



## Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 10:44 pm BST

PDB ID : 6TRD / pdb\_00006trd  
EMDB ID : EMD-10559  
Title : Cryo- EM structure of the Thermosynechococcus elongatus photosystem I in the presence of cytochrome c6  
Authors : Koelsch, A.; Radon, C.; Baumert, A.; Buerger, J.; Mielke, T.; Lisdat, F.; Zouni, A.; Wendler, P.  
Deposited on : 2019-12-18  
Resolution : 3.16 Å (reported)  
Based on initial model : 1JB0

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.4, 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 : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

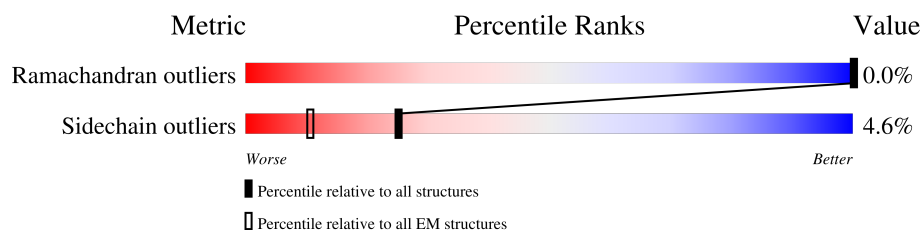
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.16 Å.

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




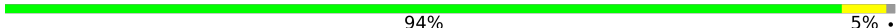






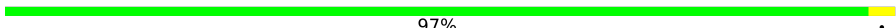
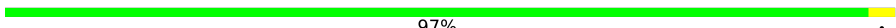
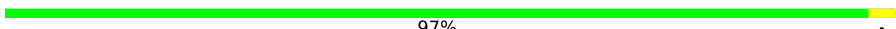






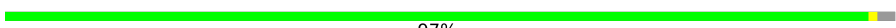
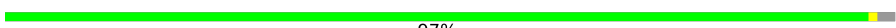
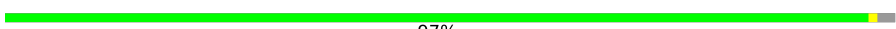





| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Ramachandran outliers | 207382                      | 16835                       |
| Sidechain outliers    | 206894                      | 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 1     | 755    | 95% . .          |
| 1   | A     | 755    | 95% . .          |
| 1   | a     | 755    | 95% . .          |
| 2   | 2     | 741    | 97% .            |
| 2   | B     | 741    | 97% .            |
| 2   | b     | 741    | 97% .            |
| 3   | 3     | 81     | 99% .            |
| 3   | C     | 81     | 99% .            |
| 3   | c     | 81     | 99% .            |
| 4   | 4     | 139    | 94% 5% .         |


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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 4   | D     | 139    |  94% 5% .       |
| 4   | d     | 139    |  94% 5% .       |
| 5   | 5     | 76     |  83% 9% 8%      |
| 5   | E     | 76     |  83% 9% 8%      |
| 5   | e     | 76     |  83% 9% 8%      |
| 6   | 6     | 141    |  89% 11%        |
| 6   | F     | 141    |  89% 11%        |
| 6   | f     | 141    |  89% 11%        |
| 7   | 7     | 38     |  97% .          |
| 7   | I     | 38     |  97% .          |
| 7   | i     | 38     |  97% .          |
| 8   | 8     | 41     |  90% 7% .      |
| 8   | J     | 41     |  90% 7% .     |
| 8   | j     | 41     |  90% 7% .     |
| 9   | 9     | 83     |  83% 10% . 5% |
| 9   | K     | 83     |  83% 10% . 5% |
| 9   | k     | 83     |  83% 10% . 5% |
| 10  | 0     | 155    |  97% ..       |
| 10  | L     | 155    |  97% ..       |
| 10  | l     | 155    |  97% ..       |
| 11  | M     | 31     |  90% 6% .     |
| 11  | m     | 31     |  90% 6% .     |
| 11  | y     | 31     |  90% 6% .     |
| 12  | X     | 36     |  64% 11% 25%  |
| 12  | x     | 36     |  64% 11% 25%  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 12  | z     | 36     |  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 13  | CL0  | 1     | 1602 | X         | -        | -       | -                |
| 13  | CL0  | A     | 801  | X         | -        | -       | -                |
| 13  | CL0  | a     | 801  | X         | -        | -       | -                |
| 14  | CLA  | 0     | 205  | X         | -        | -       | -                |
| 14  | CLA  | 0     | 206  | X         | -        | -       | -                |
| 14  | CLA  | 0     | 207  | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1601 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1603 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1604 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1605 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1606 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1607 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1608 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1609 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1610 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1611 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1612 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1613 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1614 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1615 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1616 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1617 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1618 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1619 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1620 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1621 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1622 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1623 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1624 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1625 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1626 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1627 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1628 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1629 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1630 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14  | CLA  | 1     | 1631 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1632 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1633 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1634 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1635 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1636 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1637 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1638 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1639 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1640 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1641 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1642 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1643 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1644 | X         | -        | -       | -                |
| 14  | CLA  | 1     | 1645 | X         | -        | -       | -                |
| 14  | CLA  | 2     | 802  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 803  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 804  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 805  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 806  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 807  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 808  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 809  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 810  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 811  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 812  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 813  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 814  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 815  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 816  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 817  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 818  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 819  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 820  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 821  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 822  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 823  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 824  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 825  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 826  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 827  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 828  | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14  | CLA  | 2     | 829  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 830  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 831  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 832  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 833  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 834  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 835  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 836  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 837  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 838  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 839  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 841  | X         | -        | -       | -                |
| 14  | CLA  | 2     | 842  | X         | -        | -       | -                |
| 14  | CLA  | 6     | 201  | X         | -        | -       | -                |
| 14  | CLA  | 6     | 203  | X         | -        | -       | -                |
| 14  | CLA  | 8     | 1301 | X         | -        | -       | -                |
| 14  | CLA  | 8     | 1302 | X         | -        | -       | -                |
| 14  | CLA  | 8     | 1303 | X         | -        | -       | -                |
| 14  | CLA  | 9     | 101  | X         | -        | -       | -                |
| 14  | CLA  | 9     | 103  | X         | -        | -       | -                |
| 14  | CLA  | A     | 802  | X         | -        | -       | -                |
| 14  | CLA  | A     | 803  | X         | -        | -       | -                |
| 14  | CLA  | A     | 804  | X         | -        | -       | -                |
| 14  | CLA  | A     | 805  | X         | -        | -       | -                |
| 14  | CLA  | A     | 806  | X         | -        | -       | -                |
| 14  | CLA  | A     | 807  | X         | -        | -       | -                |
| 14  | CLA  | A     | 808  | X         | -        | -       | -                |
| 14  | CLA  | A     | 809  | X         | -        | -       | -                |
| 14  | CLA  | A     | 810  | X         | -        | -       | -                |
| 14  | CLA  | A     | 811  | X         | -        | -       | -                |
| 14  | CLA  | A     | 812  | X         | -        | -       | -                |
| 14  | CLA  | A     | 813  | X         | -        | -       | -                |
| 14  | CLA  | A     | 814  | X         | -        | -       | -                |
| 14  | CLA  | A     | 815  | X         | -        | -       | -                |
| 14  | CLA  | A     | 816  | X         | -        | -       | -                |
| 14  | CLA  | A     | 817  | X         | -        | -       | -                |
| 14  | CLA  | A     | 818  | X         | -        | -       | -                |
| 14  | CLA  | A     | 819  | X         | -        | -       | -                |
| 14  | CLA  | A     | 820  | X         | -        | -       | -                |
| 14  | CLA  | A     | 821  | X         | -        | -       | -                |
| 14  | CLA  | A     | 822  | X         | -        | -       | -                |
| 14  | CLA  | A     | 823  | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 14  | CLA  | A     | 824 | X         | -        | -       | -                |
| 14  | CLA  | A     | 825 | X         | -        | -       | -                |
| 14  | CLA  | A     | 826 | X         | -        | -       | -                |
| 14  | CLA  | A     | 827 | X         | -        | -       | -                |
| 14  | CLA  | A     | 828 | X         | -        | -       | -                |
| 14  | CLA  | A     | 829 | X         | -        | -       | -                |
| 14  | CLA  | A     | 830 | X         | -        | -       | -                |
| 14  | CLA  | A     | 831 | X         | -        | -       | -                |
| 14  | CLA  | A     | 832 | X         | -        | -       | -                |
| 14  | CLA  | A     | 833 | X         | -        | -       | -                |
| 14  | CLA  | A     | 834 | X         | -        | -       | -                |
| 14  | CLA  | A     | 835 | X         | -        | -       | -                |
| 14  | CLA  | A     | 836 | X         | -        | -       | -                |
| 14  | CLA  | A     | 837 | X         | -        | -       | -                |
| 14  | CLA  | A     | 838 | X         | -        | -       | -                |
| 14  | CLA  | A     | 839 | X         | -        | -       | -                |
| 14  | CLA  | A     | 840 | X         | -        | -       | -                |
| 14  | CLA  | A     | 841 | X         | -        | -       | -                |
| 14  | CLA  | A     | 842 | X         | -        | -       | -                |
| 14  | CLA  | A     | 843 | X         | -        | -       | -                |
| 14  | CLA  | A     | 844 | X         | -        | -       | -                |
| 14  | CLA  | A     | 855 | X         | -        | -       | -                |
| 14  | CLA  | A     | 857 | X         | -        | -       | -                |
| 14  | CLA  | B     | 802 | X         | -        | -       | -                |
| 14  | CLA  | B     | 803 | X         | -        | -       | -                |
| 14  | CLA  | B     | 804 | X         | -        | -       | -                |
| 14  | CLA  | B     | 805 | X         | -        | -       | -                |
| 14  | CLA  | B     | 806 | X         | -        | -       | -                |
| 14  | CLA  | B     | 807 | X         | -        | -       | -                |
| 14  | CLA  | B     | 808 | X         | -        | -       | -                |
| 14  | CLA  | B     | 809 | X         | -        | -       | -                |
| 14  | CLA  | B     | 810 | X         | -        | -       | -                |
| 14  | CLA  | B     | 811 | X         | -        | -       | -                |
| 14  | CLA  | B     | 812 | X         | -        | -       | -                |
| 14  | CLA  | B     | 813 | X         | -        | -       | -                |
| 14  | CLA  | B     | 814 | X         | -        | -       | -                |
| 14  | CLA  | B     | 815 | X         | -        | -       | -                |
| 14  | CLA  | B     | 816 | X         | -        | -       | -                |
| 14  | CLA  | B     | 817 | X         | -        | -       | -                |
| 14  | CLA  | B     | 818 | X         | -        | -       | -                |
| 14  | CLA  | B     | 819 | X         | -        | -       | -                |
| 14  | CLA  | B     | 820 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14  | CLA  | B     | 821  | X         | -        | -       | -                |
| 14  | CLA  | B     | 822  | X         | -        | -       | -                |
| 14  | CLA  | B     | 823  | X         | -        | -       | -                |
| 14  | CLA  | B     | 824  | X         | -        | -       | -                |
| 14  | CLA  | B     | 825  | X         | -        | -       | -                |
| 14  | CLA  | B     | 826  | X         | -        | -       | -                |
| 14  | CLA  | B     | 827  | X         | -        | -       | -                |
| 14  | CLA  | B     | 828  | X         | -        | -       | -                |
| 14  | CLA  | B     | 829  | X         | -        | -       | -                |
| 14  | CLA  | B     | 830  | X         | -        | -       | -                |
| 14  | CLA  | B     | 831  | X         | -        | -       | -                |
| 14  | CLA  | B     | 832  | X         | -        | -       | -                |
| 14  | CLA  | B     | 833  | X         | -        | -       | -                |
| 14  | CLA  | B     | 834  | X         | -        | -       | -                |
| 14  | CLA  | B     | 835  | X         | -        | -       | -                |
| 14  | CLA  | B     | 836  | X         | -        | -       | -                |
| 14  | CLA  | B     | 837  | X         | -        | -       | -                |
| 14  | CLA  | B     | 838  | X         | -        | -       | -                |
| 14  | CLA  | B     | 840  | X         | -        | -       | -                |
| 14  | CLA  | B     | 841  | X         | -        | -       | -                |
| 14  | CLA  | F     | 201  | X         | -        | -       | -                |
| 14  | CLA  | F     | 203  | X         | -        | -       | -                |
| 14  | CLA  | F     | 204  | X         | -        | -       | -                |
| 14  | CLA  | J     | 101  | X         | -        | -       | -                |
| 14  | CLA  | J     | 102  | X         | -        | -       | -                |
| 14  | CLA  | K     | 101  | X         | -        | -       | -                |
| 14  | CLA  | K     | 103  | X         | -        | -       | -                |
| 14  | CLA  | L     | 203  | X         | -        | -       | -                |
| 14  | CLA  | L     | 204  | X         | -        | -       | -                |
| 14  | CLA  | L     | 205  | X         | -        | -       | -                |
| 14  | CLA  | M     | 102  | X         | -        | -       | -                |
| 14  | CLA  | X     | 1701 | X         | -        | -       | -                |
| 14  | CLA  | a     | 802  | X         | -        | -       | -                |
| 14  | CLA  | a     | 803  | X         | -        | -       | -                |
| 14  | CLA  | a     | 804  | X         | -        | -       | -                |
| 14  | CLA  | a     | 805  | X         | -        | -       | -                |
| 14  | CLA  | a     | 806  | X         | -        | -       | -                |
| 14  | CLA  | a     | 807  | X         | -        | -       | -                |
| 14  | CLA  | a     | 808  | X         | -        | -       | -                |
| 14  | CLA  | a     | 809  | X         | -        | -       | -                |
| 14  | CLA  | a     | 810  | X         | -        | -       | -                |
| 14  | CLA  | a     | 811  | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 14  | CLA  | a     | 812 | X         | -        | -       | -                |
| 14  | CLA  | a     | 813 | X         | -        | -       | -                |
| 14  | CLA  | a     | 814 | X         | -        | -       | -                |
| 14  | CLA  | a     | 815 | X         | -        | -       | -                |
| 14  | CLA  | a     | 816 | X         | -        | -       | -                |
| 14  | CLA  | a     | 817 | X         | -        | -       | -                |
| 14  | CLA  | a     | 818 | X         | -        | -       | -                |
| 14  | CLA  | a     | 819 | X         | -        | -       | -                |
| 14  | CLA  | a     | 820 | X         | -        | -       | -                |
| 14  | CLA  | a     | 821 | X         | -        | -       | -                |
| 14  | CLA  | a     | 822 | X         | -        | -       | -                |
| 14  | CLA  | a     | 823 | X         | -        | -       | -                |
| 14  | CLA  | a     | 824 | X         | -        | -       | -                |
| 14  | CLA  | a     | 825 | X         | -        | -       | -                |
| 14  | CLA  | a     | 826 | X         | -        | -       | -                |
| 14  | CLA  | a     | 827 | X         | -        | -       | -                |
| 14  | CLA  | a     | 828 | X         | -        | -       | -                |
| 14  | CLA  | a     | 829 | X         | -        | -       | -                |
| 14  | CLA  | a     | 830 | X         | -        | -       | -                |
| 14  | CLA  | a     | 831 | X         | -        | -       | -                |
| 14  | CLA  | a     | 832 | X         | -        | -       | -                |
| 14  | CLA  | a     | 833 | X         | -        | -       | -                |
| 14  | CLA  | a     | 834 | X         | -        | -       | -                |
| 14  | CLA  | a     | 835 | X         | -        | -       | -                |
| 14  | CLA  | a     | 836 | X         | -        | -       | -                |
| 14  | CLA  | a     | 837 | X         | -        | -       | -                |
| 14  | CLA  | a     | 838 | X         | -        | -       | -                |
| 14  | CLA  | a     | 839 | X         | -        | -       | -                |
| 14  | CLA  | a     | 840 | X         | -        | -       | -                |
| 14  | CLA  | a     | 841 | X         | -        | -       | -                |
| 14  | CLA  | a     | 842 | X         | -        | -       | -                |
| 14  | CLA  | a     | 843 | X         | -        | -       | -                |
| 14  | CLA  | a     | 844 | X         | -        | -       | -                |
| 14  | CLA  | b     | 802 | X         | -        | -       | -                |
| 14  | CLA  | b     | 803 | X         | -        | -       | -                |
| 14  | CLA  | b     | 804 | X         | -        | -       | -                |
| 14  | CLA  | b     | 805 | X         | -        | -       | -                |
| 14  | CLA  | b     | 806 | X         | -        | -       | -                |
| 14  | CLA  | b     | 807 | X         | -        | -       | -                |
| 14  | CLA  | b     | 808 | X         | -        | -       | -                |
| 14  | CLA  | b     | 809 | X         | -        | -       | -                |
| 14  | CLA  | b     | 810 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14  | CLA  | b     | 811  | X         | -        | -       | -                |
| 14  | CLA  | b     | 812  | X         | -        | -       | -                |
| 14  | CLA  | b     | 813  | X         | -        | -       | -                |
| 14  | CLA  | b     | 814  | X         | -        | -       | -                |
| 14  | CLA  | b     | 815  | X         | -        | -       | -                |
| 14  | CLA  | b     | 816  | X         | -        | -       | -                |
| 14  | CLA  | b     | 817  | X         | -        | -       | -                |
| 14  | CLA  | b     | 818  | X         | -        | -       | -                |
| 14  | CLA  | b     | 819  | X         | -        | -       | -                |
| 14  | CLA  | b     | 820  | X         | -        | -       | -                |
| 14  | CLA  | b     | 821  | X         | -        | -       | -                |
| 14  | CLA  | b     | 822  | X         | -        | -       | -                |
| 14  | CLA  | b     | 823  | X         | -        | -       | -                |
| 14  | CLA  | b     | 824  | X         | -        | -       | -                |
| 14  | CLA  | b     | 825  | X         | -        | -       | -                |
| 14  | CLA  | b     | 826  | X         | -        | -       | -                |
| 14  | CLA  | b     | 827  | X         | -        | -       | -                |
| 14  | CLA  | b     | 828  | X         | -        | -       | -                |
| 14  | CLA  | b     | 829  | X         | -        | -       | -                |
| 14  | CLA  | b     | 830  | X         | -        | -       | -                |
| 14  | CLA  | b     | 831  | X         | -        | -       | -                |
| 14  | CLA  | b     | 832  | X         | -        | -       | -                |
| 14  | CLA  | b     | 833  | X         | -        | -       | -                |
| 14  | CLA  | b     | 834  | X         | -        | -       | -                |
| 14  | CLA  | b     | 835  | X         | -        | -       | -                |
| 14  | CLA  | b     | 836  | X         | -        | -       | -                |
| 14  | CLA  | b     | 837  | X         | -        | -       | -                |
| 14  | CLA  | b     | 838  | X         | -        | -       | -                |
| 14  | CLA  | b     | 839  | X         | -        | -       | -                |
| 14  | CLA  | b     | 841  | X         | -        | -       | -                |
| 14  | CLA  | b     | 842  | X         | -        | -       | -                |
| 14  | CLA  | f     | 201  | X         | -        | -       | -                |
| 14  | CLA  | f     | 203  | X         | -        | -       | -                |
| 14  | CLA  | j     | 1301 | X         | -        | -       | -                |
| 14  | CLA  | j     | 1302 | X         | -        | -       | -                |
| 14  | CLA  | j     | 1303 | X         | -        | -       | -                |
| 14  | CLA  | k     | 101  | X         | -        | -       | -                |
| 14  | CLA  | k     | 103  | X         | -        | -       | -                |
| 14  | CLA  | l     | 204  | X         | -        | -       | -                |
| 14  | CLA  | l     | 205  | X         | -        | -       | -                |
| 14  | CLA  | l     | 206  | X         | -        | -       | -                |
| 14  | CLA  | x     | 1701 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 14  | CLA  | z     | 102 | X         | -        | -       | -                |

## 2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 74991 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   | A     | 746      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5826  | 3823 | 995 | 982 | 26 |         |       |
| 1   | a     | 746      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5826  | 3823 | 995 | 982 | 26 |         |       |
| 1   | 1     | 746      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5826  | 3823 | 995 | 982 | 26 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 2   | B     | 740      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5894  | 3878 | 988 | 1007 | 21 |         |       |
| 2   | b     | 740      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5894  | 3878 | 988 | 1007 | 21 |         |       |
| 2   | 2     | 740      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5894  | 3878 | 988 | 1007 | 21 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 3   | C     | 80       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 598   | 367 | 103 | 117 | 11 |         |       |
| 3   | c     | 80       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 598   | 367 | 103 | 117 | 11 |         |       |
| 3   | 3     | 80       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 598   | 367 | 103 | 117 | 11 |         |       |

