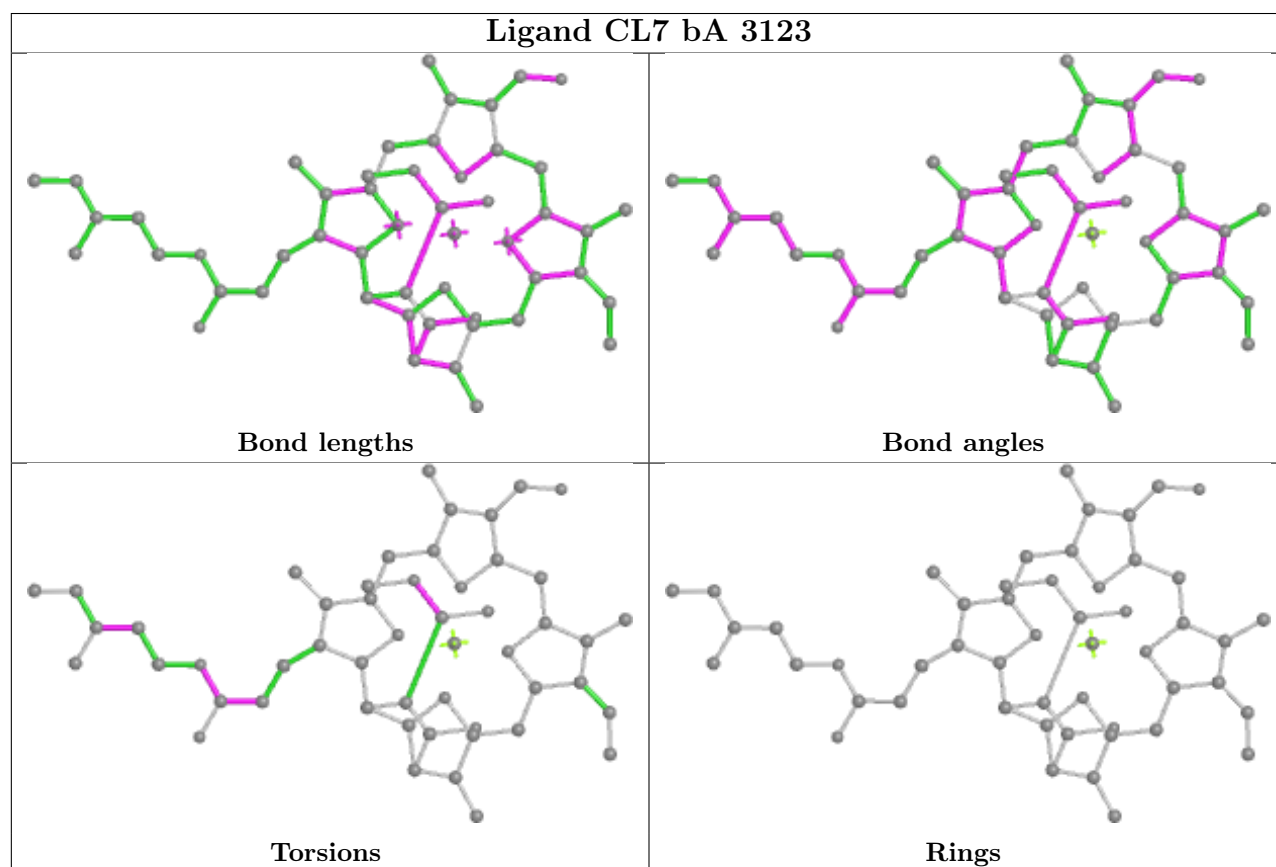
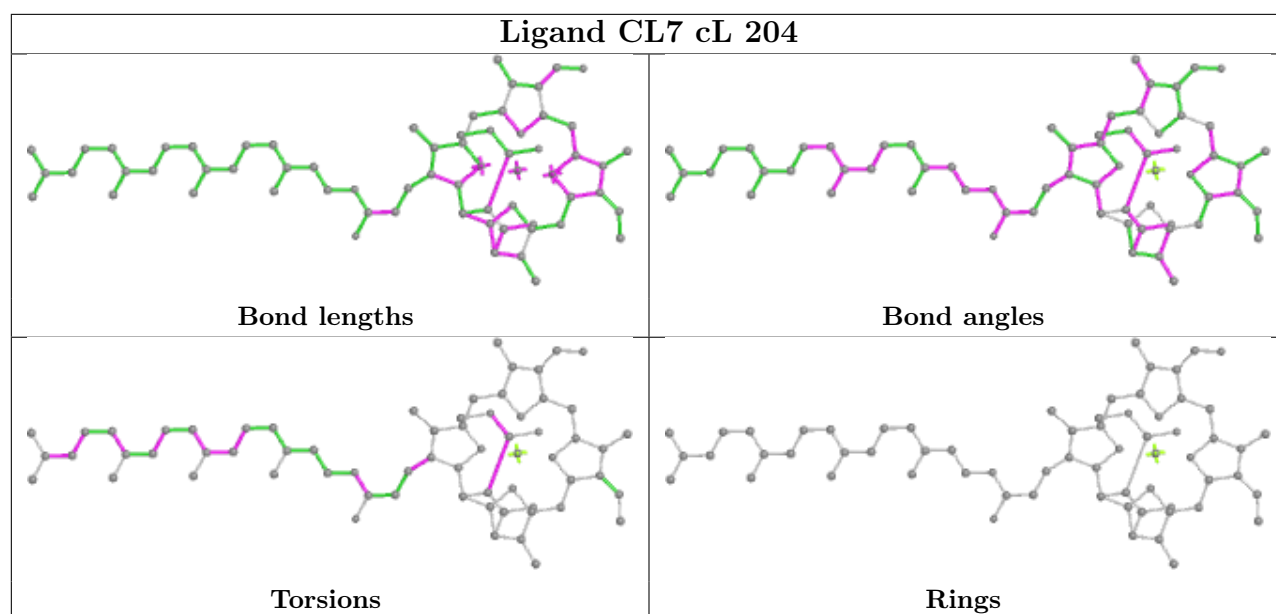
Bond angles

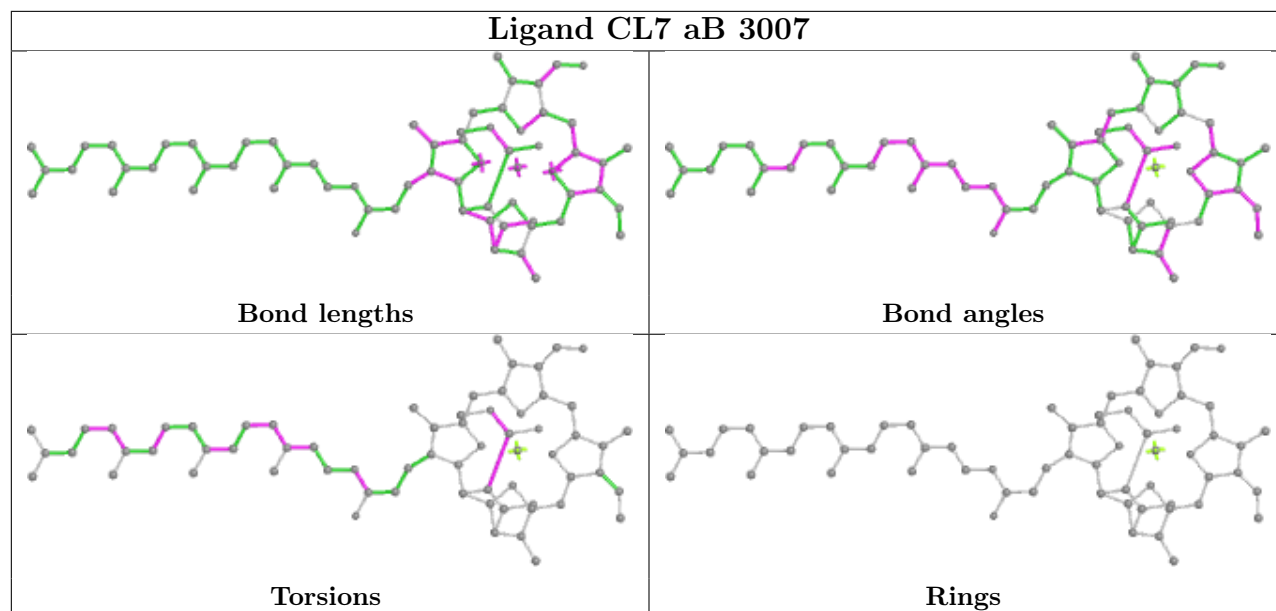


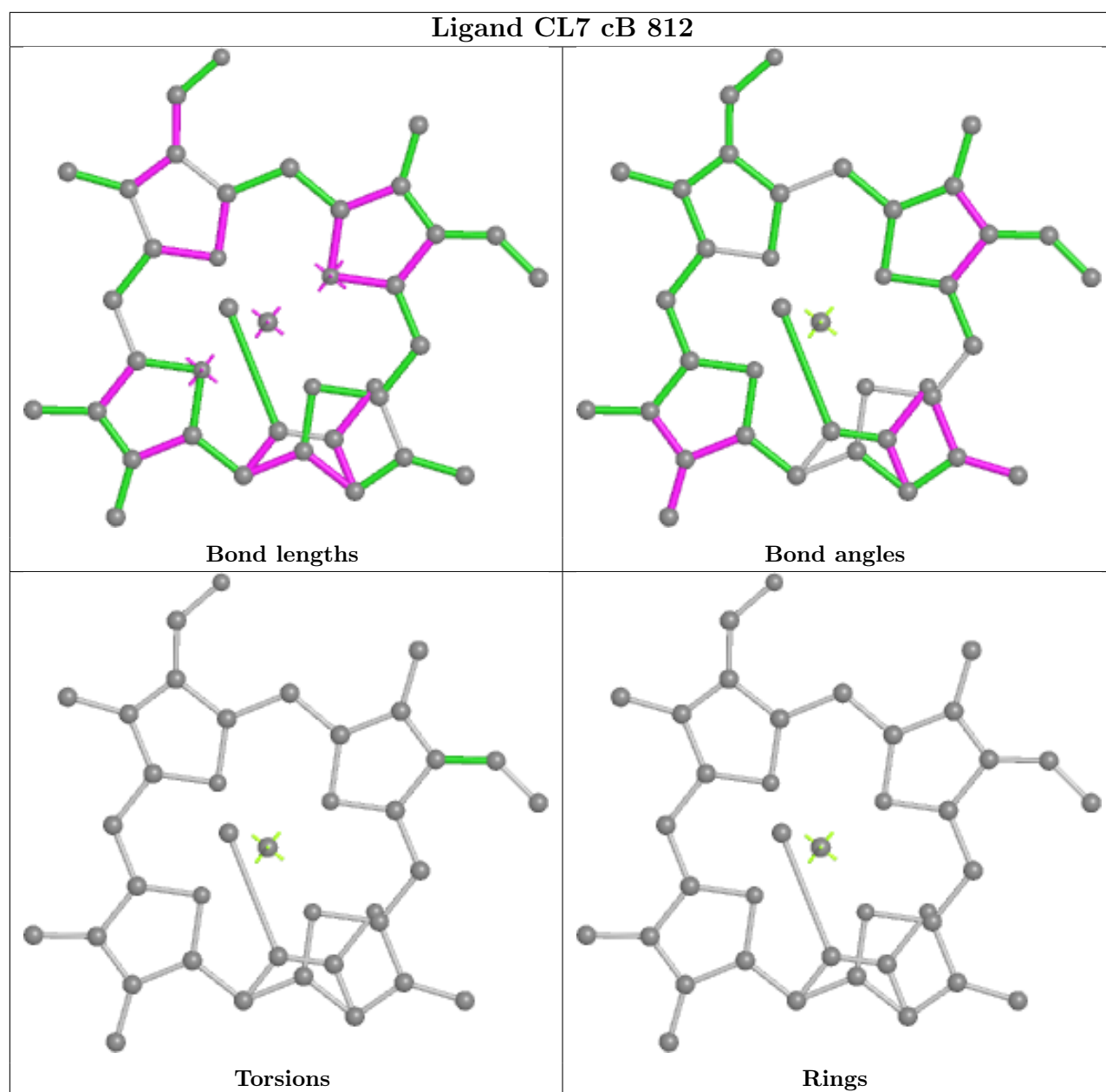
Torsions

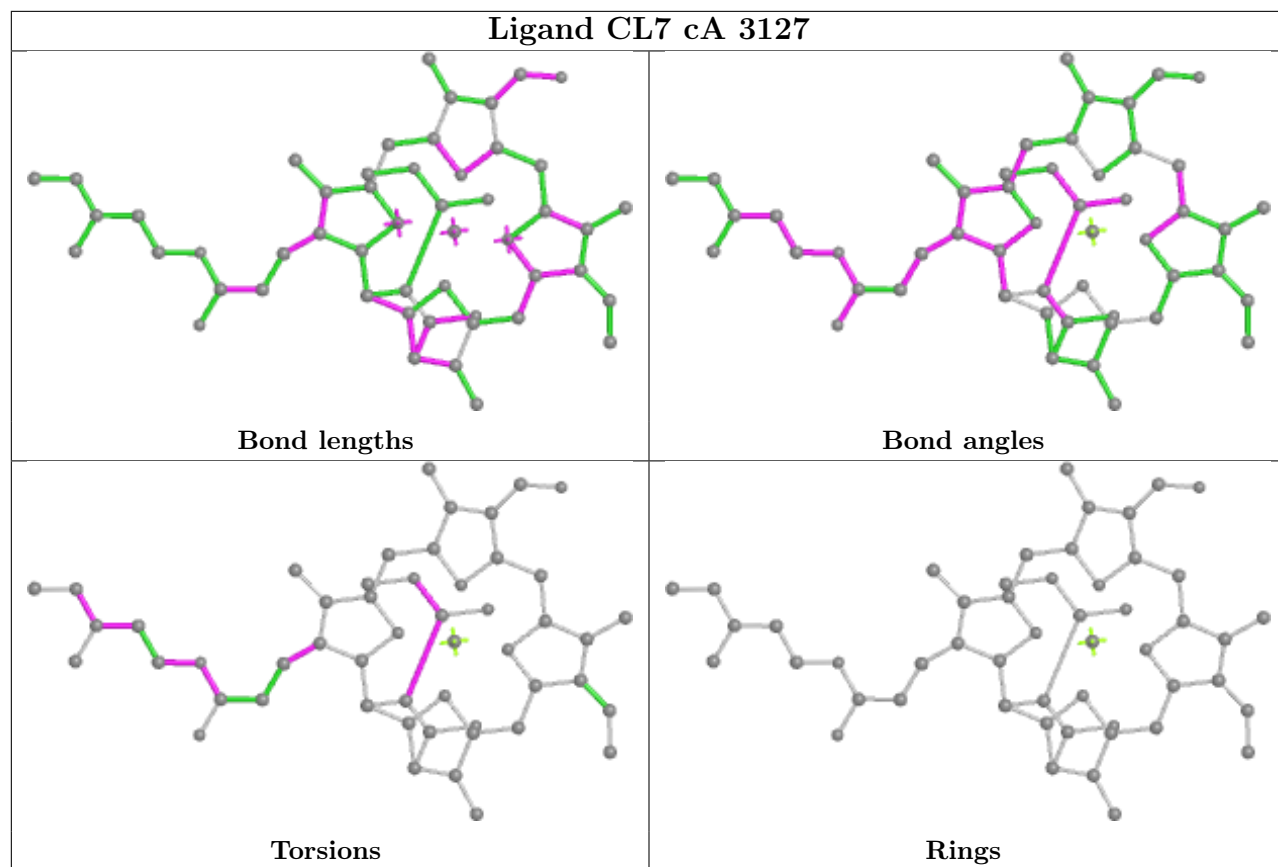


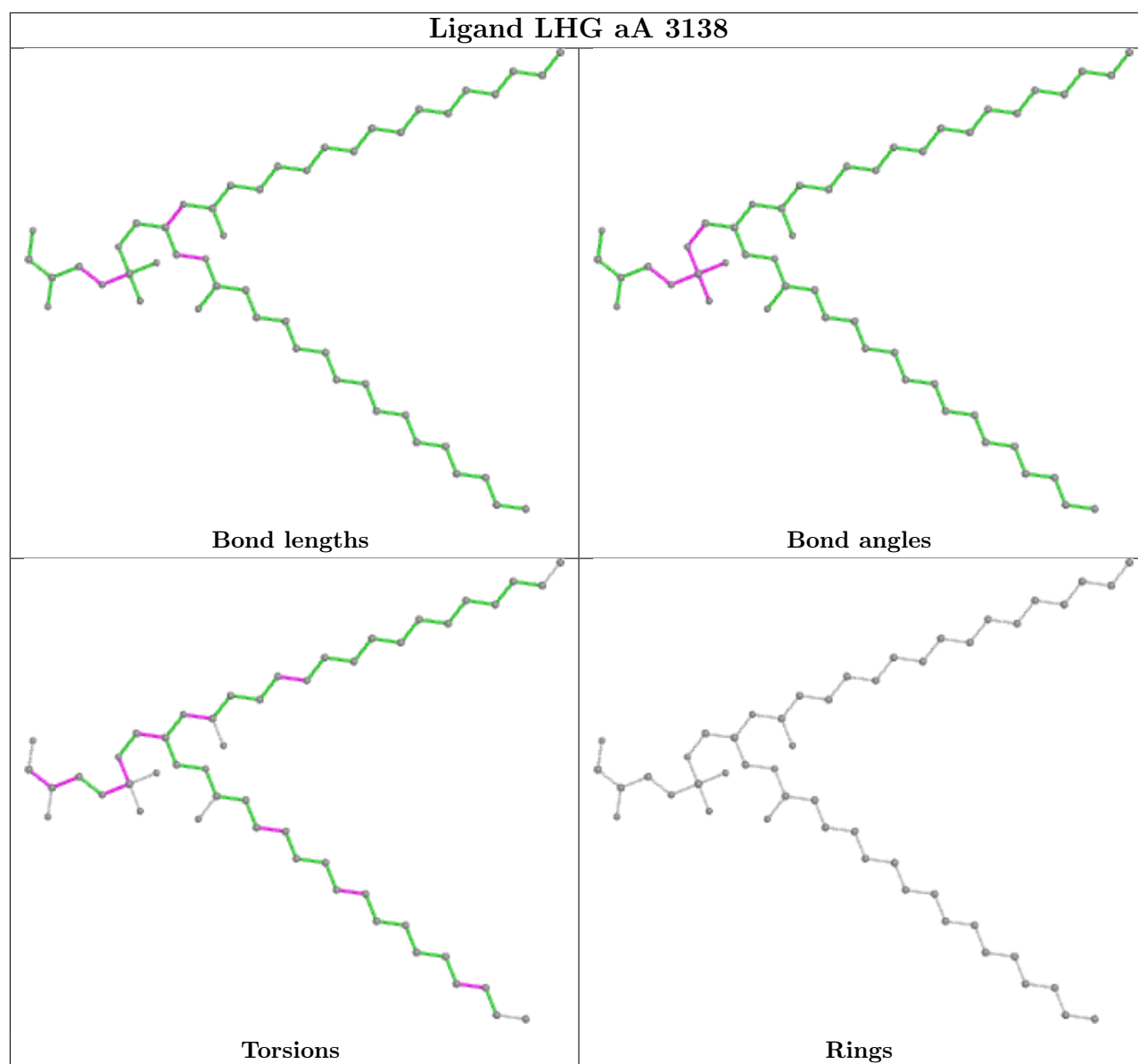
Rings

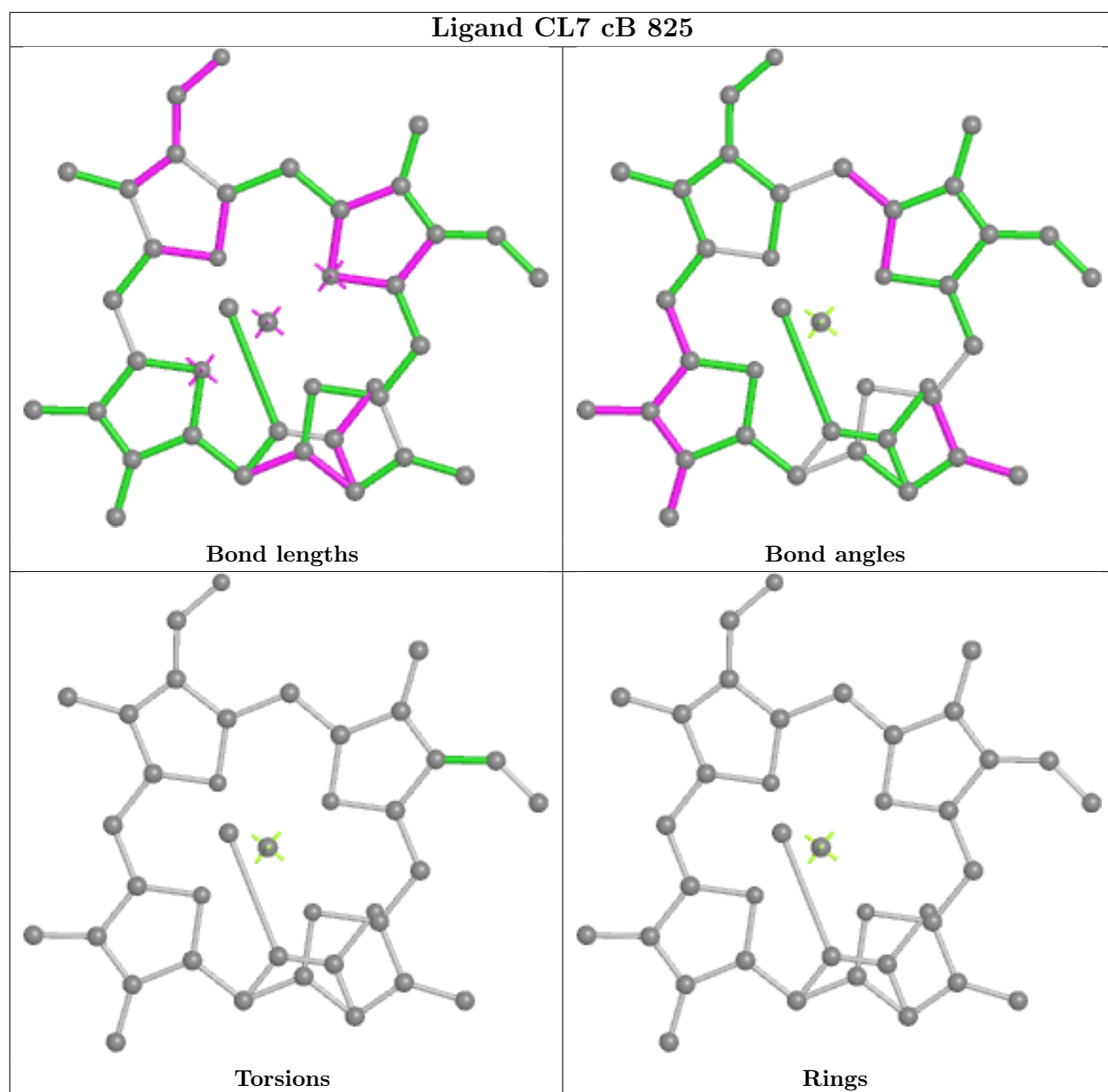


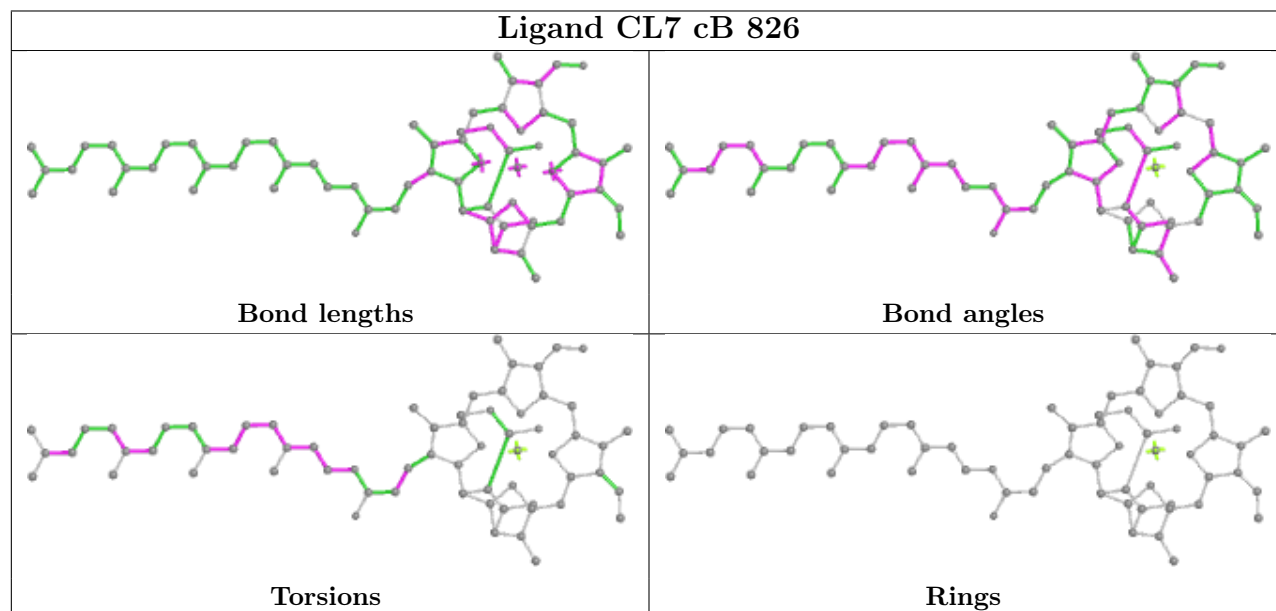
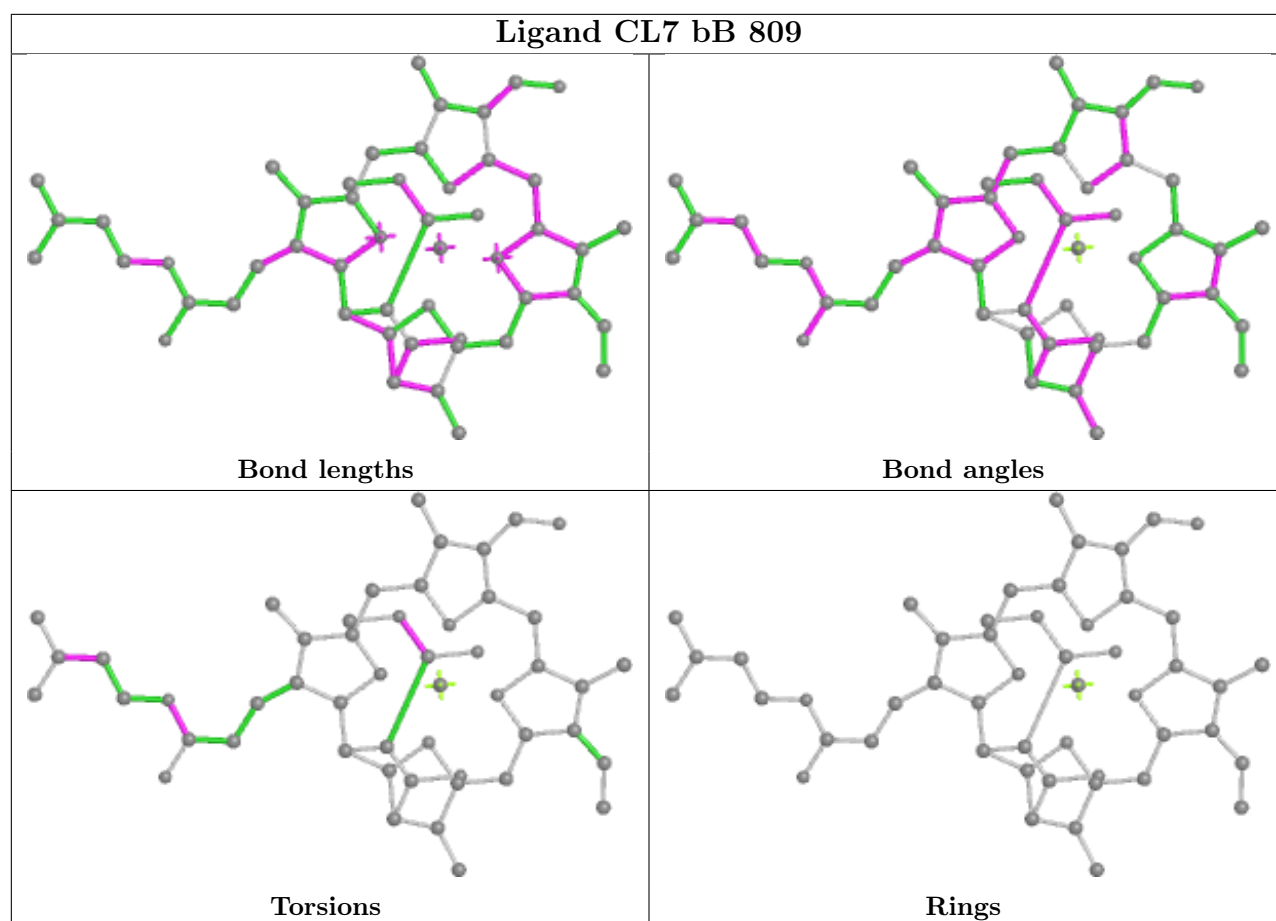


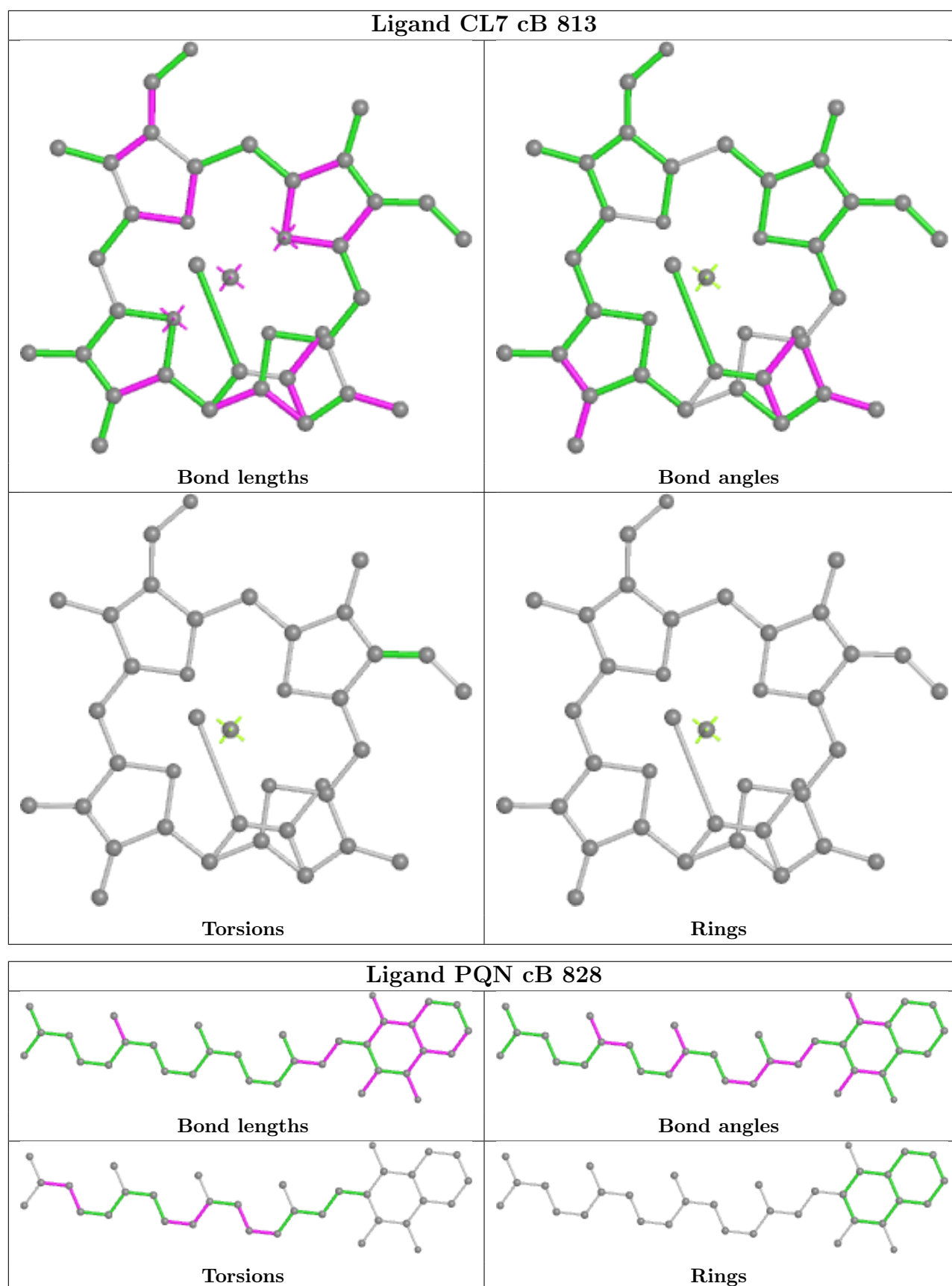


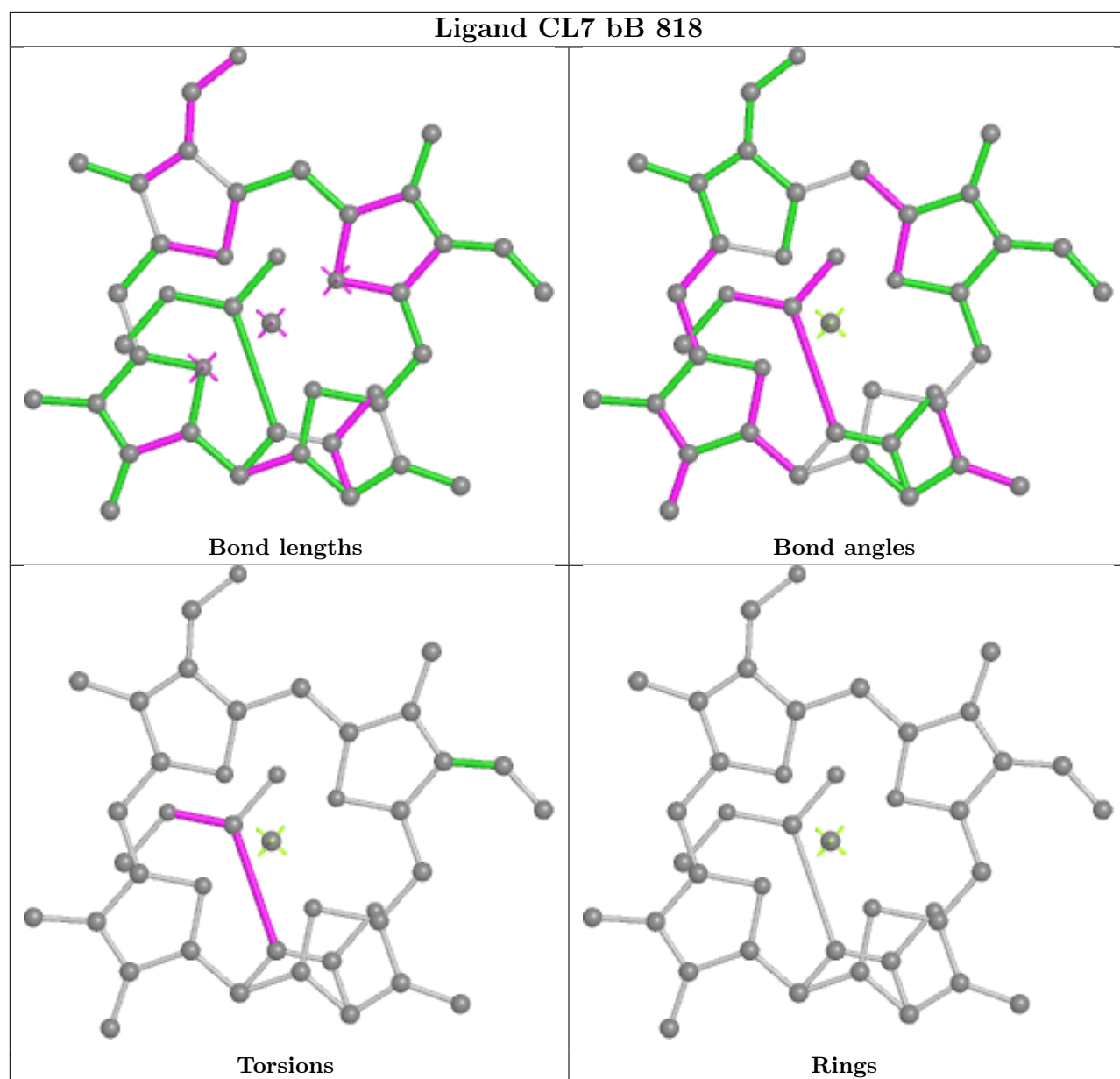




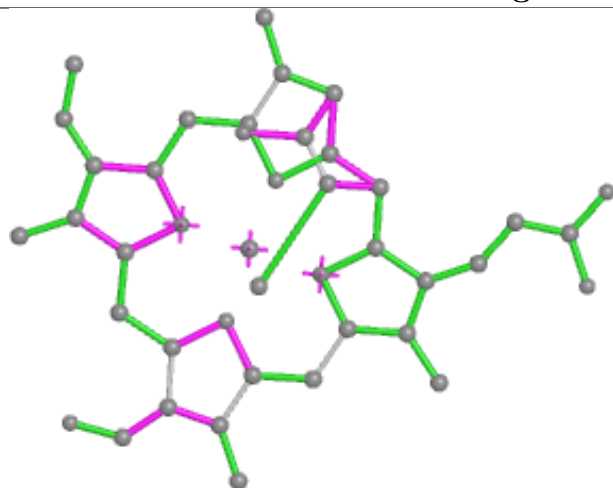




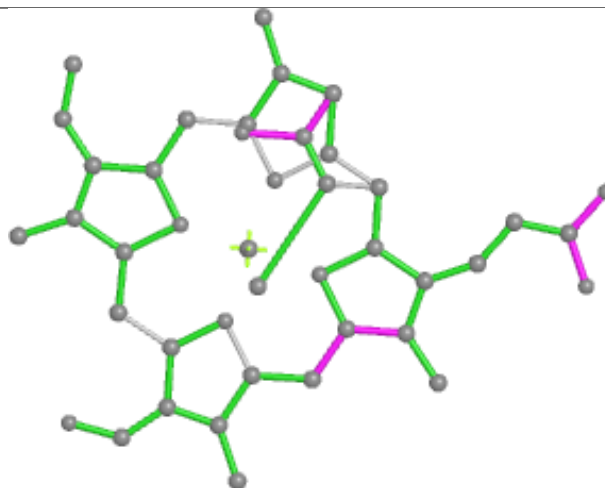




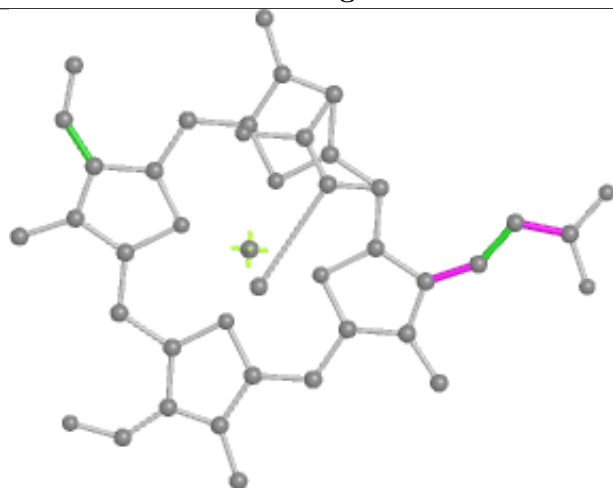
Ligand CL7 bJ 101



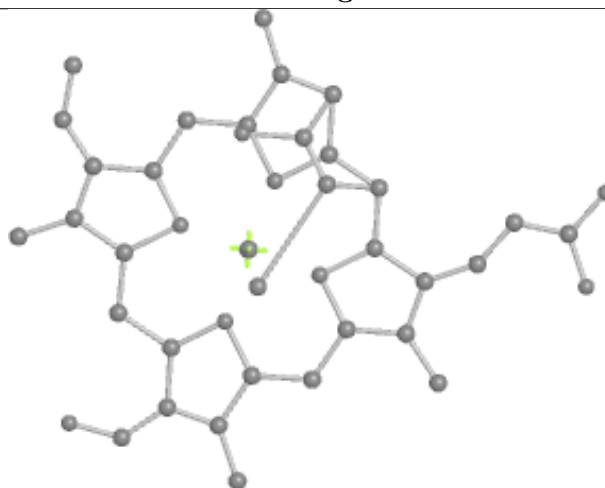
Bond lengths



Bond angles

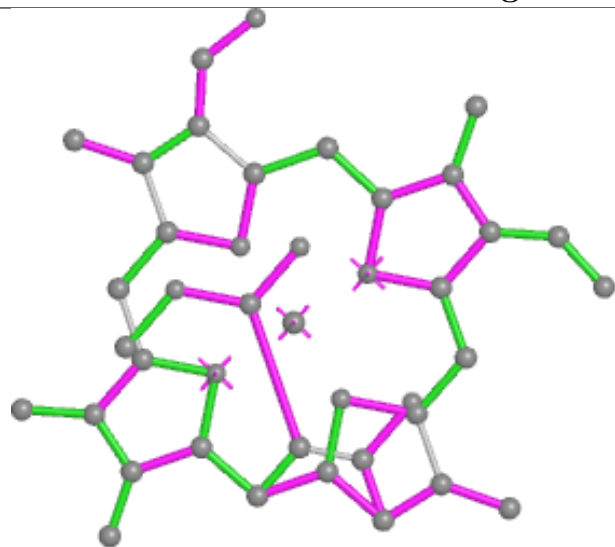


Torsions

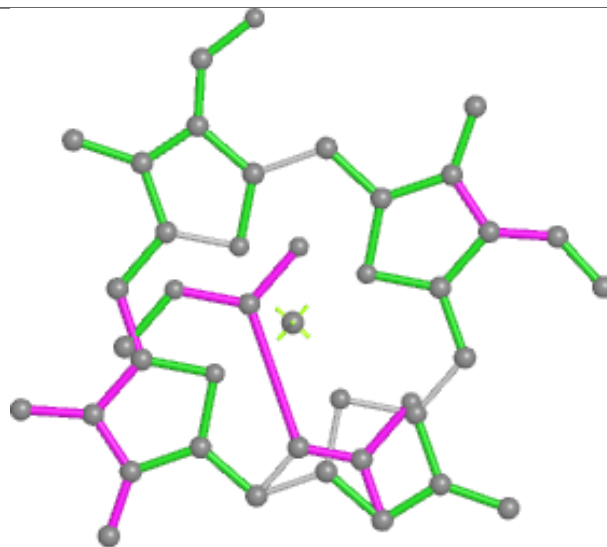


Rings

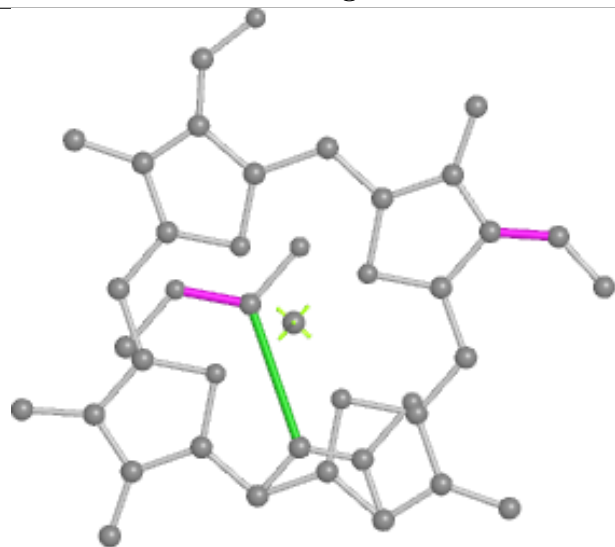
Ligand CL7 bA 3121



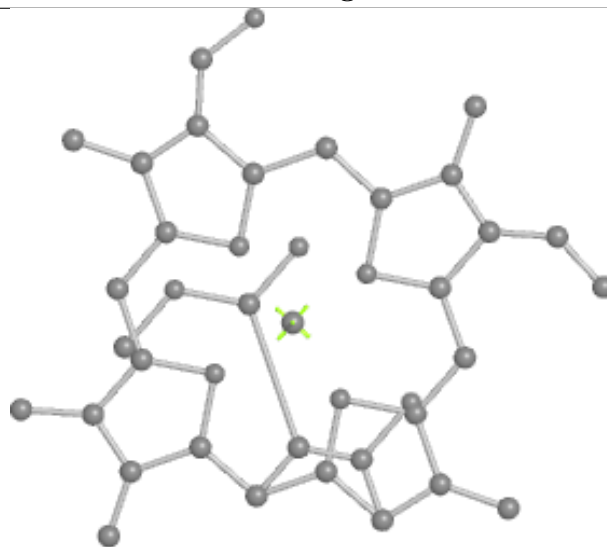
Bond lengths



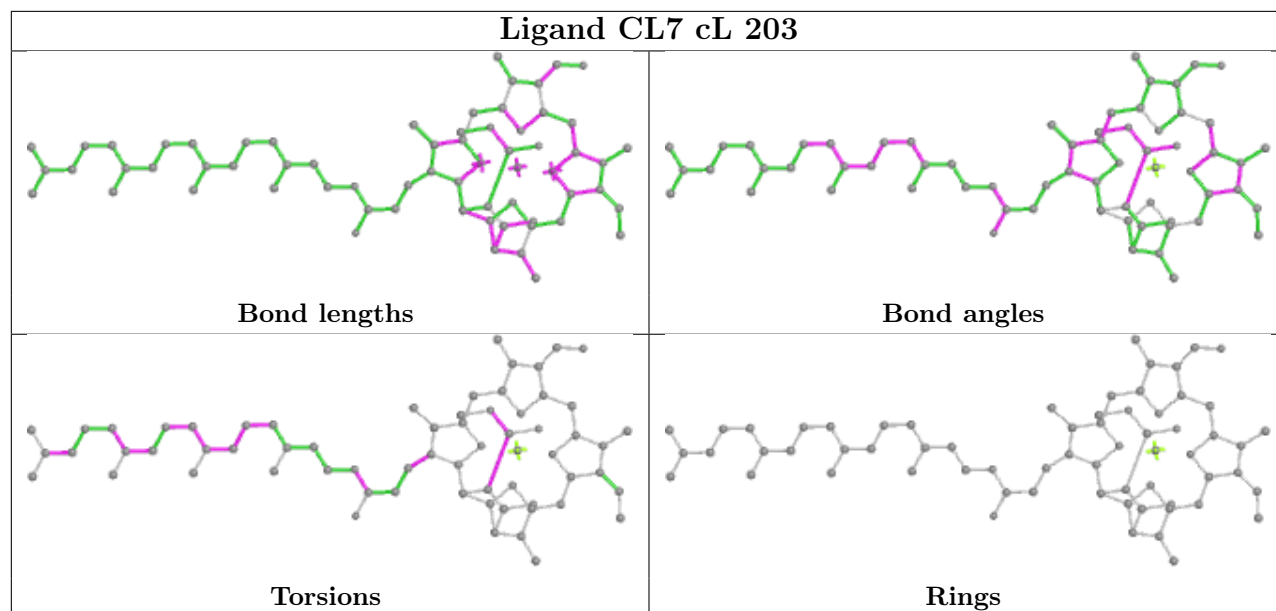
Bond angles



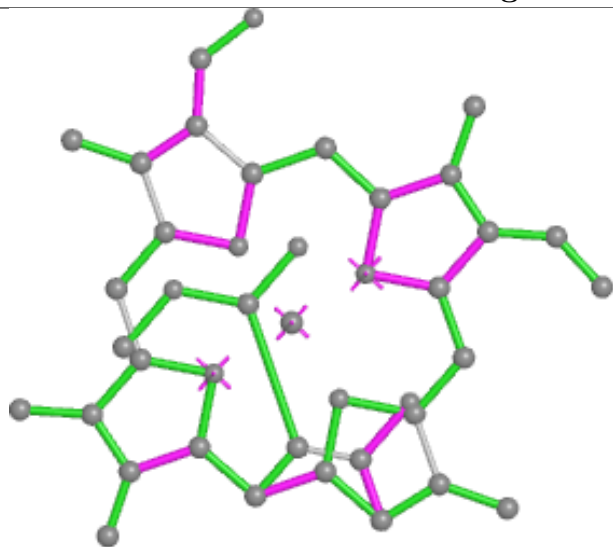
Torsions



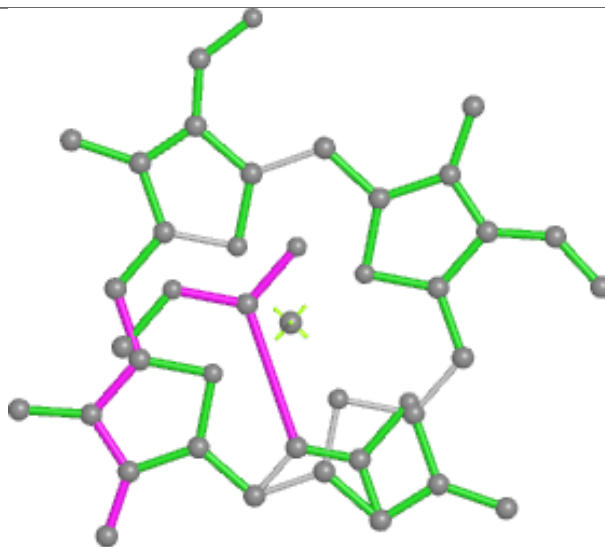
Rings



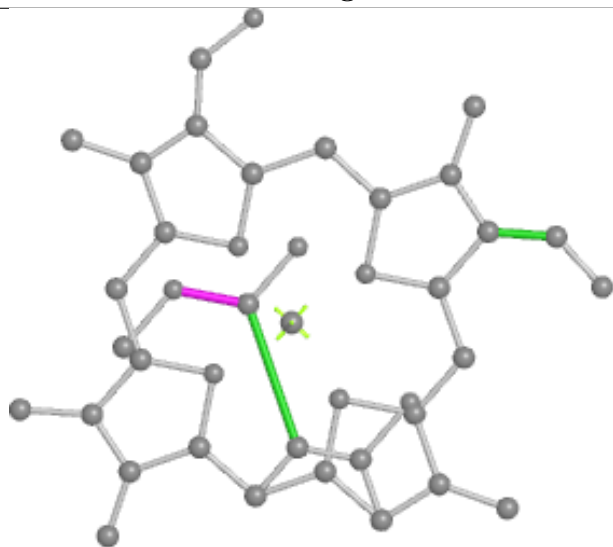
Ligand CL7 aA 3111



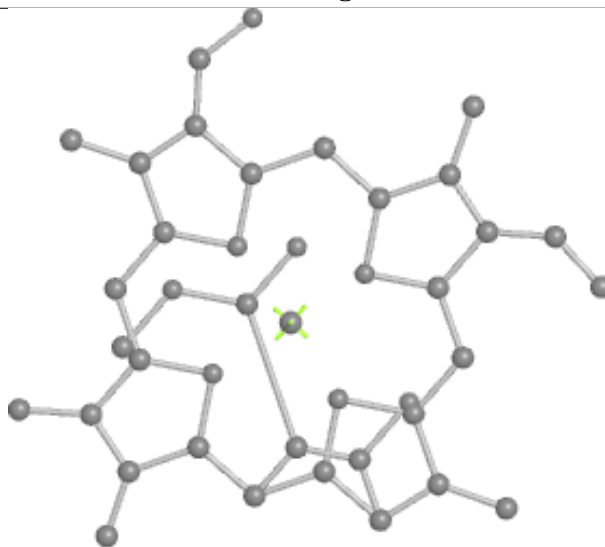
Bond lengths



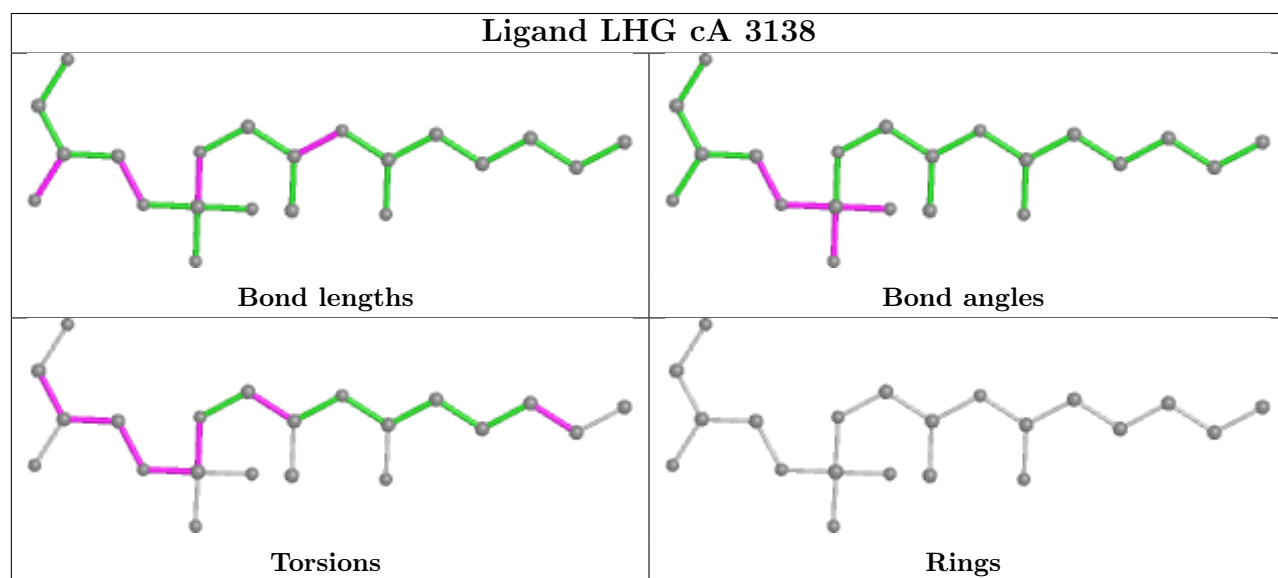
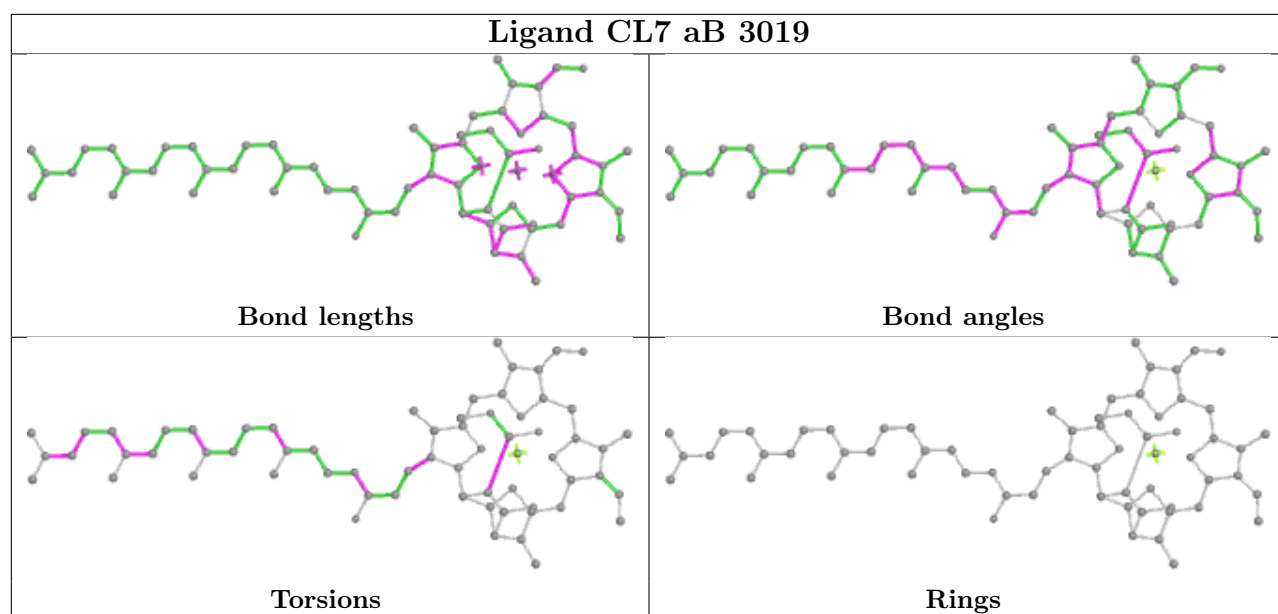
Bond angles

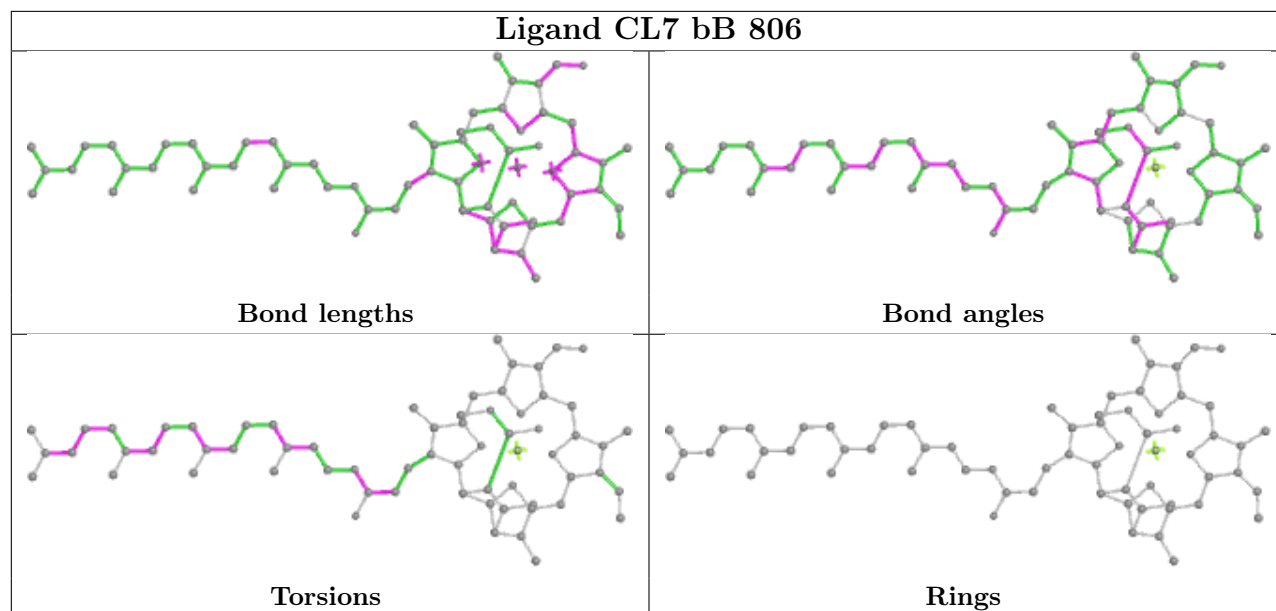


Torsions

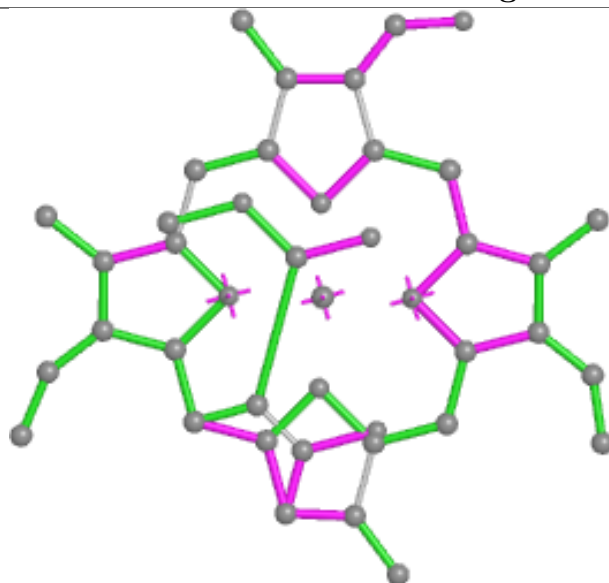


Rings

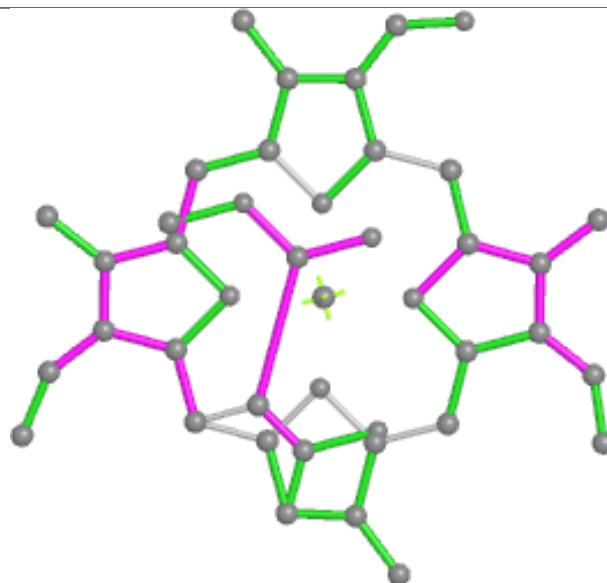




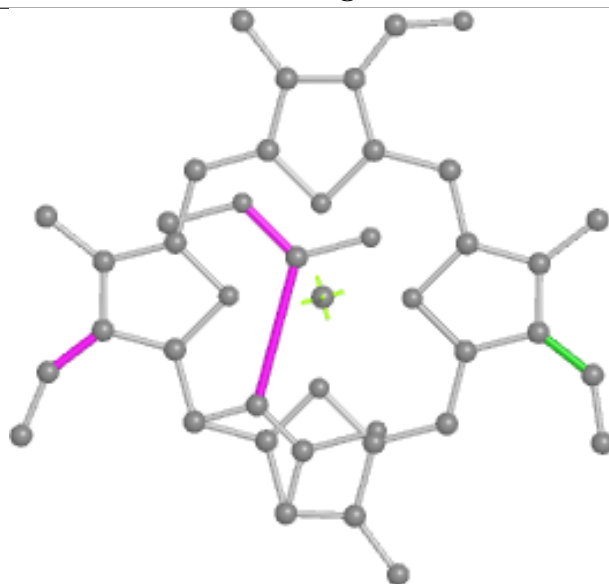
Ligand CL7 bA 3108



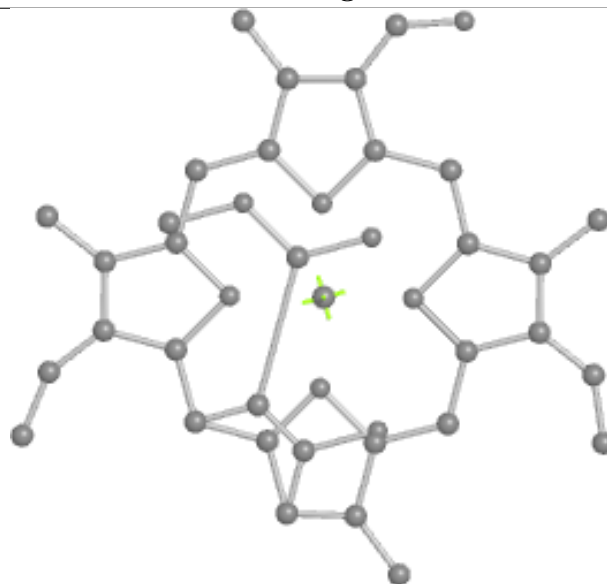
Bond lengths



Bond angles

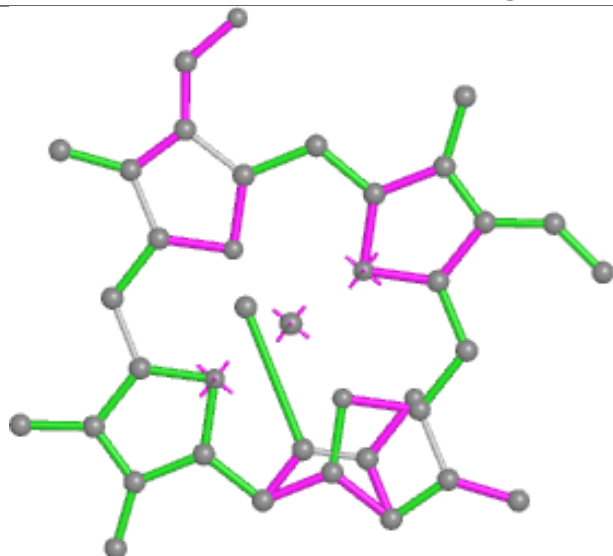


Torsions

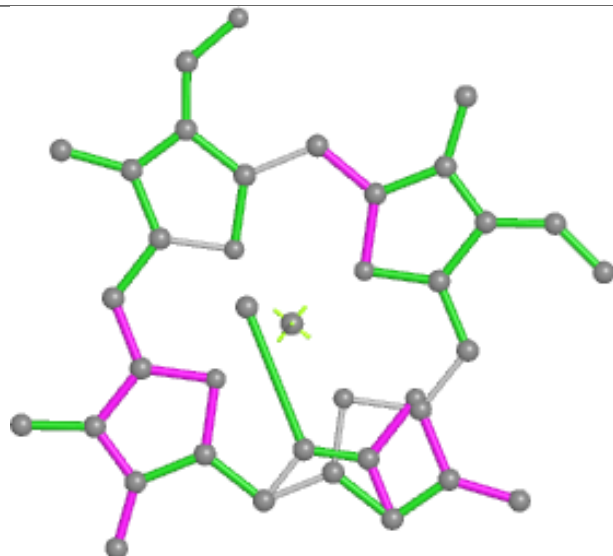


Rings

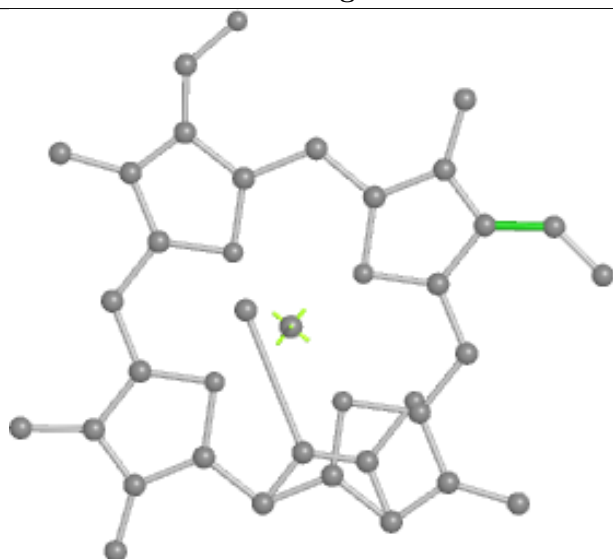
Ligand CL7 cA 3118



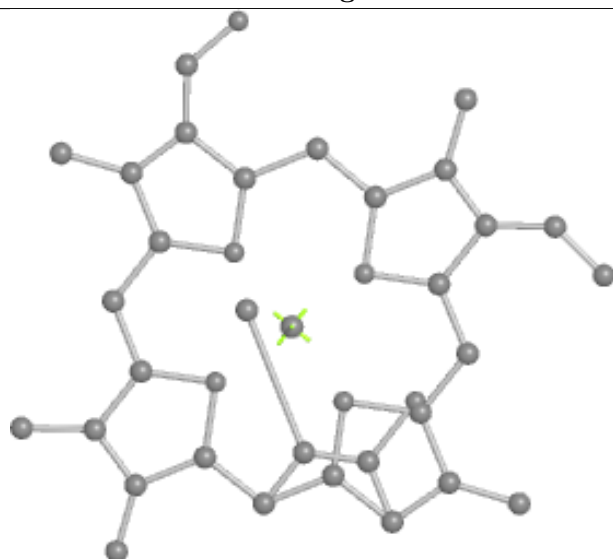
Bond lengths



Bond angles

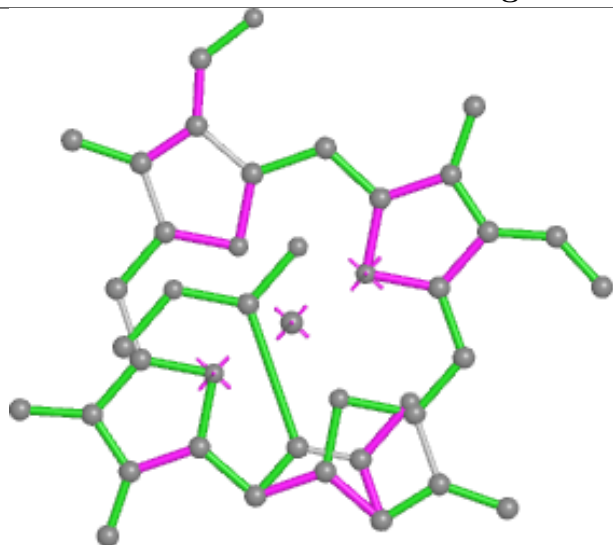


Torsions

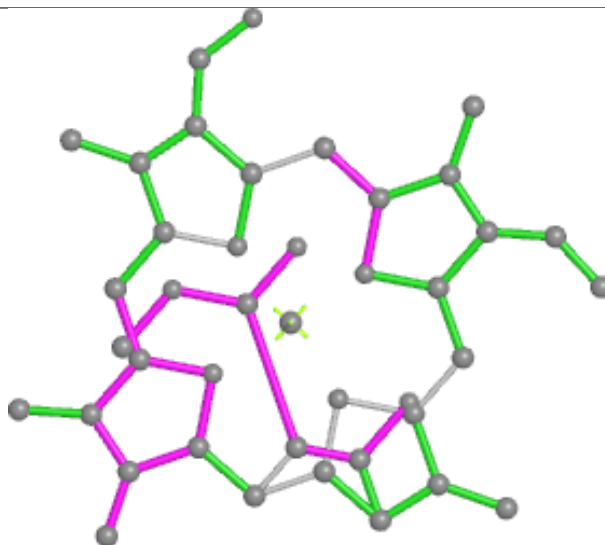


Rings

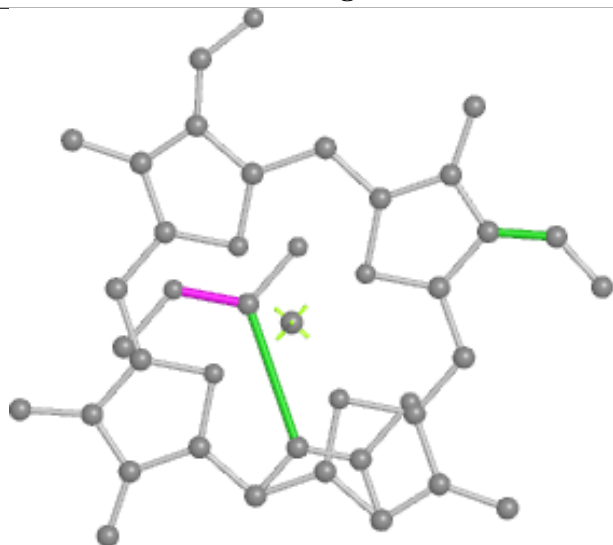
Ligand CL7 cA 3109



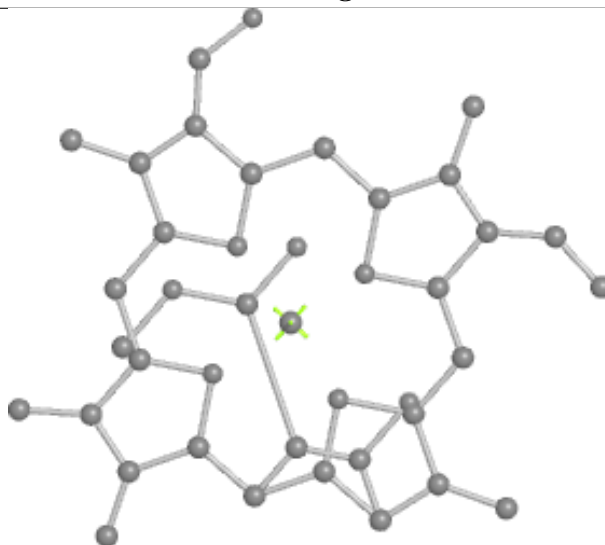
Bond lengths



Bond angles

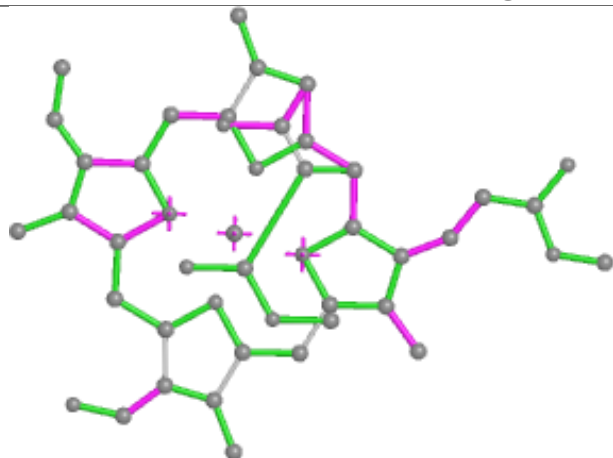


Torsions

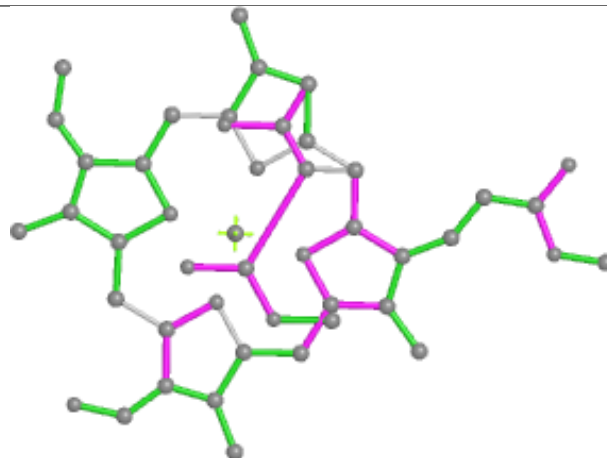


Rings

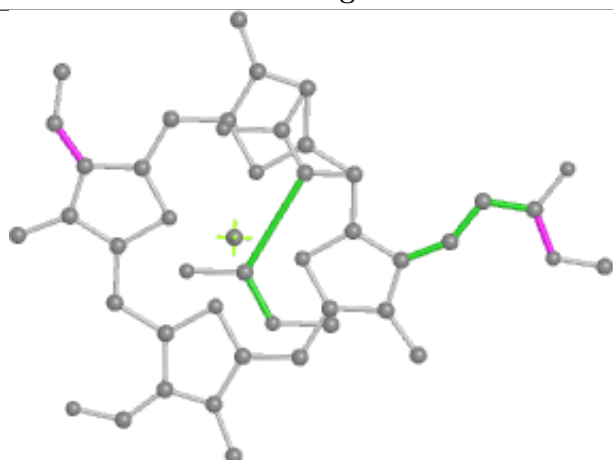
Ligand CL7 bA 3119



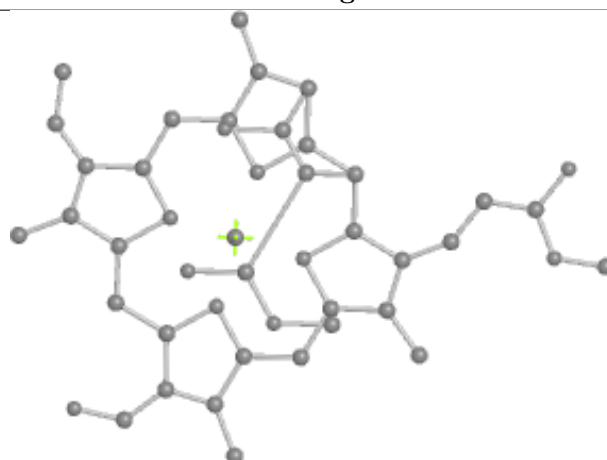
Bond lengths



Bond angles

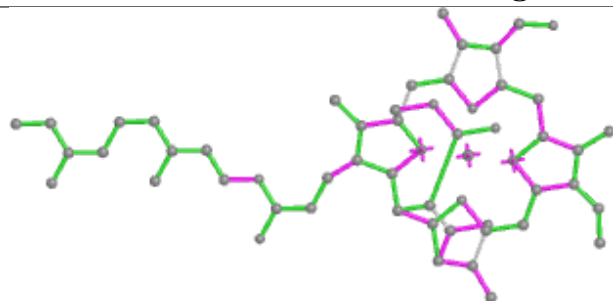


Torsions

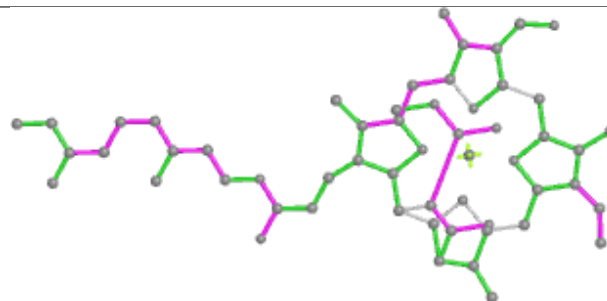


Rings

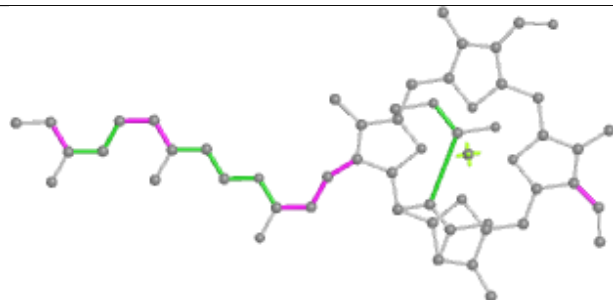
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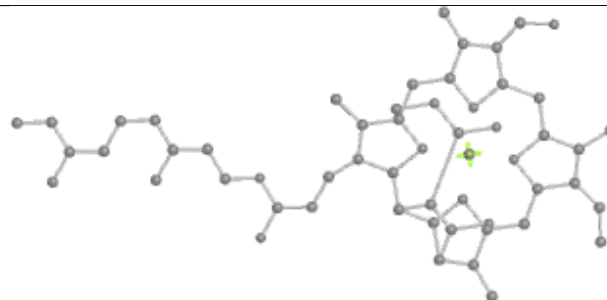
Bond lengths