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | D     | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1075  | 682 | 186 | 204 | 3 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | d     | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1075  | 682 | 186 | 204 | 3 |         |       |
| 4   | 4     | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1075  | 682 | 186 | 204 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|--|---------|-------|
| 5   | E     | 70       | Total | C   | N  | O   |  | 0       | 0     |
|     |       |          | 546   | 347 | 94 | 105 |  |         |       |
| 5   | e     | 70       | Total | C   | N  | O   |  | 0       | 0     |
|     |       |          | 546   | 347 | 94 | 105 |  |         |       |
| 5   | 5     | 70       | Total | C   | N  | O   |  | 0       | 0     |
|     |       |          | 546   | 347 | 94 | 105 |  |         |       |

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | F     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1065  | 680 | 184 | 197 | 4 |         |       |
| 6   | f     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1065  | 680 | 184 | 197 | 4 |         |       |
| 6   | 6     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1065  | 680 | 184 | 197 | 4 |         |       |

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | I     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 303   | 209 | 40 | 49 | 5 |         |       |
| 7   | i     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 303   | 209 | 40 | 49 | 5 |         |       |
| 7   | 7     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 303   | 209 | 40 | 49 | 5 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8   | J     | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 340   | 232 | 51 | 55 | 2 |         |       |
| 8   | j     | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 340   | 232 | 51 | 55 | 2 |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8   | 8     | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 340   | 232 | 51 | 55 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 9   | K     | 79       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 571   | 377 | 92 | 101 | 1 |         |       |
| 9   | k     | 79       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 571   | 377 | 92 | 101 | 1 |         |       |
| 9   | 9     | 79       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 571   | 377 | 92 | 101 | 1 |         |       |

- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | L     | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1124  | 738 | 180 | 202 | 4 |         |       |
| 10  | l     | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1124  | 738 | 180 | 202 | 4 |         |       |
| 10  | 0     | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1124  | 738 | 180 | 202 | 4 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| L     | 143     | LEU      | SER    | conflict | UNP Q8DGB4 |
| l     | 143     | LEU      | SER    | conflict | UNP Q8DGB4 |
| 0     | 143     | LEU      | SER    | conflict | UNP Q8DGB4 |

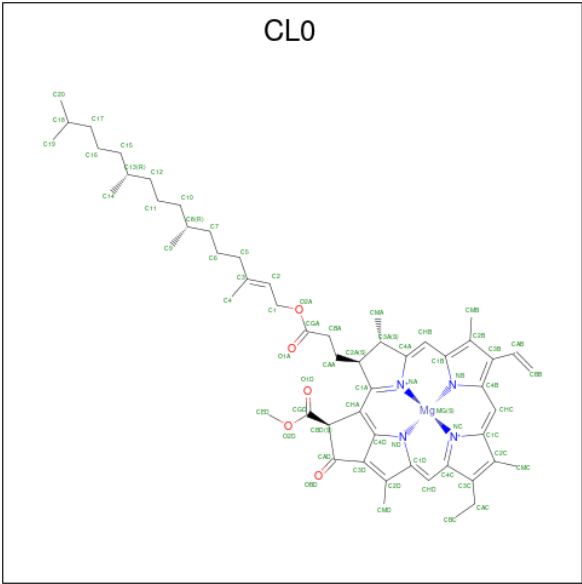
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 11  | M     | 31       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 241   | 161 | 36 | 43 | 1 |         |       |
| 11  | m     | 31       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 241   | 161 | 36 | 43 | 1 |         |       |
| 11  | y     | 31       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 241   | 161 | 36 | 43 | 1 |         |       |

- Molecule 12 is a protein called Photosystem I 4.8K protein.

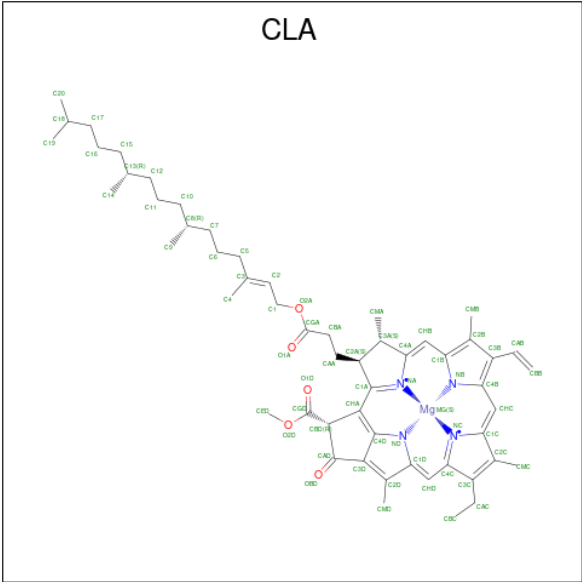
| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 12  | X     | 27       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 228   | 163 | 33 | 32 |         |       |
| 12  | x     | 27       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 228   | 163 | 33 | 32 |         |       |
| 12  | z     | 27       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 228   | 163 | 33 | 32 |         |       |

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 13  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 13  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 13  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14  | A     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>36 | C<br>30 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | F     | 1        | Total<br>58 | C<br>48 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | F     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | F     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | J     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | J     | 1        | Total<br>37 | C<br>31 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 14  | K     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | K     | 1        | Total<br>58 | C<br>48 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | L     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | L     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | L     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | M     | 1        | Total<br>36 | C<br>30 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 14  | X     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 14  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 14  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 14  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 14  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 14  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 14  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | f     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 58    | 48 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14  | f     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 14  | j     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | j     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | j     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 37    | 31 | 1  | 4 | 1 |         |
| 14  | k     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 14  | k     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 58    | 48 | 1  | 4 | 5 |         |
| 14  | l     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | l     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | l     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | x     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 36    | 30 | 1  | 4 | 1 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14  | 1     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 1     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 1     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 1     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 1     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 1     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 1     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 1     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 1     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 1     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 1     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 1     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 2     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 2     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 2     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 2     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 2     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 2     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 2     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 2     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 2     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 14  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |

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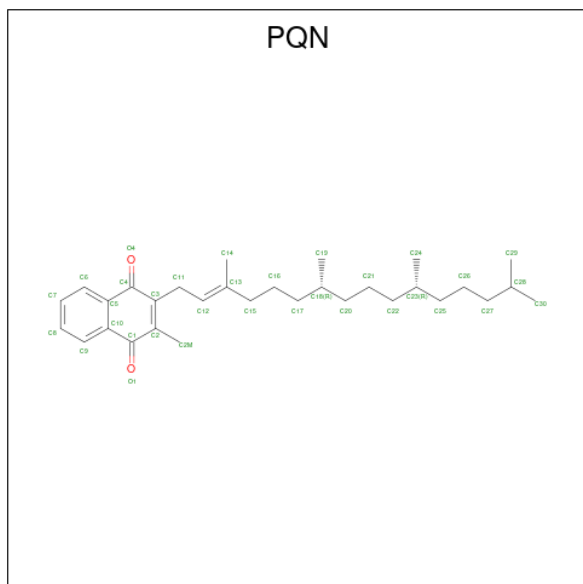
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14  | 2     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 2     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 2     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 2     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 2     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 2     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 2     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 2     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 2     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 2     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 2     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 6     | 1        | Total<br>58 | C<br>48 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 6     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 8     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 8     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 8     | 1        | Total<br>37 | C<br>31 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 14  | 9     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 9     | 1        | Total<br>58 | C<br>48 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 0     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 0     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | 0     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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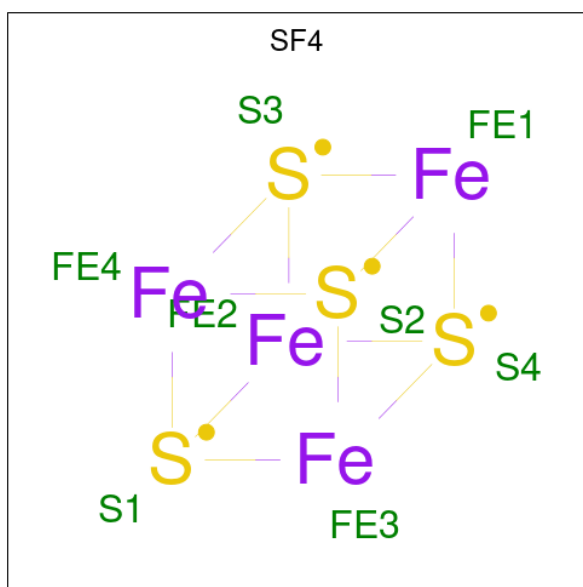
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14  | z     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ).



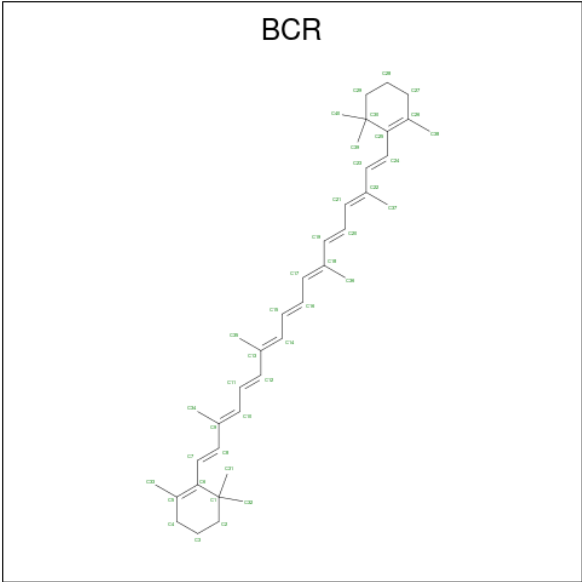
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 15  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 15  | B     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 15  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 15  | b     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 15  | 1     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 15  | 2     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $Fe_4S_4$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 16  | A     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 16  | C     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 16  | C     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 16  | a     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 16  | c     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 16  | c     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 16  | 1     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 16  | 3     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 16  | 3     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

- Molecule 17 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 17  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 17  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 17  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 17  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 17  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 17  | A     | 1        | Total | C  | 0       |
|     |       |          | 25    | 25 |         |
| 17  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 17  | B     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 17  | B     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 17  | B     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 17  | B     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 17  | B     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 17  | B     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |

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| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 17  | F     | 1        | Total C<br>40 40 | 0       |
| 17  | F     | 1        | Total C<br>40 40 | 0       |
| 17  | I     | 1        | Total C<br>40 40 | 0       |
| 17  | J     | 1        | Total C<br>40 40 | 0       |
| 17  | K     | 1        | Total C<br>40 40 | 0       |
| 17  | K     | 1        | Total C<br>25 25 | 0       |
| 17  | L     | 1        | Total C<br>40 40 | 0       |
| 17  | L     | 1        | Total C<br>40 40 | 0       |
| 17  | L     | 1        | Total C<br>40 40 | 0       |
| 17  | M     | 1        | Total C<br>40 40 | 0       |
| 17  | a     | 1        | Total C<br>40 40 | 0       |
| 17  | a     | 1        | Total C<br>40 40 | 0       |
| 17  | a     | 1        | Total C<br>40 40 | 0       |
| 17  | a     | 1        | Total C<br>40 40 | 0       |
| 17  | a     | 1        | Total C<br>40 40 | 0       |
| 17  | a     | 1        | Total C<br>25 25 | 0       |
| 17  | b     | 1        | Total C<br>40 40 | 0       |
| 17  | b     | 1        | Total C<br>40 40 | 0       |
| 17  | b     | 1        | Total C<br>40 40 | 0       |
| 17  | b     | 1        | Total C<br>40 40 | 0       |
| 17  | b     | 1        | Total C<br>40 40 | 0       |

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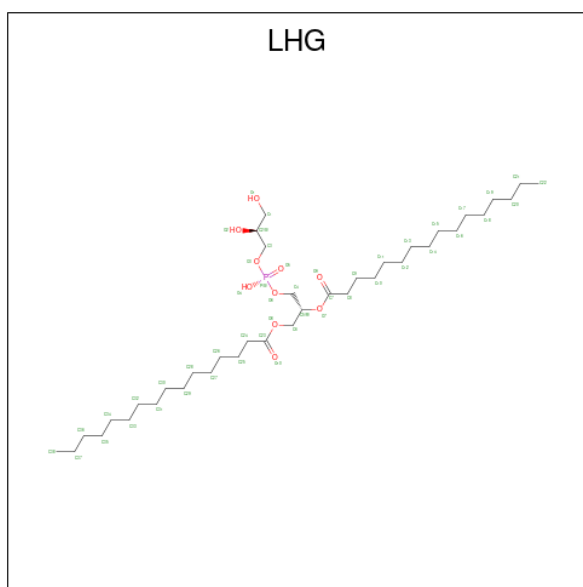
| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 17  | b     | 1        | Total C<br>40 40 | 0       |
| 17  | b     | 1        | Total C<br>40 40 | 0       |
| 17  | f     | 1        | Total C<br>40 40 | 0       |
| 17  | f     | 1        | Total C<br>40 40 | 0       |
| 17  | i     | 1        | Total C<br>40 40 | 0       |
| 17  | j     | 1        | Total C<br>40 40 | 0       |
| 17  | j     | 1        | Total C<br>40 40 | 0       |
| 17  | k     | 1        | Total C<br>40 40 | 0       |
| 17  | k     | 1        | Total C<br>25 25 | 0       |
| 17  | l     | 1        | Total C<br>40 40 | 0       |
| 17  | l     | 1        | Total C<br>40 40 | 0       |
| 17  | m     | 1        | Total C<br>40 40 | 0       |
| 17  | 1     | 1        | Total C<br>40 40 | 0       |
| 17  | 1     | 1        | Total C<br>40 40 | 0       |
| 17  | 1     | 1        | Total C<br>40 40 | 0       |
| 17  | 1     | 1        | Total C<br>40 40 | 0       |
| 17  | 1     | 1        | Total C<br>40 40 | 0       |
| 17  | 1     | 1        | Total C<br>25 25 | 0       |
| 17  | 2     | 1        | Total C<br>40 40 | 0       |
| 17  | 2     | 1        | Total C<br>40 40 | 0       |
| 17  | 2     | 1        | Total C<br>40 40 | 0       |

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| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 17  | 2     | 1        | Total C<br>40 40 | 0       |
| 17  | 2     | 1        | Total C<br>40 40 | 0       |
| 17  | 2     | 1        | Total C<br>40 40 | 0       |
| 17  | 6     | 1        | Total C<br>40 40 | 0       |
| 17  | 6     | 1        | Total C<br>40 40 | 0       |
| 17  | 7     | 1        | Total C<br>40 40 | 0       |
| 17  | 8     | 1        | Total C<br>40 40 | 0       |
| 17  | 8     | 1        | Total C<br>40 40 | 0       |
| 17  | 8     | 1        | Total C<br>40 40 | 0       |
| 17  | 9     | 1        | Total C<br>40 40 | 0       |
| 17  | 9     | 1        | Total C<br>25 25 | 0       |
| 17  | 0     | 1        | Total C<br>40 40 | 0       |
| 17  | 0     | 1        | Total C<br>40 40 | 0       |
| 17  | 0     | 1        | Total C<br>40 40 | 0       |
| 17  | 0     | 1        | Total C<br>40 40 | 0       |
| 17  | 0     | 1        | Total C<br>40 40 | 0       |
| 17  | y     | 1        | Total C<br>40 40 | 0       |

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



| Mol | Chain | Residues | Atoms       |         |         |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|
| 18  | A     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       |
| 18  | A     | 1        | Total<br>41 | C<br>30 | O<br>10 | P<br>1 | 0       |
| 18  | B     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       |
| 18  | L     | 1        | Total<br>39 | C<br>28 | O<br>10 | P<br>1 | 0       |
| 18  | M     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       |
| 18  | a     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       |
| 18  | a     | 1        | Total<br>41 | C<br>30 | O<br>10 | P<br>1 | 0       |
| 18  | b     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       |
| 18  | l     | 1        | Total<br>39 | C<br>28 | O<br>10 | P<br>1 | 0       |
| 18  | m     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       |
| 18  | 1     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       |
| 18  | 1     | 1        | Total<br>41 | C<br>30 | O<br>10 | P<br>1 | 0       |
| 18  | 0     | 1        | Total<br>39 | C<br>28 | O<br>10 | P<br>1 | 0       |
| 18  | y     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       |

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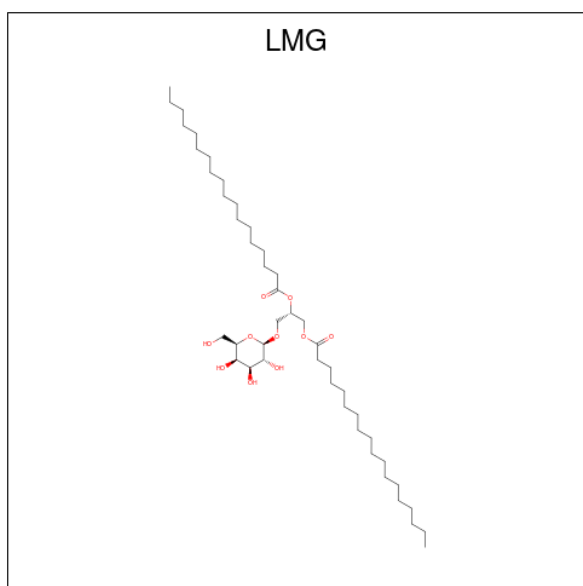
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| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 18  | z     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |

- Molecule 19 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 19  | B     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 19  | L     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 19  | b     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 19  | 1     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 19  | 2     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 19  | 0     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 20  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 45 | 10 |         |
| 20  | b     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 45 | 10 |         |

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| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 20  | 2     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 45 | 10 |         |

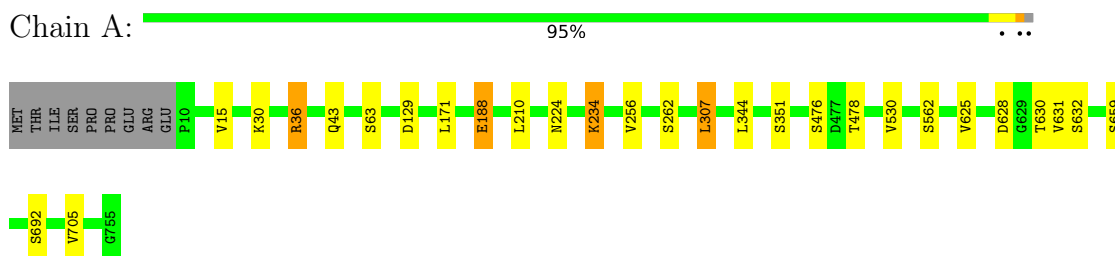
- Molecule 21 is water.

| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 21  | A     | 5        | Total | O | 0       |
|     |       |          | 5     | 5 |         |
| 21  | B     | 8        | Total | O | 0       |
|     |       |          | 8     | 8 |         |
| 21  | F     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 21  | J     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 21  | K     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 21  | L     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 21  | a     | 5        | Total | O | 0       |
|     |       |          | 5     | 5 |         |
| 21  | b     | 8        | Total | O | 0       |
|     |       |          | 8     | 8 |         |
| 21  | f     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 21  | j     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 21  | k     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 21  | l     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 21  | 1     | 5        | Total | O | 0       |
|     |       |          | 5     | 5 |         |
| 21  | 2     | 8        | Total | O | 0       |
|     |       |          | 8     | 8 |         |
| 21  | 6     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 21  | 8     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 21  | 9     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 21  | 0     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |

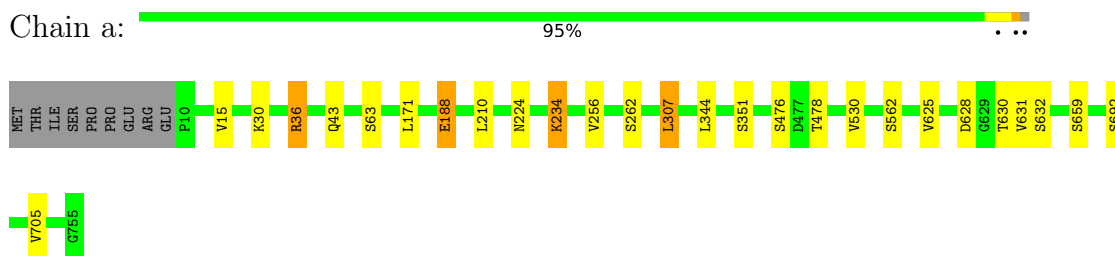
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

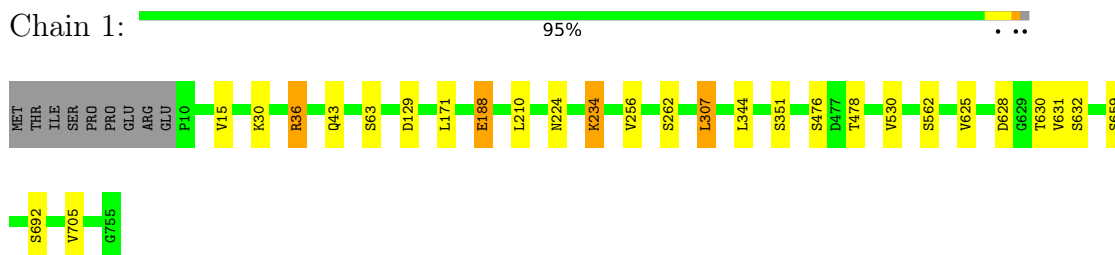
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



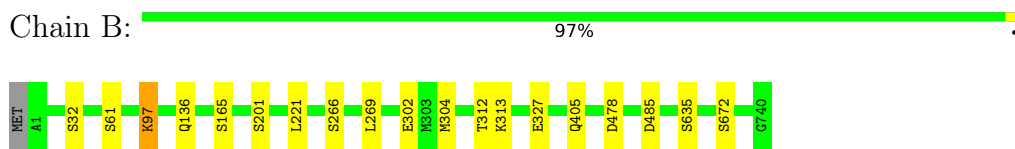
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:  97%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain 2:  97%



- Molecule 3: Photosystem I iron-sulfur center

Chain C:  99%



- Molecule 3: Photosystem I iron-sulfur center

Chain c:  99%



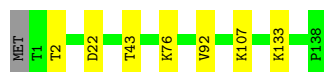
- Molecule 3: Photosystem I iron-sulfur center

Chain 3:  99%



- Molecule 4: Photosystem I reaction center subunit II

Chain D:  94% 5%



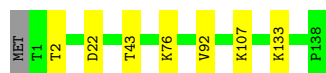
- Molecule 4: Photosystem I reaction center subunit II

Chain d:  94% 5%




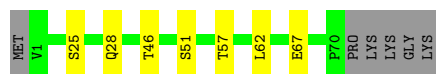
- Molecule 4: Photosystem I reaction center subunit II

Chain 4:  94% 5%




- Molecule 5: Photosystem I reaction center subunit IV

Chain E:  83% 9% 8%




- Molecule 5: Photosystem I reaction center subunit IV

Chain e:  83% 9% 8%




- Molecule 5: Photosystem I reaction center subunit IV

Chain 5:  83% 9% 8%




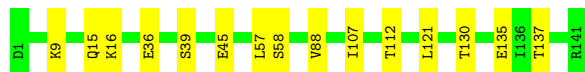
- Molecule 6: Photosystem I reaction center subunit III

Chain F:  89% 11%




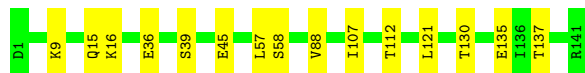
- Molecule 6: Photosystem I reaction center subunit III

Chain f:  89% 11%



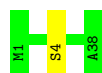
- Molecule 6: Photosystem I reaction center subunit III

Chain 6:  89% 11%



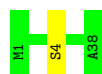
- Molecule 7: Photosystem I reaction center subunit VIII

Chain I:  97% .