Bond angles

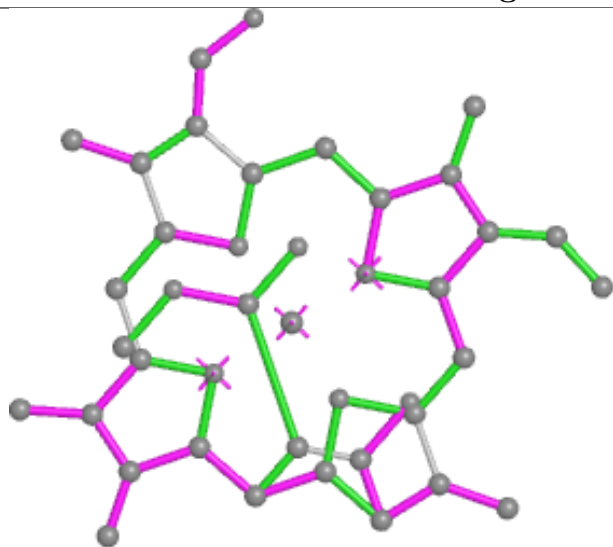


Torsions

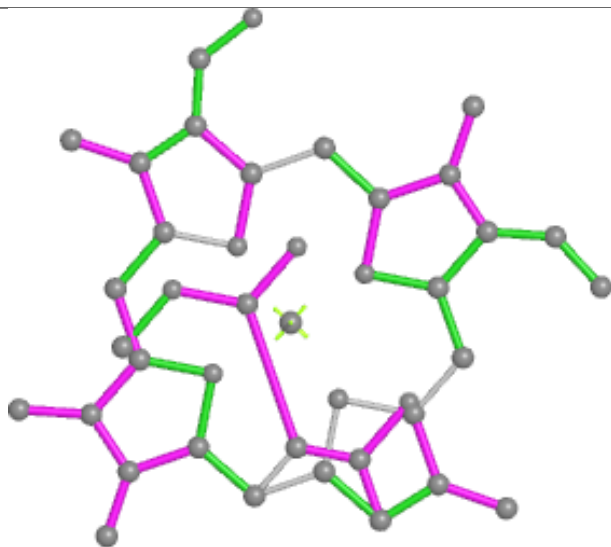


Rings

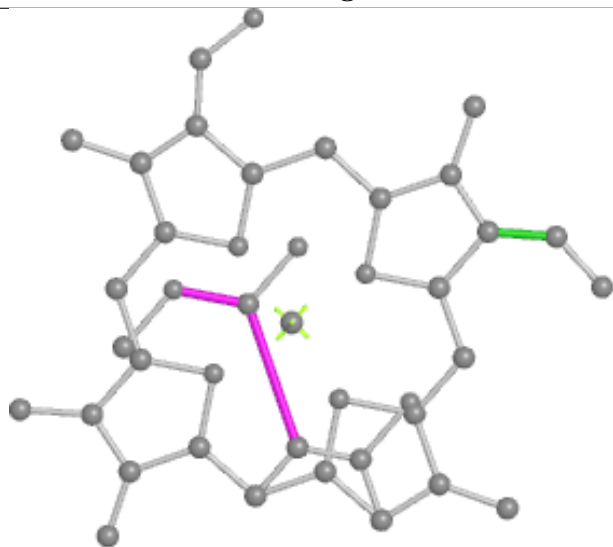
Ligand CL7 bA 3129



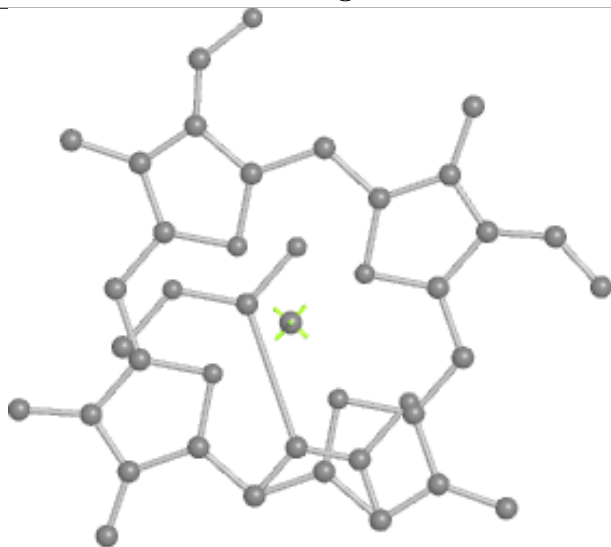
Bond lengths



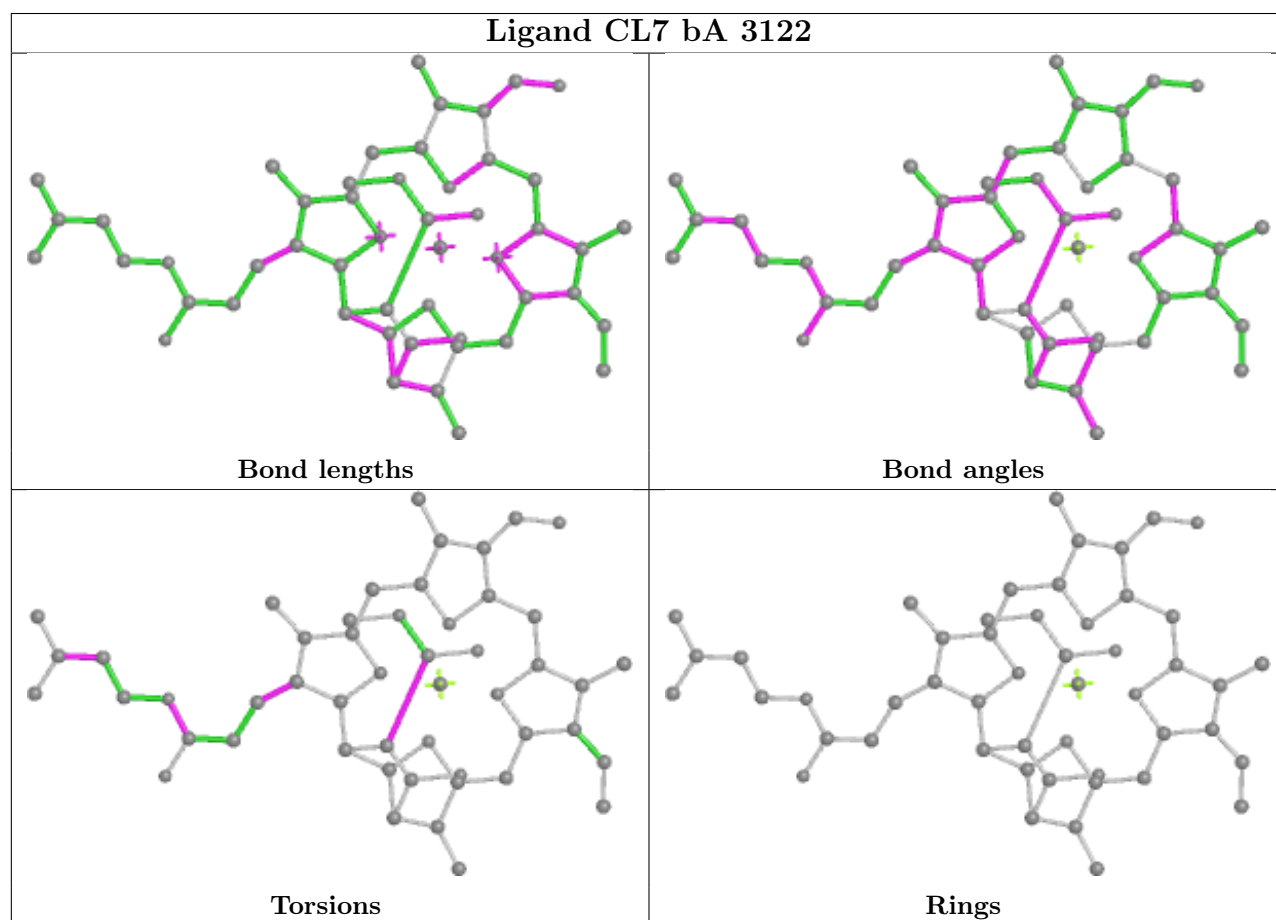
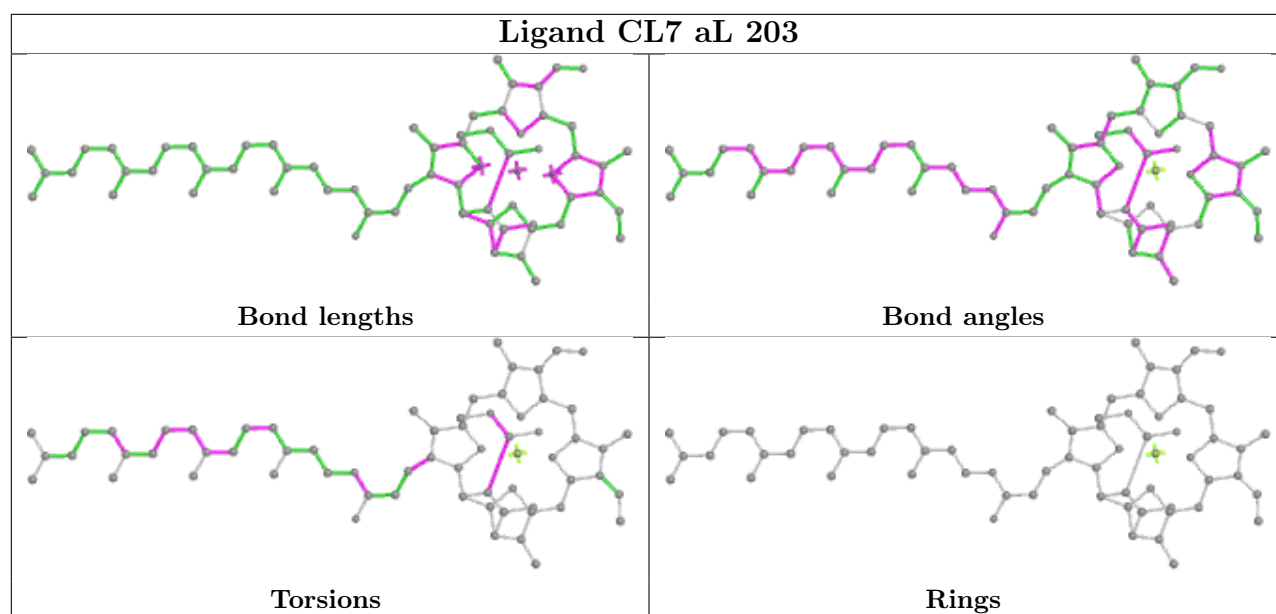
Bond angles



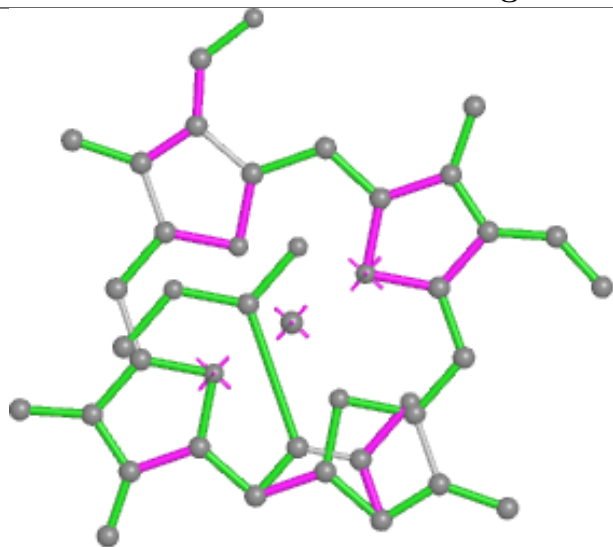
Torsions



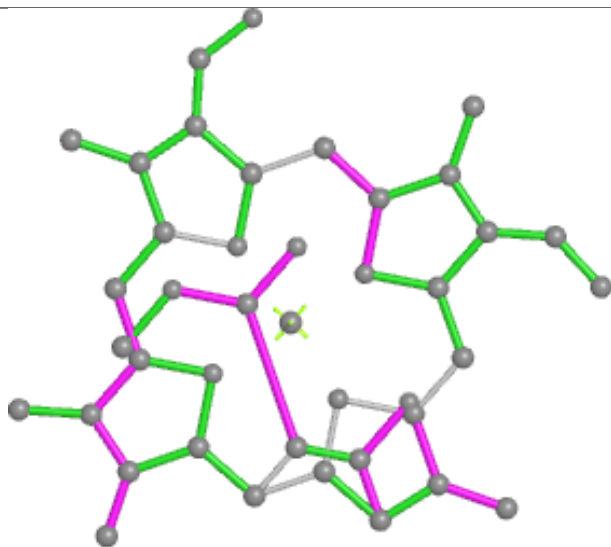
Rings



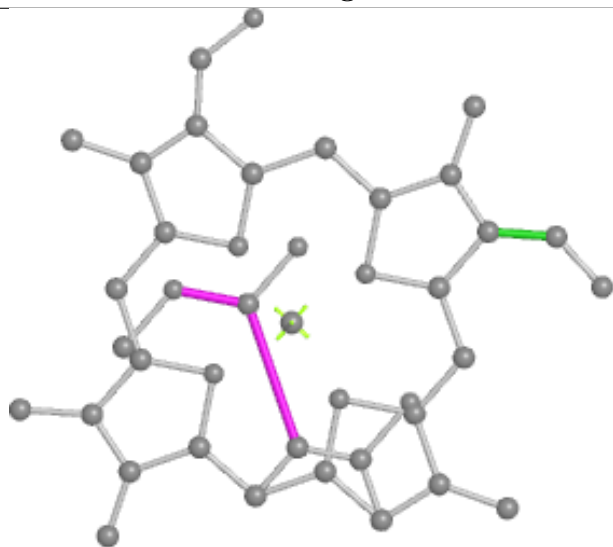
Ligand CL7 aA 3105



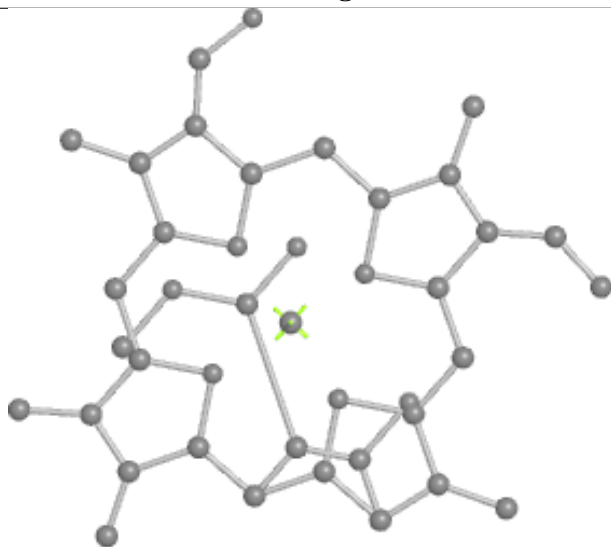
Bond lengths



Bond angles

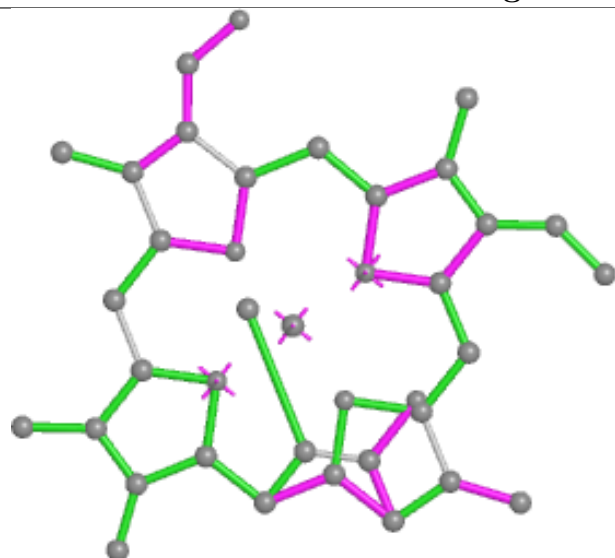


Torsions

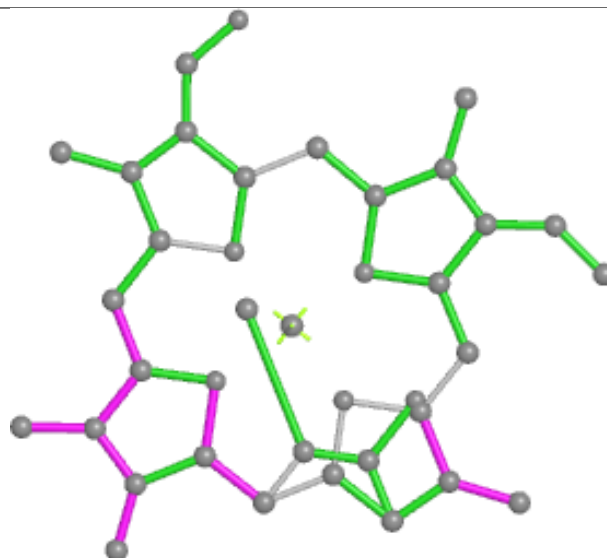


Rings

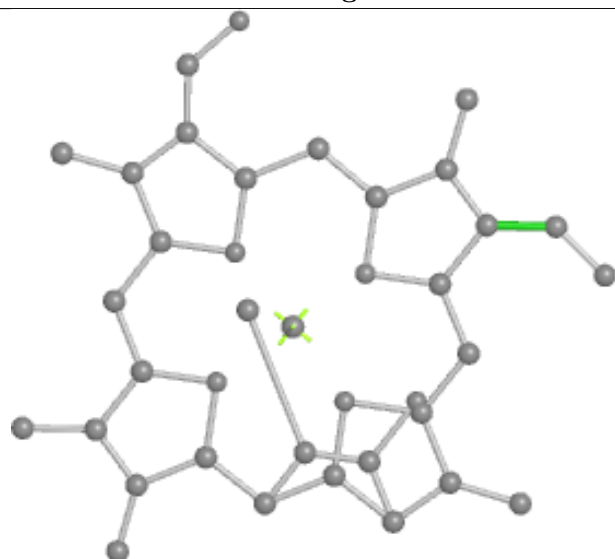
Ligand CL7 aB 3024



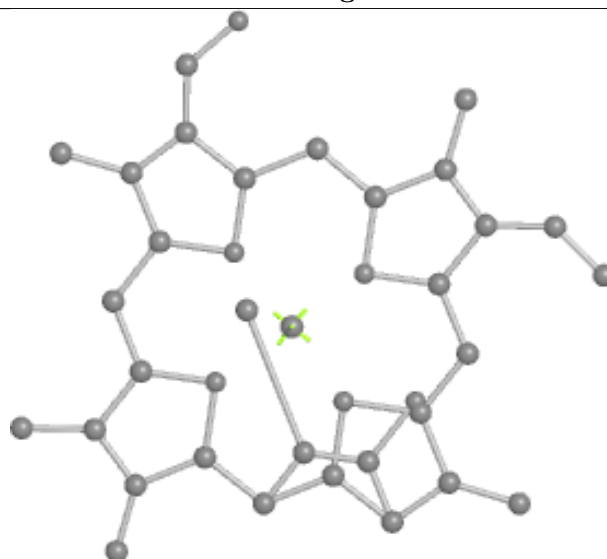
Bond lengths



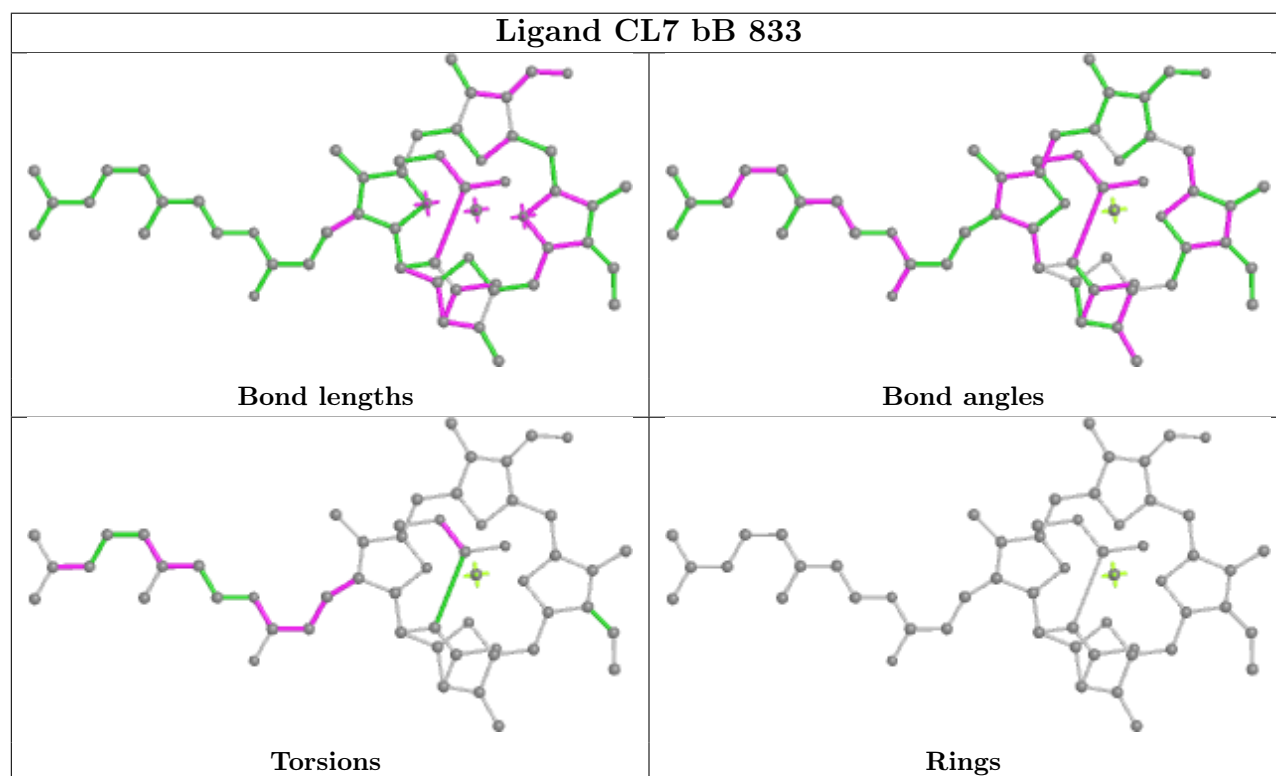
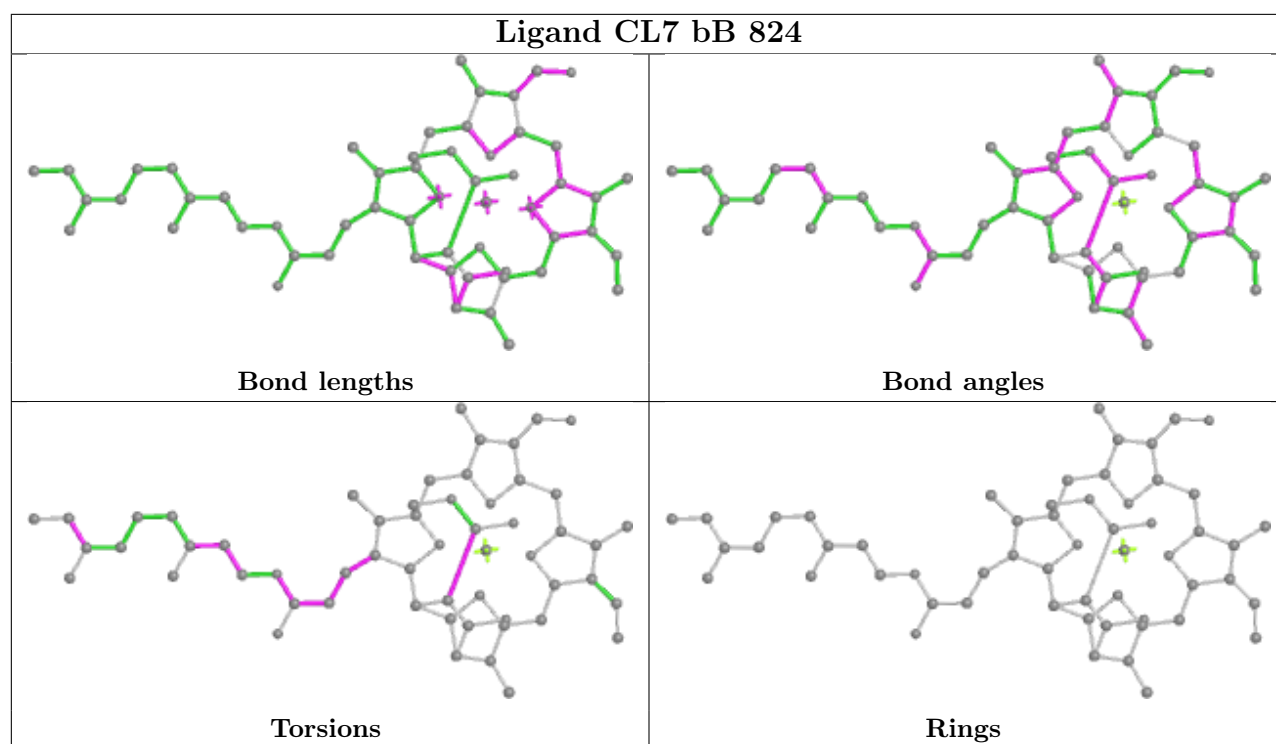
Bond angles

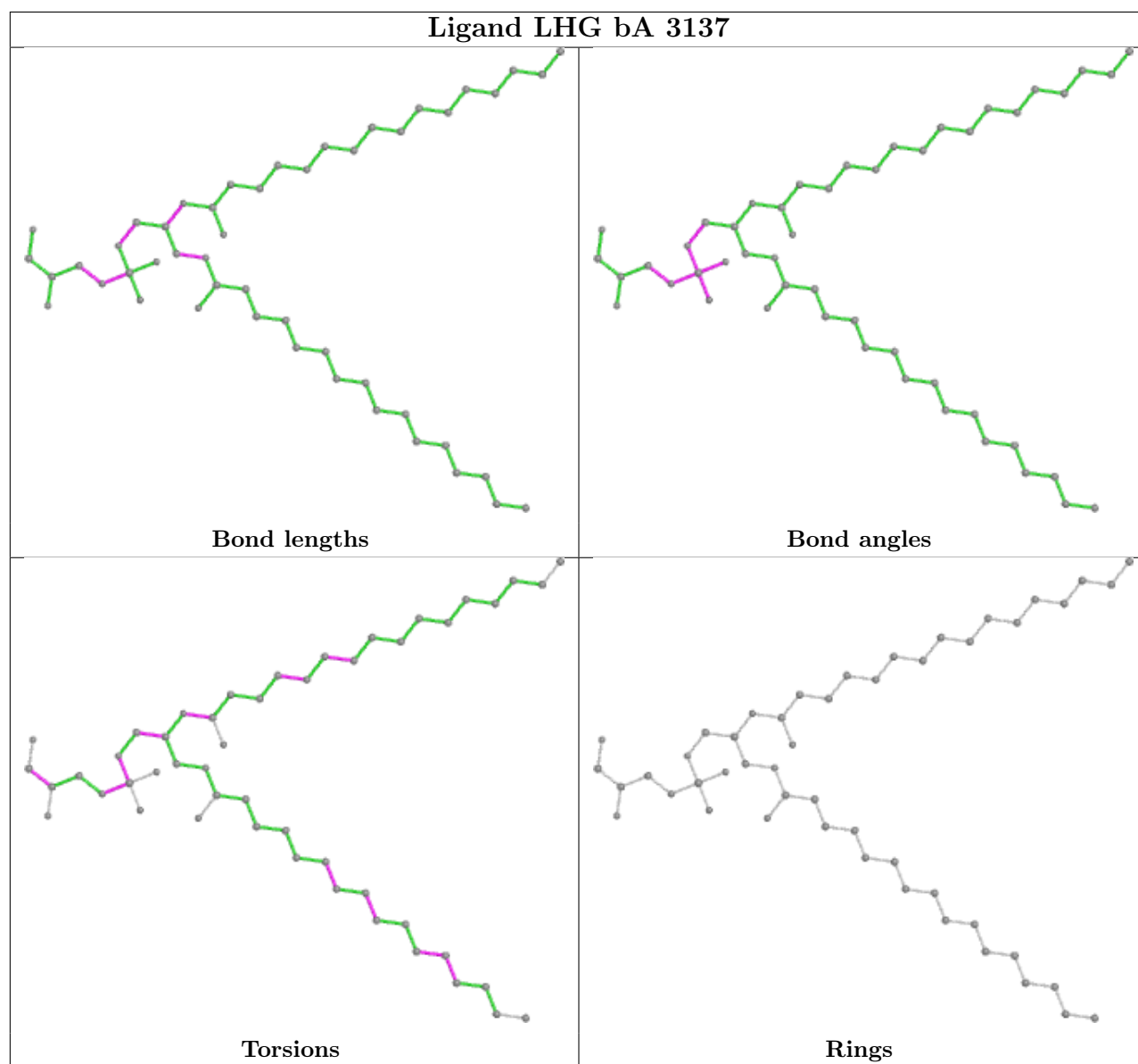
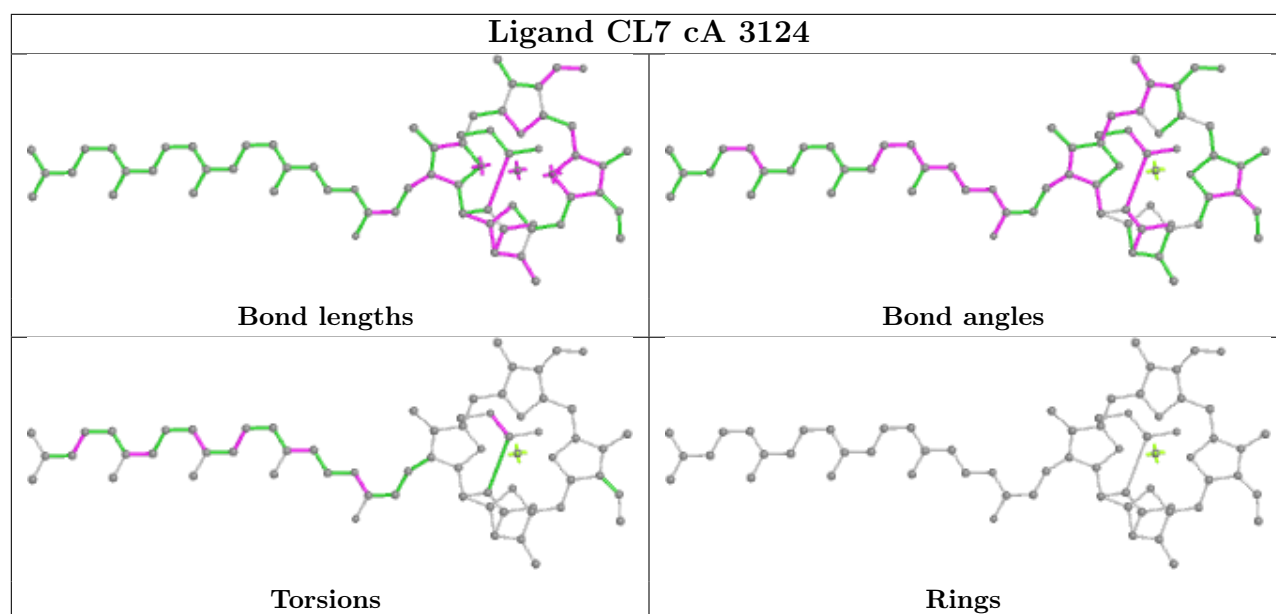