- Molecule 7: Photosystem I reaction center subunit VIII

Chain i:  97% .




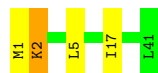
- Molecule 7: Photosystem I reaction center subunit VIII

Chain 7:  97% .




- Molecule 8: Photosystem I reaction center subunit IX

Chain J:  90% 7% .



- Molecule 8: Photosystem I reaction center subunit IX

Chain j:  90% 7% .




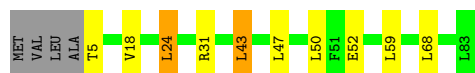
- Molecule 8: Photosystem I reaction center subunit IX

Chain 8:  90% 7% .




- Molecule 9: Photosystem I reaction center subunit PsaK

Chain K:  83% 10% 5% .




- Molecule 9: Photosystem I reaction center subunit PsaK

Chain k:  83% 10% • 5%



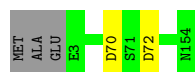
- Molecule 9: Photosystem I reaction center subunit Psak

Chain 9:  83% 10% • 5%



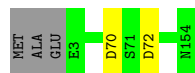
- Molecule 10: Photosystem I reaction center subunit XI

Chain L:  97% ..



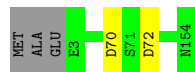
- Molecule 10: Photosystem I reaction center subunit XI

Chain l:  97% ..



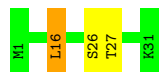
- Molecule 10: Photosystem I reaction center subunit XI

Chain 0:  97% ..



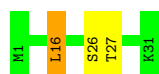
- Molecule 11: Photosystem I reaction center subunit XII

Chain M:  90% 6% •

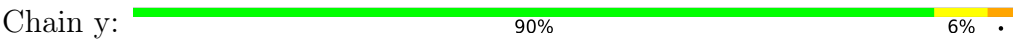


- Molecule 11: Photosystem I reaction center subunit XII

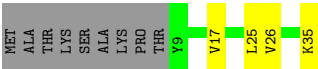
Chain m:  90% 6% •



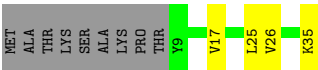
- Molecule 11: Photosystem I reaction center subunit XII



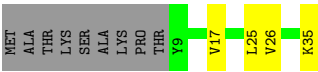
• Molecule 12: Photosystem I 4.8K protein



• Molecule 12: Photosystem I 4.8K protein



• Molecule 12: Photosystem I 4.8K protein





## 4 Experimental information

| Property                             | Value  | Source    |
|--------------------------------------|--|-----------|
| EM reconstruction method             | SINGLE PARTICLE  | Depositor |
| Imposed symmetry                     | POINT, C1  | Depositor |
| Number of particles used             | 175999   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF  | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION; CTFFIND4 was used to estimate contrast transfer function parameters. CTF correction was done in Relion 3.0. | Depositor |
| Microscope                           | FEI POLARA 300   | Depositor |
| Voltage (kV)                         | 300  | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 32   | Depositor |
| Minimum defocus (nm)                 | Not provided   |           |
| Maximum defocus (nm)                 | Not provided   |           |
| Magnification                        | Not provided   |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)  | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL0, FME, LMG, BCR, CA, PQN, SF4, LHG, CLA

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

| Mol | Chain | Bond lengths |             | Bond angles |               |
|-----|-------|--------------|-------------|-------------|---------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$   |
| 1   | 1     | 0.44         | 0/6027      | 0.54        | 6/8220 (0.1%) |
| 1   | A     | 0.44         | 0/6027      | 0.54        | 6/8220 (0.1%) |
| 1   | a     | 0.44         | 0/6027      | 0.54        | 6/8220 (0.1%) |
| 2   | 2     | 0.44         | 0/6112      | 0.51        | 4/8350 (0.0%) |
| 2   | B     | 0.44         | 0/6112      | 0.51        | 4/8350 (0.0%) |
| 2   | b     | 0.44         | 0/6112      | 0.51        | 4/8350 (0.0%) |
| 3   | 3     | 0.45         | 0/608       | 0.50        | 0/824         |
| 3   | C     | 0.45         | 0/608       | 0.49        | 0/824         |
| 3   | c     | 0.45         | 0/608       | 0.50        | 0/824         |
| 4   | 4     | 0.43         | 0/1101      | 0.70        | 2/1492 (0.1%) |
| 4   | D     | 0.43         | 0/1101      | 0.70        | 2/1492 (0.1%) |
| 4   | d     | 0.43         | 0/1101      | 0.70        | 2/1492 (0.1%) |
| 5   | 5     | 0.39         | 0/559       | 0.60        | 1/762 (0.1%)  |
| 5   | E     | 0.39         | 0/559       | 0.60        | 1/762 (0.1%)  |
| 5   | e     | 0.39         | 0/559       | 0.60        | 1/762 (0.1%)  |
| 6   | 6     | 0.44         | 0/1087      | 0.99        | 6/1476 (0.4%) |
| 6   | F     | 0.44         | 0/1087      | 0.99        | 6/1476 (0.4%) |
| 6   | f     | 0.44         | 0/1087      | 0.99        | 6/1476 (0.4%) |
| 7   | 7     | 0.50         | 0/304       | 0.56        | 0/415         |
| 7   | I     | 0.50         | 0/304       | 0.55        | 0/415         |
| 7   | i     | 0.50         | 0/304       | 0.55        | 0/415         |
| 8   | 8     | 0.37         | 0/342       | 0.65        | 1/467 (0.2%)  |
| 8   | J     | 0.37         | 0/342       | 0.65        | 1/467 (0.2%)  |
| 8   | j     | 0.37         | 0/342       | 0.65        | 1/467 (0.2%)  |
| 9   | 9     | 0.36         | 0/585       | 1.01        | 7/800 (0.9%)  |
| 9   | K     | 0.36         | 0/585       | 1.02        | 7/800 (0.9%)  |
| 9   | k     | 0.36         | 0/585       | 1.02        | 7/800 (0.9%)  |
| 10  | 0     | 0.50         | 0/1153      | 0.49        | 0/1565        |
| 10  | L     | 0.50         | 0/1153      | 0.49        | 0/1565        |
| 10  | l     | 0.50         | 0/1153      | 0.49        | 0/1565        |
| 11  | M     | 0.42         | 0/244       | 0.54        | 1/332 (0.3%)  |
| 11  | m     | 0.42         | 0/244       | 0.54        | 1/332 (0.3%)  |

| Mol | Chain | Bond lengths |         | Bond angles |                 |
|-----|-------|--------------|---------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5         |
| 11  | y     | 0.42         | 0/244   | 0.54        | 1/332 (0.3%)    |
| 12  | X     | 0.47         | 0/236   | 1.77        | 5/321 (1.6%)    |
| 12  | x     | 0.47         | 0/236   | 1.77        | 5/321 (1.6%)    |
| 12  | z     | 0.48         | 0/236   | 1.77        | 5/321 (1.6%)    |
| All | All   | 0.44         | 0/55074 | 0.63        | 99/75072 (0.1%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 9   | 9     | 0                   | 1                   |
| 9   | K     | 0                   | 1                   |
| 9   | k     | 0                   | 1                   |
| All | All   | 0                   | 3                   |

There are no bond length outliers.

All (99) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 12  | z     | 25  | LEU  | CA-CB-CG  | 17.61  | 155.81      | 115.30   |
| 12  | X     | 25  | LEU  | CA-CB-CG  | 17.61  | 155.79      | 115.30   |
| 12  | x     | 25  | LEU  | CA-CB-CG  | 17.60  | 155.77      | 115.30   |
| 6   | f     | 121 | LEU  | CA-CB-CG  | 16.85  | 154.04      | 115.30   |
| 6   | F     | 121 | LEU  | CA-CB-CG  | 16.84  | 154.03      | 115.30   |
| 6   | 6     | 121 | LEU  | CA-CB-CG  | 16.84  | 154.03      | 115.30   |
| 12  | X     | 25  | LEU  | CB-CG-CD1 | 13.33  | 133.65      | 111.00   |
| 12  | x     | 25  | LEU  | CB-CG-CD1 | 13.33  | 133.66      | 111.00   |
| 12  | z     | 25  | LEU  | CB-CG-CD1 | 13.32  | 133.65      | 111.00   |
| 9   | 9     | 59  | LEU  | CA-CB-CG  | 12.86  | 144.88      | 115.30   |
| 9   | K     | 59  | LEU  | CA-CB-CG  | 12.84  | 144.83      | 115.30   |
| 9   | k     | 59  | LEU  | CA-CB-CG  | 12.84  | 144.82      | 115.30   |
| 6   | f     | 121 | LEU  | CB-CG-CD1 | 12.49  | 132.23      | 111.00   |
| 6   | F     | 121 | LEU  | CB-CG-CD1 | 12.47  | 132.20      | 111.00   |
| 6   | 6     | 121 | LEU  | CB-CG-CD1 | 12.46  | 132.18      | 111.00   |
| 12  | z     | 25  | LEU  | CB-CG-CD2 | -12.13 | 90.38       | 111.00   |
| 12  | X     | 25  | LEU  | CB-CG-CD2 | -12.12 | 90.40       | 111.00   |
| 12  | x     | 25  | LEU  | CB-CG-CD2 | -12.12 | 90.40       | 111.00   |
| 12  | z     | 35  | LYS  | CD-CE-NZ  | 11.44  | 138.01      | 111.70   |
| 12  | x     | 35  | LYS  | CD-CE-NZ  | 11.43  | 138.00      | 111.70   |
| 12  | X     | 35  | LYS  | CD-CE-NZ  | 11.41  | 137.95      | 111.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 6   | 6     | 121 | LEU  | CB-CG-CD2 | -11.12 | 92.09       | 111.00   |
| 9   | K     | 31  | ARG  | NE-CZ-NH2 | -11.11 | 114.75      | 120.30   |
| 6   | F     | 121 | LEU  | CB-CG-CD2 | -11.10 | 92.13       | 111.00   |
| 6   | f     | 121 | LEU  | CB-CG-CD2 | -11.10 | 92.13       | 111.00   |
| 9   | k     | 31  | ARG  | NE-CZ-NH2 | -11.09 | 114.75      | 120.30   |
| 9   | 9     | 31  | ARG  | NE-CZ-NH2 | -11.04 | 114.78      | 120.30   |
| 4   | D     | 107 | LYS  | CD-CE-NZ  | -10.88 | 86.69       | 111.70   |
| 4   | 4     | 107 | LYS  | CD-CE-NZ  | -10.88 | 86.69       | 111.70   |
| 4   | d     | 107 | LYS  | CD-CE-NZ  | -10.85 | 86.75       | 111.70   |
| 4   | d     | 76  | LYS  | CD-CE-NZ  | 10.40  | 135.61      | 111.70   |
| 4   | D     | 76  | LYS  | CD-CE-NZ  | 10.39  | 135.59      | 111.70   |
| 4   | 4     | 76  | LYS  | CD-CE-NZ  | 10.38  | 135.57      | 111.70   |
| 6   | f     | 57  | LEU  | CB-CG-CD2 | 9.43   | 127.03      | 111.00   |
| 6   | F     | 57  | LEU  | CB-CG-CD2 | 9.42   | 127.01      | 111.00   |
| 6   | 6     | 57  | LEU  | CB-CG-CD2 | 9.41   | 126.99      | 111.00   |
| 1   | a     | 30  | LYS  | CD-CE-NZ  | 9.23   | 132.93      | 111.70   |
| 1   | A     | 30  | LYS  | CD-CE-NZ  | 9.22   | 132.90      | 111.70   |
| 1   | 1     | 30  | LYS  | CD-CE-NZ  | 9.22   | 132.90      | 111.70   |
| 6   | F     | 9   | LYS  | CD-CE-NZ  | -7.82  | 93.72       | 111.70   |
| 6   | 6     | 9   | LYS  | CD-CE-NZ  | -7.80  | 93.76       | 111.70   |
| 6   | f     | 9   | LYS  | CD-CE-NZ  | -7.80  | 93.77       | 111.70   |
| 9   | k     | 43  | LEU  | CB-CG-CD2 | 7.25   | 123.33      | 111.00   |
| 9   | 9     | 43  | LEU  | CB-CG-CD2 | 7.24   | 123.30      | 111.00   |
| 9   | K     | 43  | LEU  | CB-CG-CD2 | 7.23   | 123.28      | 111.00   |
| 9   | k     | 59  | LEU  | CB-CG-CD2 | -7.17  | 98.82       | 111.00   |
| 9   | K     | 59  | LEU  | CB-CG-CD2 | -7.16  | 98.83       | 111.00   |
| 9   | 9     | 59  | LEU  | CB-CG-CD2 | -7.13  | 98.89       | 111.00   |
| 9   | K     | 31  | ARG  | NE-CZ-NH1 | 6.62   | 123.61      | 120.30   |
| 9   | k     | 31  | ARG  | NE-CZ-NH1 | 6.58   | 123.59      | 120.30   |
| 9   | 9     | 31  | ARG  | NE-CZ-NH1 | 6.57   | 123.58      | 120.30   |
| 8   | j     | 5   | LEU  | CB-CG-CD2 | 6.44   | 121.95      | 111.00   |
| 8   | 8     | 5   | LEU  | CB-CG-CD2 | 6.44   | 121.94      | 111.00   |
| 8   | J     | 5   | LEU  | CB-CG-CD2 | 6.43   | 121.94      | 111.00   |
| 1   | a     | 307 | LEU  | CB-CG-CD1 | 6.21   | 121.55      | 111.00   |
| 1   | 1     | 307 | LEU  | CB-CG-CD1 | 6.20   | 121.54      | 111.00   |
| 1   | A     | 307 | LEU  | CB-CG-CD1 | 6.19   | 121.52      | 111.00   |
| 5   | 5     | 62  | LEU  | CA-CB-CG  | 5.98   | 129.05      | 115.30   |
| 5   | E     | 62  | LEU  | CA-CB-CG  | 5.96   | 129.00      | 115.30   |
| 9   | 9     | 24  | LEU  | CB-CG-CD2 | 5.94   | 121.11      | 111.00   |
| 5   | e     | 62  | LEU  | CA-CB-CG  | 5.94   | 128.96      | 115.30   |
| 9   | K     | 24  | LEU  | CB-CG-CD2 | 5.92   | 121.06      | 111.00   |
| 9   | k     | 24  | LEU  | CB-CG-CD2 | 5.91   | 121.04      | 111.00   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | 1     | 188 | GLU  | CA-CB-CG  | 5.74  | 126.02      | 113.40   |
| 1   | A     | 188 | GLU  | CA-CB-CG  | 5.73  | 126.01      | 113.40   |
| 1   | a     | 188 | GLU  | CA-CB-CG  | 5.73  | 126.01      | 113.40   |
| 1   | a     | 234 | LYS  | CD-CE-NZ  | 5.53  | 124.42      | 111.70   |
| 1   | A     | 234 | LYS  | CD-CE-NZ  | 5.52  | 124.39      | 111.70   |
| 1   | 1     | 234 | LYS  | CD-CE-NZ  | 5.52  | 124.39      | 111.70   |
| 12  | z     | 35  | LYS  | CB-CG-CD  | 5.48  | 125.85      | 111.60   |
| 12  | X     | 35  | LYS  | CB-CG-CD  | 5.48  | 125.85      | 111.60   |
| 12  | x     | 35  | LYS  | CB-CG-CD  | 5.46  | 125.81      | 111.60   |
| 2   | B     | 97  | LYS  | CB-CG-CD  | 5.41  | 125.66      | 111.60   |
| 2   | 2     | 97  | LYS  | CB-CG-CD  | 5.40  | 125.65      | 111.60   |
| 2   | b     | 97  | LYS  | CB-CG-CD  | 5.39  | 125.61      | 111.60   |
| 9   | k     | 59  | LEU  | CB-CG-CD1 | 5.38  | 120.14      | 111.00   |
| 9   | 9     | 59  | LEU  | CB-CG-CD1 | 5.37  | 120.14      | 111.00   |
| 11  | m     | 16  | LEU  | CB-CG-CD2 | 5.36  | 120.11      | 111.00   |
| 11  | y     | 16  | LEU  | CB-CG-CD2 | 5.35  | 120.10      | 111.00   |
| 9   | K     | 59  | LEU  | CB-CG-CD1 | 5.35  | 120.10      | 111.00   |
| 11  | M     | 16  | LEU  | CB-CG-CD2 | 5.33  | 120.06      | 111.00   |
| 6   | 6     | 57  | LEU  | CB-CG-CD1 | -5.24 | 102.09      | 111.00   |
| 6   | f     | 57  | LEU  | CB-CG-CD1 | -5.20 | 102.16      | 111.00   |
| 1   | a     | 36  | ARG  | NE-CZ-NH1 | -5.20 | 117.70      | 120.30   |
| 2   | B     | 221 | LEU  | CB-CG-CD1 | 5.19  | 119.82      | 111.00   |
| 6   | F     | 57  | LEU  | CB-CG-CD1 | -5.19 | 102.18      | 111.00   |
| 2   | b     | 221 | LEU  | CB-CG-CD1 | 5.18  | 119.81      | 111.00   |
| 2   | 2     | 221 | LEU  | CB-CG-CD2 | -5.18 | 102.19      | 111.00   |
| 2   | 2     | 221 | LEU  | CB-CG-CD1 | 5.18  | 119.80      | 111.00   |
| 1   | 1     | 36  | ARG  | NE-CZ-NH1 | -5.17 | 117.72      | 120.30   |
| 1   | a     | 344 | LEU  | CB-CG-CD2 | 5.16  | 119.77      | 111.00   |
| 2   | B     | 221 | LEU  | CB-CG-CD2 | -5.15 | 102.24      | 111.00   |
| 2   | b     | 221 | LEU  | CB-CG-CD2 | -5.15 | 102.24      | 111.00   |
| 1   | A     | 36  | ARG  | NE-CZ-NH1 | -5.14 | 117.73      | 120.30   |
| 1   | 1     | 344 | LEU  | CB-CG-CD2 | 5.14  | 119.75      | 111.00   |
| 1   | A     | 344 | LEU  | CB-CG-CD2 | 5.13  | 119.72      | 111.00   |
| 2   | b     | 221 | LEU  | CA-CB-CG  | 5.05  | 126.92      | 115.30   |
| 2   | B     | 221 | LEU  | CA-CB-CG  | 5.05  | 126.91      | 115.30   |
| 2   | 2     | 221 | LEU  | CA-CB-CG  | 5.03  | 126.87      | 115.30   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 9   | 9     | 47  | LEU  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 9   | K     | 47  | LEU  | Peptide |
| 9   | k     | 47  | LEU  | Peptide |

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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   | 1     | 744/755 (98%)  | 684 (92%) | 60 (8%)  | 0        | 100         | 100 |
| 1   | A     | 744/755 (98%)  | 684 (92%) | 60 (8%)  | 0        | 100         | 100 |
| 1   | a     | 744/755 (98%)  | 684 (92%) | 60 (8%)  | 0        | 100         | 100 |
| 2   | 2     | 738/741 (100%) | 679 (92%) | 59 (8%)  | 0        | 100         | 100 |
| 2   | B     | 738/741 (100%) | 679 (92%) | 59 (8%)  | 0        | 100         | 100 |
| 2   | b     | 738/741 (100%) | 679 (92%) | 59 (8%)  | 0        | 100         | 100 |
| 3   | 3     | 78/81 (96%)    | 73 (94%)  | 5 (6%)   | 0        | 100         | 100 |
| 3   | C     | 78/81 (96%)    | 73 (94%)  | 5 (6%)   | 0        | 100         | 100 |
| 3   | c     | 78/81 (96%)    | 73 (94%)  | 5 (6%)   | 0        | 100         | 100 |
| 4   | 4     | 136/139 (98%)  | 121 (89%) | 15 (11%) | 0        | 100         | 100 |
| 4   | D     | 136/139 (98%)  | 121 (89%) | 15 (11%) | 0        | 100         | 100 |
| 4   | d     | 136/139 (98%)  | 120 (88%) | 16 (12%) | 0        | 100         | 100 |
| 5   | 5     | 68/76 (90%)    | 62 (91%)  | 6 (9%)   | 0        | 100         | 100 |
| 5   | E     | 68/76 (90%)    | 62 (91%)  | 6 (9%)   | 0        | 100         | 100 |
| 5   | e     | 68/76 (90%)    | 62 (91%)  | 6 (9%)   | 0        | 100         | 100 |
| 6   | 6     | 139/141 (99%)  | 113 (81%) | 26 (19%) | 0        | 100         | 100 |
| 6   | F     | 139/141 (99%)  | 112 (81%) | 27 (19%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 6   | f     | 139/141 (99%)   | 113 (81%)  | 26 (19%) | 0        | 100         | 100 |
| 7   | 7     | 36/38 (95%)     | 33 (92%)   | 3 (8%)   | 0        | 100         | 100 |
| 7   | I     | 36/38 (95%)     | 33 (92%)   | 3 (8%)   | 0        | 100         | 100 |
| 7   | i     | 36/38 (95%)     | 33 (92%)   | 3 (8%)   | 0        | 100         | 100 |
| 8   | 8     | 39/41 (95%)     | 35 (90%)   | 3 (8%)   | 1 (3%)   | 4           | 22  |
| 8   | J     | 39/41 (95%)     | 35 (90%)   | 3 (8%)   | 1 (3%)   | 4           | 22  |
| 8   | j     | 39/41 (95%)     | 35 (90%)   | 3 (8%)   | 1 (3%)   | 4           | 22  |
| 9   | 9     | 77/83 (93%)     | 68 (88%)   | 9 (12%)  | 0        | 100         | 100 |
| 9   | K     | 77/83 (93%)     | 68 (88%)   | 9 (12%)  | 0        | 100         | 100 |
| 9   | k     | 77/83 (93%)     | 68 (88%)   | 9 (12%)  | 0        | 100         | 100 |
| 10  | 0     | 150/155 (97%)   | 143 (95%)  | 7 (5%)   | 0        | 100         | 100 |
| 10  | L     | 150/155 (97%)   | 143 (95%)  | 7 (5%)   | 0        | 100         | 100 |
| 10  | l     | 150/155 (97%)   | 143 (95%)  | 7 (5%)   | 0        | 100         | 100 |
| 11  | M     | 29/31 (94%)     | 27 (93%)   | 2 (7%)   | 0        | 100         | 100 |
| 11  | m     | 29/31 (94%)     | 27 (93%)   | 2 (7%)   | 0        | 100         | 100 |
| 11  | y     | 29/31 (94%)     | 27 (93%)   | 2 (7%)   | 0        | 100         | 100 |
| 12  | X     | 25/36 (69%)     | 23 (92%)   | 2 (8%)   | 0        | 100         | 100 |
| 12  | x     | 25/36 (69%)     | 23 (92%)   | 2 (8%)   | 0        | 100         | 100 |
| 12  | z     | 25/36 (69%)     | 23 (92%)   | 2 (8%)   | 0        | 100         | 100 |
| All | All   | 6777/6951 (98%) | 6181 (91%) | 593 (9%) | 3 (0%)   | 100         | 100 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | J     | 2   | LYS  |
| 8   | j     | 2   | LYS  |
| 8   | 8     | 2   | LYS  |

### 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   | 1     | 594/603 (98%)  | 568 (96%) | 26 (4%)  | 24          | 52  |
| 1   | A     | 594/603 (98%)  | 568 (96%) | 26 (4%)  | 24          | 52  |
| 1   | a     | 594/603 (98%)  | 569 (96%) | 25 (4%)  | 25          | 53  |
| 2   | 2     | 597/598 (100%) | 579 (97%) | 18 (3%)  | 36          | 63  |
| 2   | B     | 597/598 (100%) | 579 (97%) | 18 (3%)  | 36          | 63  |
| 2   | b     | 597/598 (100%) | 579 (97%) | 18 (3%)  | 36          | 63  |
| 3   | 3     | 67/68 (98%)    | 67 (100%) | 0        | 100         | 100 |
| 3   | C     | 67/68 (98%)    | 67 (100%) | 0        | 100         | 100 |
| 3   | c     | 67/68 (98%)    | 67 (100%) | 0        | 100         | 100 |
| 4   | 4     | 115/116 (99%)  | 110 (96%) | 5 (4%)   | 25          | 53  |
| 4   | D     | 115/116 (99%)  | 110 (96%) | 5 (4%)   | 25          | 53  |
| 4   | d     | 115/116 (99%)  | 110 (96%) | 5 (4%)   | 25          | 53  |
| 5   | 5     | 60/65 (92%)    | 54 (90%)  | 6 (10%)  | 6           | 23  |
| 5   | E     | 60/65 (92%)    | 54 (90%)  | 6 (10%)  | 6           | 23  |
| 5   | e     | 60/65 (92%)    | 54 (90%)  | 6 (10%)  | 6           | 23  |
| 6   | 6     | 109/109 (100%) | 97 (89%)  | 12 (11%) | 5           | 20  |
| 6   | F     | 109/109 (100%) | 97 (89%)  | 12 (11%) | 5           | 20  |
| 6   | f     | 109/109 (100%) | 97 (89%)  | 12 (11%) | 5           | 20  |
| 7   | 7     | 31/31 (100%)   | 30 (97%)  | 1 (3%)   | 34          | 61  |
| 7   | I     | 31/31 (100%)   | 30 (97%)  | 1 (3%)   | 34          | 61  |
| 7   | i     | 31/31 (100%)   | 30 (97%)  | 1 (3%)   | 34          | 61  |
| 8   | 8     | 35/35 (100%)   | 33 (94%)  | 2 (6%)   | 17          | 45  |
| 8   | J     | 35/35 (100%)   | 33 (94%)  | 2 (6%)   | 17          | 45  |
| 8   | j     | 35/35 (100%)   | 33 (94%)  | 2 (6%)   | 17          | 45  |
| 9   | 9     | 58/61 (95%)    | 51 (88%)  | 7 (12%)  | 4           | 17  |
| 9   | K     | 58/61 (95%)    | 51 (88%)  | 7 (12%)  | 4           | 17  |
| 9   | k     | 58/61 (95%)    | 51 (88%)  | 7 (12%)  | 4           | 17  |
| 10  | 0     | 117/120 (98%)  | 115 (98%) | 2 (2%)   | 56          | 75  |
| 10  | L     | 117/120 (98%)  | 115 (98%) | 2 (2%)   | 56          | 75  |
| 10  | l     | 117/120 (98%)  | 115 (98%) | 2 (2%)   | 56          | 75  |
| 11  | M     | 26/26 (100%)   | 23 (88%)  | 3 (12%)  | 4           | 19  |
| 11  | m     | 26/26 (100%)   | 23 (88%)  | 3 (12%)  | 4           | 19  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 11  | y     | 26/26 (100%)    | 23 (88%)   | 3 (12%)  | 4           | 19 |
| 12  | X     | 21/28 (75%)     | 19 (90%)   | 2 (10%)  | 7           | 25 |
| 12  | x     | 21/28 (75%)     | 19 (90%)   | 2 (10%)  | 7           | 25 |
| 12  | z     | 21/28 (75%)     | 19 (90%)   | 2 (10%)  | 7           | 25 |
| All | All   | 5490/5580 (98%) | 5239 (95%) | 251 (5%) | 25          | 52 |

All (251) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 15  | VAL  |
| 1   | A     | 36  | ARG  |
| 1   | A     | 43  | GLN  |
| 1   | A     | 63  | SER  |
| 1   | A     | 129 | ASP  |
| 1   | A     | 171 | LEU  |
| 1   | A     | 188 | GLU  |
| 1   | A     | 210 | LEU  |
| 1   | A     | 224 | ASN  |
| 1   | A     | 234 | LYS  |
| 1   | A     | 256 | VAL  |
| 1   | A     | 262 | SER  |
| 1   | A     | 307 | LEU  |
| 1   | A     | 351 | SER  |
| 1   | A     | 476 | SER  |
| 1   | A     | 478 | THR  |
| 1   | A     | 530 | VAL  |
| 1   | A     | 562 | SER  |
| 1   | A     | 625 | VAL  |
| 1   | A     | 628 | ASP  |
| 1   | A     | 630 | THR  |
| 1   | A     | 631 | VAL  |
| 1   | A     | 632 | SER  |
| 1   | A     | 659 | SER  |
| 1   | A     | 692 | SER  |
| 1   | A     | 705 | VAL  |
| 2   | B     | 32  | SER  |
| 2   | B     | 61  | SER  |
| 2   | B     | 97  | LYS  |
| 2   | B     | 136 | GLN  |
| 2   | B     | 165 | SER  |
| 2   | B     | 201 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 266 | SER  |
| 2   | B     | 269 | LEU  |
| 2   | B     | 302 | GLU  |
| 2   | B     | 304 | MET  |
| 2   | B     | 312 | THR  |
| 2   | B     | 313 | LYS  |
| 2   | B     | 327 | GLU  |
| 2   | B     | 405 | GLN  |
| 2   | B     | 478 | ASP  |
| 2   | B     | 485 | ASP  |
| 2   | B     | 635 | SER  |
| 2   | B     | 672 | SER  |
| 4   | D     | 2   | THR  |
| 4   | D     | 22  | ASP  |
| 4   | D     | 43  | THR  |
| 4   | D     | 92  | VAL  |
| 4   | D     | 133 | LYS  |
| 5   | E     | 25  | SER  |
| 5   | E     | 28  | GLN  |
| 5   | E     | 46  | THR  |
| 5   | E     | 51  | SER  |
| 5   | E     | 57  | THR  |
| 5   | E     | 67  | GLU  |
| 6   | F     | 15  | GLN  |
| 6   | F     | 16  | LYS  |
| 6   | F     | 36  | GLU  |
| 6   | F     | 39  | SER  |
| 6   | F     | 45  | GLU  |
| 6   | F     | 58  | SER  |
| 6   | F     | 88  | VAL  |
| 6   | F     | 107 | ILE  |
| 6   | F     | 112 | THR  |
| 6   | F     | 130 | THR  |
| 6   | F     | 135 | GLU  |
| 6   | F     | 137 | THR  |
| 7   | I     | 4   | SER  |
| 8   | J     | 2   | LYS  |
| 8   | J     | 17  | ILE  |
| 9   | K     | 5   | THR  |
| 9   | K     | 18  | VAL  |
| 9   | K     | 24  | LEU  |
| 9   | K     | 43  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | K     | 50  | LEU  |
| 9   | K     | 52  | GLU  |
| 9   | K     | 68  | LEU  |
| 10  | L     | 70  | ASP  |
| 10  | L     | 72  | ASP  |
| 11  | M     | 16  | LEU  |
| 11  | M     | 26  | SER  |
| 11  | M     | 27  | THR  |
| 12  | X     | 17  | VAL  |
| 12  | X     | 26  | VAL  |
| 1   | a     | 15  | VAL  |
| 1   | a     | 36  | ARG  |
| 1   | a     | 43  | GLN  |
| 1   | a     | 63  | SER  |
| 1   | a     | 171 | LEU  |
| 1   | a     | 188 | GLU  |
| 1   | a     | 210 | LEU  |
| 1   | a     | 224 | ASN  |
| 1   | a     | 234 | LYS  |
| 1   | a     | 256 | VAL  |
| 1   | a     | 262 | SER  |
| 1   | a     | 307 | LEU  |
| 1   | a     | 351 | SER  |
| 1   | a     | 476 | SER  |
| 1   | a     | 478 | THR  |
| 1   | a     | 530 | VAL  |
| 1   | a     | 562 | SER  |
| 1   | a     | 625 | VAL  |
| 1   | a     | 628 | ASP  |
| 1   | a     | 630 | THR  |
| 1   | a     | 631 | VAL  |
| 1   | a     | 632 | SER  |
| 1   | a     | 659 | SER  |
| 1   | a     | 692 | SER  |
| 1   | a     | 705 | VAL  |
| 2   | b     | 32  | SER  |
| 2   | b     | 61  | SER  |
| 2   | b     | 97  | LYS  |
| 2   | b     | 136 | GLN  |
| 2   | b     | 165 | SER  |
| 2   | b     | 201 | SER  |
| 2   | b     | 266 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | b     | 269 | LEU  |
| 2   | b     | 302 | GLU  |
| 2   | b     | 304 | MET  |
| 2   | b     | 312 | THR  |
| 2   | b     | 313 | LYS  |
| 2   | b     | 327 | GLU  |
| 2   | b     | 405 | GLN  |
| 2   | b     | 478 | ASP  |
| 2   | b     | 485 | ASP  |
| 2   | b     | 635 | SER  |
| 2   | b     | 672 | SER  |
| 4   | d     | 2   | THR  |
| 4   | d     | 22  | ASP  |
| 4   | d     | 43  | THR  |
| 4   | d     | 92  | VAL  |
| 4   | d     | 133 | LYS  |
| 5   | e     | 25  | SER  |
| 5   | e     | 28  | GLN  |
| 5   | e     | 46  | THR  |
| 5   | e     | 51  | SER  |
| 5   | e     | 57  | THR  |
| 5   | e     | 67  | GLU  |
| 6   | f     | 15  | GLN  |
| 6   | f     | 16  | LYS  |
| 6   | f     | 36  | GLU  |
| 6   | f     | 39  | SER  |
| 6   | f     | 45  | GLU  |
| 6   | f     | 58  | SER  |
| 6   | f     | 88  | VAL  |
| 6   | f     | 107 | ILE  |
| 6   | f     | 112 | THR  |
| 6   | f     | 130 | THR  |
| 6   | f     | 135 | GLU  |
| 6   | f     | 137 | THR  |
| 7   | i     | 4   | SER  |
| 8   | j     | 2   | LYS  |
| 8   | j     | 17  | ILE  |
| 9   | k     | 5   | THR  |
| 9   | k     | 18  | VAL  |
| 9   | k     | 24  | LEU  |
| 9   | k     | 43  | LEU  |
| 9   | k     | 50  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | k     | 52  | GLU  |
| 9   | k     | 68  | LEU  |
| 10  | l     | 70  | ASP  |
| 10  | l     | 72  | ASP  |
| 11  | m     | 16  | LEU  |
| 11  | m     | 26  | SER  |
| 11  | m     | 27  | THR  |
| 12  | x     | 17  | VAL  |
| 12  | x     | 26  | VAL  |
| 1   | 1     | 15  | VAL  |
| 1   | 1     | 36  | ARG  |
| 1   | 1     | 43  | GLN  |
| 1   | 1     | 63  | SER  |
| 1   | 1     | 129 | ASP  |
| 1   | 1     | 171 | LEU  |
| 1   | 1     | 188 | GLU  |
| 1   | 1     | 210 | LEU  |
| 1   | 1     | 224 | ASN  |
| 1   | 1     | 234 | LYS  |
| 1   | 1     | 256 | VAL  |
| 1   | 1     | 262 | SER  |
| 1   | 1     | 307 | LEU  |
| 1   | 1     | 351 | SER  |
| 1   | 1     | 476 | SER  |
| 1   | 1     | 478 | THR  |
| 1   | 1     | 530 | VAL  |
| 1   | 1     | 562 | SER  |
| 1   | 1     | 625 | VAL  |
| 1   | 1     | 628 | ASP  |
| 1   | 1     | 630 | THR  |
| 1   | 1     | 631 | VAL  |
| 1   | 1     | 632 | SER  |
| 1   | 1     | 659 | SER  |
| 1   | 1     | 692 | SER  |
| 1   | 1     | 705 | VAL  |
| 2   | 2     | 32  | SER  |
| 2   | 2     | 61  | SER  |
| 2   | 2     | 97  | LYS  |
| 2   | 2     | 136 | GLN  |
| 2   | 2     | 165 | SER  |
| 2   | 2     | 201 | SER  |
| 2   | 2     | 266 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2     | 269 | LEU  |
| 2   | 2     | 302 | GLU  |
| 2   | 2     | 304 | MET  |
| 2   | 2     | 312 | THR  |
| 2   | 2     | 313 | LYS  |
| 2   | 2     | 327 | GLU  |
| 2   | 2     | 405 | GLN  |
| 2   | 2     | 478 | ASP  |
| 2   | 2     | 485 | ASP  |
| 2   | 2     | 635 | SER  |
| 2   | 2     | 672 | SER  |
| 4   | 4     | 2   | THR  |
| 4   | 4     | 22  | ASP  |
| 4   | 4     | 43  | THR  |
| 4   | 4     | 92  | VAL  |
| 4   | 4     | 133 | LYS  |
| 5   | 5     | 25  | SER  |
| 5   | 5     | 28  | GLN  |
| 5   | 5     | 46  | THR  |
| 5   | 5     | 51  | SER  |
| 5   | 5     | 57  | THR  |
| 5   | 5     | 67  | GLU  |
| 6   | 6     | 15  | GLN  |
| 6   | 6     | 16  | LYS  |
| 6   | 6     | 36  | GLU  |
| 6   | 6     | 39  | SER  |
| 6   | 6     | 45  | GLU  |
| 6   | 6     | 58  | SER  |
| 6   | 6     | 88  | VAL  |
| 6   | 6     | 107 | ILE  |
| 6   | 6     | 112 | THR  |
| 6   | 6     | 130 | THR  |
| 6   | 6     | 135 | GLU  |
| 6   | 6     | 137 | THR  |
| 7   | 7     | 4   | SER  |
| 8   | 8     | 2   | LYS  |
| 8   | 8     | 17  | ILE  |
| 9   | 9     | 5   | THR  |
| 9   | 9     | 18  | VAL  |
| 9   | 9     | 24  | LEU  |
| 9   | 9     | 43  | LEU  |
| 9   | 9     | 50  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | 9     | 52  | GLU  |
| 9   | 9     | 68  | LEU  |
| 10  | 0     | 70  | ASP  |
| 10  | 0     | 72  | ASP  |
| 11  | y     | 16  | LEU  |
| 11  | y     | 26  | SER  |
| 11  | y     | 27  | THR  |
| 12  | z     | 17  | VAL  |
| 12  | z     | 26  | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 154 | ASN  |
| 1   | A     | 157 | GLN  |
| 1   | A     | 301 | HIS  |
| 1   | A     | 372 | GLN  |
| 1   | A     | 397 | HIS  |
| 1   | A     | 618 | GLN  |
| 1   | A     | 680 | HIS  |
| 2   | B     | 33  | HIS  |
| 2   | B     | 155 | HIS  |
| 2   | B     | 192 | HIS  |
| 2   | B     | 204 | GLN  |
| 2   | B     | 241 | HIS  |
| 2   | B     | 261 | HIS  |
| 2   | B     | 319 | ASN  |
| 2   | B     | 406 | ASN  |
| 2   | B     | 416 | GLN  |
| 2   | B     | 527 | HIS  |
| 2   | B     | 642 | ASN  |
| 2   | B     | 648 | ASN  |
| 4   | D     | 71  | GLN  |
| 5   | E     | 58  | ASN  |
| 6   | F     | 40  | GLN  |
| 8   | J     | 39  | HIS  |
| 9   | K     | 23  | ASN  |
| 10  | L     | 75  | ASN  |
| 1   | a     | 301 | HIS  |
| 1   | a     | 372 | GLN  |
| 1   | a     | 618 | GLN  |
| 2   | b     | 33  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | b     | 155 | HIS  |
| 2   | b     | 192 | HIS  |
| 2   | b     | 204 | GLN  |
| 2   | b     | 241 | HIS  |
| 2   | b     | 261 | HIS  |
| 2   | b     | 319 | ASN  |
| 2   | b     | 406 | ASN  |
| 2   | b     | 416 | GLN  |
| 2   | b     | 642 | ASN  |
| 2   | b     | 648 | ASN  |
| 4   | d     | 71  | GLN  |
| 5   | e     | 58  | ASN  |
| 9   | k     | 23  | ASN  |
| 10  | l     | 75  | ASN  |
| 1   | 1     | 198 | ASN  |
| 1   | 1     | 301 | HIS  |
| 1   | 1     | 372 | GLN  |
| 1   | 1     | 397 | HIS  |
| 1   | 1     | 618 | GLN  |
| 2   | 2     | 33  | HIS  |
| 2   | 2     | 155 | HIS  |
| 2   | 2     | 192 | HIS  |
| 2   | 2     | 204 | GLN  |
| 2   | 2     | 241 | HIS  |
| 2   | 2     | 261 | HIS  |
| 2   | 2     | 319 | ASN  |
| 2   | 2     | 406 | ASN  |
| 2   | 2     | 416 | GLN  |
| 2   | 2     | 642 | ASN  |
| 2   | 2     | 648 | ASN  |
| 4   | 4     | 71  | GLN  |
| 4   | 4     | 113 | ASN  |
| 5   | 5     | 58  | ASN  |
| 6   | 6     | 40  | GLN  |
| 8   | 8     | 39  | HIS  |
| 9   | 9     | 23  | ASN  |
| 10  | 0     | 75  | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 7   | FME  | 7     | 1   | 7    | 8,9,10       | 0.98 | 0           | 7,9,11      | 0.83 | 0           |
| 8   | FME  | J     | 1   | 8    | 8,9,10       | 1.01 | 0           | 7,9,11      | 1.37 | 2 (28%)     |
| 7   | FME  | I     | 1   | 7    | 8,9,10       | 0.98 | 0           | 7,9,11      | 0.83 | 0           |
| 8   | FME  | 8     | 1   | 8    | 8,9,10       | 1.02 | 0           | 7,9,11      | 1.37 | 2 (28%)     |
| 7   | FME  | i     | 1   | 7    | 8,9,10       | 1.00 | 0           | 7,9,11      | 0.82 | 0           |
| 8   | FME  | j     | 1   | 8    | 8,9,10       | 1.01 | 0           | 7,9,11      | 1.37 | 2 (28%)     |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 7   | FME  | 7     | 1   | 7    | -       | 1/7/9/11 | -     |
| 8   | FME  | J     | 1   | 8    | -       | 1/7/9/11 | -     |
| 7   | FME  | I     | 1   | 7    | -       | 1/7/9/11 | -     |
| 8   | FME  | 8     | 1   | 8    | -       | 1/7/9/11 | -     |
| 7   | FME  | i     | 1   | 7    | -       | 1/7/9/11 | -     |
| 8   | FME  | j     | 1   | 8    | -       | 1/7/9/11 | -     |