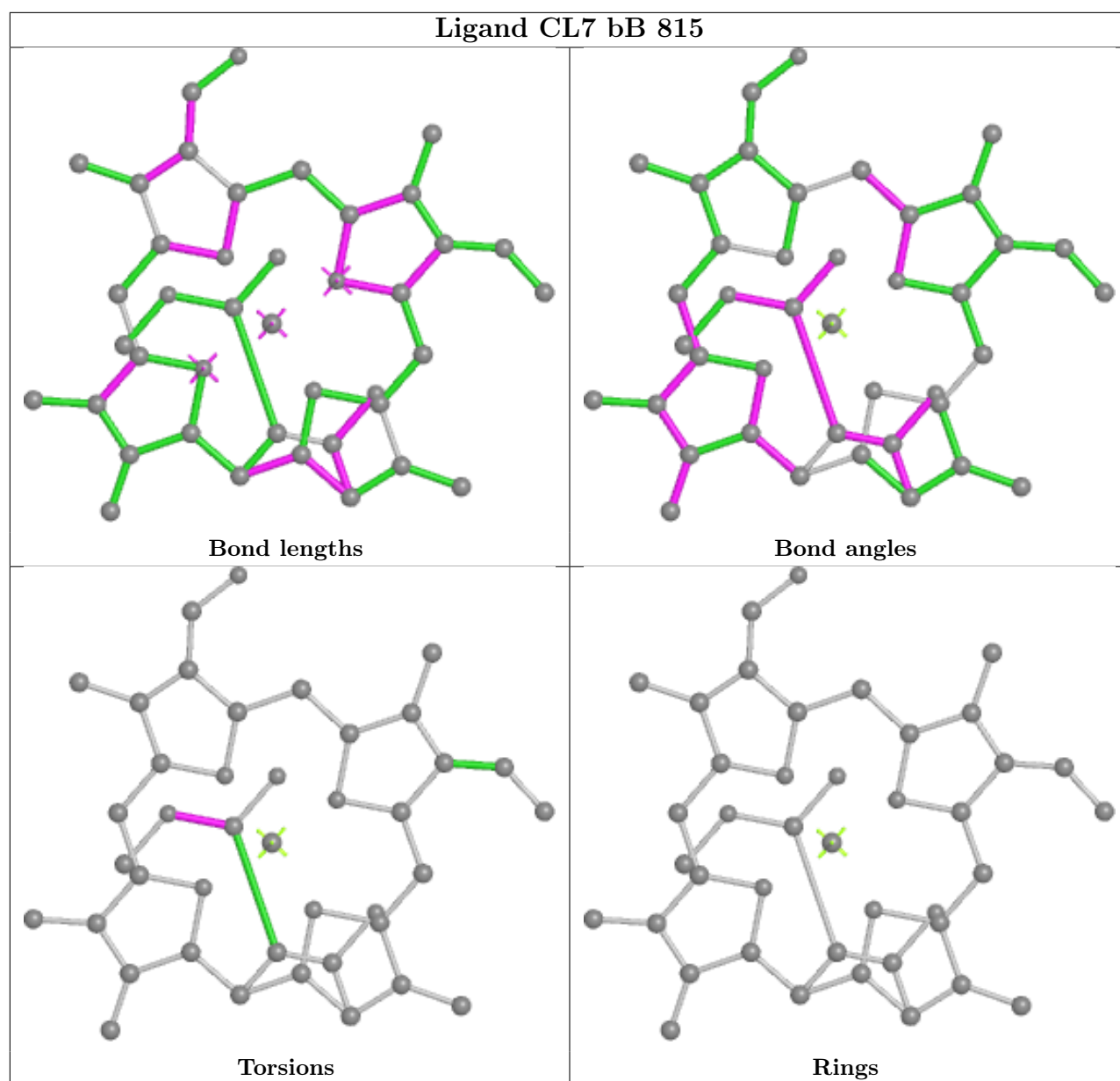
Torsions



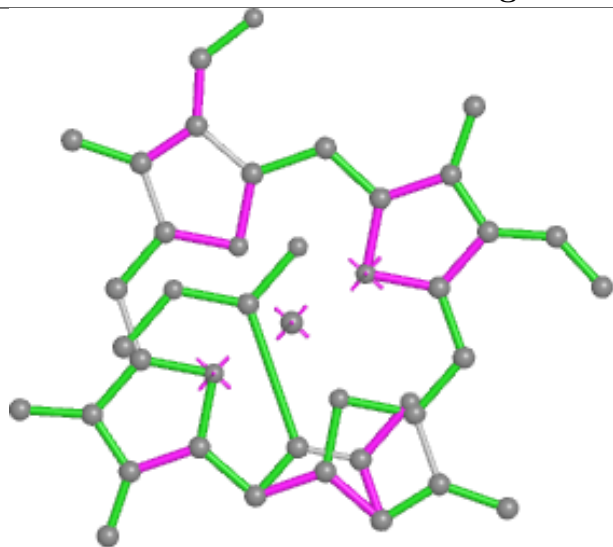
Rings



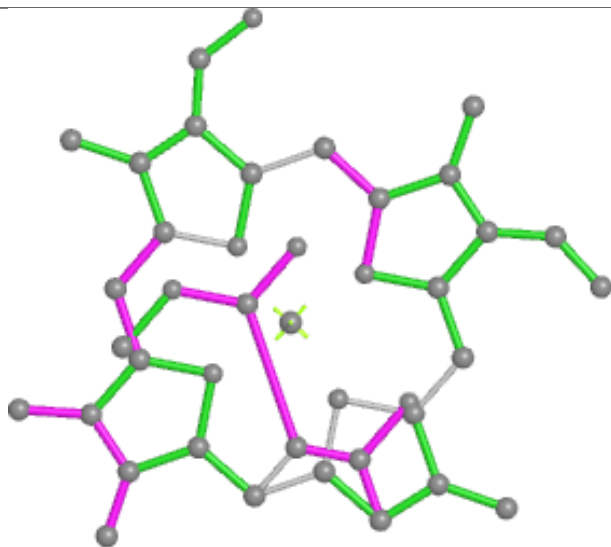




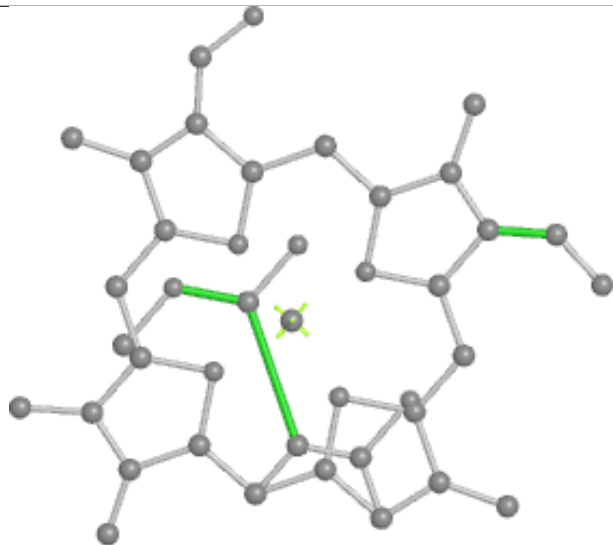
Ligand CL7 bA 3113



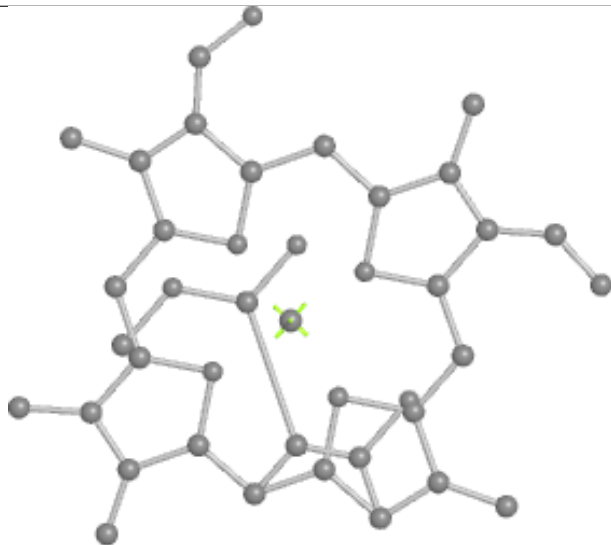
Bond lengths



Bond angles

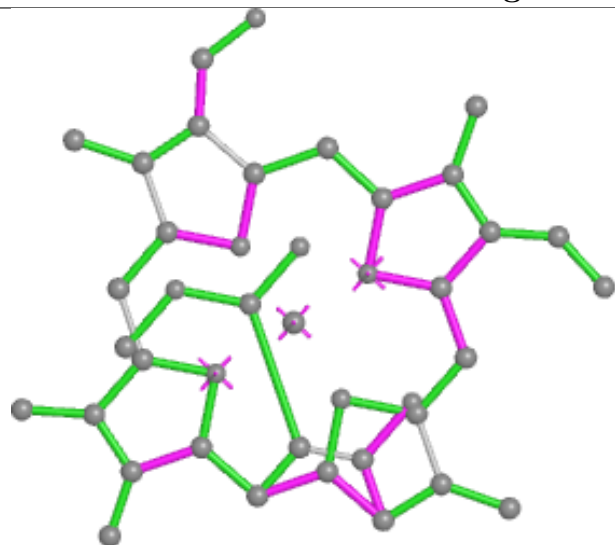


Torsions

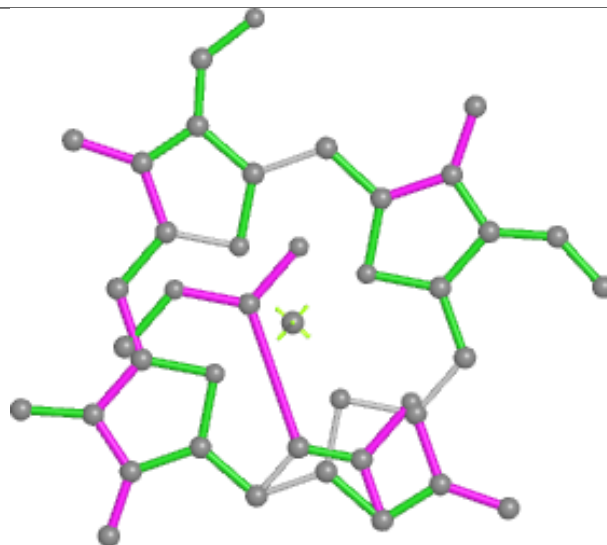


Rings

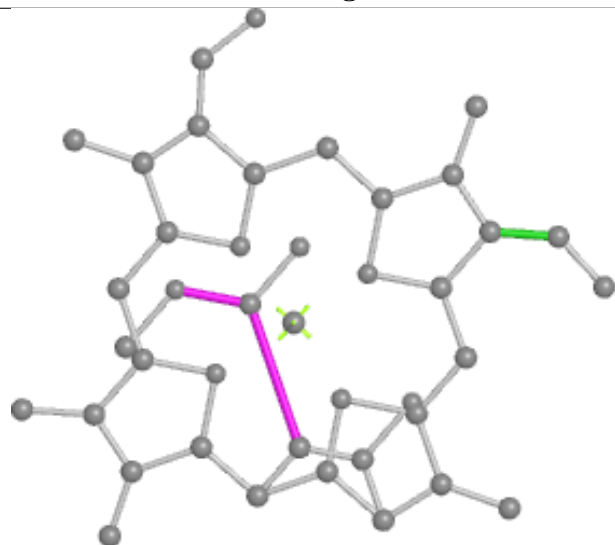
Ligand CL7 aB 3021



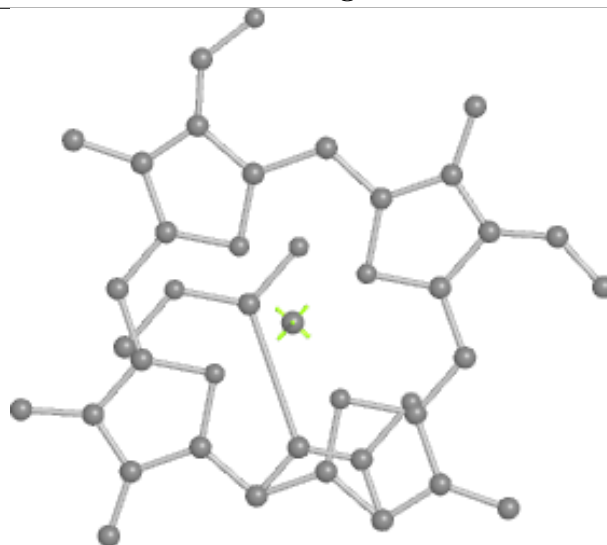
Bond lengths



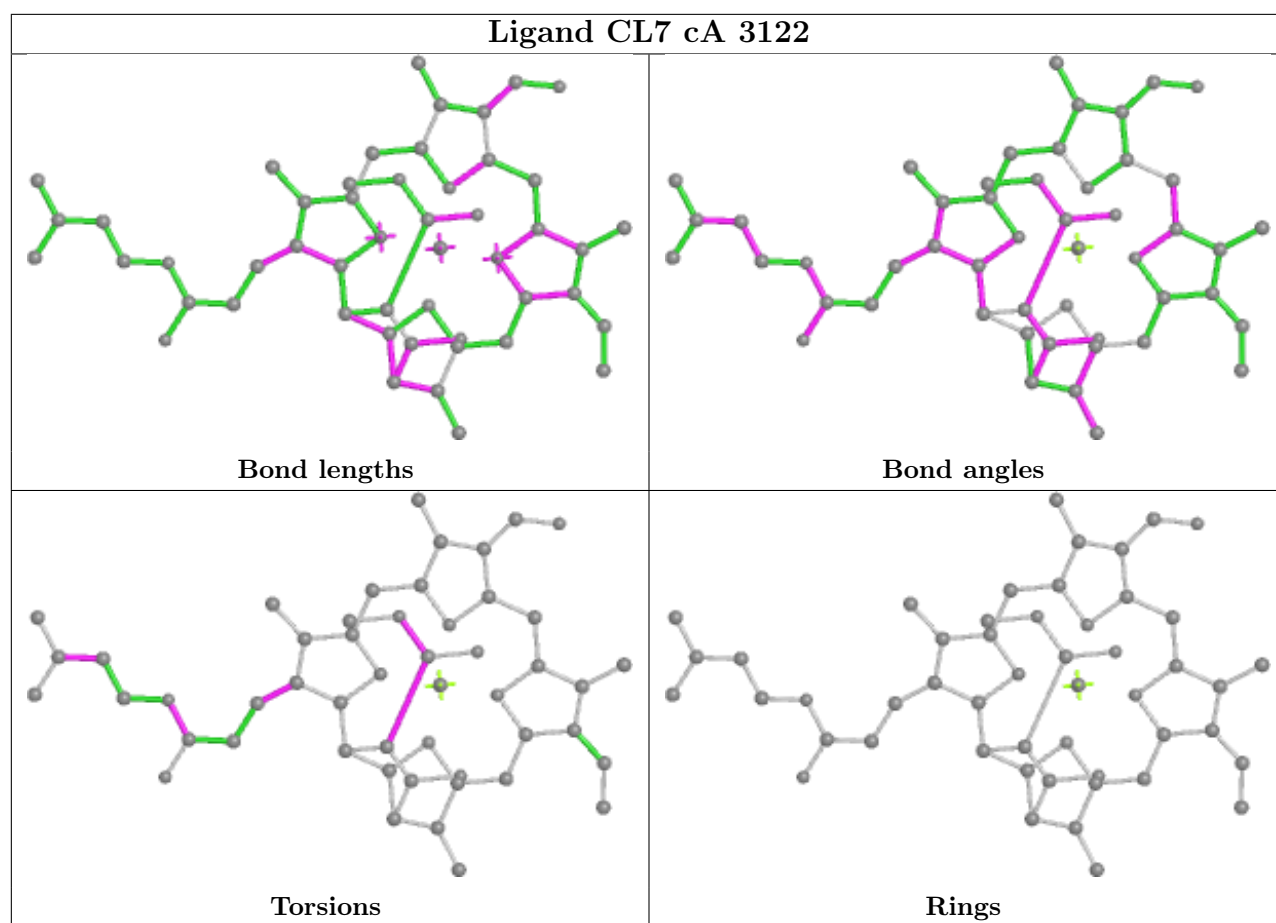
Bond angles

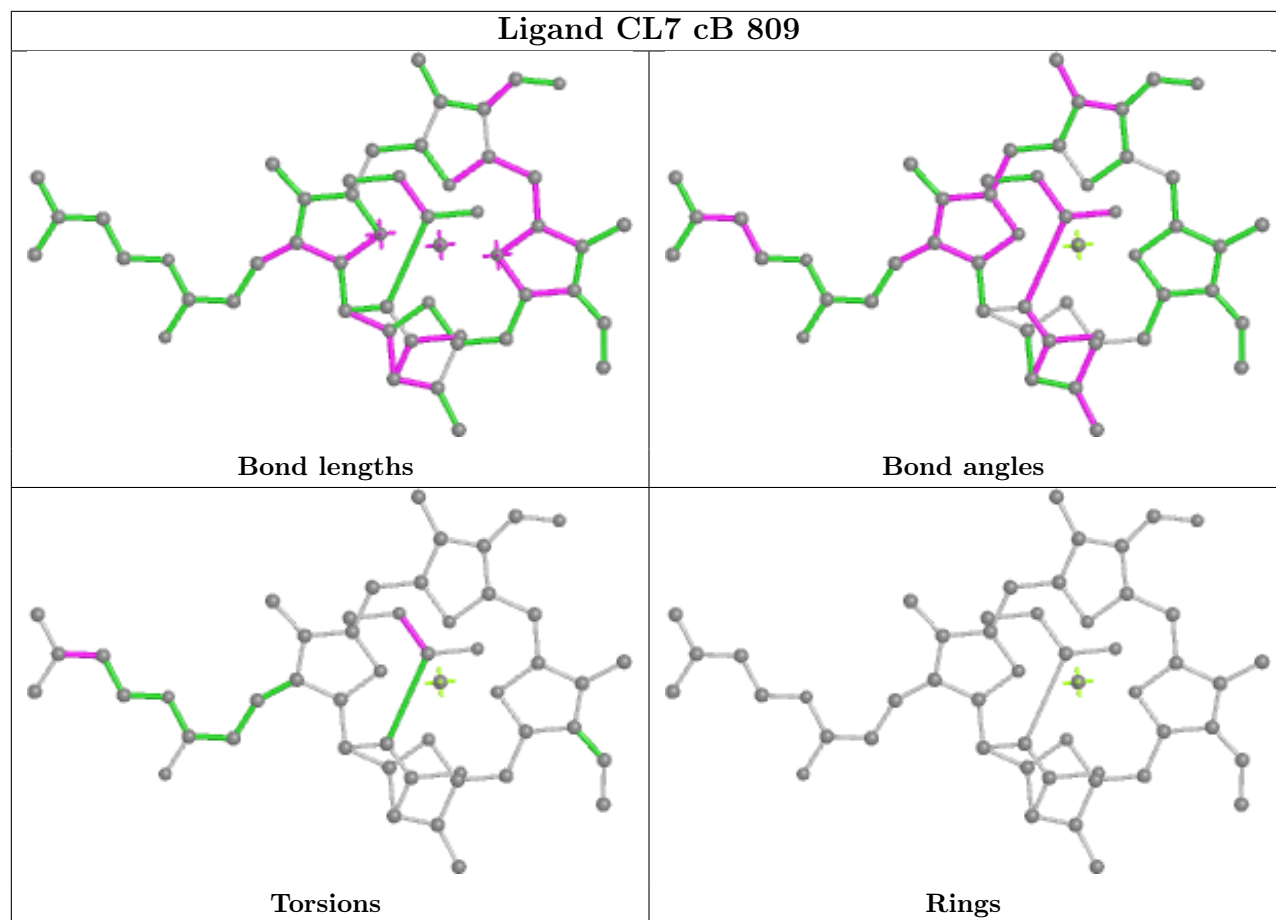


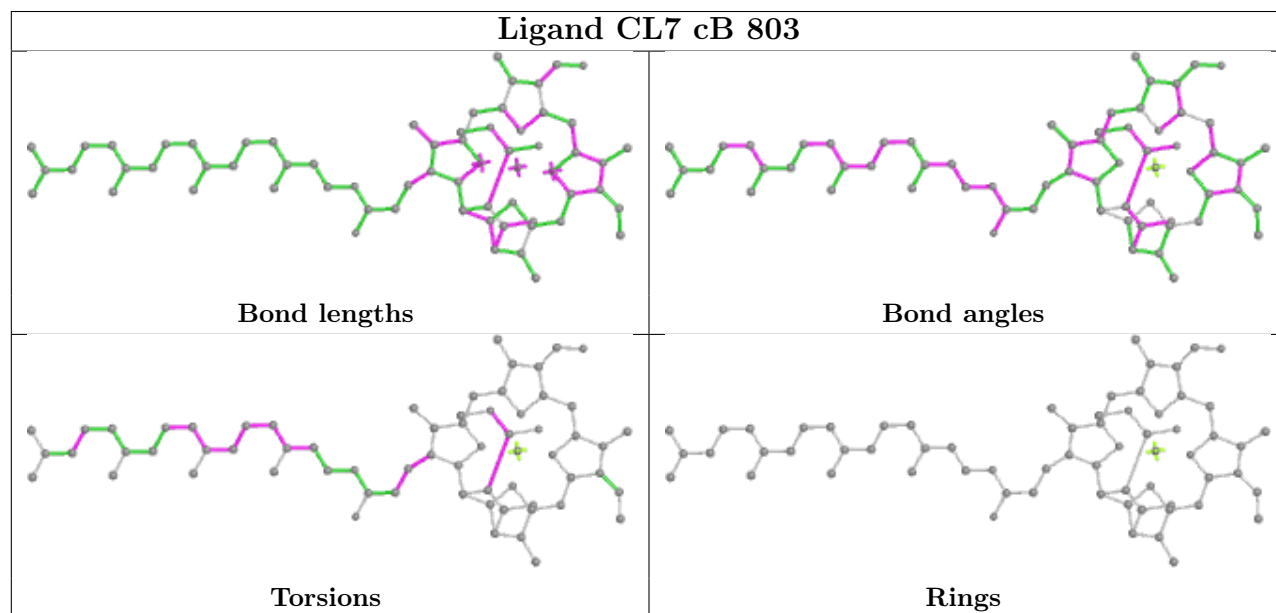
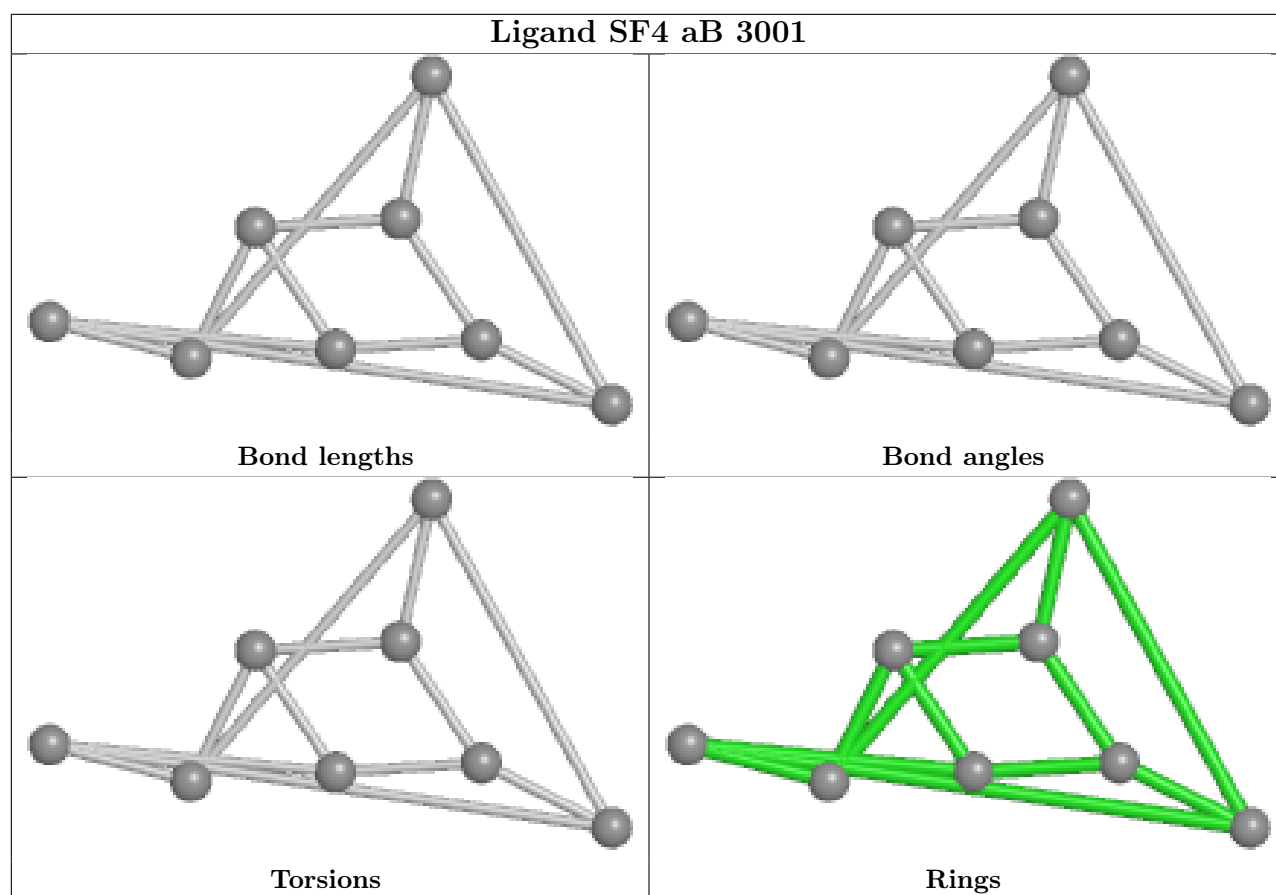
Torsions



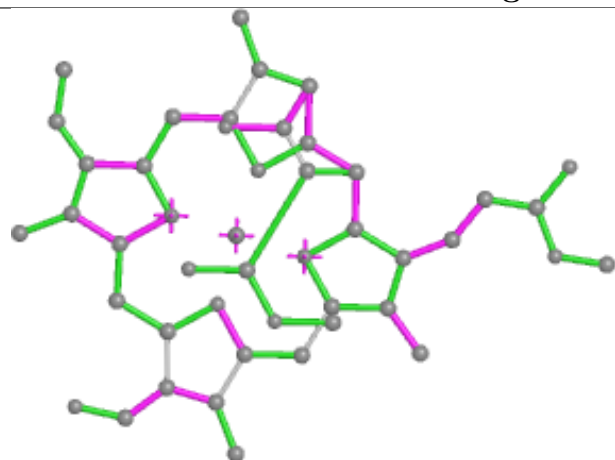
Rings



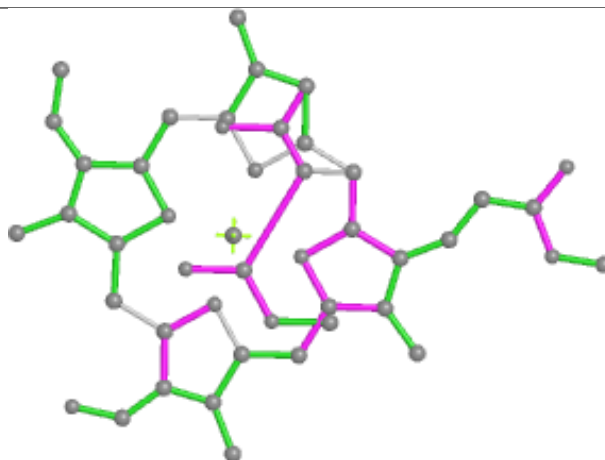




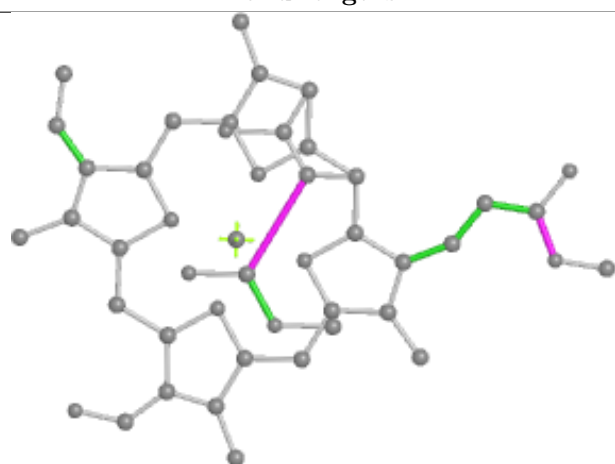
Ligand CL7 aA 3120



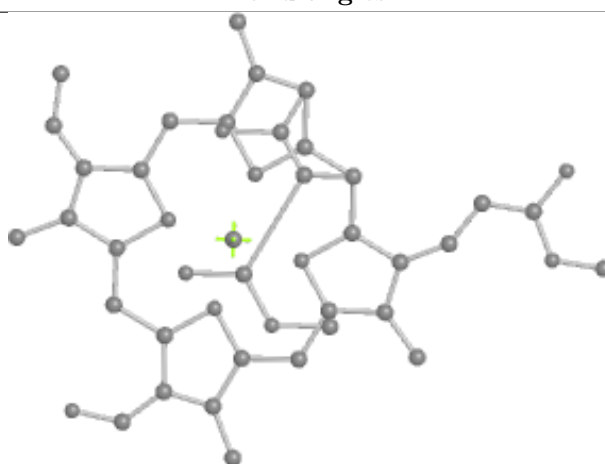
Bond lengths



Bond angles

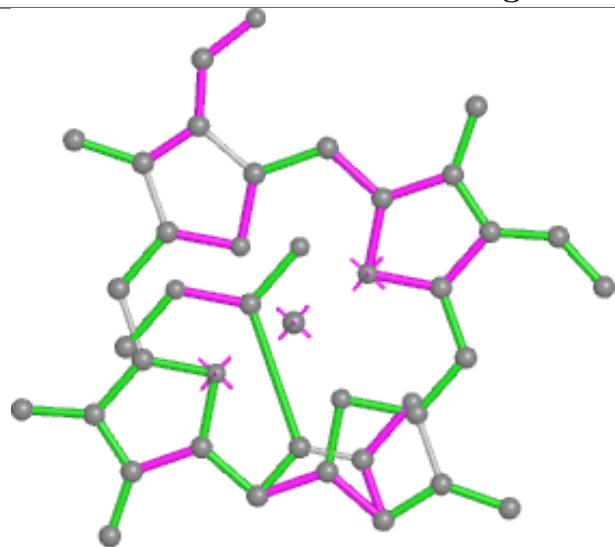


Torsions

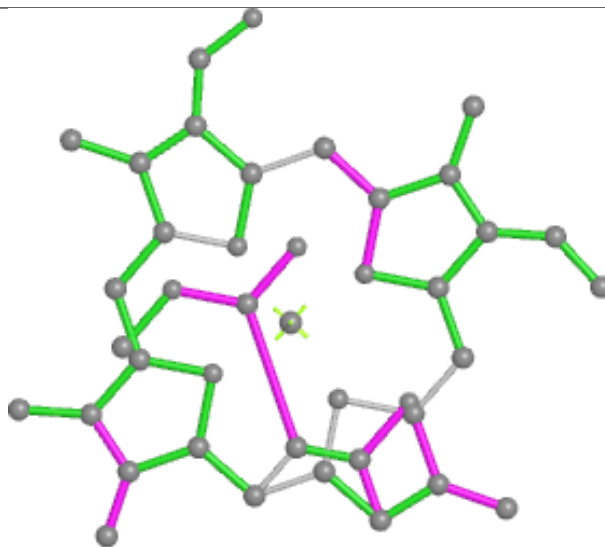


Rings

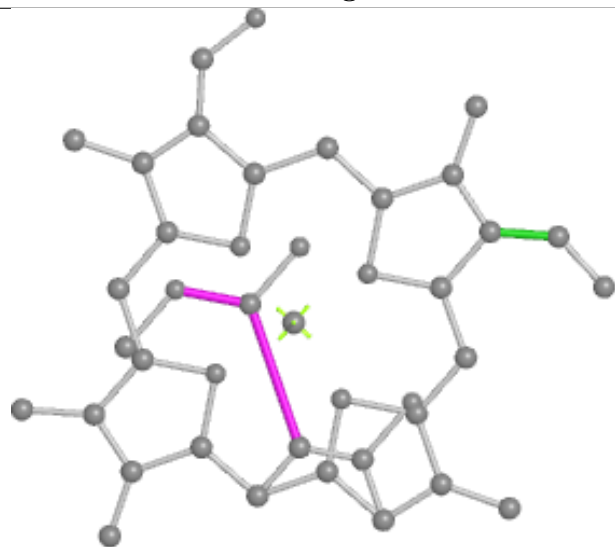
Ligand CL7 aA 3131



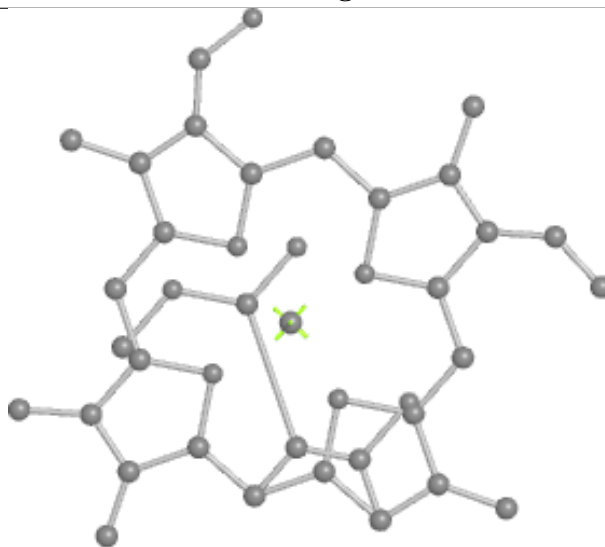
Bond lengths



Bond angles

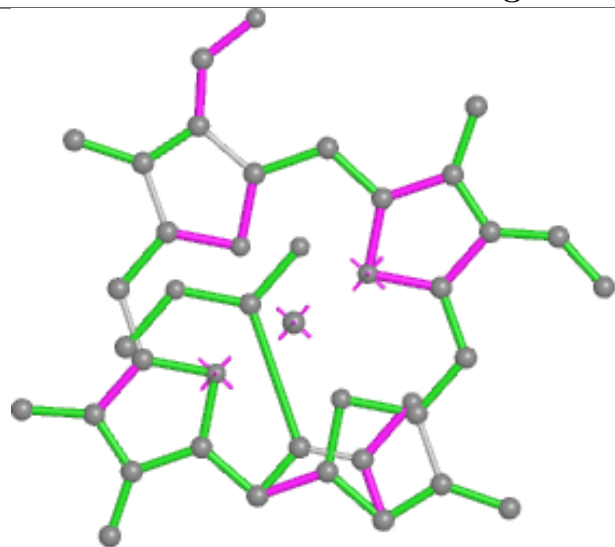


Torsions

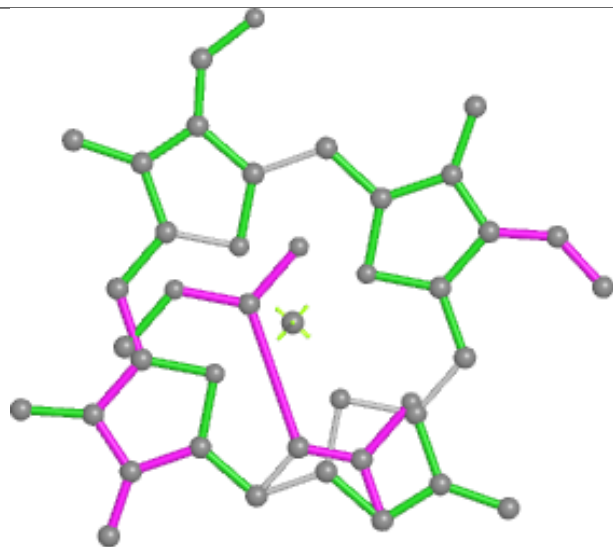


Rings

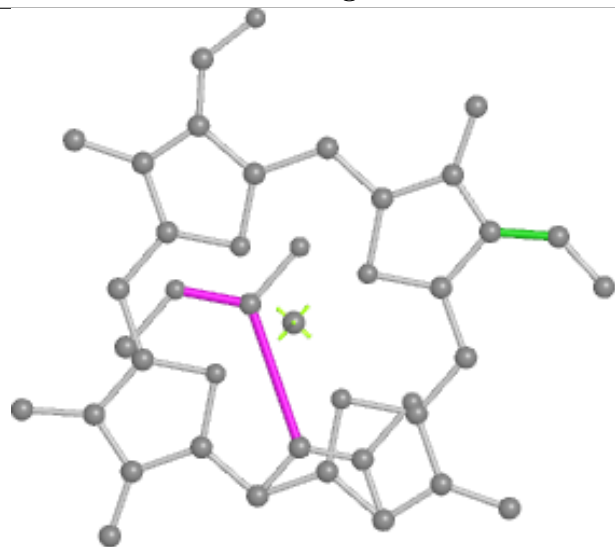
Ligand CL7 cA 3133



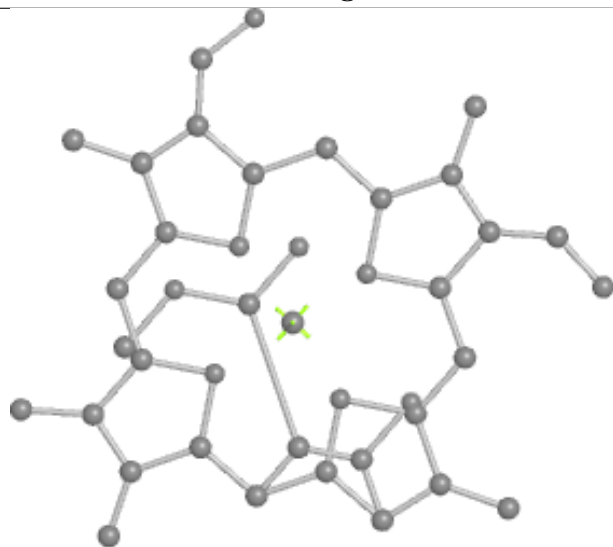
Bond lengths



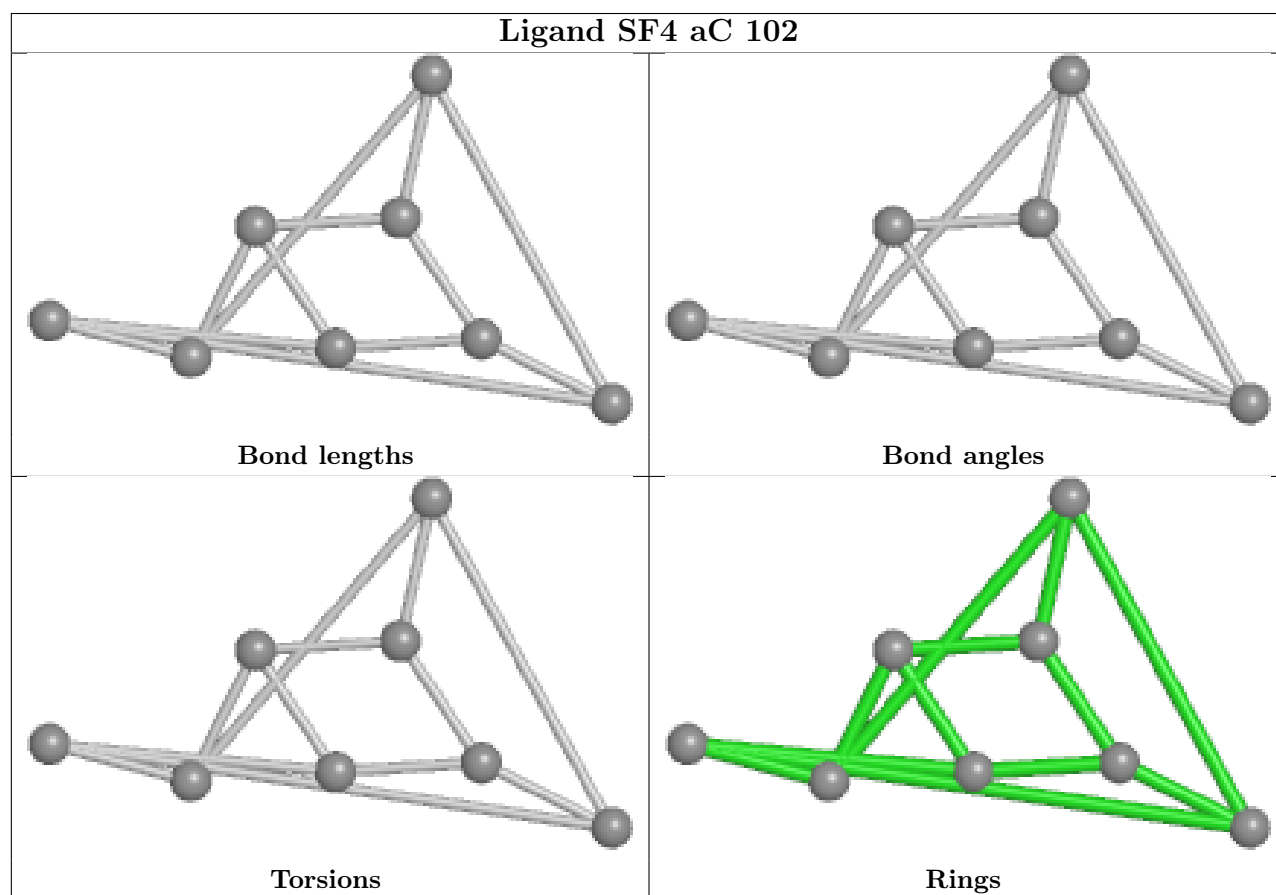
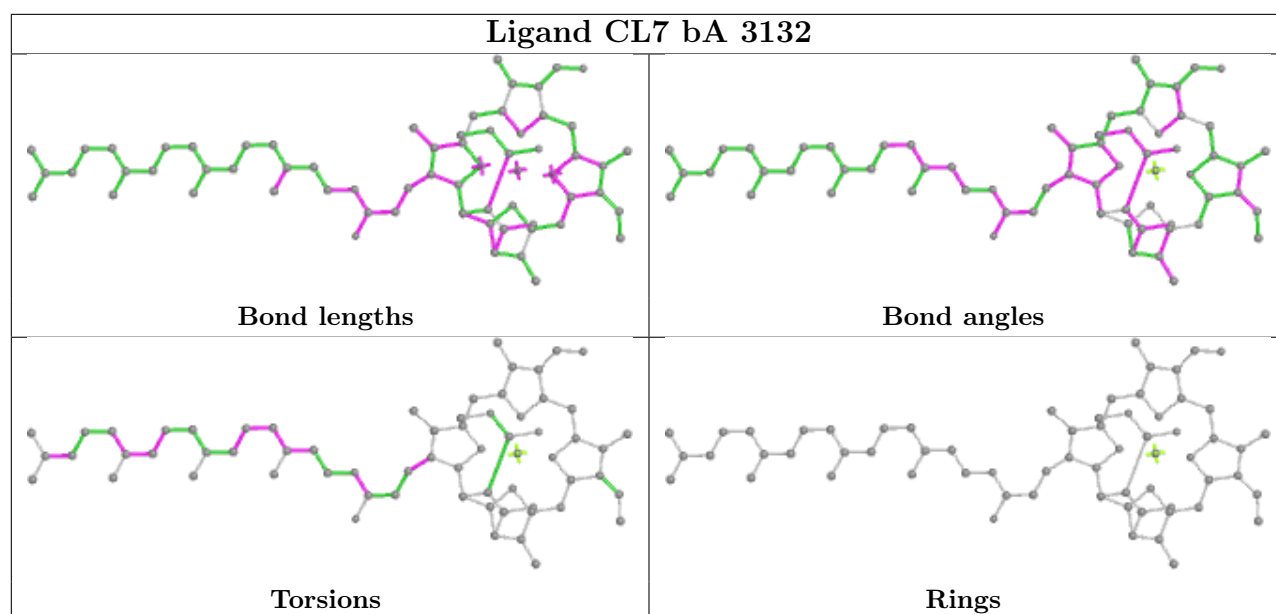
Bond angles



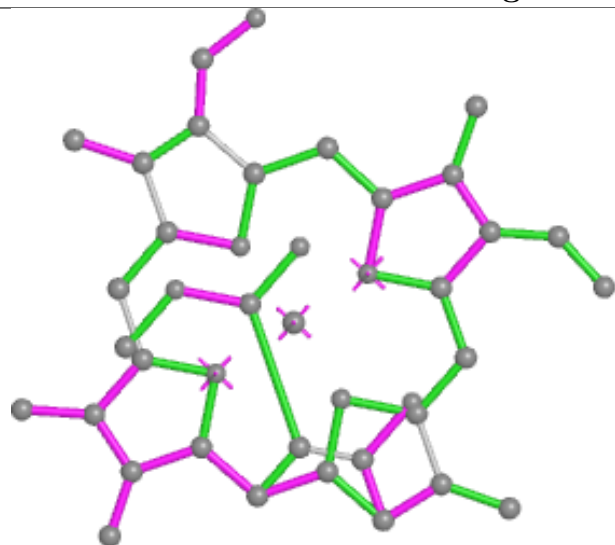
Torsions



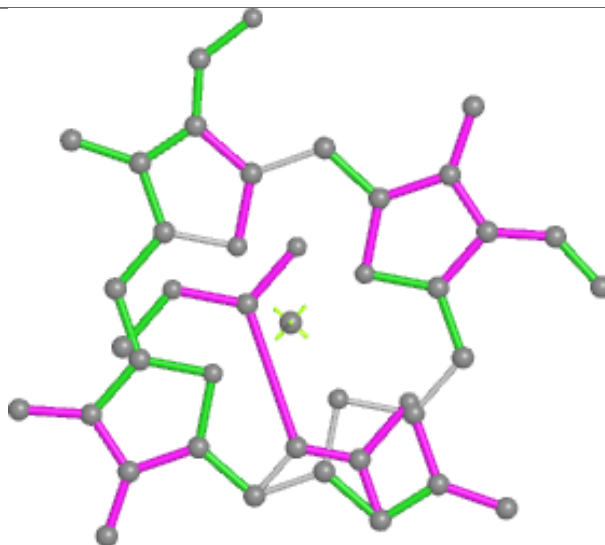
Rings



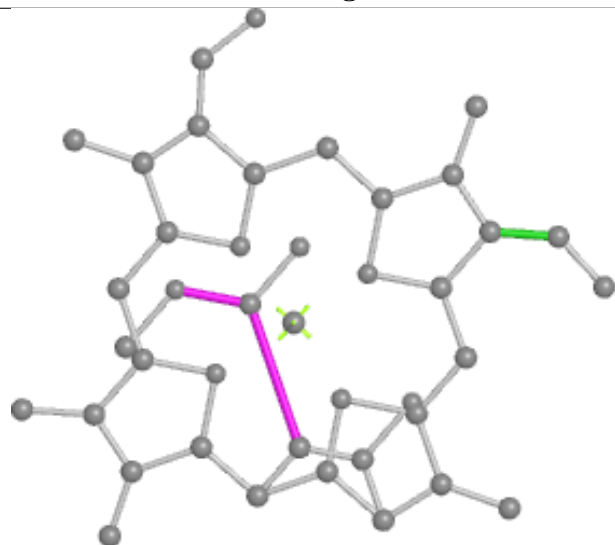
Ligand CL7 aA 3130



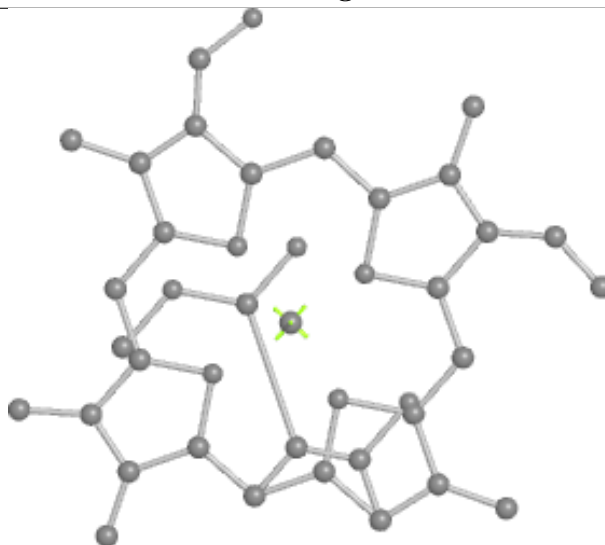
Bond lengths



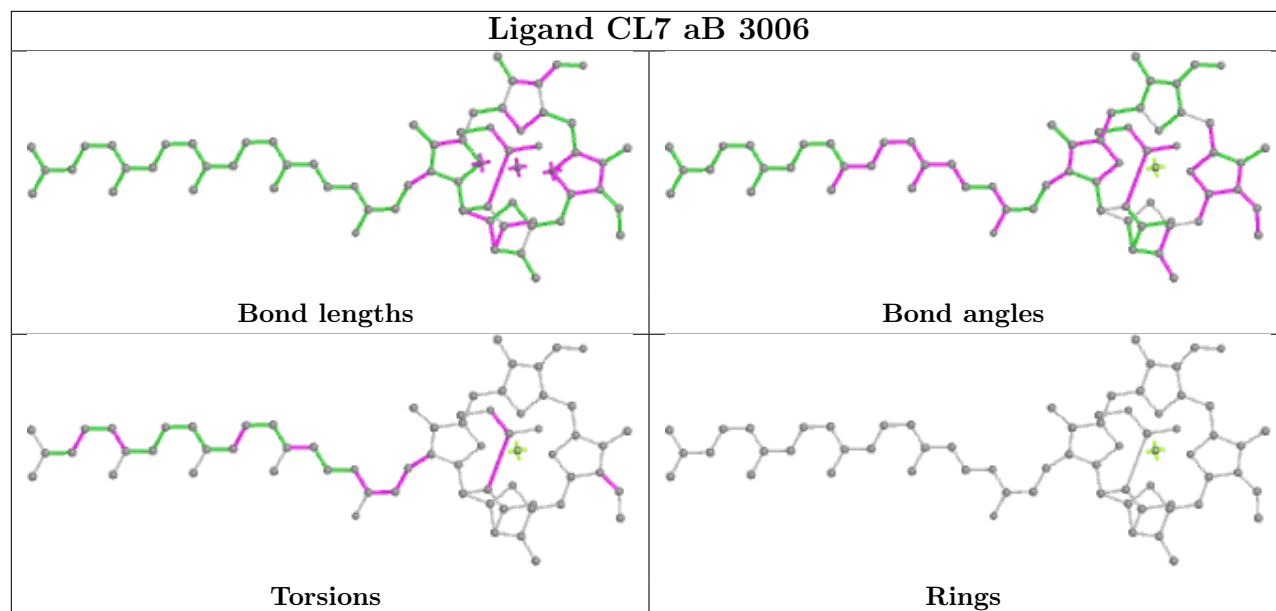
Bond angles

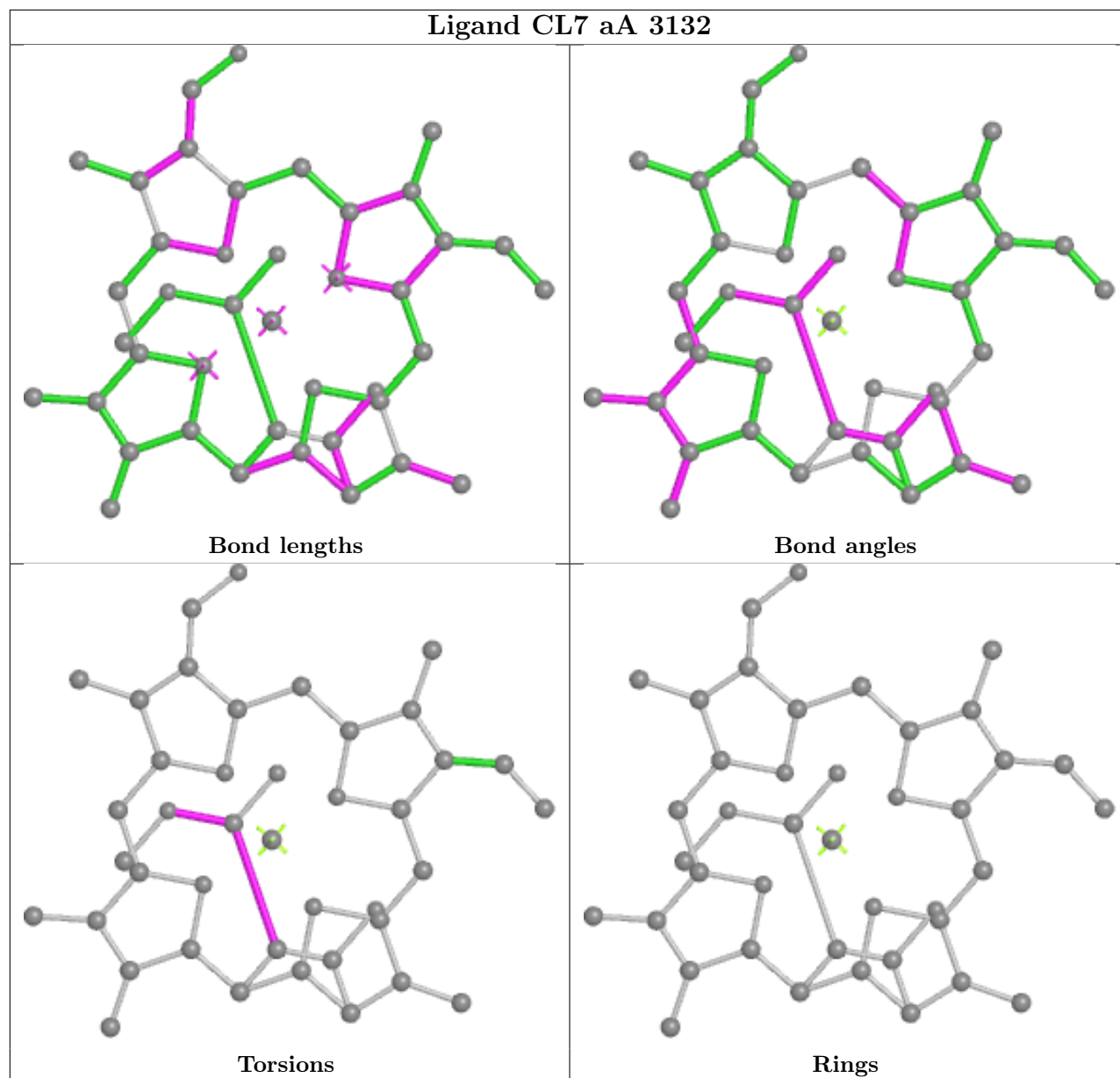


Torsions

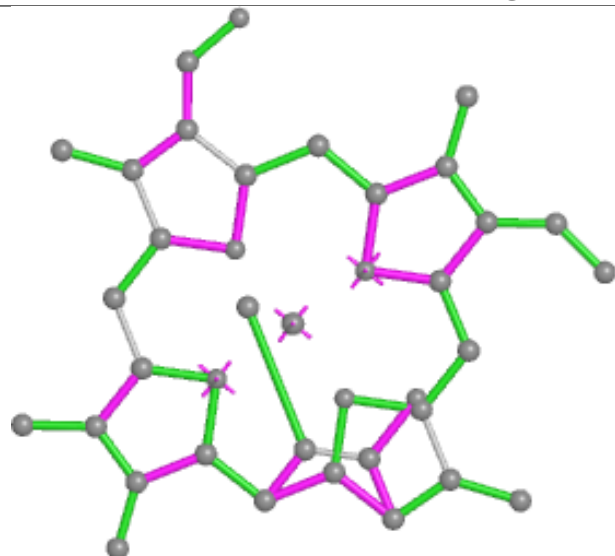


Rings

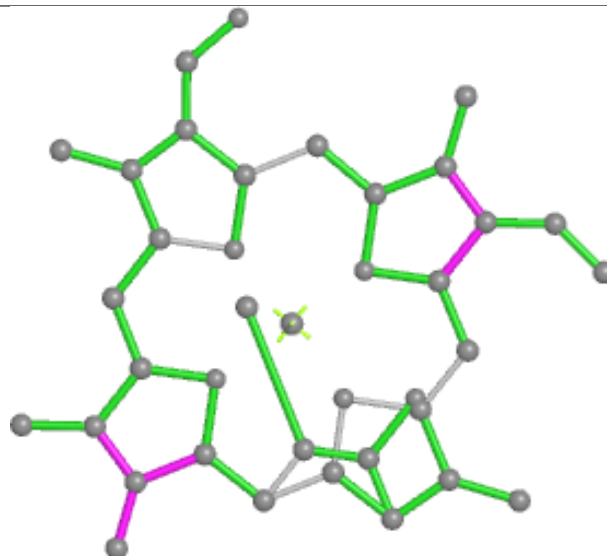




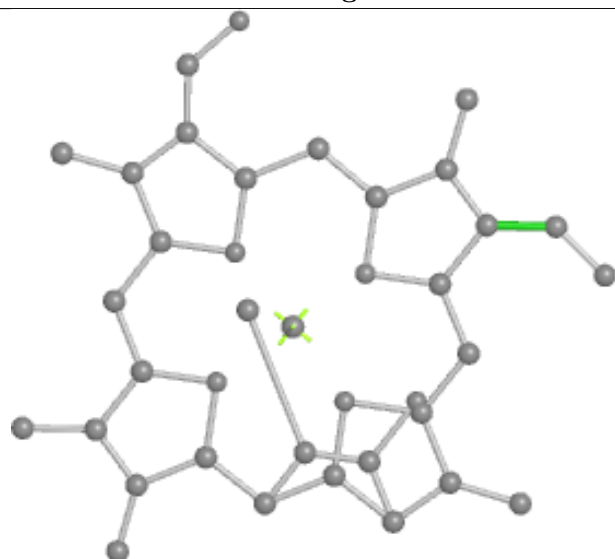
Ligand CL7 aB 3011



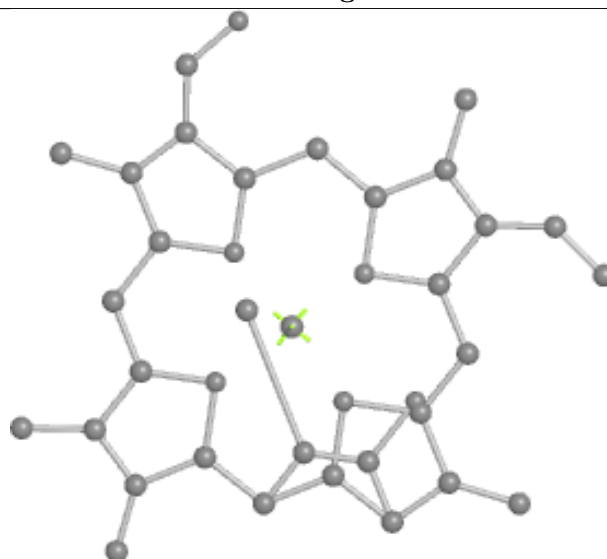
Bond lengths



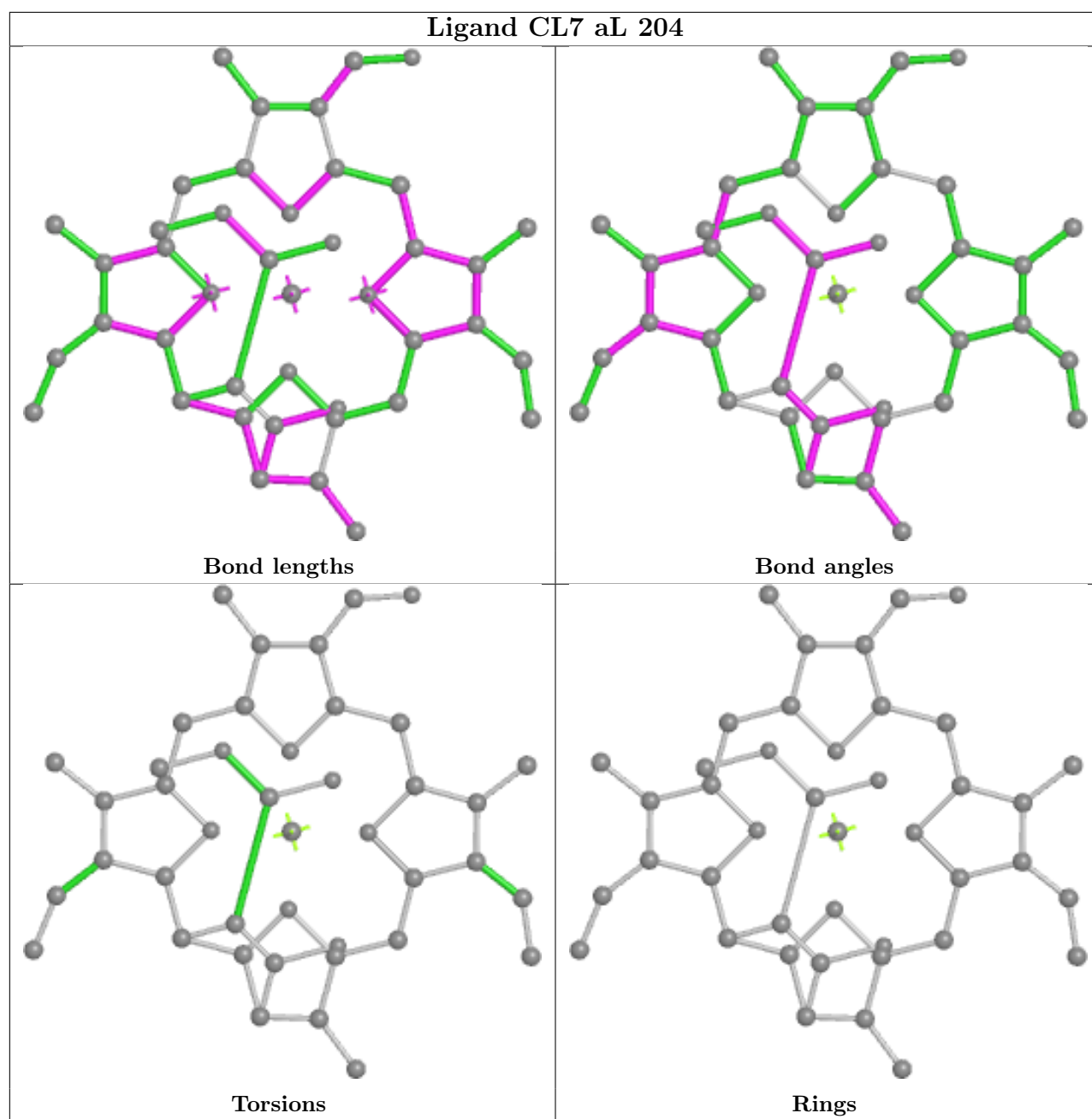
Bond angles

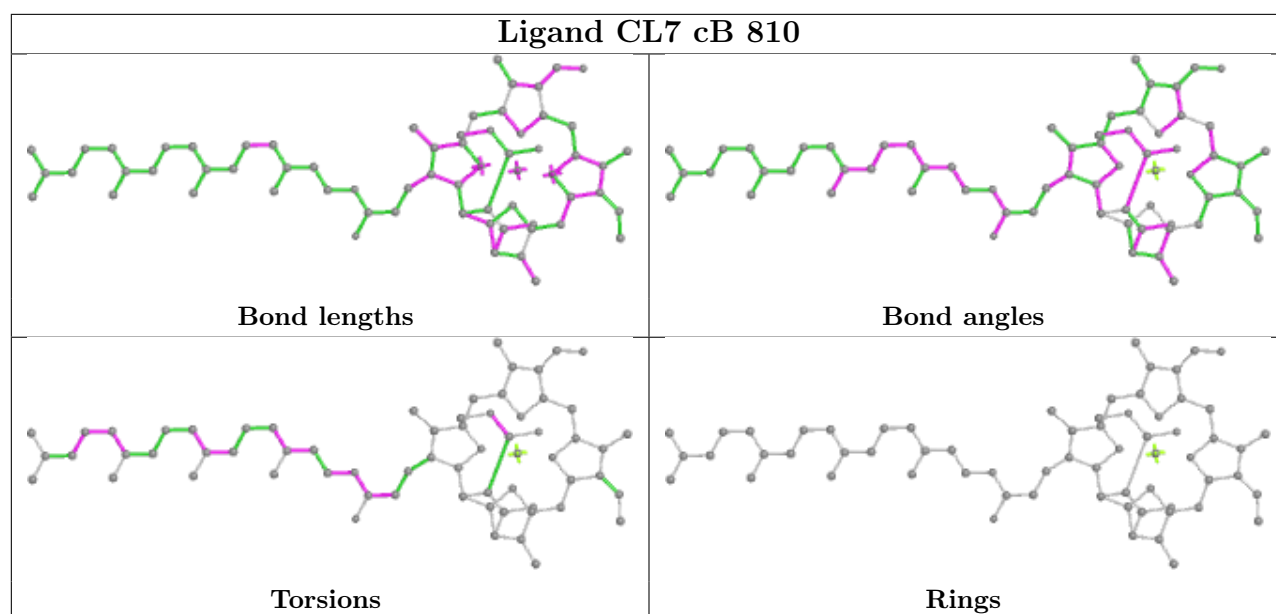


Torsions

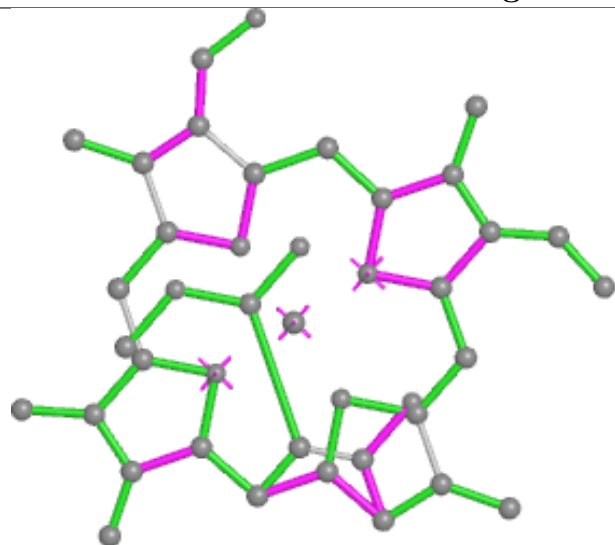


Rings

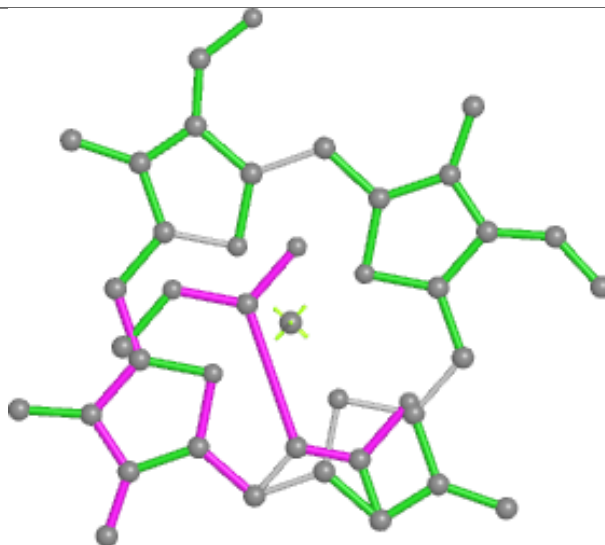




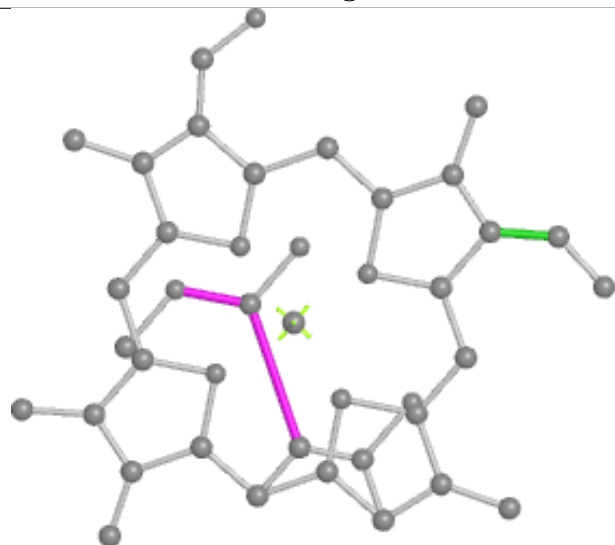
Ligand CL7 aA 3146



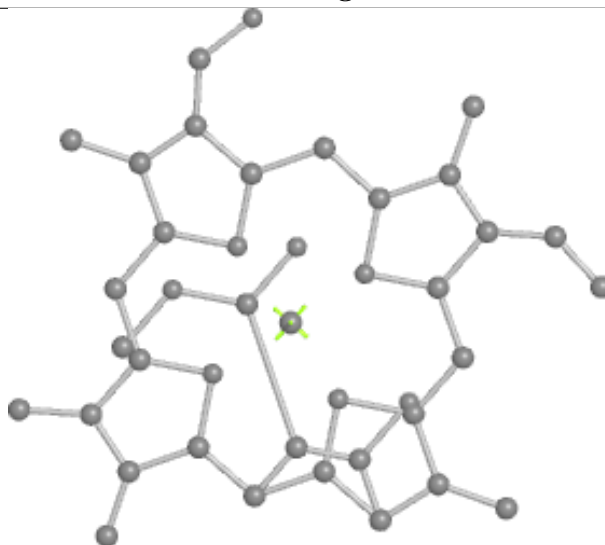
Bond lengths



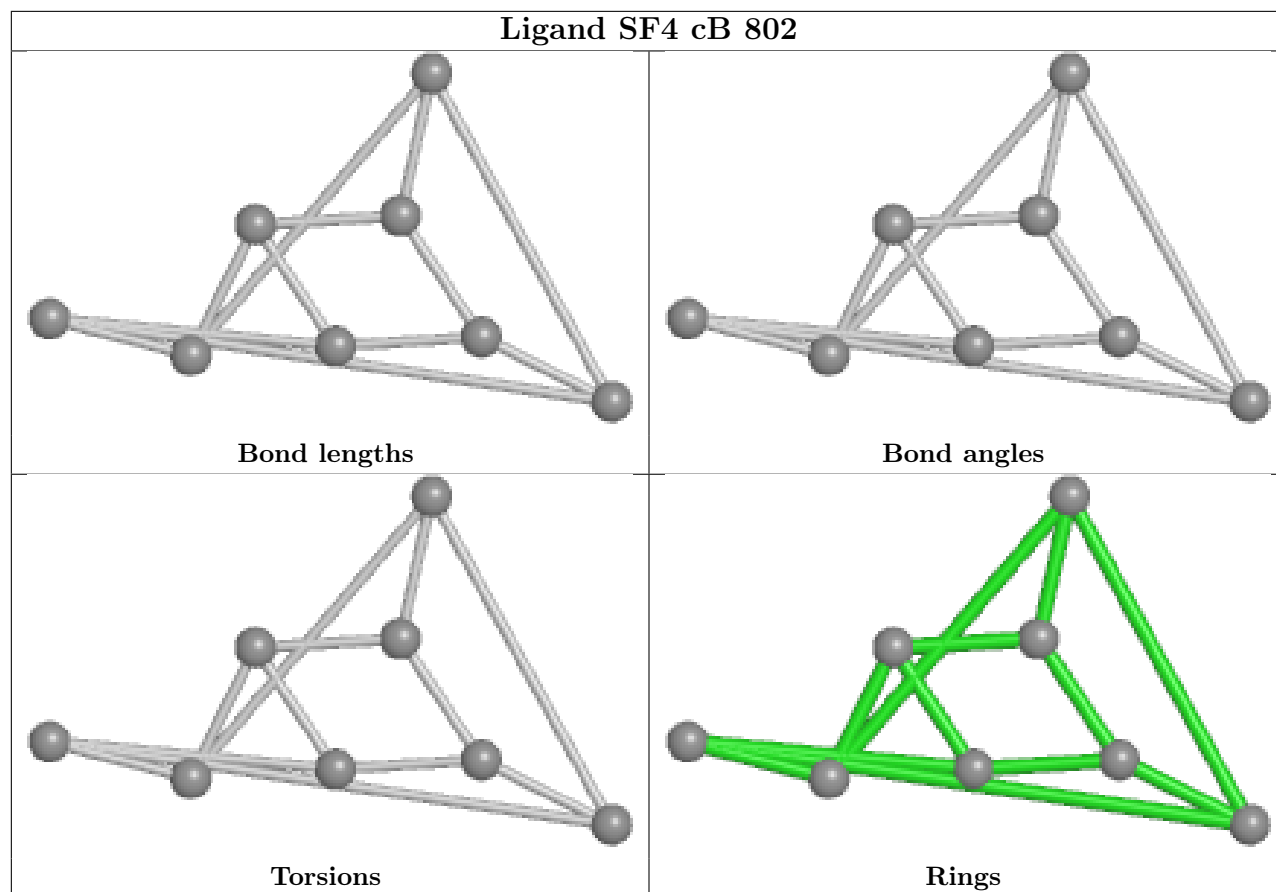
Bond angles



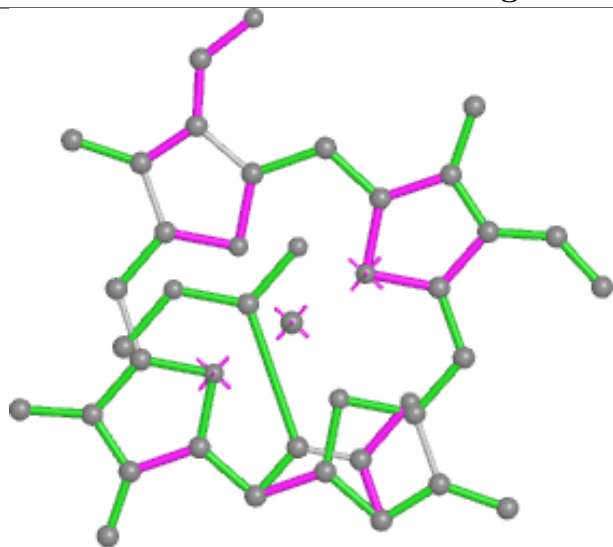
Torsions



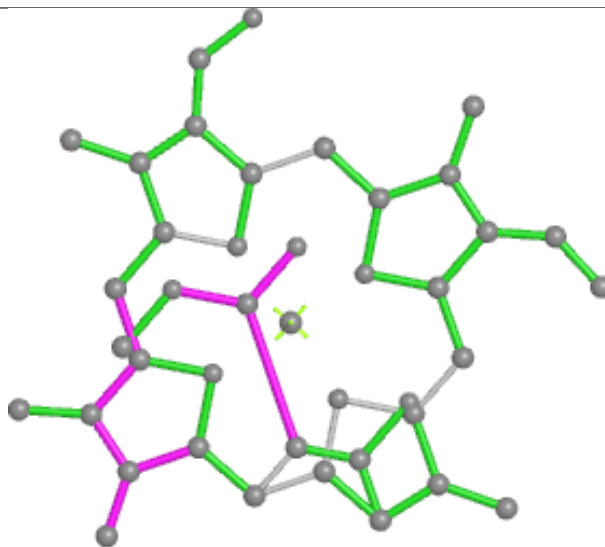
Rings



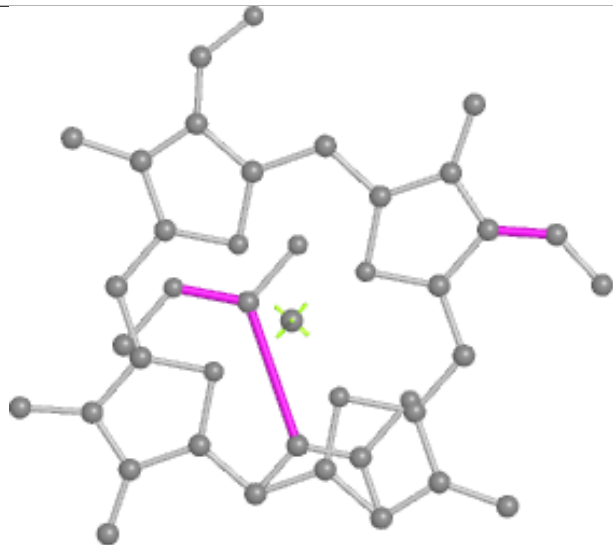
Ligand CL7 aA 3134



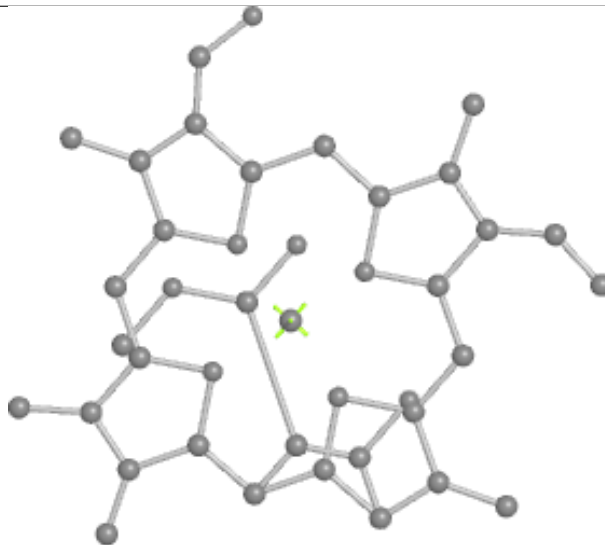
Bond lengths



Bond angles

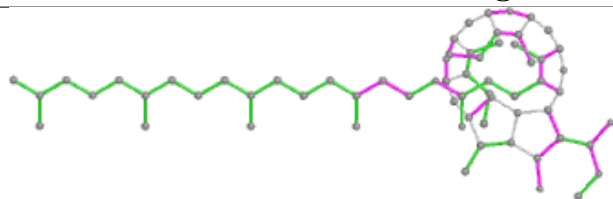


Torsions