There are no bond length outliers.

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 8   | j     | 1   | FME  | C-CA-N | 2.57  | 114.36      | 109.73   |
| 8   | 8     | 1   | FME  | C-CA-N | 2.56  | 114.36      | 109.73   |
| 8   | J     | 1   | FME  | C-CA-N | 2.56  | 114.34      | 109.73   |
| 8   | j     | 1   | FME  | O-C-CA | -2.06 | 119.38      | 124.78   |
| 8   | J     | 1   | FME  | O-C-CA | -2.06 | 119.38      | 124.78   |
| 8   | 8     | 1   | FME  | O-C-CA | -2.05 | 119.39      | 124.78   |

There are no chirality outliers.

All (6) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms      |
|-----|-------|-----|------|------------|
| 8   | J     | 1   | FME  | CB-CA-N-CN |
| 8   | j     | 1   | FME  | CB-CA-N-CN |
| 8   | 8     | 1   | FME  | CB-CA-N-CN |
| 7   | I     | 1   | FME  | N-CA-CB-CG |
| 7   | i     | 1   | FME  | N-CA-CB-CG |
| 7   | 7     | 1   | FME  | N-CA-CB-CG |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 402 ligands modelled in this entry, 6 are monoatomic - leaving 396 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 | $\# Z  > 2$ |
| 17  | BCR  | a     | 848  | -    | 41,41,41     | 1.19 | 3 (7%)      | 56,56,56    | 1.23 | 6 (10%)     |
| 14  | CLA  | a     | 842  | -    | 65,73,73     | 1.48 | 8 (12%)     | 76,113,113  | 1.50 | 9 (11%)     |
| 14  | CLA  | A     | 833  | -    | 65,73,73     | 1.45 | 10 (15%)    | 76,113,113  | 1.38 | 6 (7%)      |
| 14  | CLA  | 1     | 1615 | -    | 65,73,73     | 1.49 | 9 (13%)     | 76,113,113  | 1.34 | 7 (9%)      |
| 14  | CLA  | 1     | 1625 | -    | 65,73,73     | 1.52 | 8 (12%)     | 76,113,113  | 1.39 | 9 (11%)     |
| 14  | CLA  | 1     | 206  | 21   | 65,73,73     | 1.45 | 10 (15%)    | 76,113,113  | 1.49 | 10 (13%)    |
| 14  | CLA  | 2     | 826  | 21   | 65,73,73     | 1.50 | 9 (13%)     | 76,113,113  | 1.53 | 10 (13%)    |
| 14  | CLA  | 6     | 201  | 21   | 58,66,73     | 1.58 | 7 (12%)     | 67,104,113  | 1.47 | 8 (11%)     |
| 14  | CLA  | 2     | 835  | -    | 65,73,73     | 1.47 | 6 (9%)      | 76,113,113  | 1.44 | 9 (11%)     |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | A     | 835  | -    | 65,73,73     | 1.44 | 9 (13%)  | 76,113,113  | 1.44 | 6 (7%)   |
| 17  | BCR  | 1     | 1653 | -    | 25,25,41     | 1.13 | 1 (4%)   | 33,33,56    | 1.28 | 4 (12%)  |
| 14  | CLA  | 2     | 837  | 21   | 45,53,73     | 1.81 | 7 (15%)  | 52,89,113   | 1.51 | 5 (9%)   |
| 17  | BCR  | J     | 103  | -    | 41,41,41     | 1.16 | 3 (7%)   | 56,56,56    | 1.19 | 6 (10%)  |
| 14  | CLA  | a     | 816  | -    | 65,73,73     | 1.47 | 6 (9%)   | 76,113,113  | 1.39 | 7 (9%)   |
| 14  | CLA  | b     | 802  | 21   | 65,73,73     | 1.42 | 7 (10%)  | 76,113,113  | 1.60 | 8 (10%)  |
| 14  | CLA  | k     | 101  | -    | 46,54,73     | 1.74 | 7 (15%)  | 53,90,113   | 1.57 | 7 (13%)  |
| 14  | CLA  | 1     | 1606 | 14   | 59,67,73     | 1.51 | 7 (11%)  | 68,105,113  | 1.54 | 8 (11%)  |
| 14  | CLA  | 1     | 1641 | -    | 65,73,73     | 1.49 | 9 (13%)  | 76,113,113  | 1.44 | 8 (10%)  |
| 15  | PQN  | A     | 845  | -    | 34,34,34     | 0.39 | 0        | 42,45,45    | 0.35 | 0        |
| 14  | CLA  | 2     | 825  | 2    | 65,73,73     | 1.46 | 8 (12%)  | 76,113,113  | 1.47 | 8 (10%)  |
| 14  | CLA  | 1     | 1629 | -    | 65,73,73     | 1.47 | 7 (10%)  | 76,113,113  | 1.38 | 8 (10%)  |
| 14  | CLA  | l     | 205  | -    | 65,73,73     | 1.46 | 10 (15%) | 76,113,113  | 1.53 | 9 (11%)  |
| 17  | BCR  | L     | 206  | -    | 41,41,41     | 1.21 | 3 (7%)   | 56,56,56    | 1.34 | 7 (12%)  |
| 17  | BCR  | j     | 1305 | -    | 41,41,41     | 1.22 | 2 (4%)   | 56,56,56    | 1.28 | 8 (14%)  |
| 14  | CLA  | a     | 804  | -    | 65,73,73     | 1.41 | 7 (10%)  | 76,113,113  | 1.50 | 7 (9%)   |
| 14  | CLA  | 2     | 823  | 21   | 55,63,73     | 1.62 | 7 (12%)  | 64,101,113  | 1.46 | 6 (9%)   |
| 15  | PQN  | 1     | 1646 | -    | 34,34,34     | 0.40 | 0        | 42,45,45    | 0.36 | 0        |
| 14  | CLA  | a     | 817  | 21   | 65,73,73     | 1.48 | 7 (10%)  | 76,113,113  | 1.35 | 7 (9%)   |
| 14  | CLA  | 1     | 1603 | -    | 65,73,73     | 1.44 | 8 (12%)  | 76,113,113  | 1.54 | 8 (10%)  |
| 15  | PQN  | 2     | 843  | -    | 34,34,34     | 0.45 | 0        | 42,45,45    | 0.38 | 0        |
| 14  | CLA  | 1     | 1627 | 21   | 65,73,73     | 1.45 | 9 (13%)  | 76,113,113  | 1.50 | 9 (11%)  |
| 14  | CLA  | a     | 843  | 21   | 65,73,73     | 1.50 | 9 (13%)  | 76,113,113  | 1.42 | 7 (9%)   |
| 17  | BCR  | A     | 850  | -    | 41,41,41     | 1.33 | 3 (7%)   | 56,56,56    | 1.29 | 7 (12%)  |
| 17  | BCR  | k     | 102  | -    | 41,41,41     | 1.18 | 2 (4%)   | 56,56,56    | 1.31 | 7 (12%)  |
| 14  | CLA  | 0     | 205  | 10   | 65,73,73     | 1.52 | 9 (13%)  | 76,113,113  | 1.37 | 8 (10%)  |
| 13  | CL0  | A     | 801  | -    | 65,73,73     | 1.45 | 10 (15%) | 76,113,113  | 1.46 | 8 (10%)  |
| 14  | CLA  | f     | 203  | -    | 50,58,73     | 1.72 | 5 (10%)  | 58,95,113   | 1.53 | 8 (13%)  |
| 17  | BCR  | 6     | 202  | -    | 41,41,41     | 1.25 | 3 (7%)   | 56,56,56    | 1.25 | 6 (10%)  |
| 18  | LHG  | B     | 850  | -    | 48,48,48     | 0.61 | 1 (2%)   | 51,54,54    | 1.20 | 5 (9%)   |
| 14  | CLA  | F     | 204  | -    | 50,58,73     | 1.72 | 5 (10%)  | 58,95,113   | 1.52 | 8 (13%)  |
| 16  | SF4  | A     | 846  | 2,1  | 0,12,12      | -    | -        | -           | -    | -        |
| 17  | BCR  | a     | 851  | -    | 41,41,41     | 1.27 | 3 (7%)   | 56,56,56    | 1.29 | 7 (12%)  |
| 15  | PQN  | B     | 842  | -    | 34,34,34     | 0.45 | 0        | 42,45,45    | 0.38 | 0        |
| 14  | CLA  | b     | 839  | -    | 65,73,73     | 1.47 | 9 (13%)  | 76,113,113  | 1.39 | 5 (6%)   |
| 14  | CLA  | B     | 818  | -    | 65,73,73     | 1.44 | 8 (12%)  | 76,113,113  | 1.51 | 9 (11%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | a     | 813  | -    | 45,53,73     | 1.77 | 8 (17%)  | 52,89,113   | 1.63 | 7 (13%)  |
| 18  | LHG  | y     | 101  | -    | 48,48,48     | 0.71 | 2 (4%)   | 51,54,54    | 1.22 | 3 (5%)   |
| 18  | LHG  | a     | 853  | -    | 48,48,48     | 0.74 | 1 (2%)   | 51,54,54    | 1.23 | 4 (7%)   |
| 14  | CLA  | b     | 808  | -    | 65,73,73     | 1.48 | 9 (13%)  | 76,113,113  | 1.44 | 9 (11%)  |
| 14  | CLA  | L     | 205  | 21   | 65,73,73     | 1.45 | 10 (15%) | 76,113,113  | 1.49 | 10 (13%) |
| 14  | CLA  | A     | 843  | 21   | 65,73,73     | 1.49 | 9 (13%)  | 76,113,113  | 1.42 | 7 (9%)   |
| 14  | CLA  | b     | 825  | 2    | 65,73,73     | 1.47 | 7 (10%)  | 76,113,113  | 1.48 | 8 (10%)  |
| 14  | CLA  | 2     | 831  | -    | 55,63,73     | 1.60 | 9 (16%)  | 64,101,113  | 1.50 | 9 (14%)  |
| 14  | CLA  | a     | 810  | 1    | 65,73,73     | 1.47 | 7 (10%)  | 76,113,113  | 1.45 | 7 (9%)   |
| 14  | CLA  | 1     | 1621 | -    | 65,73,73     | 1.44 | 7 (10%)  | 76,113,113  | 1.58 | 9 (11%)  |
| 17  | BCR  | K     | 104  | -    | 25,25,41     | 1.15 | 1 (4%)   | 33,33,56    | 1.15 | 4 (12%)  |
| 14  | CLA  | 2     | 817  | -    | 65,73,73     | 1.45 | 6 (9%)   | 76,113,113  | 1.48 | 8 (10%)  |
| 14  | CLA  | B     | 813  | -    | 65,73,73     | 1.46 | 8 (12%)  | 76,113,113  | 1.44 | 9 (11%)  |
| 14  | CLA  | b     | 818  | -    | 65,73,73     | 1.51 | 9 (13%)  | 76,113,113  | 1.49 | 9 (11%)  |
| 14  | CLA  | A     | 820  | -    | 65,73,73     | 1.45 | 7 (10%)  | 76,113,113  | 1.58 | 9 (11%)  |
| 14  | CLA  | a     | 829  | -    | 65,73,73     | 1.46 | 7 (10%)  | 76,113,113  | 1.47 | 8 (10%)  |
| 20  | LMG  | B     | 849  | -    | 55,55,55     | 0.92 | 4 (7%)   | 63,63,63    | 1.35 | 10 (15%) |
| 17  | BCR  | B     | 845  | -    | 41,41,41     | 1.26 | 3 (7%)   | 56,56,56    | 1.24 | 6 (10%)  |
| 14  | CLA  | A     | 857  | -    | 36,44,73     | 1.96 | 7 (19%)  | 40,76,113   | 1.65 | 5 (12%)  |
| 14  | CLA  | b     | 832  | -    | 49,57,73     | 1.65 | 7 (14%)  | 55,93,113   | 1.65 | 6 (10%)  |
| 14  | CLA  | 1     | 1623 | 21   | 65,73,73     | 1.48 | 7 (10%)  | 76,113,113  | 1.46 | 7 (9%)   |
| 14  | CLA  | 1     | 1607 | -    | 65,73,73     | 1.45 | 10 (15%) | 76,113,113  | 1.58 | 12 (15%) |
| 14  | CLA  | 8     | 1302 | -    | 45,53,73     | 1.79 | 6 (13%)  | 52,89,113   | 1.58 | 8 (15%)  |
| 14  | CLA  | a     | 835  | -    | 65,73,73     | 1.44 | 9 (13%)  | 76,113,113  | 1.45 | 7 (9%)   |
| 17  | BCR  | 1     | 1652 | -    | 41,41,41     | 1.27 | 2 (4%)   | 56,56,56    | 1.29 | 7 (12%)  |
| 14  | CLA  | a     | 806  | -    | 65,73,73     | 1.46 | 10 (15%) | 76,113,113  | 1.59 | 12 (15%) |
| 14  | CLA  | 2     | 805  | -    | 65,73,73     | 1.50 | 9 (13%)  | 76,113,113  | 1.46 | 11 (14%) |
| 14  | CLA  | b     | 815  | -    | 65,73,73     | 1.44 | 8 (12%)  | 76,113,113  | 1.43 | 8 (10%)  |
| 17  | BCR  | I     | 101  | -    | 41,41,41     | 1.28 | 4 (9%)   | 56,56,56    | 1.25 | 3 (5%)   |
| 17  | BCR  | b     | 845  | -    | 41,41,41     | 1.17 | 3 (7%)   | 56,56,56    | 1.19 | 3 (5%)   |
| 14  | CLA  | B     | 823  | -    | 45,53,73     | 1.75 | 7 (15%)  | 52,89,113   | 1.71 | 7 (13%)  |
| 14  | CLA  | a     | 838  | -    | 65,73,73     | 1.42 | 7 (10%)  | 76,113,113  | 1.61 | 7 (9%)   |
| 14  | CLA  | 1     | 1644 | 21   | 65,73,73     | 1.50 | 9 (13%)  | 76,113,113  | 1.42 | 7 (9%)   |
| 14  | CLA  | 2     | 814  | -    | 65,73,73     | 1.45 | 8 (12%)  | 76,113,113  | 1.45 | 9 (11%)  |
| 14  | CLA  | a     | 805  | 14   | 59,67,73     | 1.51 | 7 (11%)  | 68,105,113  | 1.54 | 8 (11%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 18  | LHG  | m     | 101  | -    | 48,48,48     | 0.70 | 2 (4%)   | 51,54,54    | 1.22 | 3 (5%)   |
| 14  | CLA  | j     | 1302 | -    | 45,53,73     | 1.78 | 5 (11%)  | 52,89,113   | 1.59 | 8 (15%)  |
| 14  | CLA  | 1     | 1640 | -    | 65,73,73     | 1.44 | 9 (13%)  | 76,113,113  | 1.48 | 9 (11%)  |
| 18  | LHG  | b     | 851  | -    | 48,48,48     | 0.61 | 1 (2%)   | 51,54,54    | 1.20 | 5 (9%)   |
| 14  | CLA  | B     | 820  | -    | 65,73,73     | 1.50 | 7 (10%)  | 76,113,113  | 1.33 | 7 (9%)   |
| 14  | CLA  | 2     | 830  | -    | 65,73,73     | 1.43 | 12 (18%) | 76,113,113  | 1.57 | 10 (13%) |
| 14  | CLA  | b     | 823  | 21   | 55,63,73     | 1.62 | 7 (12%)  | 64,101,113  | 1.48 | 6 (9%)   |
| 14  | CLA  | b     | 834  | -    | 65,73,73     | 1.47 | 9 (13%)  | 76,113,113  | 1.45 | 7 (9%)   |
| 17  | BCR  | f     | 202  | -    | 41,41,41     | 1.24 | 3 (7%)   | 56,56,56    | 1.26 | 6 (10%)  |
| 14  | CLA  | 1     | 1645 | 18   | 45,53,73     | 1.73 | 7 (15%)  | 52,89,113   | 1.69 | 7 (13%)  |
| 14  | CLA  | a     | 814  | -    | 65,73,73     | 1.50 | 9 (13%)  | 76,113,113  | 1.34 | 8 (10%)  |
| 16  | SF4  | 3     | 101  | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 14  | CLA  | 1     | 1636 | -    | 65,73,73     | 1.44 | 9 (13%)  | 76,113,113  | 1.45 | 6 (7%)   |
| 14  | CLA  | a     | 832  | -    | 60,68,73     | 1.52 | 10 (16%) | 70,107,113  | 1.44 | 6 (8%)   |
| 14  | CLA  | A     | 806  | -    | 65,73,73     | 1.46 | 10 (15%) | 76,113,113  | 1.58 | 12 (15%) |
| 14  | CLA  | A     | 838  | -    | 65,73,73     | 1.41 | 7 (10%)  | 76,113,113  | 1.61 | 7 (9%)   |
| 14  | CLA  | 2     | 810  | 2    | 65,73,73     | 1.46 | 11 (16%) | 76,113,113  | 1.60 | 9 (11%)  |
| 14  | CLA  | A     | 805  | 14   | 59,67,73     | 1.51 | 7 (11%)  | 68,105,113  | 1.55 | 8 (11%)  |
| 14  | CLA  | b     | 841  | 21   | 65,73,73     | 1.47 | 9 (13%)  | 76,113,113  | 1.43 | 10 (13%) |
| 18  | LHG  | l     | 201  | -    | 38,38,48     | 0.73 | 0        | 41,44,54    | 1.26 | 3 (7%)   |
| 14  | CLA  | 1     | 1624 | -    | 45,53,73     | 1.76 | 7 (15%)  | 52,89,113   | 1.67 | 8 (15%)  |
| 17  | BCR  | 2     | 844  | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.22 | 4 (7%)   |
| 20  | LMG  | b     | 850  | -    | 55,55,55     | 0.92 | 4 (7%)   | 63,63,63    | 1.35 | 10 (15%) |
| 14  | CLA  | B     | 815  | -    | 65,73,73     | 1.45 | 7 (10%)  | 76,113,113  | 1.39 | 7 (9%)   |
| 14  | CLA  | B     | 811  | -    | 65,73,73     | 1.44 | 7 (10%)  | 76,113,113  | 1.54 | 9 (11%)  |
| 14  | CLA  | b     | 833  | -    | 65,73,73     | 1.49 | 8 (12%)  | 76,113,113  | 1.44 | 8 (10%)  |
| 14  | CLA  | A     | 811  | -    | 49,57,73     | 1.70 | 9 (18%)  | 55,93,113   | 1.48 | 8 (14%)  |
| 14  | CLA  | b     | 836  | 21   | 50,58,73     | 1.69 | 9 (18%)  | 58,95,113   | 1.52 | 8 (13%)  |
| 14  | CLA  | 1     | 1617 | -    | 65,73,73     | 1.47 | 6 (9%)   | 76,113,113  | 1.38 | 7 (9%)   |
| 14  | CLA  | 2     | 839  | -    | 65,73,73     | 1.46 | 9 (13%)  | 76,113,113  | 1.40 | 6 (7%)   |
| 14  | CLA  | b     | 821  | -    | 65,73,73     | 1.50 | 7 (10%)  | 76,113,113  | 1.34 | 8 (10%)  |
| 14  | CLA  | B     | 803  | -    | 65,73,73     | 1.43 | 10 (15%) | 76,113,113  | 1.52 | 8 (10%)  |
| 14  | CLA  | 1     | 1633 | -    | 60,68,73     | 1.52 | 10 (16%) | 70,107,113  | 1.44 | 6 (8%)   |
| 14  | CLA  | L     | 203  | 10   | 65,73,73     | 1.51 | 9 (13%)  | 76,113,113  | 1.38 | 8 (10%)  |
| 14  | CLA  | a     | 809  | 1    | 65,73,73     | 1.46 | 9 (13%)  | 76,113,113  | 1.51 | 9 (11%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | 1     | 1604 | 21   | 65,73,73     | 1.54 | 9 (13%)  | 76,113,113  | 1.30 | 8 (10%)  |
| 14  | CLA  | 2     | 819  | -    | 65,73,73     | 1.44 | 8 (12%)  | 76,113,113  | 1.52 | 10 (13%) |
| 13  | CL0  | 1     | 1602 | -    | 65,73,73     | 1.45 | 10 (15%) | 76,113,113  | 1.47 | 8 (10%)  |
| 17  | BCR  | 0     | 209  | -    | 41,41,41     | 1.18 | 3 (7%)   | 56,56,56    | 1.28 | 7 (12%)  |
| 14  | CLA  | b     | 807  | -    | 65,73,73     | 1.47 | 9 (13%)  | 76,113,113  | 1.41 | 8 (10%)  |
| 14  | CLA  | a     | 830  | -    | 65,73,73     | 1.41 | 9 (13%)  | 76,113,113  | 1.54 | 7 (9%)   |
| 14  | CLA  | a     | 841  | -    | 65,73,73     | 1.46 | 8 (12%)  | 76,113,113  | 1.46 | 8 (10%)  |
| 14  | CLA  | 2     | 840  | -    | 47,55,73     | 1.80 | 9 (19%)  | 54,91,113   | 1.48 | 8 (14%)  |
| 14  | CLA  | 2     | 804  | -    | 65,73,73     | 1.42 | 10 (15%) | 76,113,113  | 1.50 | 8 (10%)  |