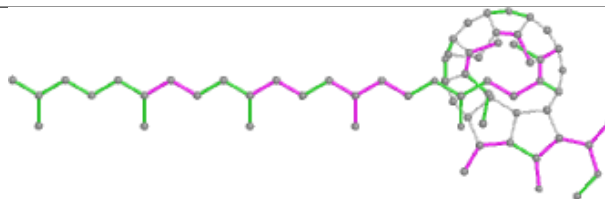


Rings

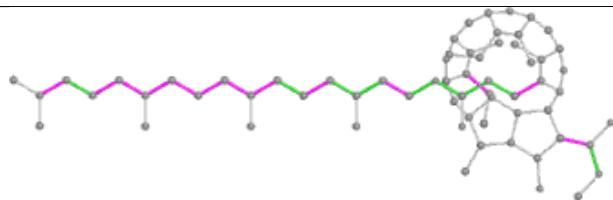
Ligand PHO aB 3004



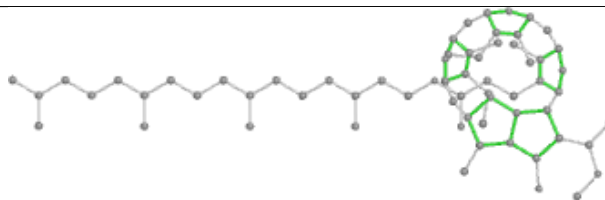
Bond lengths



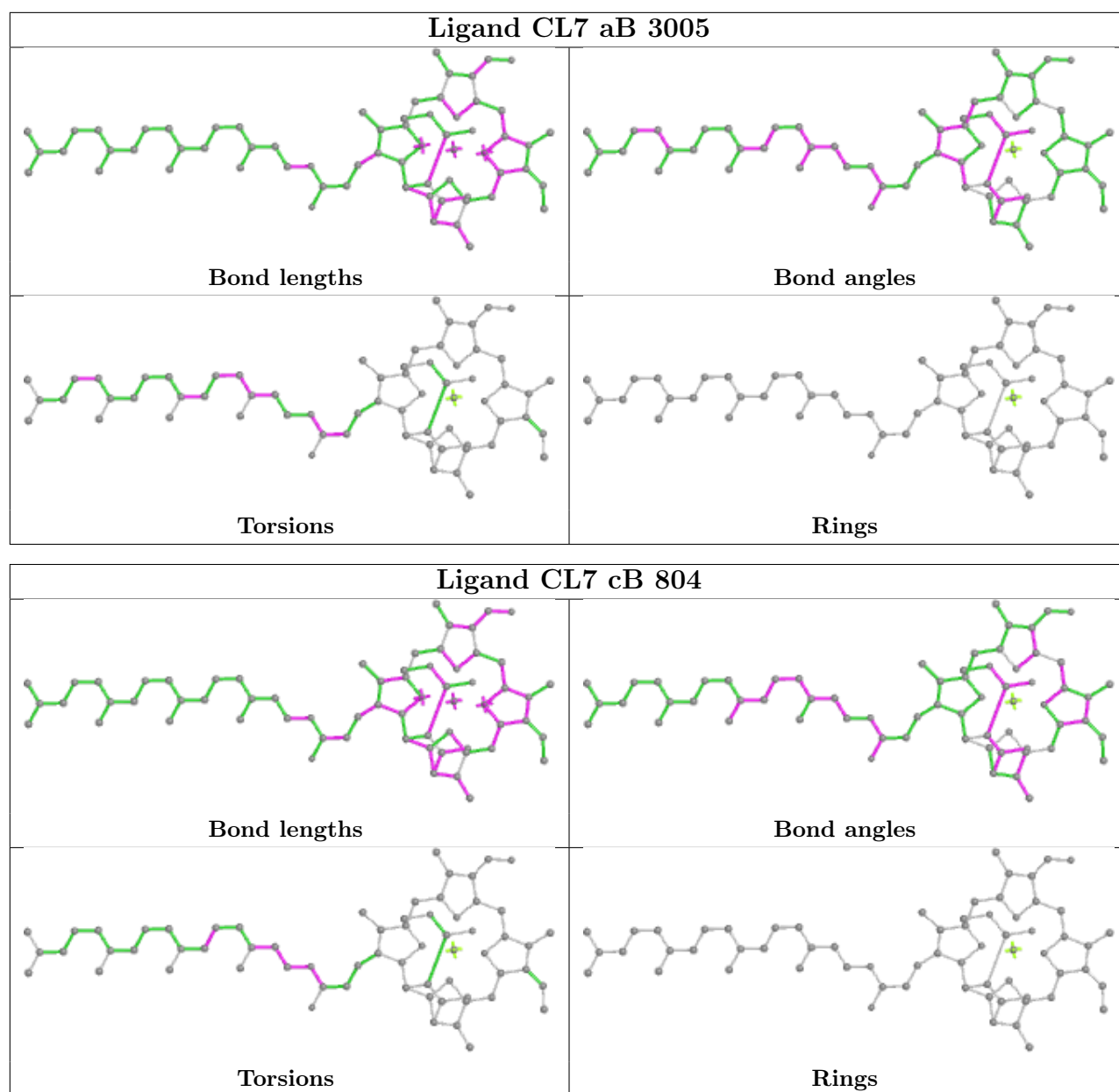
Bond angles



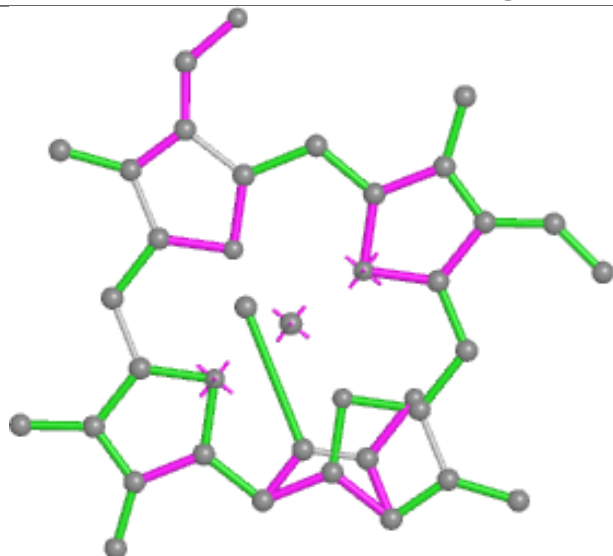
Torsions



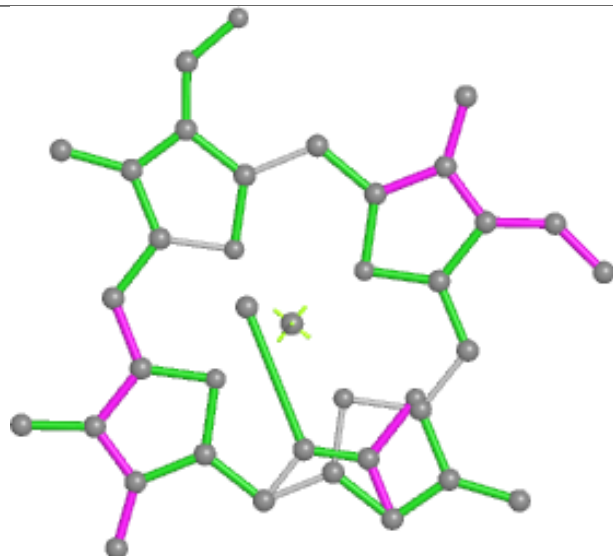
Rings



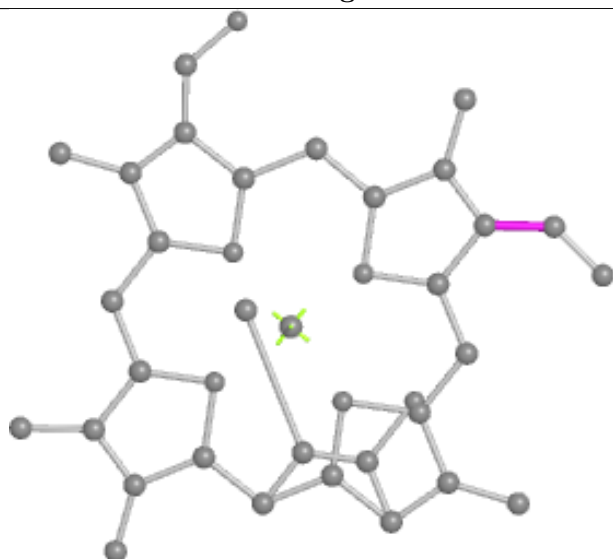
Ligand CL7 bA 3115



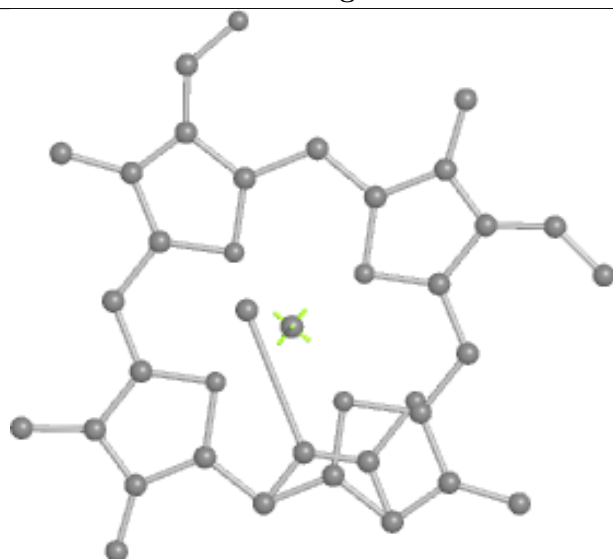
Bond lengths



Bond angles

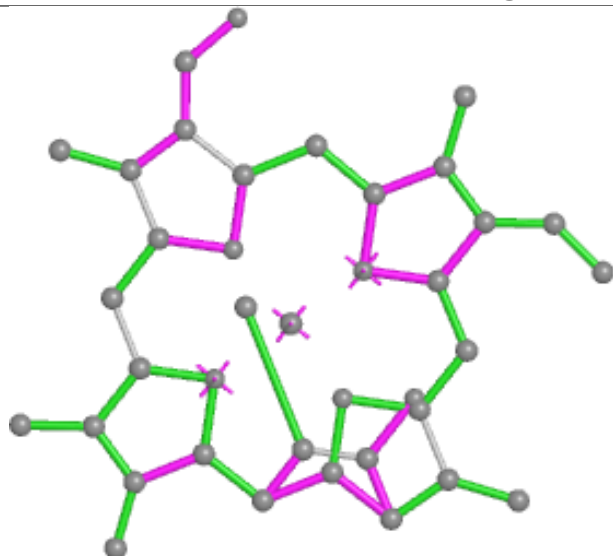


Torsions

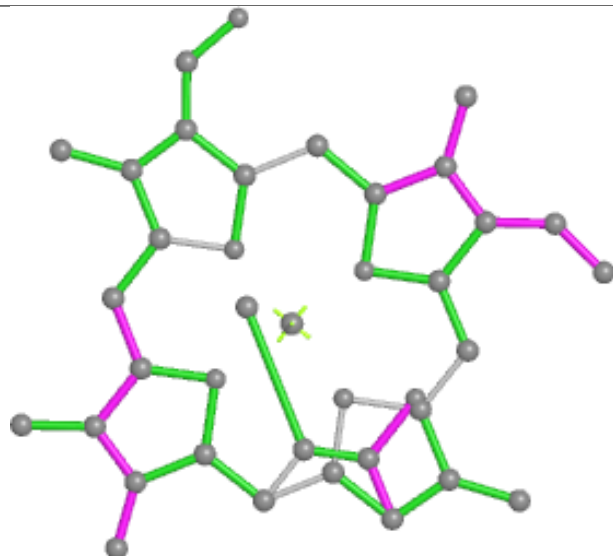


Rings

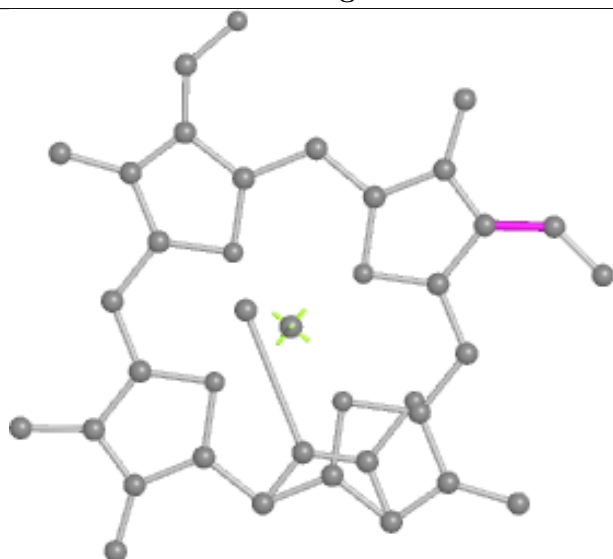
Ligand CL7 aA 3116



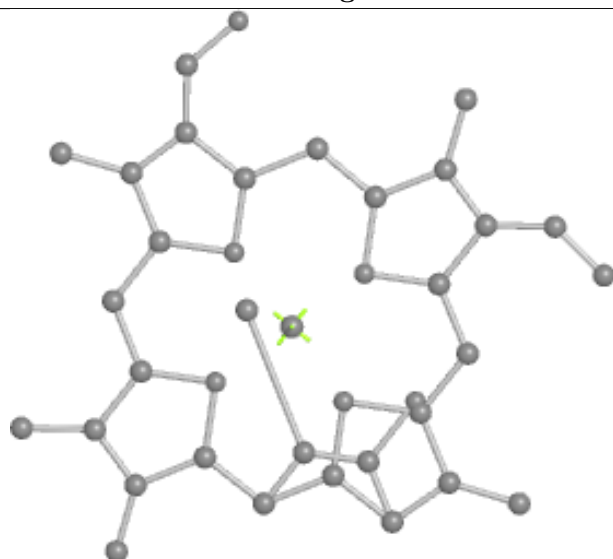
Bond lengths



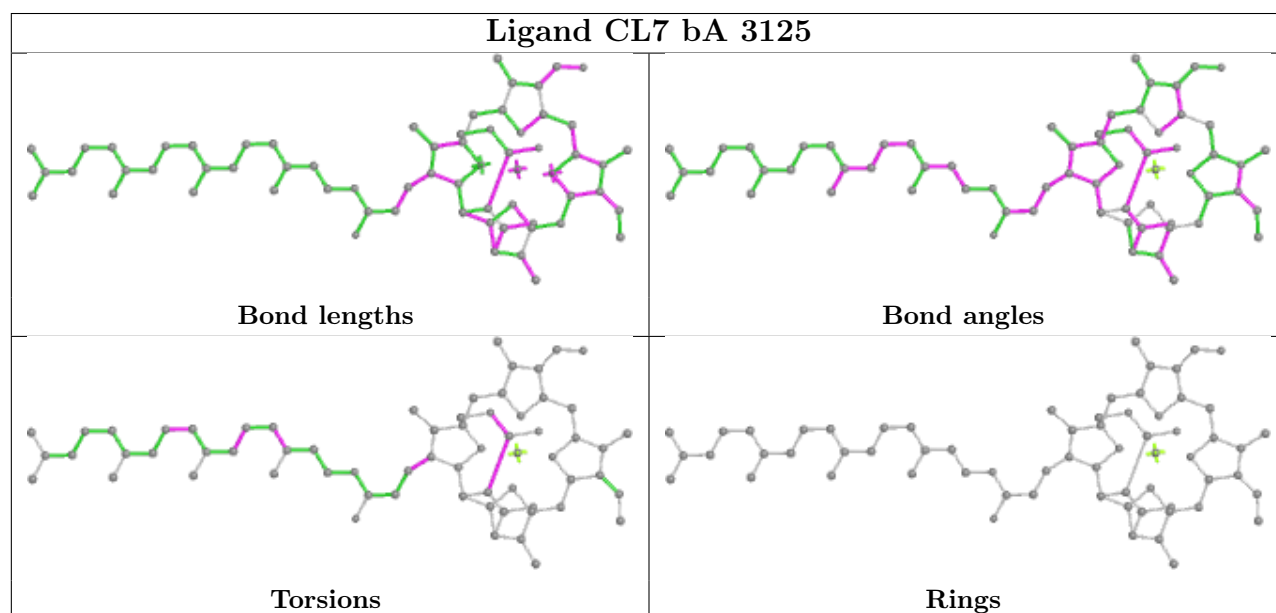
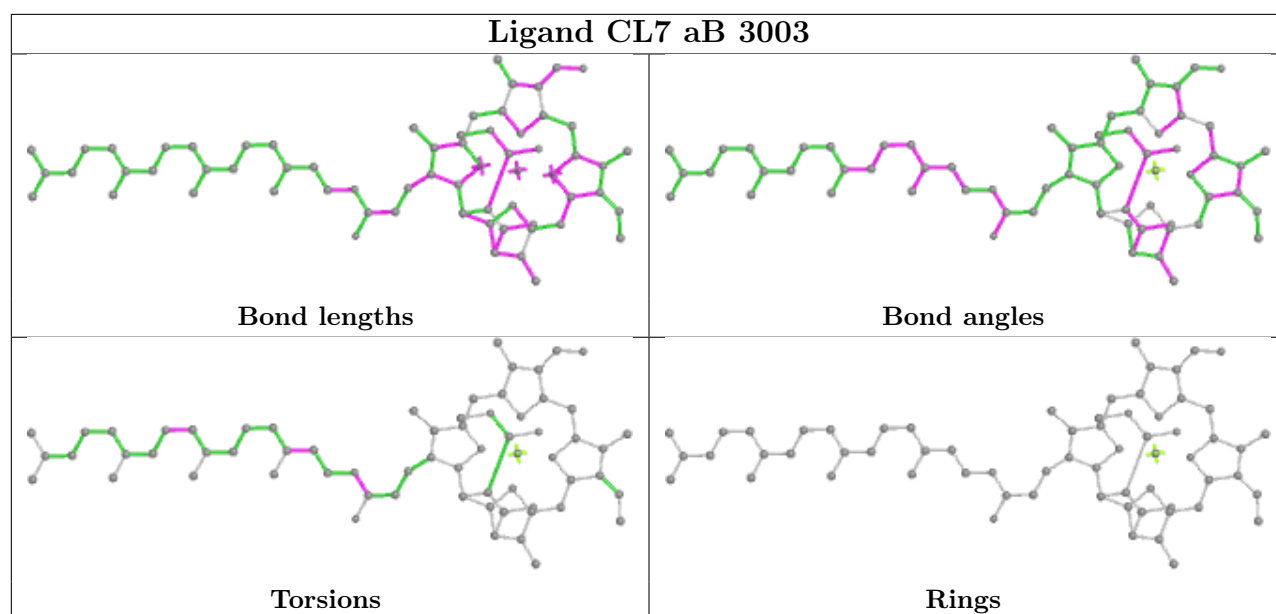
Bond angles

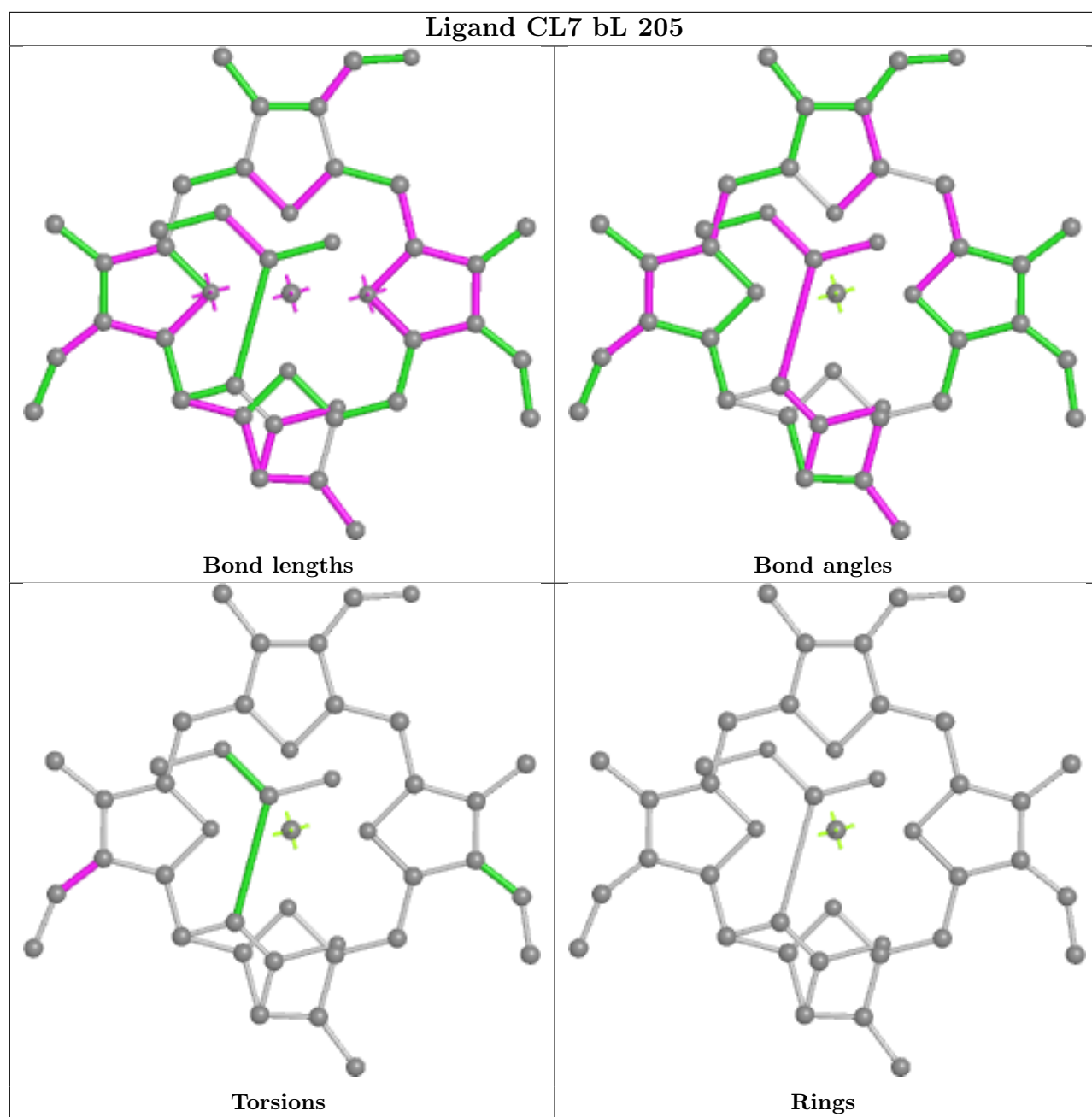


Torsions

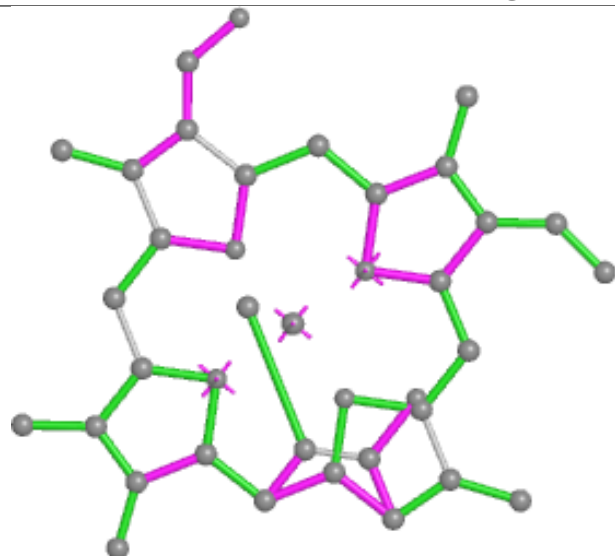


Rings

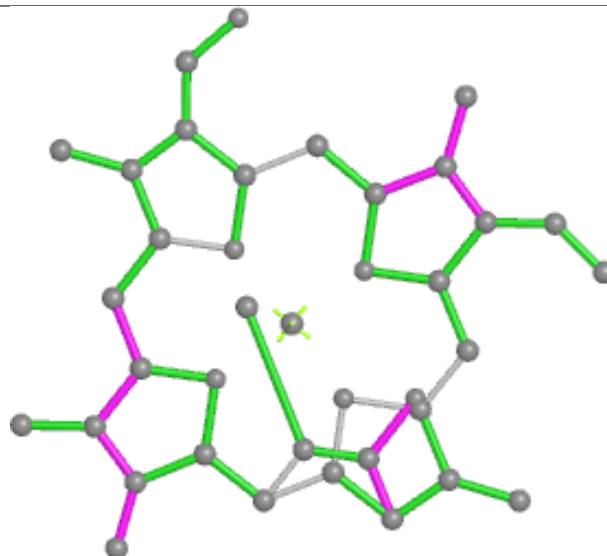




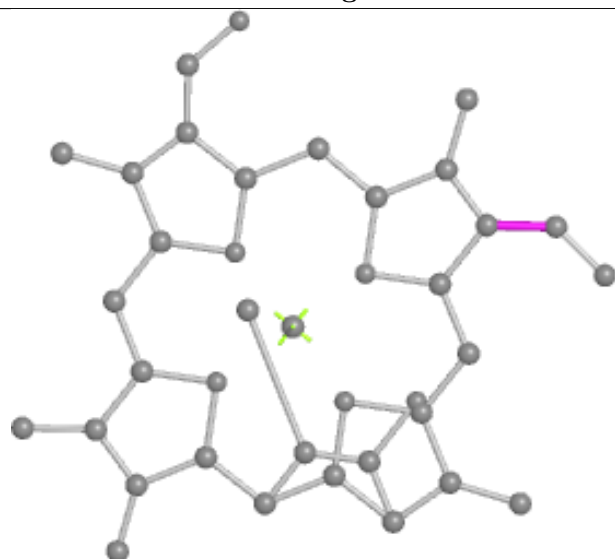
Ligand CL7 cA 3115



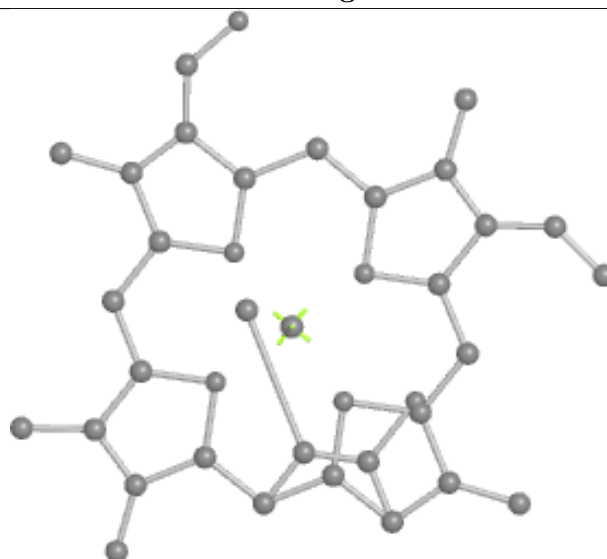
Bond lengths



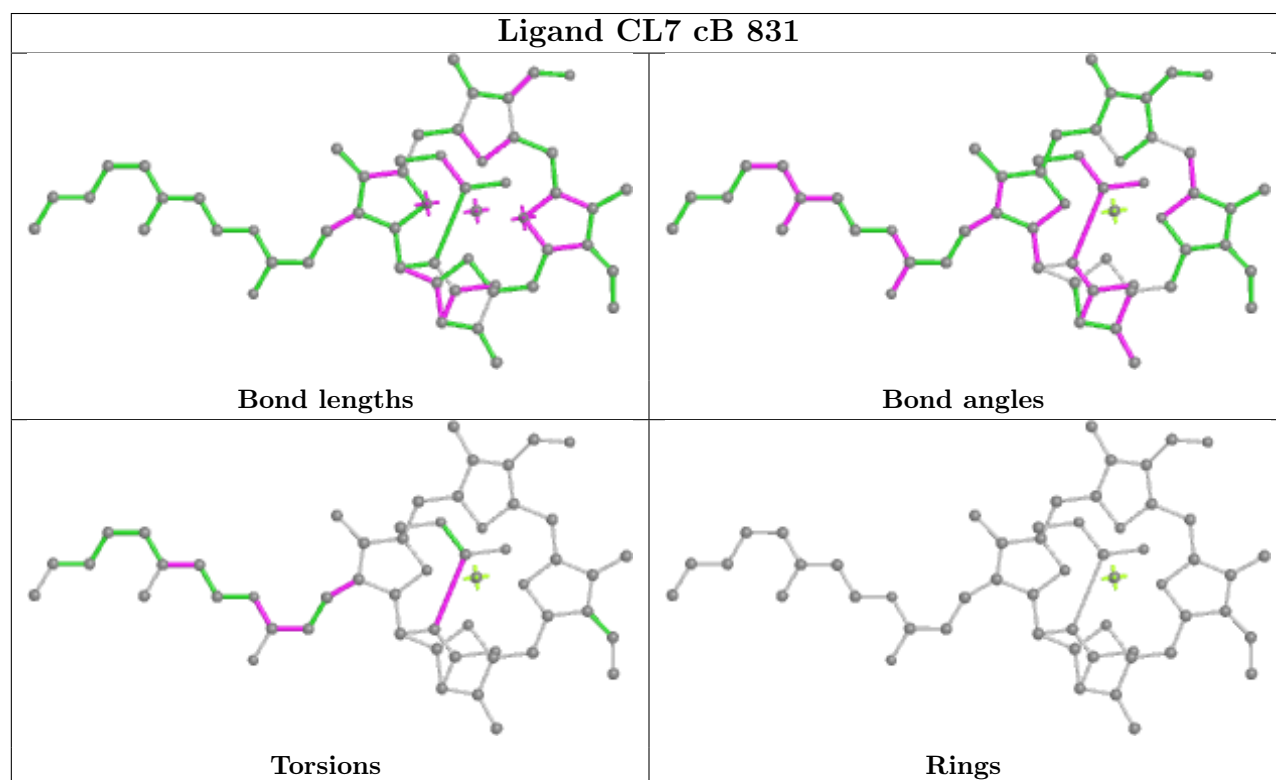
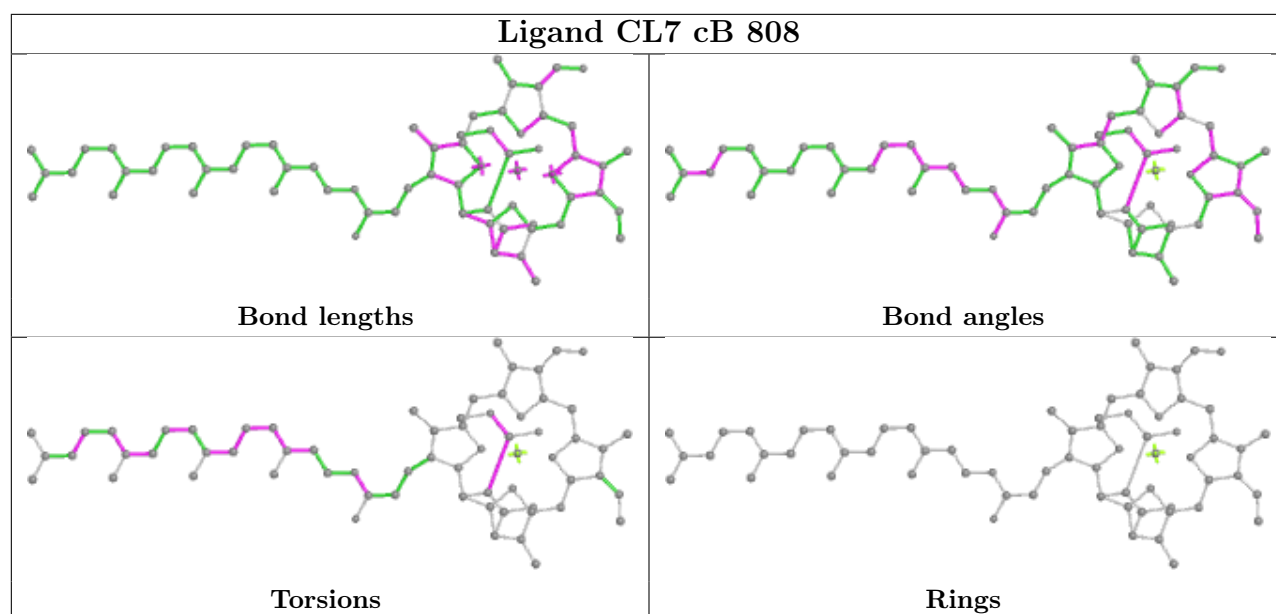
Bond angles

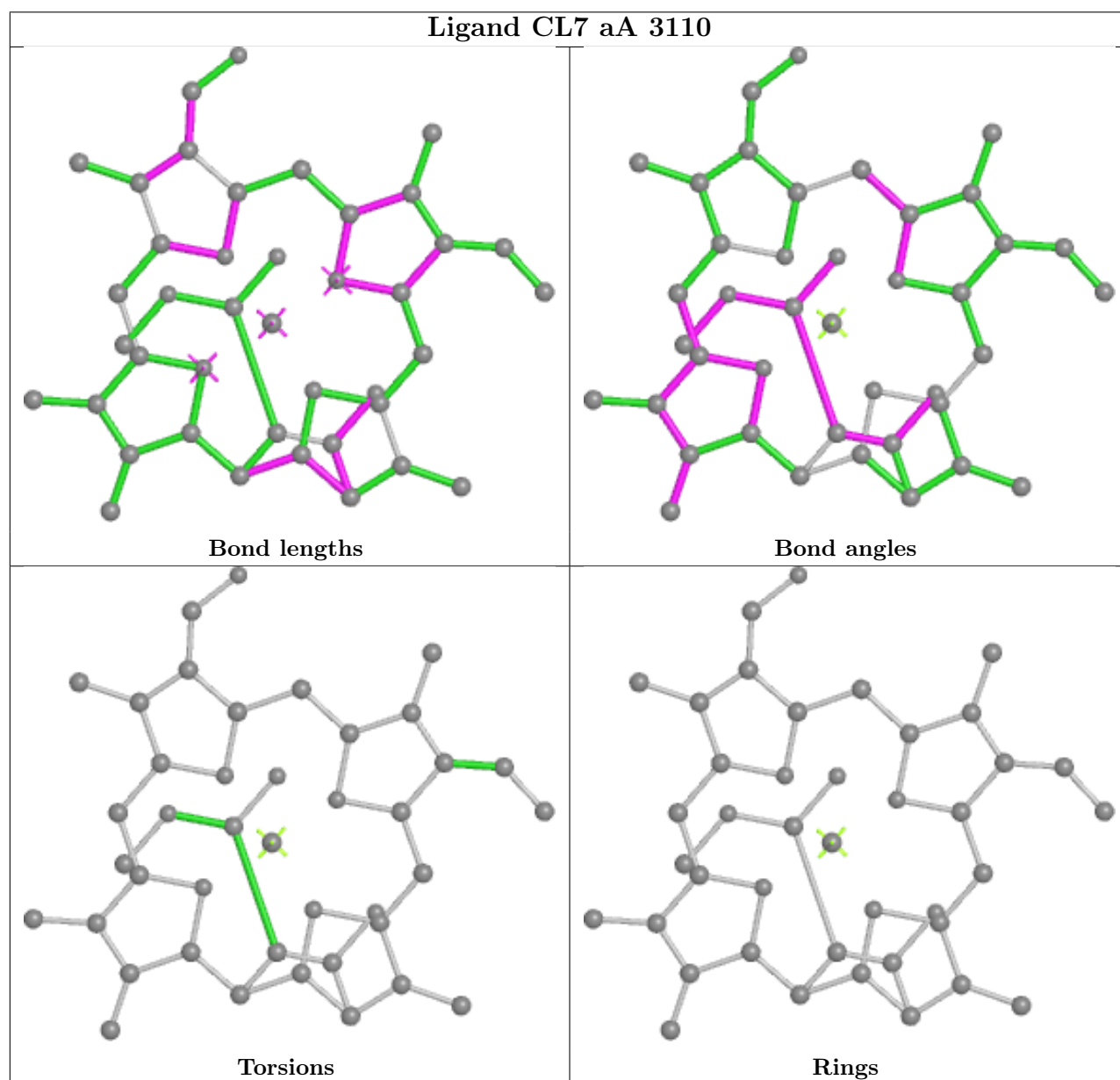
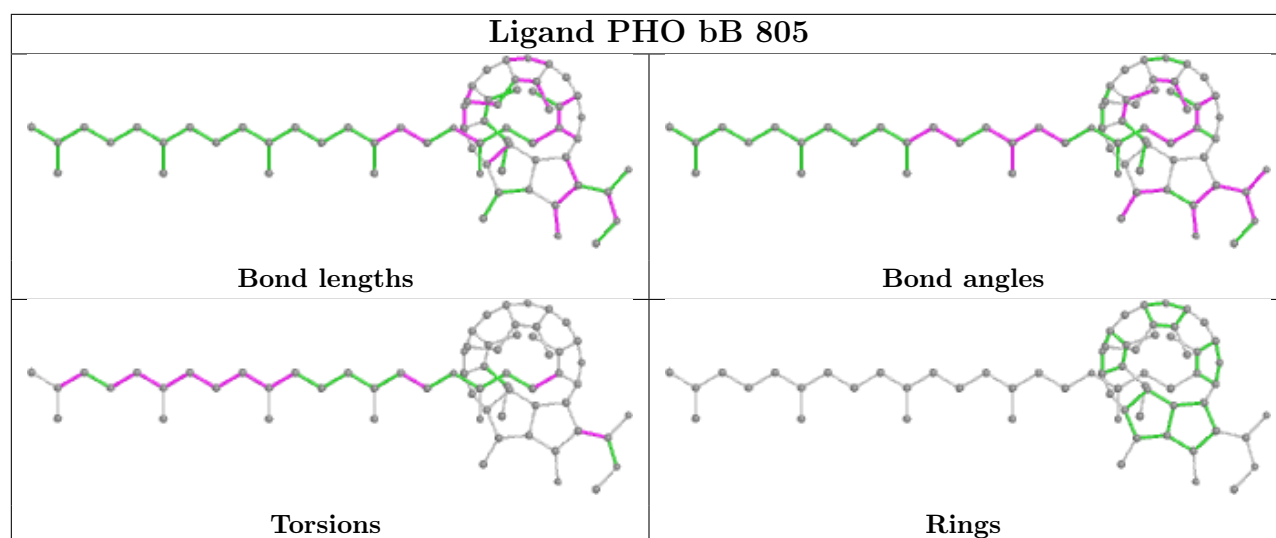


Torsions

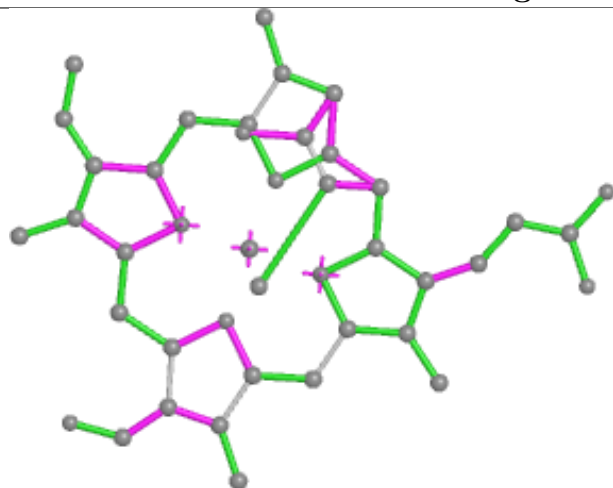


Rings

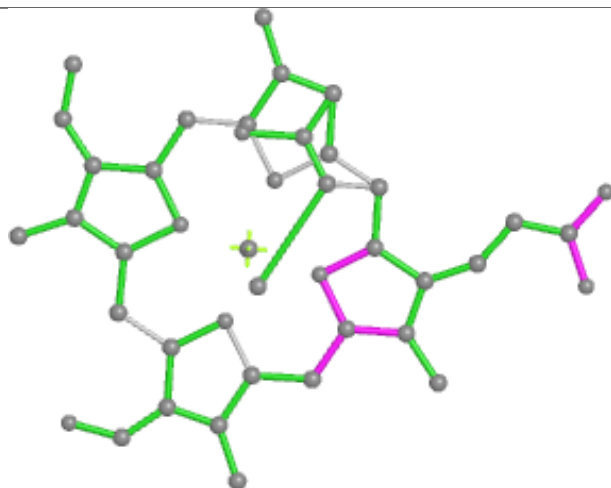




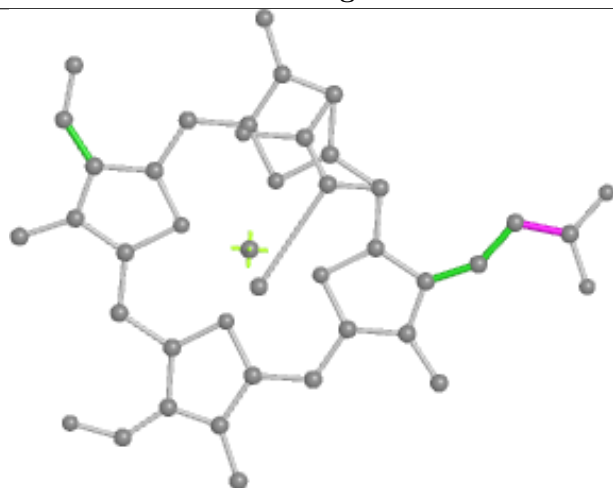
Ligand CL7 aJ 101



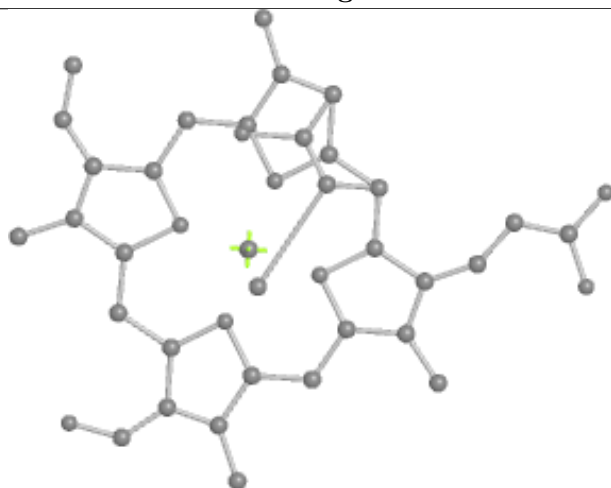
Bond lengths



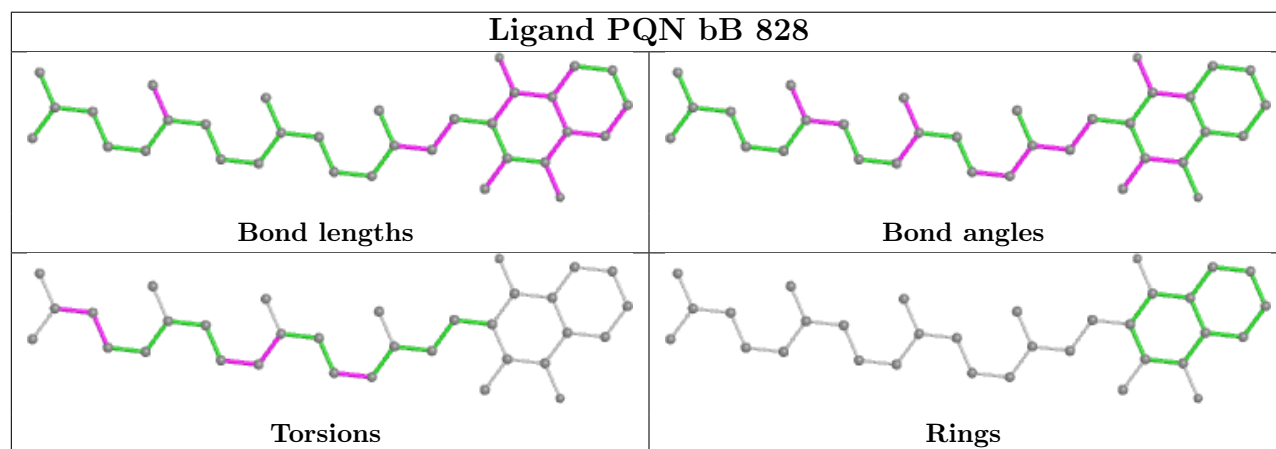
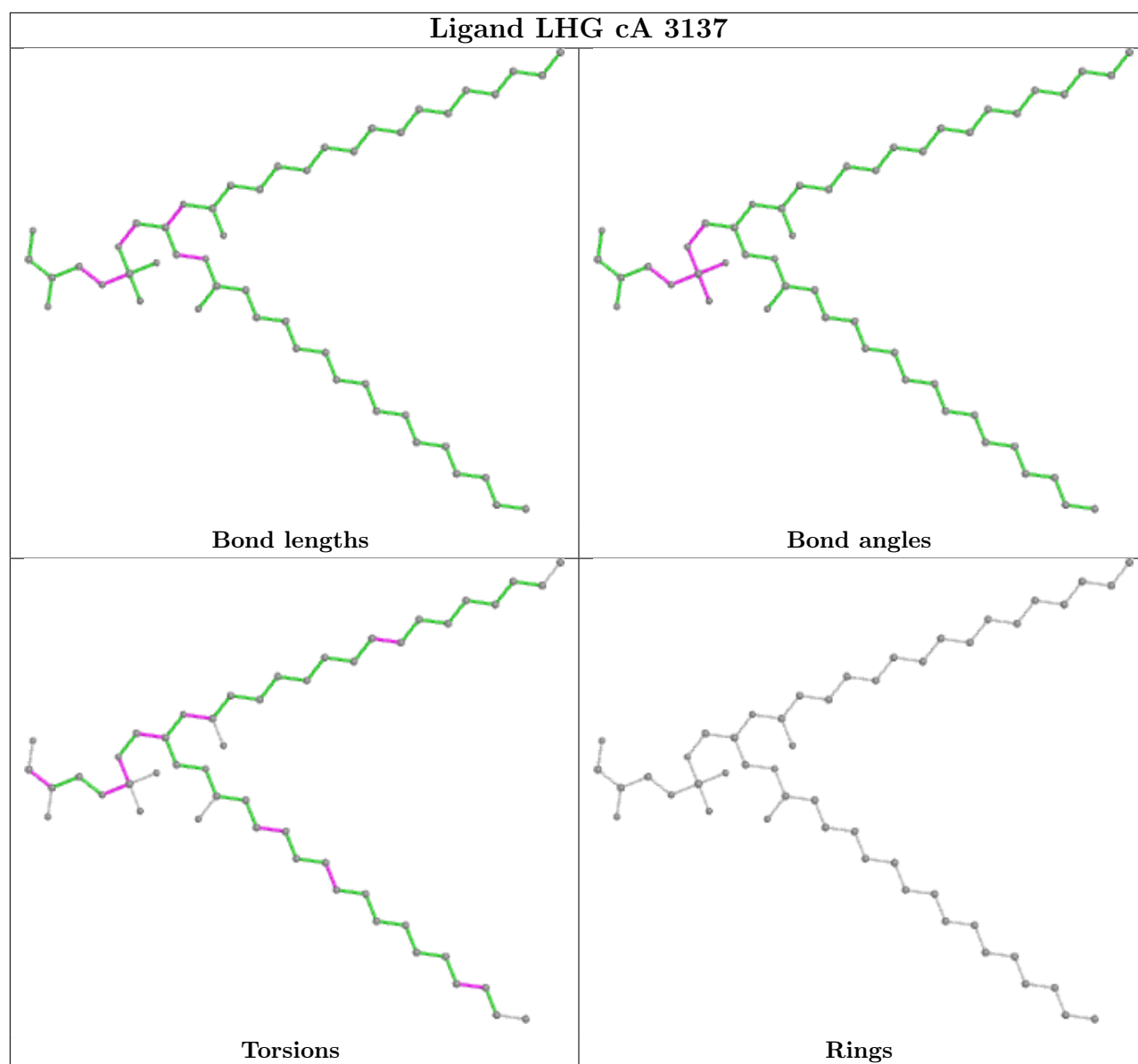
Bond angles



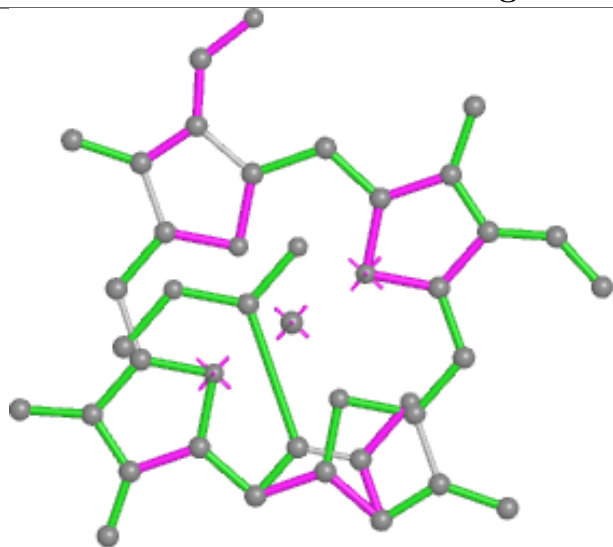
Torsions



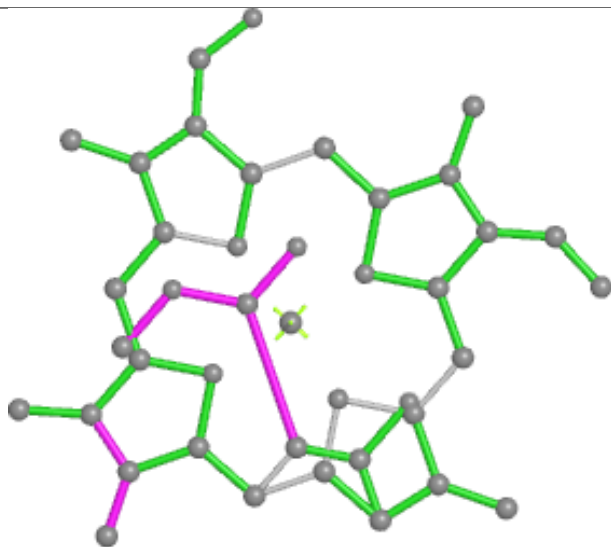
Rings



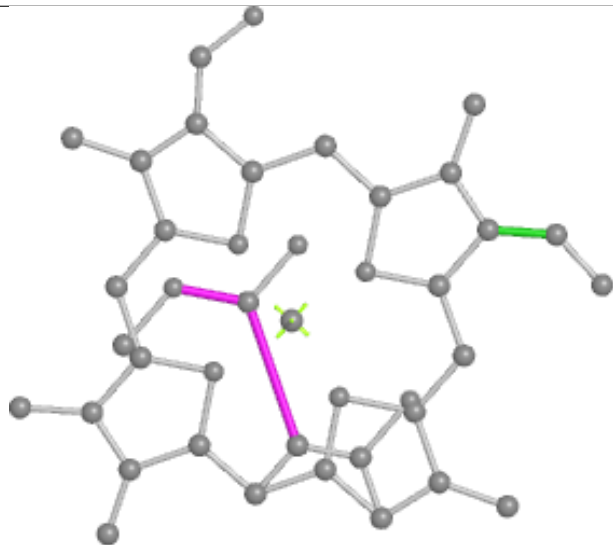
Ligand CL7 bA 3145



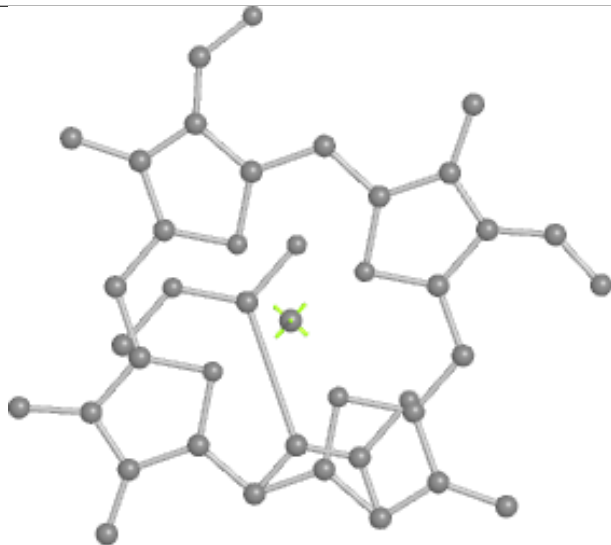
Bond lengths



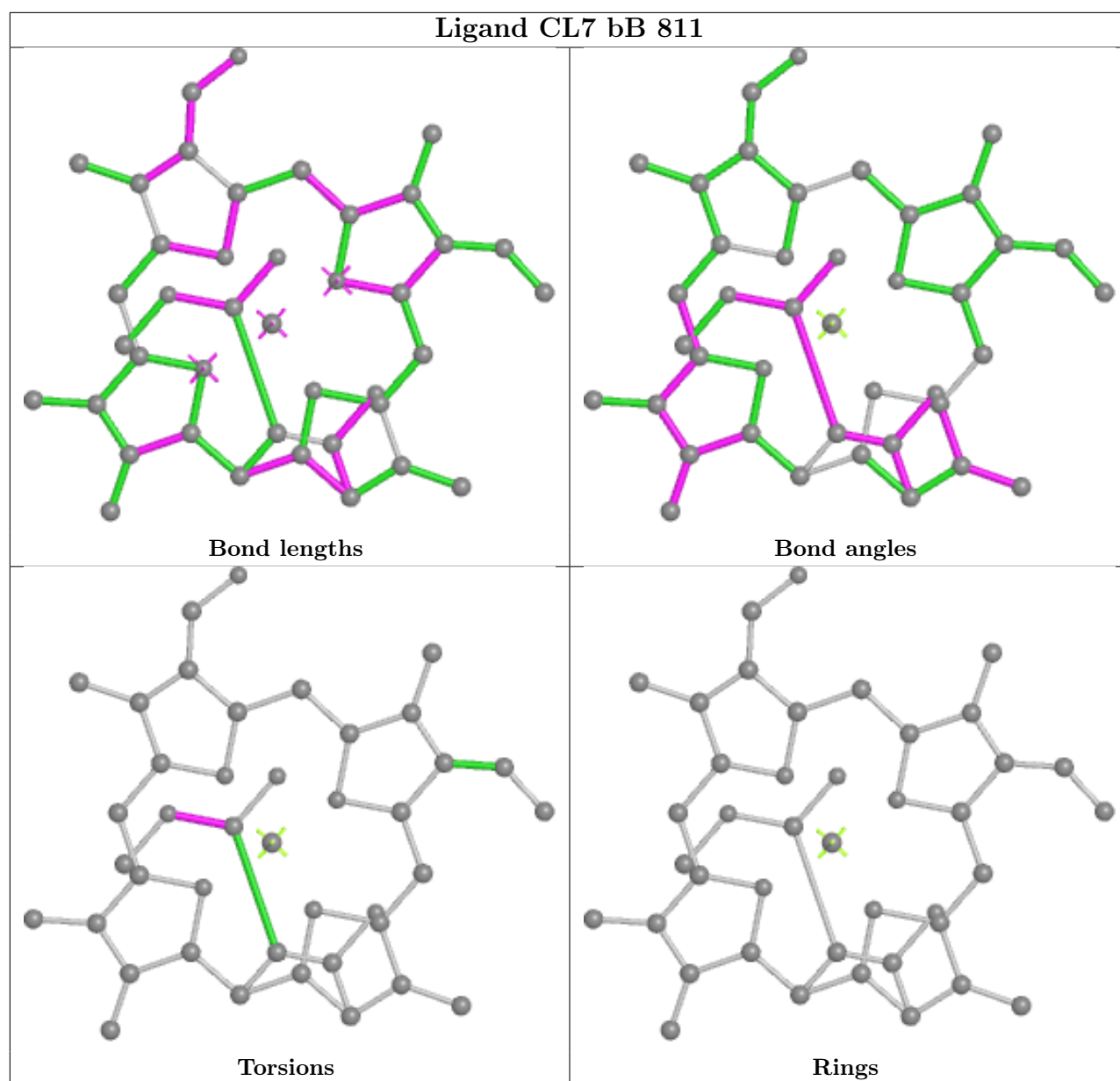
Bond angles



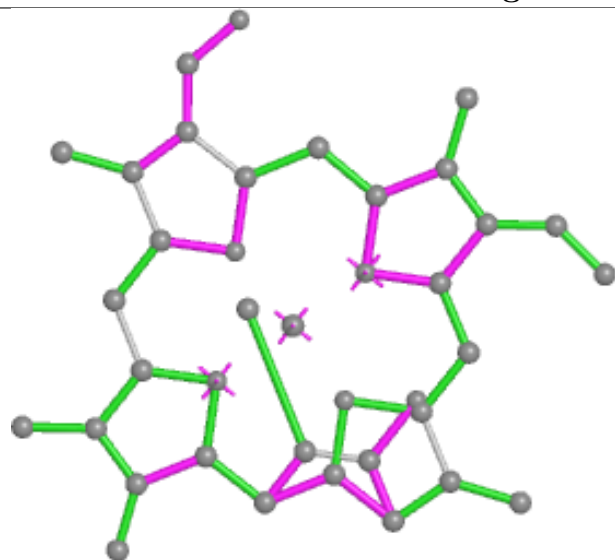
Torsions



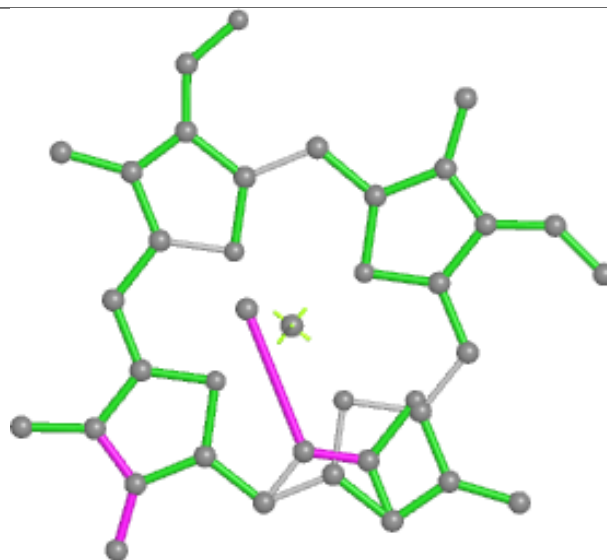
Rings



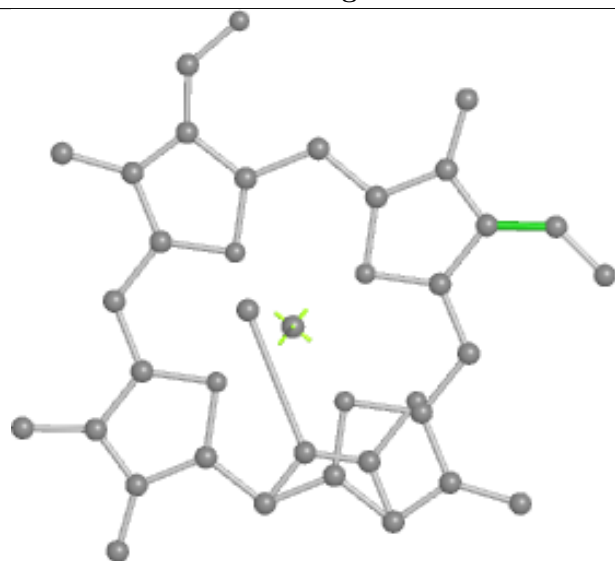
Ligand CL7 aA 3112



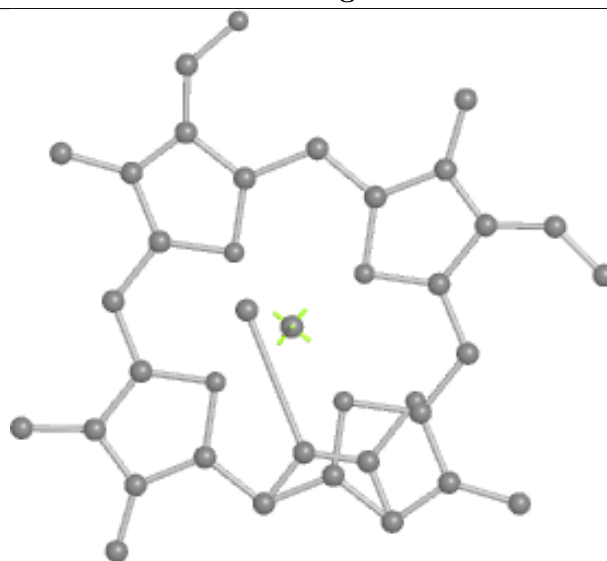
Bond lengths



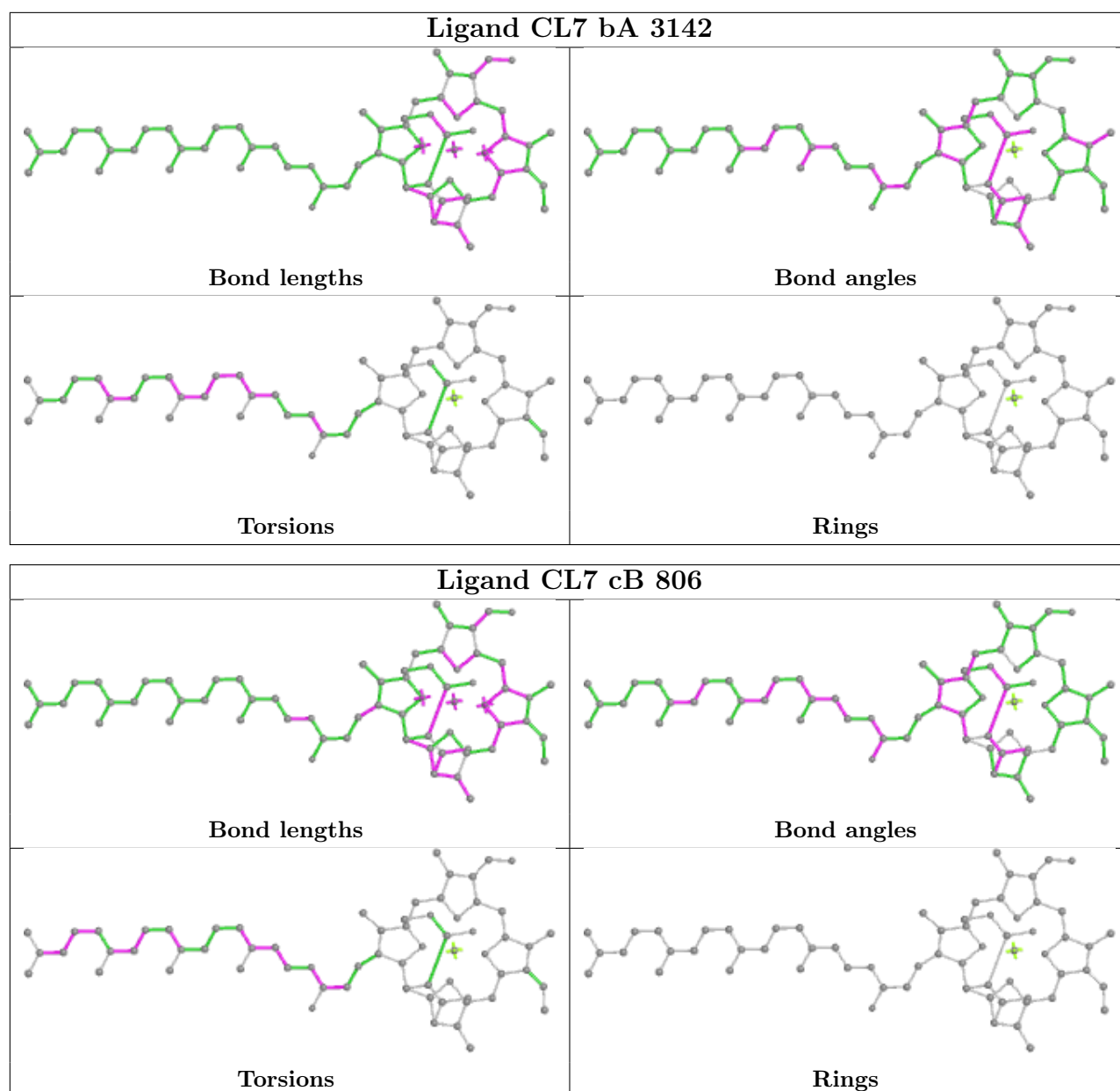
Bond angles



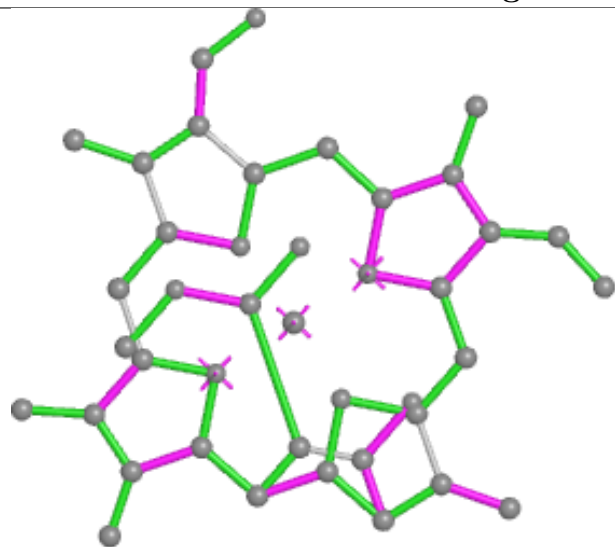
Torsions



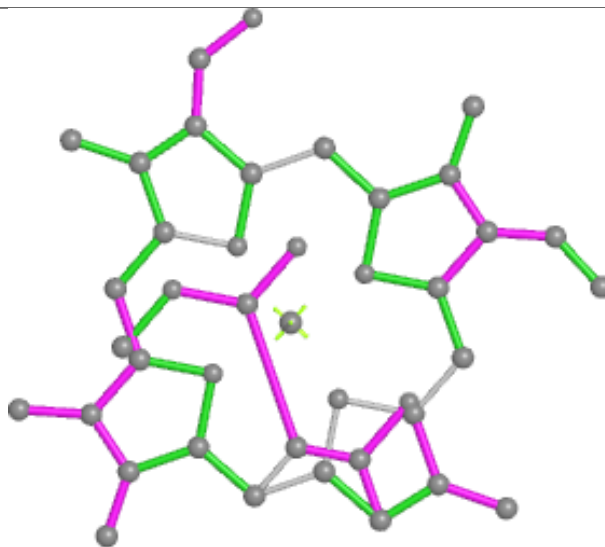
Rings



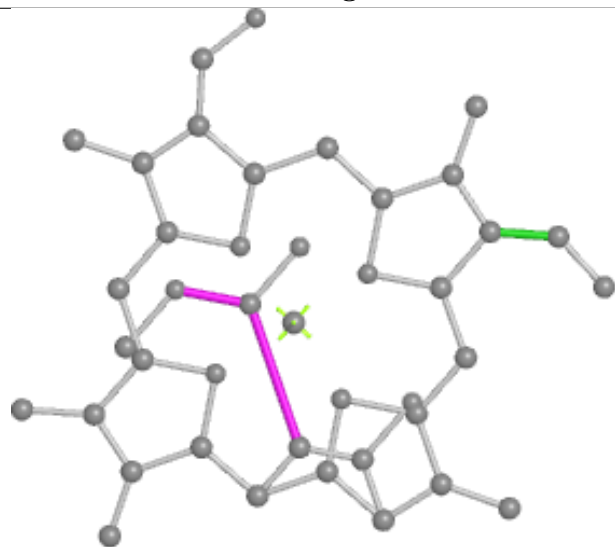
Ligand CL7 aA 3106



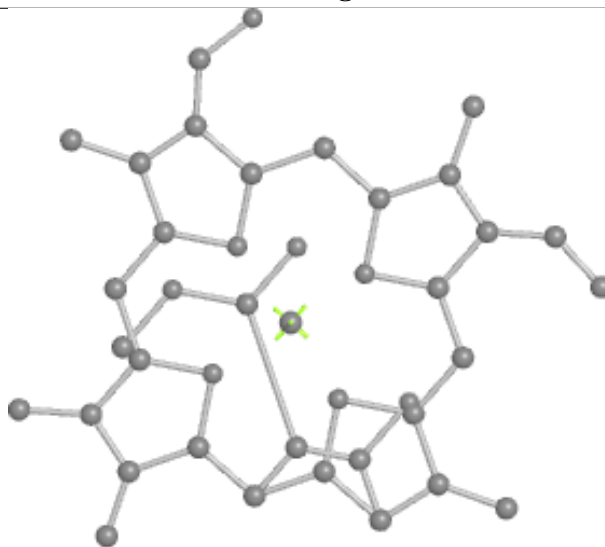
Bond lengths



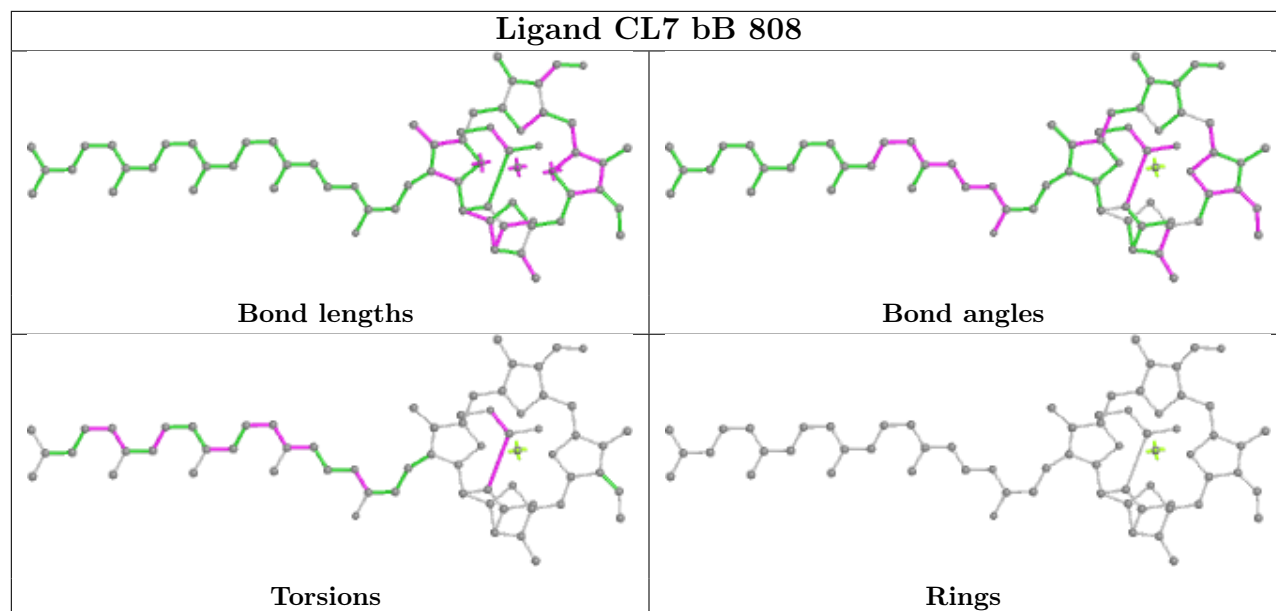
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

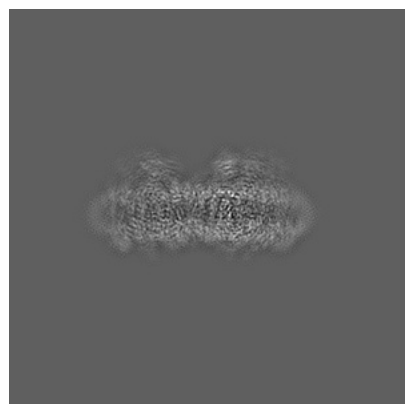
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30420. These allow visual inspection of the internal detail of the map and identification of artifacts.