| 14  | CLA  | a     | 828  | -    | 65,73,73     | 1.47 | 7 (10%)  | 76,113,113  | 1.38 | 8 (10%)  |
| 16  | SF4  | C     | 102  | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 14  | CLA  | 1     | 1642 | -    | 65,73,73     | 1.46 | 8 (12%)  | 76,113,113  | 1.46 | 8 (10%)  |
| 14  | CLA  | 1     | 1626 | -    | 65,73,73     | 1.45 | 9 (13%)  | 76,113,113  | 1.45 | 9 (11%)  |
| 17  | BCR  | F     | 205  | -    | 41,41,41     | 1.18 | 2 (4%)   | 56,56,56    | 1.36 | 8 (14%)  |
| 17  | BCR  | l     | 207  | -    | 41,41,41     | 1.21 | 3 (7%)   | 56,56,56    | 1.34 | 7 (12%)  |
| 14  | CLA  | b     | 810  | 2    | 65,73,73     | 1.46 | 11 (16%) | 76,113,113  | 1.61 | 10 (13%) |
| 14  | CLA  | 1     | 1635 | -    | 65,73,73     | 1.45 | 8 (12%)  | 76,113,113  | 1.59 | 12 (15%) |
| 17  | BCR  | 2     | 848  | -    | 41,41,41     | 1.28 | 3 (7%)   | 56,56,56    | 1.31 | 8 (14%)  |
| 17  | BCR  | 1     | 1651 | -    | 41,41,41     | 1.35 | 4 (9%)   | 56,56,56    | 1.28 | 7 (12%)  |
| 14  | CLA  | 2     | 841  | 21   | 65,73,73     | 1.47 | 9 (13%)  | 76,113,113  | 1.43 | 10 (13%) |
| 14  | CLA  | X     | 1701 | 12   | 45,53,73     | 1.81 | 6 (13%)  | 52,89,113   | 1.60 | 6 (11%)  |
| 14  | CLA  | b     | 824  | -    | 45,53,73     | 1.74 | 7 (15%)  | 52,89,113   | 1.71 | 7 (13%)  |
| 17  | BCR  | b     | 847  | -    | 41,41,41     | 1.15 | 3 (7%)   | 56,56,56    | 1.25 | 8 (14%)  |
| 14  | CLA  | 1     | 1638 | 1    | 45,53,73     | 1.78 | 7 (15%)  | 52,89,113   | 1.53 | 8 (15%)  |
| 17  | BCR  | A     | 852  | -    | 25,25,41     | 1.13 | 1 (4%)   | 33,33,56    | 1.28 | 4 (12%)  |
| 14  | CLA  | A     | 842  | -    | 65,73,73     | 1.47 | 9 (13%)  | 76,113,113  | 1.50 | 9 (11%)  |
| 14  | CLA  | 2     | 836  | 21   | 50,58,73     | 1.70 | 9 (18%)  | 58,95,113   | 1.53 | 8 (13%)  |
| 18  | LHG  | A     | 854  | 14   | 40,40,48     | 0.77 | 1 (2%)   | 43,46,54    | 1.22 | 4 (9%)   |
| 17  | BCR  | B     | 844  | -    | 41,41,41     | 1.17 | 3 (7%)   | 56,56,56    | 1.19 | 3 (5%)   |
| 14  | CLA  | 2     | 821  | -    | 65,73,73     | 1.49 | 7 (10%)  | 76,113,113  | 1.32 | 7 (9%)   |
| 17  | BCR  | A     | 848  | -    | 41,41,41     | 1.18 | 3 (7%)   | 56,56,56    | 1.23 | 6 (10%)  |
| 18  | LHG  | 0     | 202  | -    | 38,38,48     | 0.73 | 1 (2%)   | 41,44,54    | 1.26 | 3 (7%)   |
| 17  | BCR  | b     | 849  | -    | 41,41,41     | 1.39 | 4 (9%)   | 56,56,56    | 1.29 | 6 (10%)  |
| 16  | SF4  | 3     | 102  | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 14  | CLA  | b     | 820  | 21   | 65,73,73     | 1.54 | 7 (10%)  | 76,113,113  | 1.35 | 9 (11%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 17  | BCR  | a     | 849  | -    | 41,41,41     | 1.22 | 2 (4%)   | 56,56,56    | 1.20 | 6 (10%)  |
| 14  | CLA  | B     | 835  | 21   | 50,58,73     | 1.70 | 9 (18%)  | 58,95,113   | 1.53 | 8 (13%)  |
| 14  | CLA  | a     | 808  | -    | 51,59,73     | 1.66 | 9 (17%)  | 59,96,113   | 1.53 | 8 (13%)  |
| 14  | CLA  | a     | 825  | -    | 65,73,73     | 1.46 | 8 (12%)  | 76,113,113  | 1.45 | 8 (10%)  |
| 14  | CLA  | B     | 819  | 21   | 65,73,73     | 1.55 | 8 (12%)  | 76,113,113  | 1.35 | 9 (11%)  |
| 14  | CLA  | A     | 819  | -    | 65,73,73     | 1.49 | 8 (12%)  | 76,113,113  | 1.47 | 9 (11%)  |
| 14  | CLA  | a     | 823  | -    | 45,53,73     | 1.75 | 6 (13%)  | 52,89,113   | 1.68 | 8 (15%)  |
| 14  | CLA  | 8     | 1301 | 21   | 45,53,73     | 1.77 | 7 (15%)  | 52,89,113   | 1.68 | 7 (13%)  |
| 14  | CLA  | A     | 837  | 1    | 45,53,73     | 1.79 | 7 (15%)  | 52,89,113   | 1.54 | 8 (15%)  |
| 14  | CLA  | b     | 831  | -    | 55,63,73     | 1.60 | 9 (16%)  | 64,101,113  | 1.49 | 9 (14%)  |
| 14  | CLA  | 2     | 812  | -    | 65,73,73     | 1.44 | 7 (10%)  | 76,113,113  | 1.55 | 9 (11%)  |
| 14  | CLA  | B     | 808  | -    | 65,73,73     | 1.43 | 8 (12%)  | 76,113,113  | 1.54 | 10 (13%) |
| 14  | CLA  | B     | 804  | -    | 65,73,73     | 1.49 | 9 (13%)  | 76,113,113  | 1.46 | 11 (14%) |
| 14  | CLA  | b     | 827  | -    | 65,73,73     | 1.48 | 8 (12%)  | 76,113,113  | 1.43 | 8 (10%)  |
| 14  | CLA  | M     | 102  | -    | 36,44,73     | 1.96 | 7 (19%)  | 40,76,113   | 1.64 | 5 (12%)  |
| 14  | CLA  | A     | 804  | -    | 65,73,73     | 1.42 | 7 (10%)  | 76,113,113  | 1.50 | 7 (9%)   |
| 14  | CLA  | a     | 802  | -    | 65,73,73     | 1.45 | 8 (12%)  | 76,113,113  | 1.54 | 8 (10%)  |
| 15  | PQN  | b     | 843  | -    | 34,34,34     | 0.45 | 0        | 42,45,45    | 0.38 | 0        |
| 14  | CLA  | 1     | 1639 | -    | 65,73,73     | 1.42 | 8 (12%)  | 76,113,113  | 1.61 | 7 (9%)   |
| 14  | CLA  | A     | 831  | -    | 65,73,73     | 1.51 | 11 (16%) | 76,113,113  | 1.49 | 9 (11%)  |
| 17  | BCR  | 8     | 1306 | -    | 41,41,41     | 1.21 | 2 (4%)   | 56,56,56    | 1.34 | 9 (16%)  |
| 17  | BCR  | l     | 202  | -    | 41,41,41     | 1.39 | 4 (9%)   | 56,56,56    | 1.32 | 7 (12%)  |
| 17  | BCR  | m     | 102  | -    | 41,41,41     | 1.24 | 3 (7%)   | 56,56,56    | 1.22 | 5 (8%)   |
| 14  | CLA  | A     | 818  | -    | 65,73,73     | 1.46 | 6 (9%)   | 76,113,113  | 1.44 | 7 (9%)   |
| 14  | CLA  | 1     | 1628 | 21   | 65,73,73     | 1.46 | 9 (13%)  | 76,113,113  | 1.52 | 10 (13%) |
| 14  | CLA  | F     | 201  | 21   | 58,66,73     | 1.59 | 7 (12%)  | 67,104,113  | 1.47 | 8 (11%)  |
| 14  | CLA  | a     | 821  | -    | 65,73,73     | 1.45 | 6 (9%)   | 76,113,113  | 1.52 | 7 (9%)   |
| 14  | CLA  | A     | 826  | 21   | 65,73,73     | 1.46 | 9 (13%)  | 76,113,113  | 1.49 | 9 (11%)  |
| 14  | CLA  | 2     | 838  | -    | 60,68,73     | 1.56 | 9 (15%)  | 70,107,113  | 1.47 | 7 (10%)  |
| 14  | CLA  | B     | 836  | 21   | 45,53,73     | 1.82 | 7 (15%)  | 52,89,113   | 1.52 | 5 (9%)   |
| 14  | CLA  | a     | 827  | 21   | 65,73,73     | 1.45 | 9 (13%)  | 76,113,113  | 1.52 | 10 (13%) |
| 14  | CLA  | 2     | 803  | -    | 65,73,73     | 1.45 | 10 (15%) | 76,113,113  | 1.45 | 8 (10%)  |
| 14  | CLA  | A     | 810  | 1    | 65,73,73     | 1.47 | 7 (10%)  | 76,113,113  | 1.46 | 7 (9%)   |
| 14  | CLA  | a     | 826  | 21   | 65,73,73     | 1.46 | 9 (13%)  | 76,113,113  | 1.50 | 9 (11%)  |
| 14  | CLA  | x     | 1701 | 12   | 45,53,73     | 1.79 | 6 (13%)  | 52,89,113   | 1.61 | 6 (11%)  |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 17  | BCR  | 0     | 201  | -    | 41,41,41     | 1.18 | 3 (7%)   | 56,56,56    | 1.28 | 7 (12%)  |
| 14  | CLA  | 2     | 824  | -    | 45,53,73     | 1.75 | 7 (15%)  | 52,89,113   | 1.71 | 7 (13%)  |
| 17  | BCR  | 1     | 1649 | -    | 41,41,41     | 1.19 | 3 (7%)   | 56,56,56    | 1.22 | 6 (10%)  |
| 17  | BCR  | 0     | 208  | -    | 41,41,41     | 1.22 | 3 (7%)   | 56,56,56    | 1.34 | 7 (12%)  |
| 14  | CLA  | 1     | 1605 | -    | 65,73,73     | 1.42 | 7 (10%)  | 76,113,113  | 1.49 | 7 (9%)   |
| 14  | CLA  | B     | 827  | -    | 65,73,73     | 1.50 | 8 (12%)  | 76,113,113  | 1.43 | 7 (9%)   |
| 14  | CLA  | A     | 809  | 1    | 65,73,73     | 1.45 | 8 (12%)  | 76,113,113  | 1.51 | 8 (10%)  |
| 14  | CLA  | B     | 829  | -    | 65,73,73     | 1.44 | 12 (18%) | 76,113,113  | 1.57 | 10 (13%) |
| 17  | BCR  | a     | 850  | -    | 41,41,41     | 1.34 | 4 (9%)   | 56,56,56    | 1.29 | 7 (12%)  |
| 14  | CLA  | A     | 825  | -    | 65,73,73     | 1.46 | 9 (13%)  | 76,113,113  | 1.47 | 9 (11%)  |
| 14  | CLA  | A     | 829  | -    | 65,73,73     | 1.45 | 7 (10%)  | 76,113,113  | 1.47 | 8 (10%)  |
| 14  | CLA  | 9     | 103  | 21   | 58,66,73     | 1.56 | 7 (12%)  | 67,104,113  | 1.50 | 9 (13%)  |
| 14  | CLA  | b     | 803  | -    | 65,73,73     | 1.43 | 10 (15%) | 76,113,113  | 1.44 | 8 (10%)  |
| 14  | CLA  | 2     | 833  | -    | 65,73,73     | 1.49 | 8 (12%)  | 76,113,113  | 1.44 | 8 (10%)  |
| 14  | CLA  | 2     | 827  | -    | 65,73,73     | 1.48 | 8 (12%)  | 76,113,113  | 1.42 | 8 (10%)  |
| 14  | CLA  | a     | 834  | -    | 65,73,73     | 1.45 | 7 (10%)  | 76,113,113  | 1.59 | 12 (15%) |
| 17  | BCR  | a     | 852  | -    | 25,25,41     | 1.12 | 1 (4%)   | 33,33,56    | 1.29 | 4 (12%)  |
| 18  | LHG  | M     | 101  | -    | 48,48,48     | 0.70 | 2 (4%)   | 51,54,54    | 1.22 | 3 (5%)   |
| 14  | CLA  | b     | 822  | -    | 45,53,73     | 1.73 | 7 (15%)  | 52,89,113   | 1.78 | 9 (17%)  |
| 14  | CLA  | 2     | 818  | -    | 65,73,73     | 1.50 | 9 (13%)  | 76,113,113  | 1.49 | 9 (11%)  |
| 14  | CLA  | B     | 839  | -    | 47,55,73     | 1.80 | 9 (19%)  | 54,91,113   | 1.48 | 8 (14%)  |
| 17  | BCR  | A     | 856  | -    | 41,41,41     | 1.23 | 3 (7%)   | 56,56,56    | 1.28 | 8 (14%)  |
| 14  | CLA  | a     | 836  | -    | 65,73,73     | 1.48 | 9 (13%)  | 76,113,113  | 1.44 | 7 (9%)   |
| 17  | BCR  | b     | 844  | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.21 | 4 (7%)   |
| 16  | SF4  | c     | 102  | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 16  | SF4  | c     | 101  | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 17  | BCR  | B     | 843  | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.21 | 4 (7%)   |
| 14  | CLA  | 2     | 822  | -    | 45,53,73     | 1.72 | 7 (15%)  | 52,89,113   | 1.78 | 9 (17%)  |
| 14  | CLA  | K     | 103  | 21   | 58,66,73     | 1.56 | 7 (12%)  | 67,104,113  | 1.50 | 9 (13%)  |
| 14  | CLA  | B     | 810  | 2    | 65,73,73     | 1.44 | 9 (13%)  | 76,113,113  | 1.52 | 9 (11%)  |
| 16  | SF4  | C     | 101  | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 17  | BCR  | F     | 202  | -    | 41,41,41     | 1.25 | 3 (7%)   | 56,56,56    | 1.25 | 6 (10%)  |
| 14  | CLA  | b     | 811  | 2    | 65,73,73     | 1.44 | 9 (13%)  | 76,113,113  | 1.52 | 8 (10%)  |
| 14  | CLA  | A     | 828  | -    | 65,73,73     | 1.46 | 7 (10%)  | 76,113,113  | 1.39 | 8 (10%)  |
| 14  | CLA  | a     | 815  | -    | 65,73,73     | 1.50 | 7 (10%)  | 76,113,113  | 1.40 | 7 (9%)   |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | A     | 844  | 18   | 45,53,73     | 1.72 | 7 (15%)  | 52,89,113   | 1.69 | 7 (13%)  |
| 14  | CLA  | b     | 835  | -    | 65,73,73     | 1.47 | 6 (9%)   | 76,113,113  | 1.44 | 9 (11%)  |
| 14  | CLA  | B     | 816  | -    | 65,73,73     | 1.44 | 6 (9%)   | 76,113,113  | 1.48 | 8 (10%)  |
| 14  | CLA  | 2     | 809  | -    | 65,73,73     | 1.44 | 8 (12%)  | 76,113,113  | 1.54 | 10 (13%) |
| 14  | CLA  | a     | 803  | 21   | 65,73,73     | 1.54 | 9 (13%)  | 76,113,113  | 1.29 | 6 (7%)   |
| 14  | CLA  | 2     | 807  | -    | 65,73,73     | 1.48 | 9 (13%)  | 76,113,113  | 1.40 | 8 (10%)  |
| 14  | CLA  | B     | 837  | -    | 60,68,73     | 1.56 | 9 (15%)  | 70,107,113  | 1.46 | 7 (10%)  |
| 14  | CLA  | 1     | 1632 | -    | 65,73,73     | 1.51 | 9 (13%)  | 76,113,113  | 1.50 | 9 (11%)  |
| 14  | CLA  | a     | 822  | 21   | 65,73,73     | 1.47 | 7 (10%)  | 76,113,113  | 1.46 | 7 (9%)   |
| 14  | CLA  | z     | 102  | 12   | 45,53,73     | 1.80 | 6 (13%)  | 52,89,113   | 1.61 | 6 (11%)  |
| 14  | CLA  | 1     | 1611 | 1    | 65,73,73     | 1.47 | 7 (10%)  | 76,113,113  | 1.44 | 7 (9%)   |
| 14  | CLA  | b     | 805  | -    | 65,73,73     | 1.49 | 9 (13%)  | 76,113,113  | 1.46 | 12 (15%) |
| 14  | CLA  | B     | 838  | -    | 65,73,73     | 1.47 | 9 (13%)  | 76,113,113  | 1.40 | 6 (7%)   |
| 14  | CLA  | A     | 814  | -    | 65,73,73     | 1.49 | 9 (13%)  | 76,113,113  | 1.33 | 8 (10%)  |
| 14  | CLA  | f     | 201  | 21   | 58,66,73     | 1.58 | 7 (12%)  | 67,104,113  | 1.47 | 8 (11%)  |
| 14  | CLA  | 1     | 1643 | -    | 65,73,73     | 1.47 | 8 (12%)  | 76,113,113  | 1.50 | 9 (11%)  |
| 17  | BCR  | M     | 103  | -    | 41,41,41     | 1.23 | 3 (7%)   | 56,56,56    | 1.22 | 5 (8%)   |
| 14  | CLA  | B     | 805  | -    | 65,73,73     | 1.44 | 7 (10%)  | 76,113,113  | 1.57 | 8 (10%)  |
| 14  | CLA  | a     | 807  | -    | 65,73,73     | 1.44 | 8 (12%)  | 76,113,113  | 1.53 | 5 (6%)   |
| 14  | CLA  | B     | 822  | 21   | 55,63,73     | 1.63 | 7 (12%)  | 64,101,113  | 1.47 | 6 (9%)   |
| 17  | BCR  | a     | 847  | -    | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.30 | 7 (12%)  |
| 14  | CLA  | a     | 833  | -    | 65,73,73     | 1.45 | 10 (15%) | 76,113,113  | 1.39 | 6 (7%)   |
| 14  | CLA  | B     | 807  | -    | 65,73,73     | 1.48 | 9 (13%)  | 76,113,113  | 1.43 | 10 (13%) |
| 14  | CLA  | 2     | 808  | -    | 65,73,73     | 1.48 | 9 (13%)  | 76,113,113  | 1.43 | 9 (11%)  |
| 14  | CLA  | B     | 814  | -    | 65,73,73     | 1.44 | 7 (10%)  | 76,113,113  | 1.44 | 8 (10%)  |
| 14  | CLA  | B     | 809  | 2    | 65,73,73     | 1.45 | 10 (15%) | 76,113,113  | 1.61 | 10 (13%) |
| 14  | CLA  | B     | 833  | -    | 65,73,73     | 1.48 | 9 (13%)  | 76,113,113  | 1.45 | 7 (9%)   |
| 17  | BCR  | B     | 851  | -    | 41,41,41     | 1.21 | 2 (4%)   | 56,56,56    | 1.34 | 9 (16%)  |
| 17  | BCR  | f     | 204  | -    | 41,41,41     | 1.19 | 2 (4%)   | 56,56,56    | 1.36 | 8 (14%)  |
| 14  | CLA  | B     | 830  | -    | 55,63,73     | 1.60 | 9 (16%)  | 64,101,113  | 1.50 | 9 (14%)  |
| 16  | SF4  | 1     | 1647 | 2,1  | 0,12,12      | -    | -        | -           | -    | -        |
| 14  | CLA  | b     | 819  | -    | 65,73,73     | 1.43 | 7 (10%)  | 76,113,113  | 1.51 | 9 (11%)  |
| 14  | CLA  | b     | 809  | -    | 65,73,73     | 1.43 | 8 (12%)  | 76,113,113  | 1.53 | 10 (13%) |
| 14  | CLA  | B     | 806  | -    | 65,73,73     | 1.48 | 9 (13%)  | 76,113,113  | 1.40 | 8 (10%)  |
| 17  | BCR  | 1     | 1648 | -    | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.31 | 7 (12%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | 8     | 1303 | -    | 38,45,73     | 1.91 | 8 (21%)  | 43,78,113   | 1.68 | 7 (16%)  |
| 14  | CLA  | A     | 830  | -    | 65,73,73     | 1.41 | 9 (13%)  | 76,113,113  | 1.54 | 7 (9%)   |
| 14  | CLA  | 1     | 1613 | 14   | 65,73,73     | 1.47 | 7 (10%)  | 76,113,113  | 1.36 | 7 (9%)   |
| 14  | CLA  | 2     | 815  | -    | 65,73,73     | 1.45 | 8 (12%)  | 76,113,113  | 1.44 | 8 (10%)  |
| 14  | CLA  | A     | 839  | -    | 65,73,73     | 1.44 | 9 (13%)  | 76,113,113  | 1.47 | 9 (11%)  |
| 14  | CLA  | 1     | 1612 | -    | 49,57,73     | 1.71 | 9 (18%)  | 55,93,113   | 1.49 | 8 (14%)  |
| 14  | CLA  | A     | 821  | -    | 65,73,73     | 1.45 | 6 (9%)   | 76,113,113  | 1.51 | 7 (9%)   |
| 14  | CLA  | A     | 840  | -    | 65,73,73     | 1.49 | 9 (13%)  | 76,113,113  | 1.43 | 8 (10%)  |
| 14  | CLA  | 1     | 1622 | -    | 65,73,73     | 1.45 | 6 (9%)   | 76,113,113  | 1.52 | 7 (9%)   |
| 14  | CLA  | F     | 203  | 21   | 45,53,73     | 1.77 | 7 (15%)  | 52,89,113   | 1.68 | 7 (13%)  |
| 14  | CLA  | b     | 830  | -    | 65,73,73     | 1.44 | 12 (18%) | 76,113,113  | 1.57 | 10 (13%) |
| 14  | CLA  | A     | 808  | -    | 51,59,73     | 1.66 | 8 (15%)  | 59,96,113   | 1.54 | 8 (13%)  |
| 14  | CLA  | 0     | 207  | 21   | 65,73,73     | 1.45 | 10 (15%) | 76,113,113  | 1.50 | 9 (11%)  |
| 17  | BCR  | 9     | 102  | -    | 41,41,41     | 1.18 | 2 (4%)   | 56,56,56    | 1.32 | 7 (12%)  |
| 13  | CL0  | a     | 801  | -    | 65,73,73     | 1.44 | 10 (15%) | 76,113,113  | 1.46 | 8 (10%)  |
| 14  | CLA  | B     | 828  | -    | 65,73,73     | 1.51 | 8 (12%)  | 76,113,113  | 1.30 | 7 (9%)   |
| 14  | CLA  | 1     | 1610 | 1    | 65,73,73     | 1.46 | 8 (12%)  | 76,113,113  | 1.51 | 9 (11%)  |
| 17  | BCR  | 2     | 845  | -    | 41,41,41     | 1.17 | 3 (7%)   | 56,56,56    | 1.19 | 3 (5%)   |
| 14  | CLA  | a     | 824  | -    | 65,73,73     | 1.52 | 8 (12%)  | 76,113,113  | 1.39 | 9 (11%)  |
| 14  | CLA  | 2     | 816  | -    | 65,73,73     | 1.46 | 7 (10%)  | 76,113,113  | 1.39 | 7 (9%)   |
| 14  | CLA  | A     | 816  | -    | 65,73,73     | 1.47 | 6 (9%)   | 76,113,113  | 1.39 | 7 (9%)   |
| 17  | BCR  | j     | 1304 | -    | 41,41,41     | 1.17 | 3 (7%)   | 56,56,56    | 1.19 | 7 (12%)  |
| 14  | CLA  | 2     | 802  | 21   | 65,73,73     | 1.42 | 8 (12%)  | 76,113,113  | 1.60 | 8 (10%)  |
| 17  | BCR  | L     | 201  | -    | 41,41,41     | 1.39 | 4 (9%)   | 56,56,56    | 1.33 | 7 (12%)  |
| 14  | CLA  | A     | 832  | -    | 60,68,73     | 1.53 | 10 (16%) | 70,107,113  | 1.43 | 6 (8%)   |
| 15  | PQN  | a     | 845  | -    | 34,34,34     | 0.40 | 0        | 42,45,45    | 0.35 | 0        |
| 17  | BCR  | B     | 846  | -    | 41,41,41     | 1.16 | 3 (7%)   | 56,56,56    | 1.24 | 7 (12%)  |
| 14  | CLA  | A     | 803  | 21   | 65,73,73     | 1.54 | 9 (13%)  | 76,113,113  | 1.30 | 8 (10%)  |
| 17  | BCR  | A     | 851  | -    | 41,41,41     | 1.27 | 2 (4%)   | 56,56,56    | 1.30 | 7 (12%)  |
| 14  | CLA  | b     | 813  | -    | 45,53,73     | 1.80 | 8 (17%)  | 52,89,113   | 1.62 | 7 (13%)  |
| 17  | BCR  | 8     | 1305 | -    | 41,41,41     | 1.22 | 2 (4%)   | 56,56,56    | 1.28 | 8 (14%)  |
| 14  | CLA  | k     | 103  | 21   | 58,66,73     | 1.57 | 7 (12%)  | 67,104,113  | 1.50 | 9 (13%)  |
| 14  | CLA  | 2     | 806  | -    | 65,73,73     | 1.44 | 7 (10%)  | 76,113,113  | 1.58 | 8 (10%)  |
| 14  | CLA  | L     | 204  | -    | 65,73,73     | 1.46 | 10 (15%) | 76,113,113  | 1.53 | 9 (11%)  |
| 14  | CLA  | 1     | 1637 | -    | 65,73,73     | 1.48 | 9 (13%)  | 76,113,113  | 1.44 | 7 (9%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 17  | BCR  | 8     | 1304 | -    | 41,41,41     | 1.17 | 3 (7%)   | 56,56,56    | 1.20 | 7 (12%)  |
| 14  | CLA  | 2     | 813  | -    | 45,53,73     | 1.80 | 8 (17%)  | 52,89,113   | 1.61 | 7 (13%)  |
| 14  | CLA  | B     | 840  | 21   | 65,73,73     | 1.47 | 9 (13%)  | 76,113,113  | 1.43 | 10 (13%) |
| 17  | BCR  | B     | 848  | -    | 41,41,41     | 1.39 | 4 (9%)   | 56,56,56    | 1.29 | 6 (10%)  |
| 14  | CLA  | J     | 102  | -    | 38,45,73     | 1.92 | 8 (21%)  | 43,78,113   | 1.68 | 7 (16%)  |
| 14  | CLA  | B     | 817  | -    | 65,73,73     | 1.52 | 9 (13%)  | 76,113,113  | 1.49 | 9 (11%)  |
| 14  | CLA  | 1     | 1608 | -    | 65,73,73     | 1.43 | 7 (10%)  | 76,113,113  | 1.53 | 5 (6%)   |
| 17  | BCR  | i     | 101  | -    | 41,41,41     | 1.29 | 4 (9%)   | 56,56,56    | 1.24 | 3 (5%)   |
| 17  | BCR  | b     | 846  | -    | 41,41,41     | 1.25 | 3 (7%)   | 56,56,56    | 1.24 | 6 (10%)  |
| 14  | CLA  | A     | 817  | 21   | 65,73,73     | 1.48 | 7 (10%)  | 76,113,113  | 1.35 | 7 (9%)   |
| 14  | CLA  | 1     | 1614 | -    | 45,53,73     | 1.78 | 8 (17%)  | 52,89,113   | 1.64 | 8 (15%)  |
| 14  | CLA  | 1     | 1619 | -    | 65,73,73     | 1.45 | 6 (9%)   | 76,113,113  | 1.45 | 7 (9%)   |
| 14  | CLA  | b     | 812  | -    | 65,73,73     | 1.45 | 7 (10%)  | 76,113,113  | 1.54 | 10 (13%) |
| 14  | CLA  | b     | 840  | -    | 47,55,73     | 1.79 | 9 (19%)  | 54,91,113   | 1.48 | 7 (12%)  |
| 14  | CLA  | A     | 834  | -    | 65,73,73     | 1.45 | 7 (10%)  | 76,113,113  | 1.58 | 13 (17%) |
| 14  | CLA  | A     | 802  | -    | 65,73,73     | 1.45 | 8 (12%)  | 76,113,113  | 1.54 | 8 (10%)  |
| 18  | LHG  | a     | 854  | 14   | 40,40,48     | 0.77 | 1 (2%)   | 43,46,54    | 1.21 | 4 (9%)   |
| 17  | BCR  | b     | 852  | -    | 41,41,41     | 1.21 | 2 (4%)   | 56,56,56    | 1.33 | 9 (16%)  |
| 14  | CLA  | K     | 101  | -    | 46,54,73     | 1.74 | 7 (15%)  | 53,90,113   | 1.57 | 7 (13%)  |
| 17  | BCR  | b     | 848  | -    | 41,41,41     | 1.27 | 3 (7%)   | 56,56,56    | 1.31 | 9 (16%)  |
| 14  | CLA  | a     | 839  | -    | 65,73,73     | 1.45 | 9 (13%)  | 76,113,113  | 1.48 | 9 (11%)  |
| 14  | CLA  | b     | 842  | -    | 65,73,73     | 1.48 | 9 (13%)  | 76,113,113  | 1.47 | 7 (9%)   |
| 14  | CLA  | 2     | 829  | -    | 65,73,73     | 1.51 | 8 (12%)  | 76,113,113  | 1.30 | 7 (9%)   |
| 14  | CLA  | 1     | 1609 | -    | 51,59,73     | 1.66 | 9 (17%)  | 59,96,113   | 1.55 | 8 (13%)  |
| 14  | CLA  | 1     | 1618 | 21   | 65,73,73     | 1.47 | 7 (10%)  | 76,113,113  | 1.36 | 7 (9%)   |
| 14  | CLA  | A     | 823  | -    | 45,53,73     | 1.75 | 6 (13%)  | 52,89,113   | 1.67 | 8 (15%)  |
| 14  | CLA  | 1     | 1616 | -    | 65,73,73     | 1.50 | 8 (12%)  | 76,113,113  | 1.40 | 7 (9%)   |
| 14  | CLA  | A     | 841  | -    | 65,73,73     | 1.45 | 8 (12%)  | 76,113,113  | 1.46 | 8 (10%)  |
| 14  | CLA  | a     | 831  | -    | 65,73,73     | 1.51 | 10 (15%) | 76,113,113  | 1.49 | 9 (11%)  |
| 14  | CLA  | b     | 816  | -    | 65,73,73     | 1.45 | 7 (10%)  | 76,113,113  | 1.39 | 7 (9%)   |
| 14  | CLA  | l     | 204  | 10   | 65,73,73     | 1.52 | 9 (13%)  | 76,113,113  | 1.38 | 8 (10%)  |
| 20  | LMG  | 2     | 850  | -    | 55,55,55     | 0.92 | 4 (7%)   | 63,63,63    | 1.35 | 9 (14%)  |
| 14  | CLA  | A     | 824  | -    | 65,73,73     | 1.52 | 8 (12%)  | 76,113,113  | 1.38 | 9 (11%)  |
| 14  | CLA  | A     | 815  | -    | 65,73,73     | 1.50 | 8 (12%)  | 76,113,113  | 1.40 | 7 (9%)   |
| 14  | CLA  | B     | 825  | 21   | 65,73,73     | 1.51 | 9 (13%)  | 76,113,113  | 1.53 | 10 (13%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 17  | BCR  | y     | 102  | -    | 41,41,41     | 1.24 | 3 (7%)   | 56,56,56    | 1.22 | 5 (8%)   |
| 18  | LHG  | A     | 853  | -    | 48,48,48     | 0.75 | 2 (4%)   | 51,54,54    | 1.23 | 4 (7%)   |
| 14  | CLA  | 2     | 828  | -    | 65,73,73     | 1.51 | 8 (12%)  | 76,113,113  | 1.43 | 7 (9%)   |
| 14  | CLA  | 1     | 1631 | -    | 65,73,73     | 1.41 | 9 (13%)  | 76,113,113  | 1.54 | 6 (7%)   |
| 18  | LHG  | 1     | 1654 | -    | 48,48,48     | 0.75 | 1 (2%)   | 51,54,54    | 1.23 | 4 (7%)   |
| 14  | CLA  | A     | 836  | -    | 65,73,73     | 1.48 | 9 (13%)  | 76,113,113  | 1.44 | 7 (9%)   |
| 18  | LHG  | L     | 208  | -    | 38,38,48     | 0.73 | 0        | 41,44,54    | 1.26 | 3 (7%)   |
| 14  | CLA  | J     | 101  | -    | 45,53,73     | 1.78 | 5 (11%)  | 52,89,113   | 1.58 | 8 (15%)  |
| 14  | CLA  | B     | 821  | -    | 45,53,73     | 1.73 | 7 (15%)  | 52,89,113   | 1.78 | 9 (17%)  |
| 14  | CLA  | 1     | 1620 | -    | 65,73,73     | 1.50 | 8 (12%)  | 76,113,113  | 1.47 | 9 (11%)  |
| 14  | CLA  | a     | 812  | 14   | 65,73,73     | 1.47 | 7 (10%)  | 76,113,113  | 1.36 | 6 (7%)   |
| 14  | CLA  | 2     | 811  | 2    | 65,73,73     | 1.45 | 9 (13%)  | 76,113,113  | 1.51 | 9 (11%)  |
| 14  | CLA  | b     | 837  | 21   | 45,53,73     | 1.82 | 7 (15%)  | 52,89,113   | 1.53 | 5 (9%)   |
| 14  | CLA  | a     | 820  | -    | 65,73,73     | 1.45 | 7 (10%)  | 76,113,113  | 1.58 | 9 (11%)  |
| 17  | BCR  | A     | 849  | -    | 41,41,41     | 1.23 | 2 (4%)   | 56,56,56    | 1.20 | 6 (10%)  |
| 14  | CLA  | j     | 1301 | 21   | 45,53,73     | 1.77 | 7 (15%)  | 52,89,113   | 1.68 | 7 (13%)  |
| 14  | CLA  | B     | 802  | -    | 65,73,73     | 1.43 | 10 (15%) | 76,113,113  | 1.44 | 8 (10%)  |
| 14  | CLA  | 1     | 1634 | -    | 65,73,73     | 1.45 | 10 (15%) | 76,113,113  | 1.39 | 6 (7%)   |
| 14  | CLA  | A     | 827  | 21   | 65,73,73     | 1.46 | 10 (15%) | 76,113,113  | 1.53 | 10 (13%) |
| 14  | CLA  | 1     | 1630 | -    | 65,73,73     | 1.45 | 7 (10%)  | 76,113,113  | 1.47 | 8 (10%)  |
| 14  | CLA  | b     | 804  | -    | 65,73,73     | 1.43 | 11 (16%) | 76,113,113  | 1.51 | 8 (10%)  |
| 14  | CLA  | B     | 826  | -    | 65,73,73     | 1.48 | 8 (12%)  | 76,113,113  | 1.43 | 8 (10%)  |
| 14  | CLA  | A     | 807  | -    | 65,73,73     | 1.44 | 8 (12%)  | 76,113,113  | 1.53 | 6 (7%)   |
| 14  | CLA  | 2     | 832  | -    | 49,57,73     | 1.65 | 7 (14%)  | 55,93,113   | 1.65 | 6 (10%)  |
| 14  | CLA  | a     | 811  | -    | 49,57,73     | 1.70 | 8 (16%)  | 55,93,113   | 1.49 | 8 (14%)  |
| 17  | BCR  | 6     | 204  | -    | 41,41,41     | 1.18 | 2 (4%)   | 56,56,56    | 1.36 | 8 (14%)  |
| 14  | CLA  | 1     | 1601 | -    | 36,44,73     | 1.95 | 7 (19%)  | 40,76,113   | 1.64 | 5 (12%)  |
| 16  | SF4  | a     | 846  | 2,1  | 0,12,12      | -    | -        | -           | -    | -        |
| 18  | LHG  | 1     | 1655 | 14   | 40,40,48     | 0.77 | 1 (2%)   | 43,46,54    | 1.21 | 4 (9%)   |
| 14  | CLA  | a     | 818  | -    | 65,73,73     | 1.46 | 6 (9%)   | 76,113,113  | 1.45 | 7 (9%)   |
| 14  | CLA  | B     | 812  | -    | 45,53,73     | 1.78 | 8 (17%)  | 52,89,113   | 1.62 | 7 (13%)  |
| 14  | CLA  | 2     | 820  | 21   | 65,73,73     | 1.55 | 8 (12%)  | 76,113,113  | 1.35 | 9 (11%)  |
| 17  | BCR  | 2     | 847  | -    | 41,41,41     | 1.16 | 3 (7%)   | 56,56,56    | 1.25 | 7 (12%)  |
| 17  | BCR  | 9     | 104  | -    | 25,25,41     | 1.14 | 1 (4%)   | 33,33,56    | 1.15 | 4 (12%)  |
| 14  | CLA  | A     | 812  | 14   | 65,73,73     | 1.46 | 7 (10%)  | 76,113,113  | 1.35 | 7 (9%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | 2     | 842  | -    | 65,73,73     | 1.48 | 9 (13%)  | 76,113,113  | 1.47 | 7 (9%)   |
| 14  | CLA  | b     | 806  | -    | 65,73,73     | 1.44 | 7 (10%)  | 76,113,113  | 1.57 | 8 (10%)  |
| 14  | CLA  | b     | 814  | -    | 65,73,73     | 1.45 | 8 (12%)  | 76,113,113  | 1.45 | 9 (11%)  |
| 17  | BCR  | K     | 102  | -    | 41,41,41     | 1.18 | 2 (4%)   | 56,56,56    | 1.31 | 7 (12%)  |
| 14  | CLA  | B     | 832  | -    | 65,73,73     | 1.50 | 8 (12%)  | 76,113,113  | 1.44 | 8 (10%)  |
| 14  | CLA  | a     | 837  | 1    | 45,53,73     | 1.79 | 7 (15%)  | 52,89,113   | 1.54 | 8 (15%)  |
| 14  | CLA  | b     | 826  | 21   | 65,73,73     | 1.51 | 9 (13%)  | 76,113,113  | 1.53 | 10 (13%) |
| 17  | BCR  | L     | 207  | -    | 41,41,41     | 1.18 | 3 (7%)   | 56,56,56    | 1.28 | 7 (12%)  |
| 14  | CLA  | 0     | 206  | -    | 65,73,73     | 1.45 | 10 (15%) | 76,113,113  | 1.52 | 9 (11%)  |
| 14  | CLA  | b     | 838  | -    | 60,68,73     | 1.56 | 9 (15%)  | 70,107,113  | 1.47 | 7 (10%)  |
| 14  | CLA  | B     | 831  | -    | 49,57,73     | 1.66 | 7 (14%)  | 55,93,113   | 1.66 | 7 (12%)  |
| 17  | BCR  | 2     | 849  | -    | 41,41,41     | 1.39 | 4 (9%)   | 56,56,56    | 1.29 | 6 (10%)  |
| 14  | CLA  | 2     | 834  | -    | 65,73,73     | 1.47 | 9 (13%)  | 76,113,113  | 1.45 | 7 (9%)   |
| 14  | CLA  | 9     | 101  | -    | 46,54,73     | 1.73 | 7 (15%)  | 53,90,113   | 1.58 | 7 (13%)  |
| 17  | BCR  | A     | 847  | -    | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.31 | 7 (12%)  |
| 14  | CLA  | b     | 829  | -    | 65,73,73     | 1.51 | 8 (12%)  | 76,113,113  | 1.30 | 6 (7%)   |
| 14  | CLA  | b     | 817  | -    | 65,73,73     | 1.45 | 6 (9%)   | 76,113,113  | 1.47 | 8 (10%)  |
| 17  | BCR  | 7     | 101  | -    | 41,41,41     | 1.29 | 4 (9%)   | 56,56,56    | 1.24 | 3 (5%)   |
| 14  | CLA  | A     | 813  | -    | 45,53,73     | 1.78 | 8 (17%)  | 52,89,113   | 1.63 | 8 (15%)  |
| 14  | CLA  | B     | 834  | -    | 65,73,73     | 1.47 | 6 (9%)   | 76,113,113  | 1.45 | 9 (11%)  |
| 17  | BCR  | 2     | 846  | -    | 41,41,41     | 1.26 | 3 (7%)   | 56,56,56    | 1.25 | 6 (10%)  |
| 14  | CLA  | A     | 822  | 21   | 65,73,73     | 1.47 | 7 (10%)  | 76,113,113  | 1.46 | 7 (9%)   |
| 17  | BCR  | k     | 104  | -    | 25,25,41     | 1.14 | 1 (4%)   | 33,33,56    | 1.15 | 4 (12%)  |
| 14  | CLA  | B     | 824  | 2    | 65,73,73     | 1.46 | 7 (10%)  | 76,113,113  | 1.47 | 8 (10%)  |
| 14  | CLA  | 6     | 203  | -    | 50,58,73     | 1.72 | 5 (10%)  | 58,95,113   | 1.52 | 8 (13%)  |
| 18  | LHG  | z     | 101  | -    | 48,48,48     | 0.61 | 1 (2%)   | 51,54,54    | 1.20 | 5 (9%)   |
| 14  | CLA  | B     | 841  | -    | 65,73,73     | 1.48 | 9 (13%)  | 76,113,113  | 1.47 | 7 (9%)   |
| 14  | CLA  | b     | 828  | -    | 65,73,73     | 1.50 | 8 (12%)  | 76,113,113  | 1.43 | 7 (9%)   |
| 14  | CLA  | j     | 1303 | -    | 38,45,73     | 1.92 | 8 (21%)  | 43,78,113   | 1.67 | 7 (16%)  |
| 17  | BCR  | 0     | 203  | -    | 41,41,41     | 1.39 | 4 (9%)   | 56,56,56    | 1.33 | 7 (12%)  |
| 14  | CLA  | a     | 819  | -    | 65,73,73     | 1.49 | 8 (12%)  | 76,113,113  | 1.47 | 10 (13%) |
| 17  | BCR  | 1     | 1650 | -    | 41,41,41     | 1.22 | 2 (4%)   | 56,56,56    | 1.20 | 6 (10%)  |
| 14  | CLA  | a     | 840  | -    | 65,73,73     | 1.49 | 9 (13%)  | 76,113,113  | 1.44 | 8 (10%)  |
| 14  | CLA  | A     | 855  | 21   | 65,73,73     | 1.43 | 7 (10%)  | 76,113,113  | 1.61 | 8 (10%)  |
| 14  | CLA  | a     | 844  | 18   | 45,53,73     | 1.73 | 7 (15%)  | 52,89,113   | 1.70 | 7 (13%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 17  | BCR  | B     | 847 | -    | 41,41,41     | 1.27 | 3 (7%)   | 56,56,56    | 1.31 | 9 (16%)  |