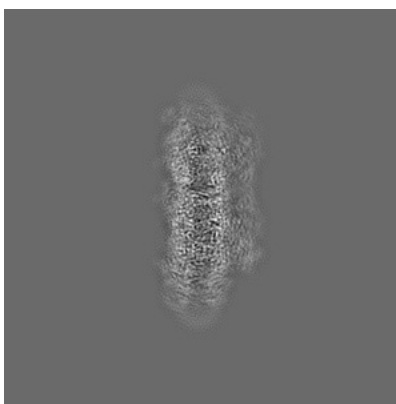
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

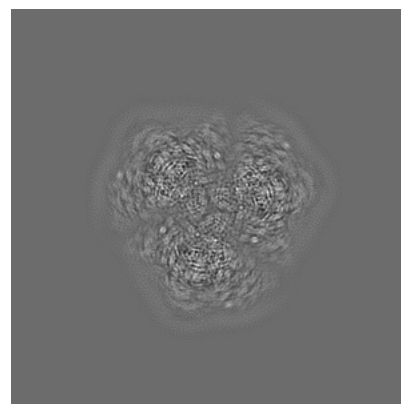
6.1.1 Primary map



X

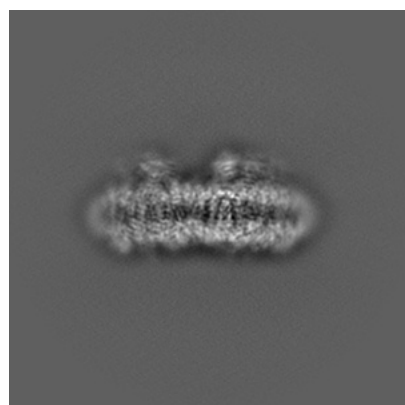


Y

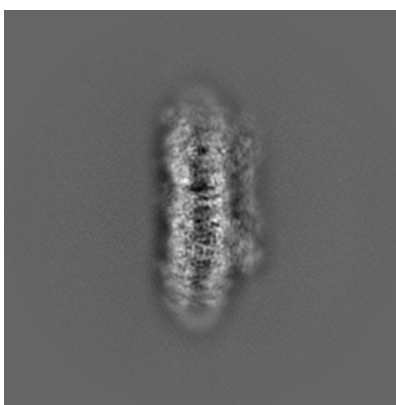


Z

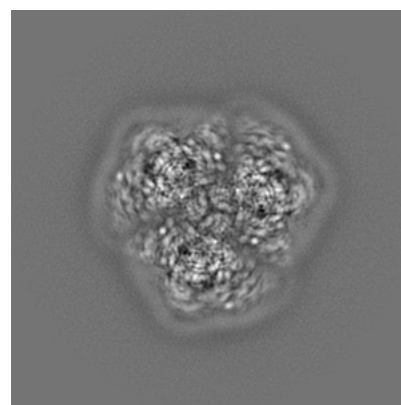
6.1.2 Raw map



X



Y

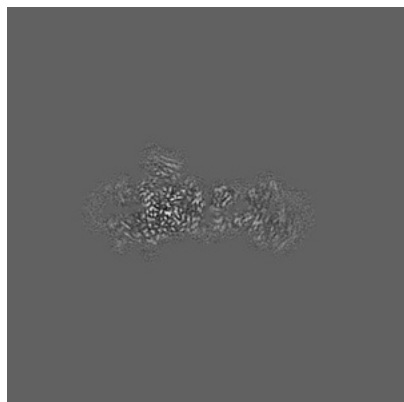


Z

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

6.2 Central slices [i](#)

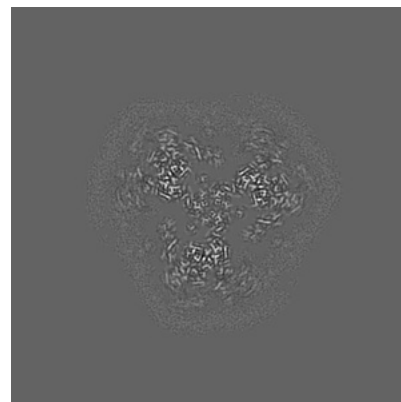
6.2.1 Primary map



X Index: 165

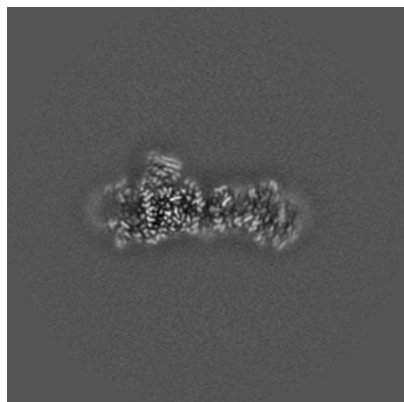


Y Index: 165

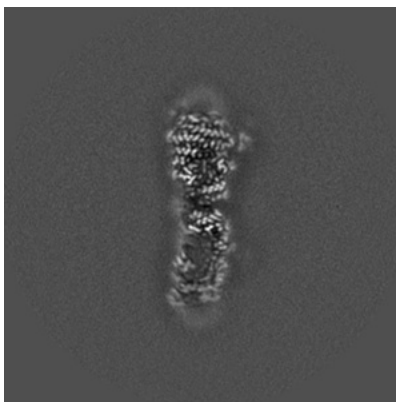


Z Index: 165

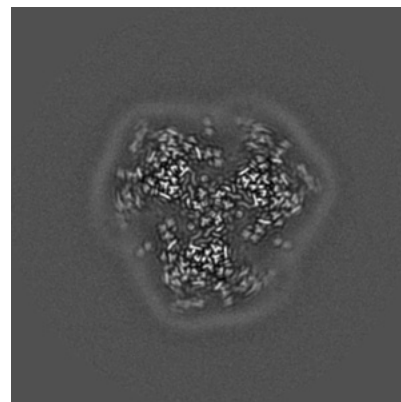
6.2.2 Raw map



X Index: 165



Y Index: 165

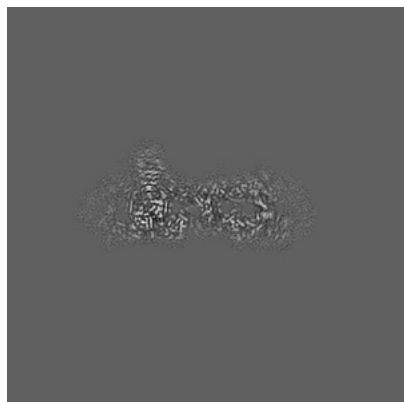


Z Index: 165

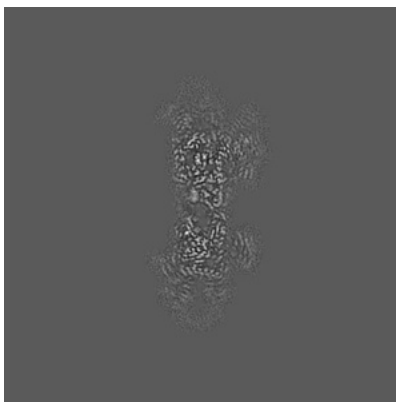
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

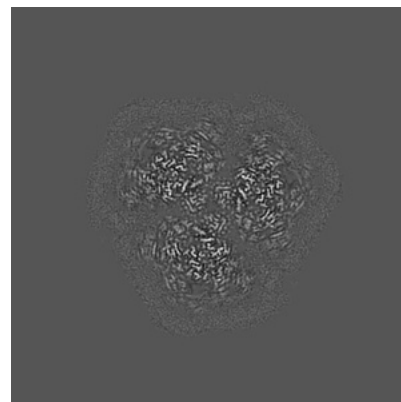
6.3.1 Primary map



X Index: 153

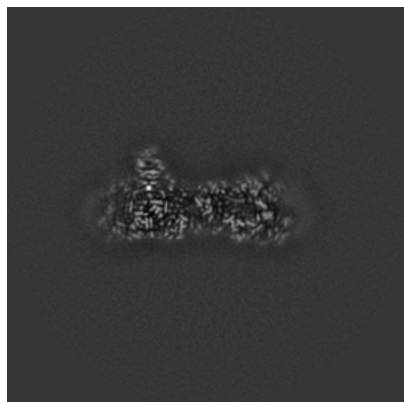


Y Index: 181

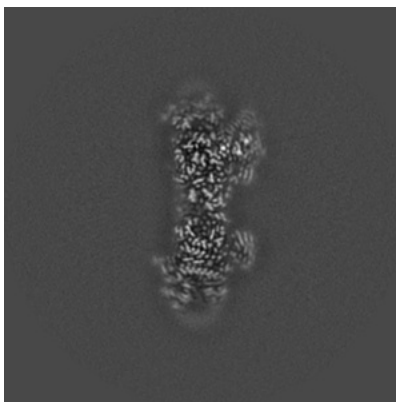


Z Index: 155

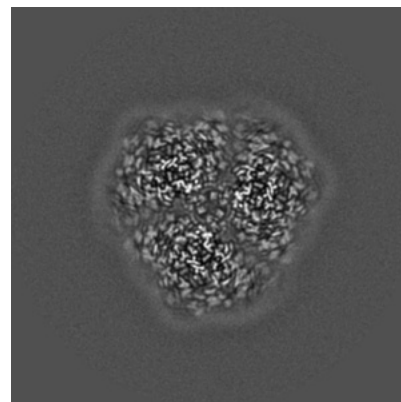
6.3.2 Raw map



X Index: 153



Y Index: 180

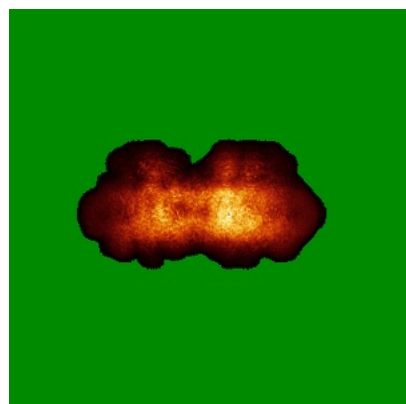


Z Index: 152

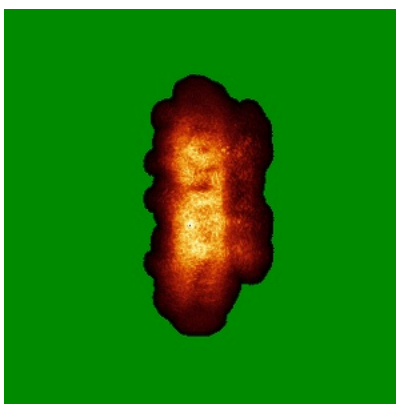
The images above show the largest variance slices of the map in three orthogonal directions.

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

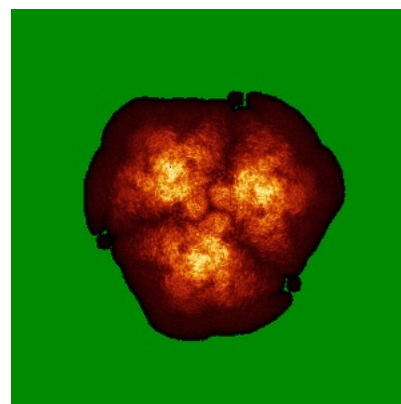
6.4.1 Primary map



X

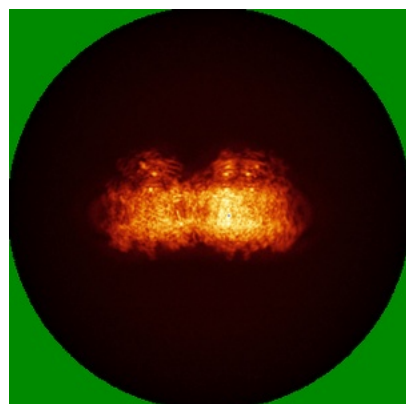


Y

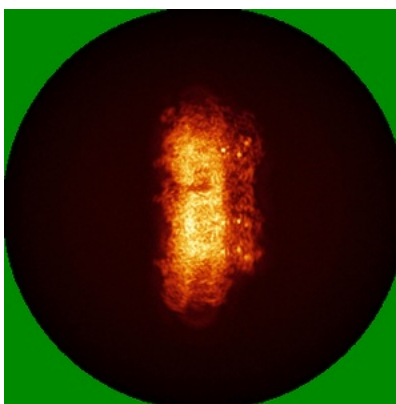


Z

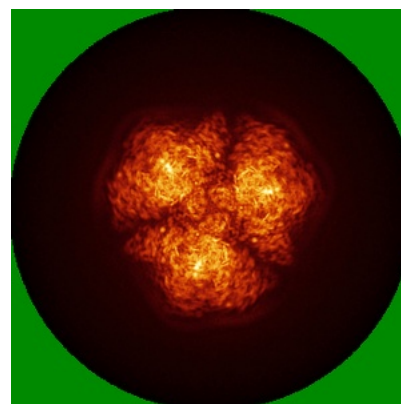
6.4.2 Raw map



X



Y

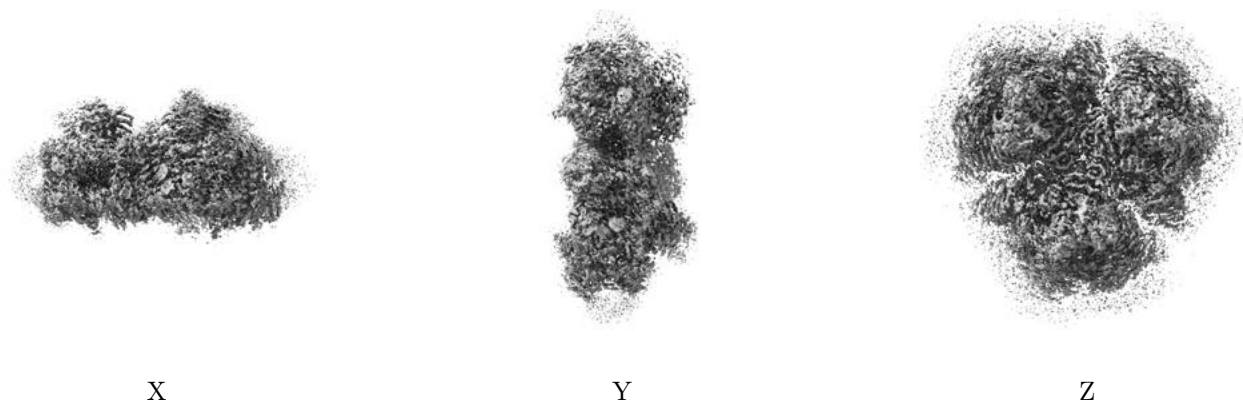


Z

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

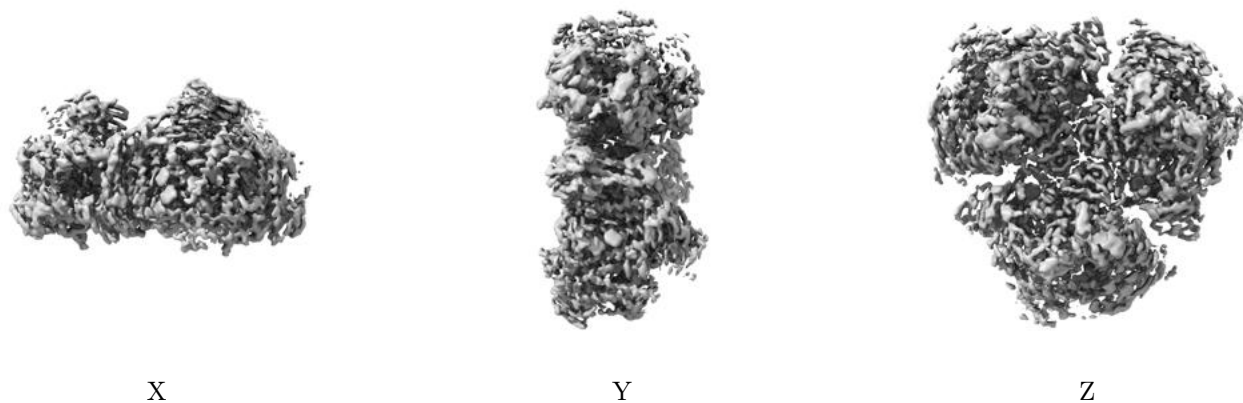
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00637. 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.

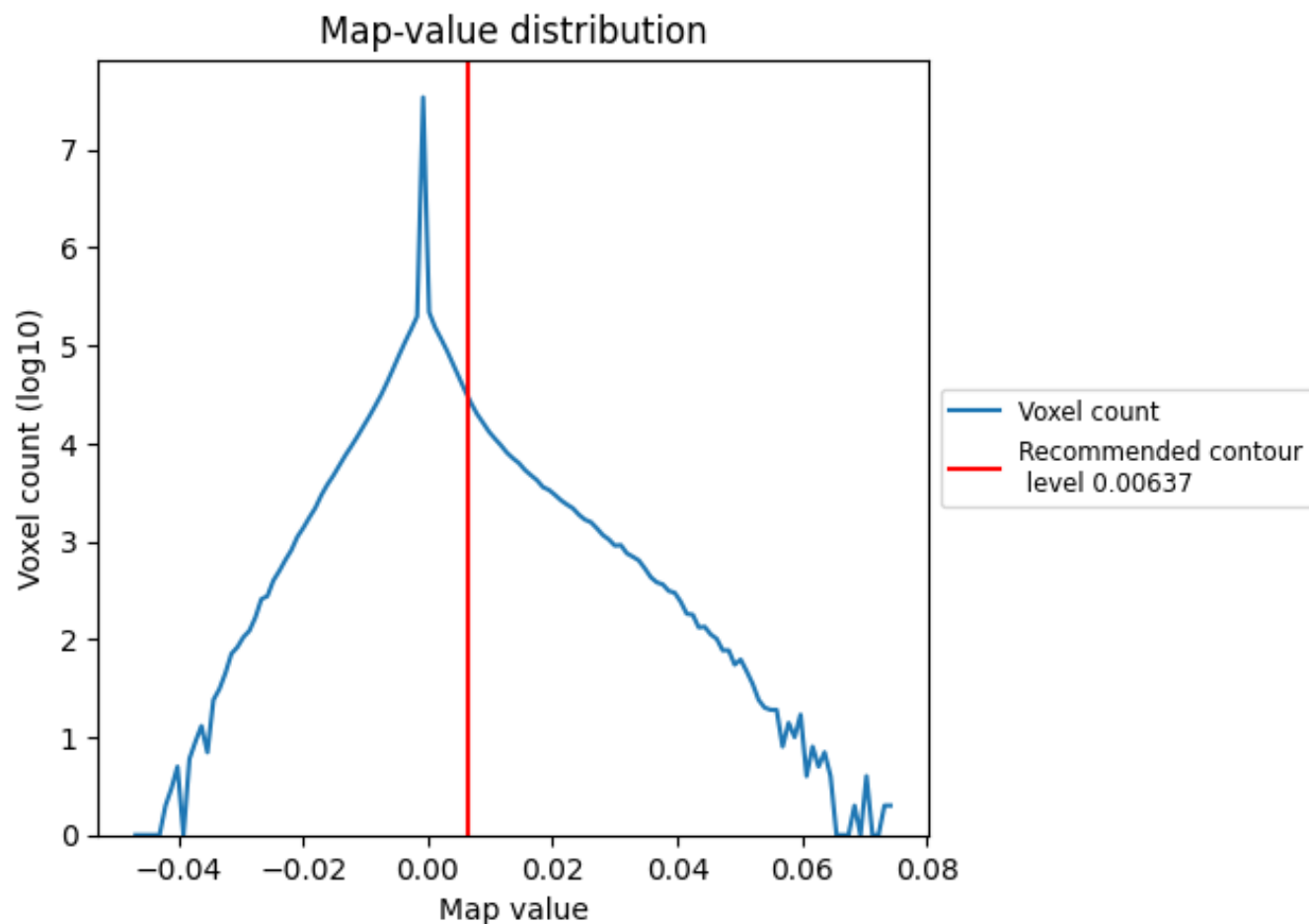
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

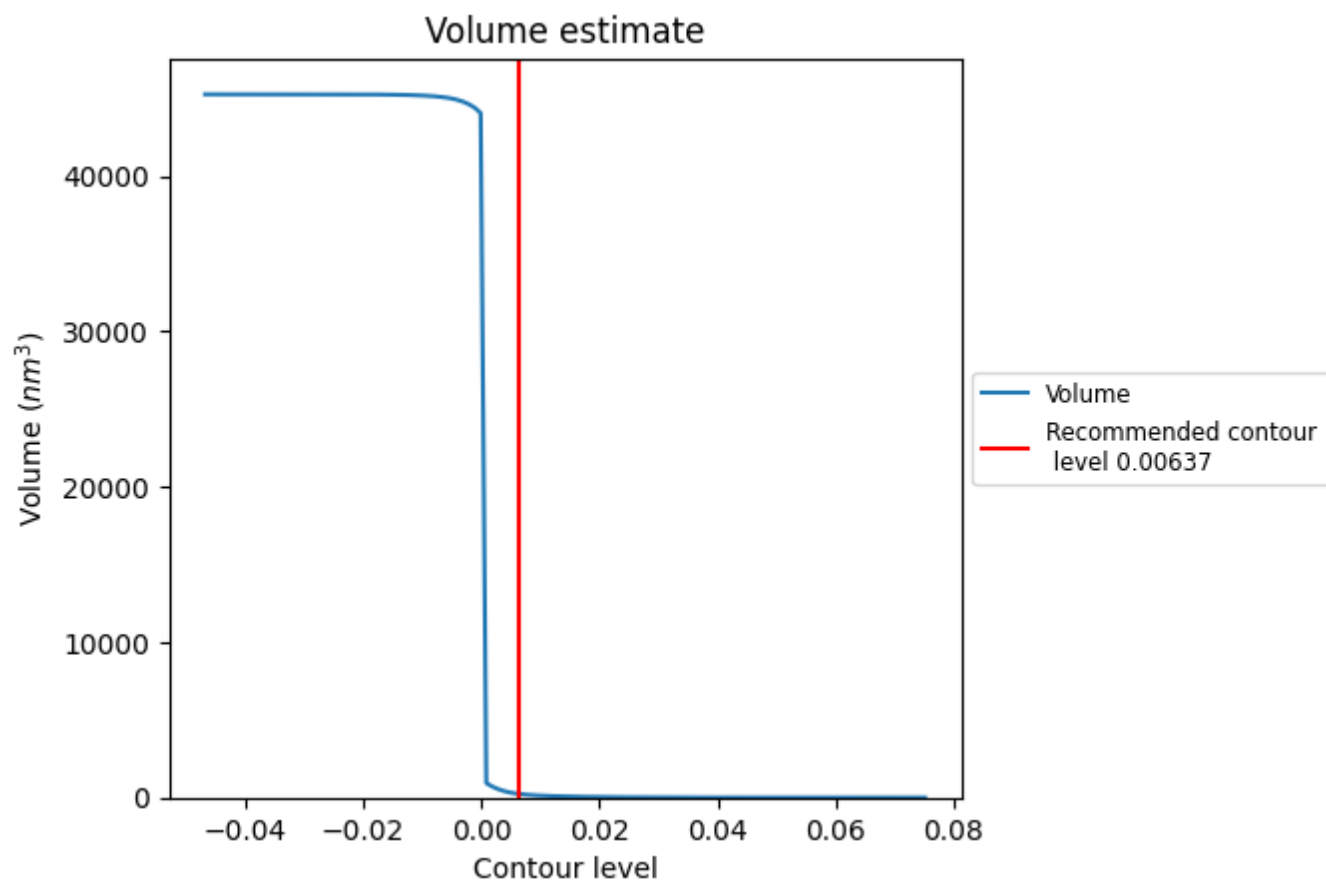
This section contains the results of statistical analysis of the map.

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.

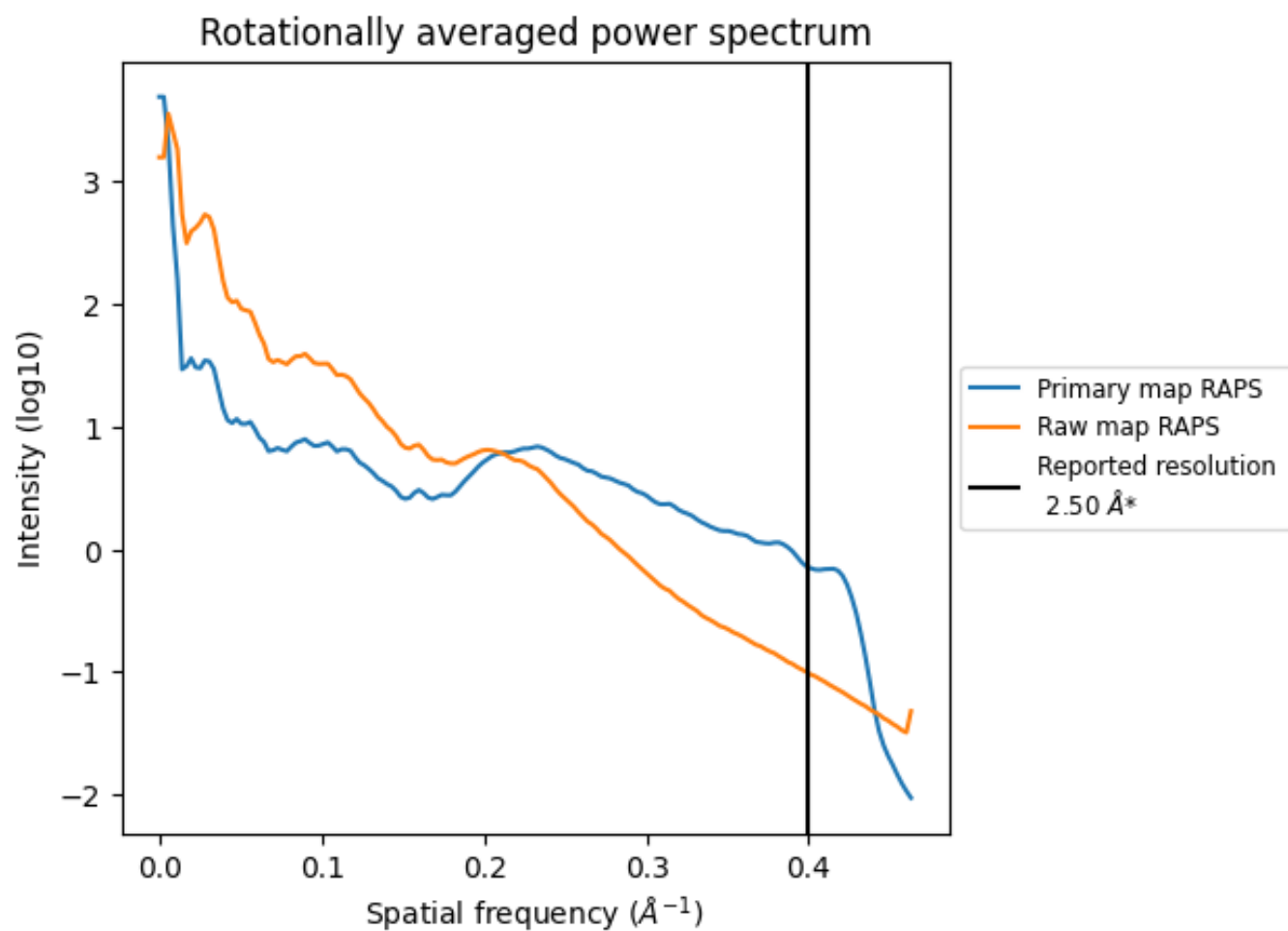
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 234 nm³; this corresponds to an approximate mass of 211 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 ⓘ

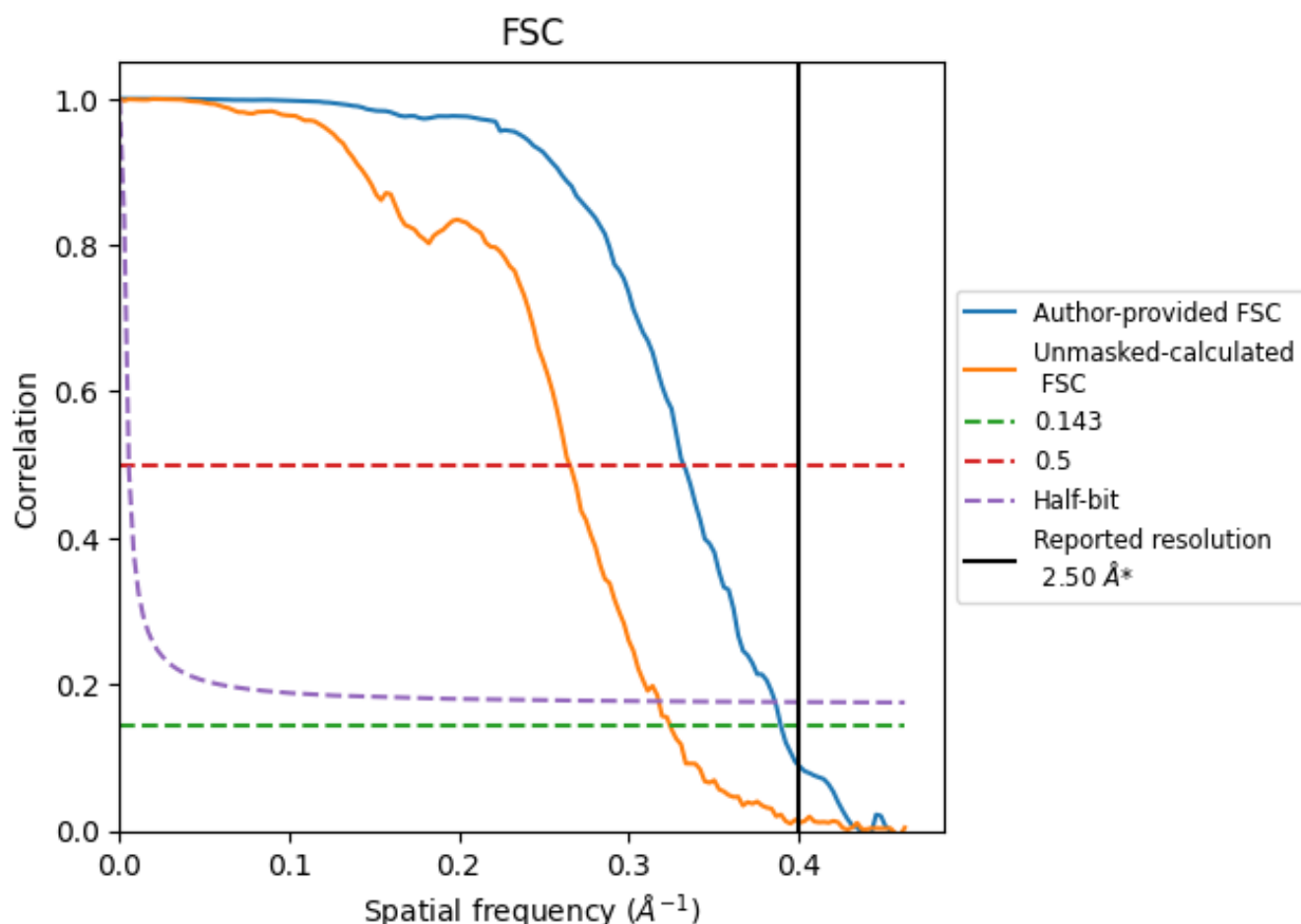


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.400 \AA^{-1}

8.2 Resolution estimates [i](#)

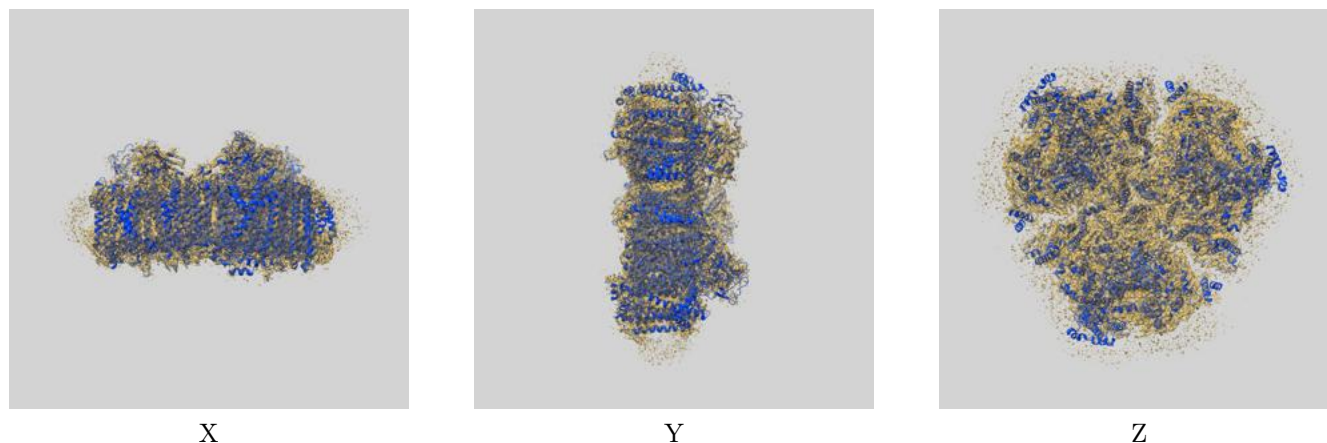
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.50 | - | - |
| Author-provided FSC curve | 2.56 | 3.01 | 2.59 |
| Unmasked-calculated* | 3.08 | 3.77 | 3.15 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.08 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

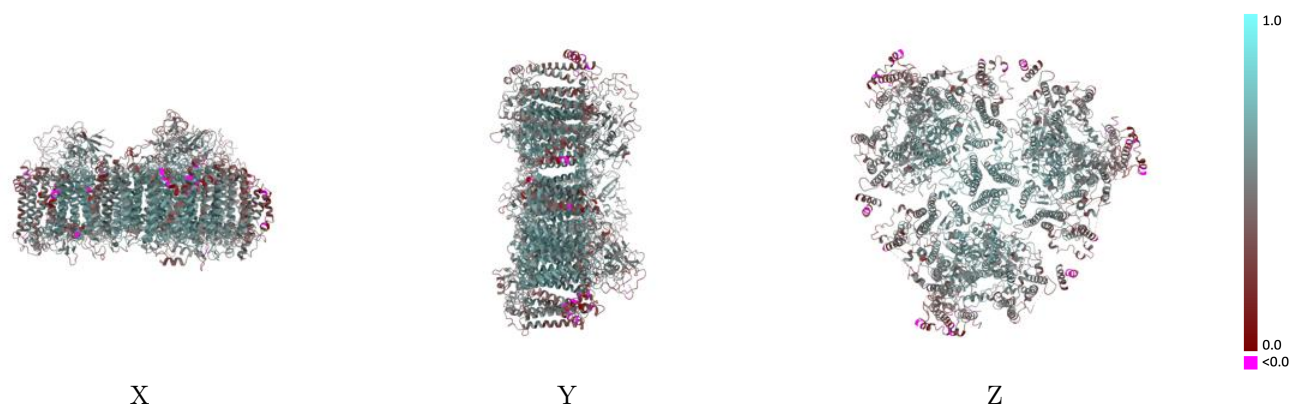
This section contains information regarding the fit between EMDB map EMD-30420 and PDB model 7COY. Per-residue inclusion information can be found in section [3](#) on page [30](#).

9.1 Map-model overlay [i](#)



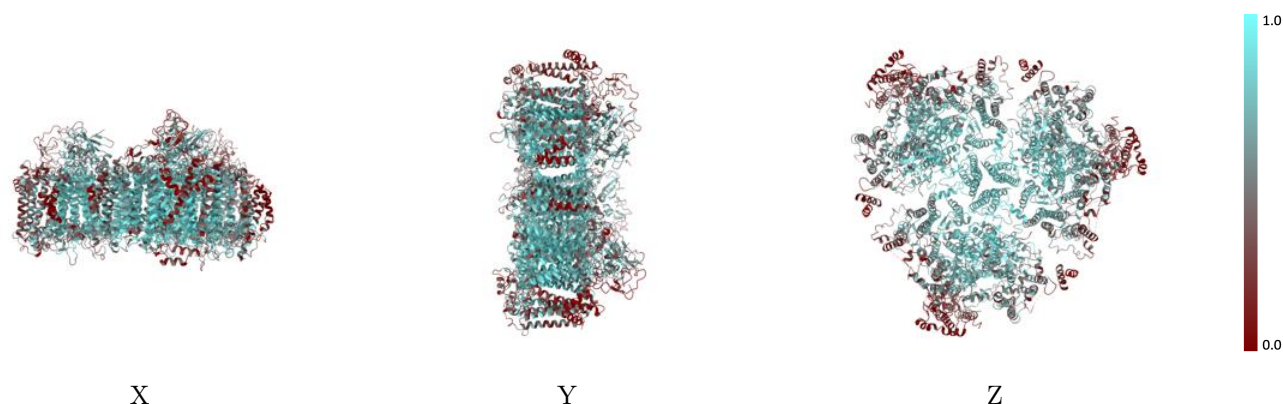
The images above show the 3D surface view of the map at the recommended contour level 0.00637 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



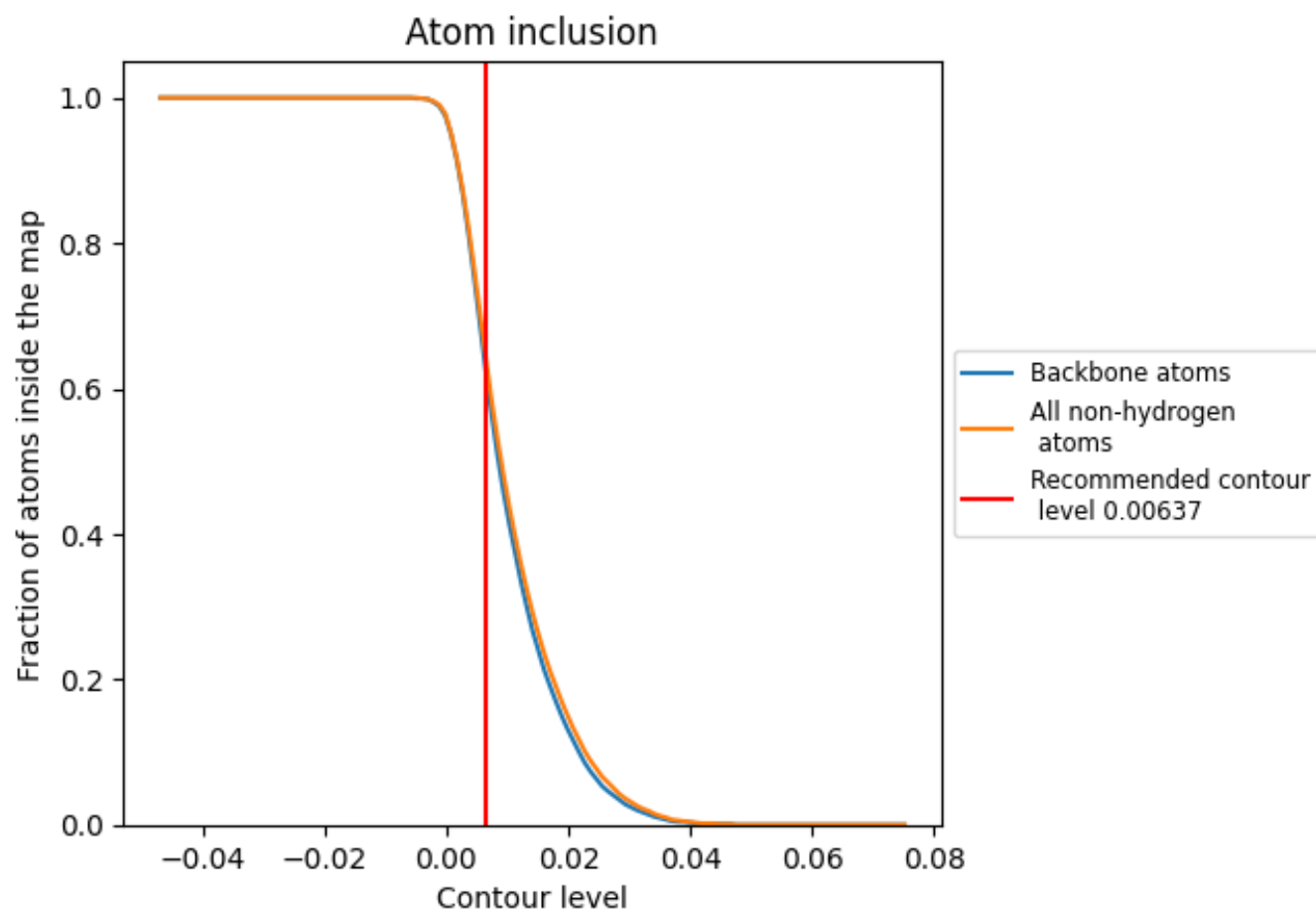
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00637).





































































9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 65% 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 (0.00637) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.6510 |  0.5530 |
| aA |  0.6990 |  0.5750 |
| aB |  0.6990 |  0.5740 |
| aC |  0.6750 |  0.5290 |
| aD |  0.5080 |  0.4760 |
| aE |  0.2160 |  0.3930 |
| aF |  0.2070 |  0.3320 |
| aI |  0.7970 |  0.6330 |
| aJ |  0.2620 |  0.4220 |
| aK |  0.0880 |  0.2480 |
| aL |  0.8270 |  0.6390 |
| aM |  0.5560 |  0.5030 |
| bA |  0.7030 |  0.5760 |
| bB |  0.6980 |  0.5740 |
| bC |  0.6780 |  0.5310 |
| bD |  0.5080 |  0.4790 |
| bE |  0.2070 |  0.4020 |
| bF |  0.1950 |  0.3290 |
| bI |  0.8040 |  0.6290 |
| bJ |  0.2590 |  0.4280 |
| bK |  0.0830 |  0.2480 |
| bL |  0.8320 |  0.6390 |
| bM |  0.5560 |  0.5060 |
| cA |  0.7070 |  0.5790 |
| cB |  0.6980 |  0.5740 |
| cC |  0.6900 |  0.5280 |
| cD |  0.5100 |  0.4790 |
| cE |  0.2000 |  0.3950 |
| cF |  0.1960 |  0.3370 |
| cI |  0.8170 |  0.6330 |
| cJ |  0.2650 |  0.4260 |
| cK |  0.0720 |  0.2680 |
| cL |  0.8340 |  0.6370 |
| cM |  0.5320 |  0.4980 |