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   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 17  | BCR  | a     | 848  | -    | -         | 15/29/63/63   | 0/2/2/2 |
| 14  | CLA  | a     | 842  | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 14  | CLA  | A     | 833  | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 14  | CLA  | 1     | 1615 | -    | 1/1/15/20 | 15/37/115/115 | -       |
| 14  | CLA  | 1     | 1625 | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 14  | CLA  | l     | 206  | 21   | 1/1/15/20 | 11/37/115/115 | -       |
| 14  | CLA  | 2     | 826  | 21   | 1/1/15/20 | 11/37/115/115 | -       |
| 14  | CLA  | 6     | 201  | 21   | 1/1/13/20 | 6/29/107/115  | -       |
| 14  | CLA  | 2     | 835  | -    | 1/1/15/20 | 9/37/115/115  | -       |
| 14  | CLA  | A     | 835  | -    | 1/1/15/20 | 8/37/115/115  | -       |
| 17  | BCR  | 1     | 1653 | -    | -         | 11/18/35/63   | 0/1/1/2 |
| 14  | CLA  | 2     | 837  | 21   | 1/1/11/20 | 3/13/91/115   | -       |
| 17  | BCR  | J     | 103  | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 14  | CLA  | a     | 816  | -    | 1/1/15/20 | 19/37/115/115 | -       |
| 14  | CLA  | b     | 802  | 21   | 1/1/15/20 | 18/37/115/115 | -       |
| 14  | CLA  | k     | 101  | -    | 1/1/11/20 | 10/15/93/115  | -       |
| 14  | CLA  | 1     | 1606 | 14   | 1/1/13/20 | 10/30/108/115 | -       |
| 14  | CLA  | 1     | 1641 | -    | 1/1/15/20 | 17/37/115/115 | -       |
| 15  | PQN  | A     | 845  | -    | -         | 1/23/43/43    | 0/2/2/2 |
| 14  | CLA  | 2     | 825  | 2    | 1/1/15/20 | 14/37/115/115 | -       |
| 14  | CLA  | 1     | 1629 | -    | 1/1/15/20 | 7/37/115/115  | -       |
| 14  | CLA  | l     | 205  | -    | 1/1/15/20 | 11/37/115/115 | -       |
| 17  | BCR  | L     | 206  | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 17  | BCR  | j     | 1305 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 14  | CLA  | a     | 804  | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 14  | CLA  | 2     | 823  | 21   | 1/1/13/20 | 5/25/103/115  | -       |
| 15  | PQN  | 1     | 1646 | -    | -         | 1/23/43/43    | 0/2/2/2 |
| 14  | CLA  | a     | 817  | 21   | 1/1/15/20 | 12/37/115/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | 1     | 1603 | -    | 1/1/15/20 | 15/37/115/115 | -       |
| 15  | PQN  | 2     | 843  | -    | -         | 1/23/43/43    | 0/2/2/2 |
| 14  | CLA  | 1     | 1627 | 21   | 1/1/15/20 | 13/37/115/115 | -       |
| 14  | CLA  | a     | 843  | 21   | 1/1/15/20 | 16/37/115/115 | -       |
| 17  | BCR  | A     | 850  | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 17  | BCR  | k     | 102  | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 14  | CLA  | 0     | 205  | 10   | 1/1/15/20 | 17/37/115/115 | -       |
| 13  | CL0  | A     | 801  | -    | 3/3/20/25 | 10/37/135/135 | -       |
| 14  | CLA  | f     | 203  | -    | 1/1/12/20 | 6/19/97/115   | -       |
| 17  | BCR  | 6     | 202  | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 18  | LHG  | B     | 850  | -    | -         | 18/53/53/53   | -       |
| 14  | CLA  | F     | 204  | -    | 1/1/12/20 | 6/19/97/115   | -       |
| 16  | SF4  | A     | 846  | 2,1  | -         | -             | 0/6/5/5 |
| 17  | BCR  | a     | 851  | -    | -         | 18/29/63/63   | 0/2/2/2 |
| 15  | PQN  | B     | 842  | -    | -         | 1/23/43/43    | 0/2/2/2 |
| 14  | CLA  | b     | 839  | -    | 1/1/15/20 | 9/37/115/115  | -       |
| 14  | CLA  | B     | 818  | -    | 1/1/15/20 | 17/37/115/115 | -       |
| 14  | CLA  | a     | 813  | -    | 1/1/11/20 | 4/13/91/115   | -       |
| 18  | LHG  | y     | 101  | -    | -         | 27/53/53/53   | -       |
| 18  | LHG  | a     | 853  | -    | -         | 21/53/53/53   | -       |
| 14  | CLA  | b     | 808  | -    | 1/1/15/20 | 6/37/115/115  | -       |
| 14  | CLA  | L     | 205  | 21   | 1/1/15/20 | 11/37/115/115 | -       |
| 14  | CLA  | A     | 843  | 21   | 1/1/15/20 | 16/37/115/115 | -       |
| 14  | CLA  | b     | 825  | 2    | 1/1/15/20 | 14/37/115/115 | -       |
| 14  | CLA  | 2     | 831  | -    | 1/1/13/20 | 13/25/103/115 | -       |
| 14  | CLA  | a     | 810  | 1    | 1/1/15/20 | 12/37/115/115 | -       |
| 14  | CLA  | 1     | 1621 | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 17  | BCR  | K     | 104  | -    | -         | 4/18/35/63    | 0/1/1/2 |
| 14  | CLA  | 2     | 817  | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 14  | CLA  | B     | 813  | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 14  | CLA  | b     | 818  | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 14  | CLA  | A     | 820  | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 14  | CLA  | a     | 829  | -    | 1/1/15/20 | 14/37/115/115 | -       |
| 20  | LMG  | B     | 849  | -    | -         | 27/50/70/70   | 0/1/1/1 |
| 17  | BCR  | B     | 845  | -    | -         | 11/29/63/63   | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | A     | 857  | -    | 1/1/7/20  | 0/2/72/115    | -       |
| 14  | CLA  | b     | 832  | -    | 1/1/11/20 | 10/18/96/115  | -       |
| 14  | CLA  | 1     | 1623 | 21   | 1/1/15/20 | 12/37/115/115 | -       |
| 14  | CLA  | 1     | 1607 | -    | 1/1/15/20 | 21/37/115/115 | -       |
| 14  | CLA  | 8     | 1302 | -    | 1/1/11/20 | 5/13/91/115   | -       |
| 14  | CLA  | a     | 835  | -    | 1/1/15/20 | 8/37/115/115  | -       |
| 17  | BCR  | 1     | 1652 | -    | -         | 18/29/63/63   | 0/2/2/2 |
| 14  | CLA  | a     | 806  | -    | 1/1/15/20 | 21/37/115/115 | -       |
| 14  | CLA  | 2     | 805  | -    | 1/1/15/20 | 17/37/115/115 | -       |
| 14  | CLA  | b     | 815  | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 17  | BCR  | I     | 101  | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 17  | BCR  | b     | 845  | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 14  | CLA  | B     | 823  | -    | 1/1/11/20 | 5/13/91/115   | -       |
| 14  | CLA  | a     | 838  | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 14  | CLA  | 1     | 1644 | 21   | 1/1/15/20 | 16/37/115/115 | -       |
| 14  | CLA  | 2     | 814  | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 14  | CLA  | a     | 805  | 14   | 1/1/13/20 | 10/30/108/115 | -       |
| 18  | LHG  | m     | 101  | -    | -         | 27/53/53/53   | -       |
| 14  | CLA  | j     | 1302 | -    | 1/1/11/20 | 5/13/91/115   | -       |
| 14  | CLA  | 1     | 1640 | -    | 1/1/15/20 | 20/37/115/115 | -       |
| 18  | LHG  | b     | 851  | -    | -         | 18/53/53/53   | -       |
| 14  | CLA  | B     | 820  | -    | 1/1/15/20 | 19/37/115/115 | -       |
| 14  | CLA  | 2     | 830  | -    | 1/1/15/20 | 7/37/115/115  | -       |
| 14  | CLA  | b     | 823  | 21   | 1/1/13/20 | 5/25/103/115  | -       |
| 14  | CLA  | b     | 834  | -    | 1/1/15/20 | 11/37/115/115 | -       |
| 17  | BCR  | f     | 202  | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 14  | CLA  | 1     | 1645 | 18   | 1/1/11/20 | 5/13/91/115   | -       |
| 14  | CLA  | a     | 814  | -    | 1/1/15/20 | 15/37/115/115 | -       |
| 14  | CLA  | 1     | 1636 | -    | 1/1/15/20 | 8/37/115/115  | -       |
| 16  | SF4  | 3     | 101  | 3    | -         | -             | 0/6/5/5 |
| 14  | CLA  | a     | 832  | -    | 1/1/14/20 | 6/31/109/115  | -       |
| 14  | CLA  | A     | 806  | -    | 1/1/15/20 | 21/37/115/115 | -       |
| 14  | CLA  | A     | 838  | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 14  | CLA  | 2     | 810  | 2    | 1/1/15/20 | 11/37/115/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | A     | 805  | 14   | 1/1/13/20 | 10/30/108/115 | -       |
| 14  | CLA  | b     | 841  | 21   | 1/1/15/20 | 7/37/115/115  | -       |
| 18  | LHG  | l     | 201  | -    | -         | 27/43/43/53   | -       |
| 14  | CLA  | 1     | 1624 | -    | 1/1/11/20 | 8/13/91/115   | -       |
| 17  | BCR  | 2     | 844  | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 20  | LMG  | b     | 850  | -    | -         | 27/50/70/70   | 0/1/1/1 |
| 14  | CLA  | B     | 815  | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 14  | CLA  | B     | 811  | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 14  | CLA  | b     | 833  | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 14  | CLA  | A     | 811  | -    | 1/1/11/20 | 8/18/96/115   | -       |
| 14  | CLA  | b     | 836  | 21   | 1/1/12/20 | 9/19/97/115   | -       |
| 14  | CLA  | 1     | 1617 | -    | 1/1/15/20 | 19/37/115/115 | -       |
| 14  | CLA  | 2     | 839  | -    | 1/1/15/20 | 9/37/115/115  | -       |
| 14  | CLA  | b     | 821  | -    | 1/1/15/20 | 19/37/115/115 | -       |
| 14  | CLA  | B     | 803  | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 14  | CLA  | 1     | 1633 | -    | 1/1/14/20 | 6/31/109/115  | -       |
| 14  | CLA  | L     | 203  | 10   | 1/1/15/20 | 17/37/115/115 | -       |
| 14  | CLA  | a     | 809  | 1    | 1/1/15/20 | 11/37/115/115 | -       |
| 14  | CLA  | 1     | 1604 | 21   | 1/1/15/20 | 6/37/115/115  | -       |
| 14  | CLA  | 2     | 819  | -    | 1/1/15/20 | 17/37/115/115 | -       |
| 13  | CL0  | 1     | 1602 | -    | 3/3/20/25 | 10/37/135/135 | -       |
| 17  | BCR  | 0     | 209  | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 14  | CLA  | b     | 807  | -    | 1/1/15/20 | 9/37/115/115  | -       |
| 14  | CLA  | a     | 830  | -    | 1/1/15/20 | 15/37/115/115 | -       |
| 14  | CLA  | a     | 841  | -    | 1/1/15/20 | 14/37/115/115 | -       |
| 14  | CLA  | 2     | 840  | -    | -         | 2/16/94/115   | -       |
| 14  | CLA  | 2     | 804  | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 14  | CLA  | a     | 828  | -    | 1/1/15/20 | 7/37/115/115  | -       |
| 16  | SF4  | C     | 102  | 3    | -         | -             | 0/6/5/5 |
| 14  | CLA  | 1     | 1642 | -    | 1/1/15/20 | 14/37/115/115 | -       |
| 14  | CLA  | 1     | 1626 | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 17  | BCR  | F     | 205  | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 17  | BCR  | l     | 207  | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 14  | CLA  | b     | 810  | 2    | 1/1/15/20 | 11/37/115/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | 1     | 1635 | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 17  | BCR  | 2     | 848  | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 17  | BCR  | 1     | 1651 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 14  | CLA  | 2     | 841  | 21   | 1/1/15/20 | 7/37/115/115  | -       |
| 14  | CLA  | X     | 1701 | 12   | 1/1/11/20 | 7/13/91/115   | -       |
| 14  | CLA  | b     | 824  | -    | 1/1/11/20 | 5/13/91/115   | -       |
| 17  | BCR  | b     | 847  | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 14  | CLA  | 1     | 1638 | 1    | 1/1/11/20 | 5/13/91/115   | -       |
| 17  | BCR  | A     | 852  | -    | -         | 11/18/35/63   | 0/1/1/2 |
| 14  | CLA  | A     | 842  | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 14  | CLA  | 2     | 836  | 21   | 1/1/12/20 | 9/19/97/115   | -       |
| 18  | LHG  | A     | 854  | 14   | -         | 13/45/45/53   | -       |
| 17  | BCR  | B     | 844  | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 14  | CLA  | 2     | 821  | -    | 1/1/15/20 | 19/37/115/115 | -       |
| 17  | BCR  | A     | 848  | -    | -         | 15/29/63/63   | 0/2/2/2 |
| 18  | LHG  | 0     | 202  | -    | -         | 27/43/43/53   | -       |
| 17  | BCR  | b     | 849  | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 16  | SF4  | 3     | 102  | 3    | -         | -             | 0/6/5/5 |
| 14  | CLA  | b     | 820  | 21   | 1/1/15/20 | 15/37/115/115 | -       |
| 17  | BCR  | a     | 849  | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 14  | CLA  | B     | 835  | 21   | 1/1/12/20 | 9/19/97/115   | -       |
| 14  | CLA  | a     | 808  | -    | 1/1/12/20 | 4/21/99/115   | -       |
| 14  | CLA  | a     | 825  | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 14  | CLA  | B     | 819  | 21   | 1/1/15/20 | 15/37/115/115 | -       |
| 14  | CLA  | A     | 819  | -    | 1/1/15/20 | 17/37/115/115 | -       |
| 14  | CLA  | a     | 823  | -    | 1/1/11/20 | 8/13/91/115   | -       |
| 14  | CLA  | 8     | 1301 | 21   | 1/1/11/20 | 2/13/91/115   | -       |
| 14  | CLA  | A     | 837  | 1    | 1/1/11/20 | 5/13/91/115   | -       |
| 14  | CLA  | b     | 831  | -    | 1/1/13/20 | 13/25/103/115 | -       |
| 14  | CLA  | 2     | 812  | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 14  | CLA  | B     | 808  | -    | 1/1/15/20 | 8/37/115/115  | -       |
| 14  | CLA  | B     | 804  | -    | 1/1/15/20 | 17/37/115/115 | -       |
| 14  | CLA  | b     | 827  | -    | 1/1/15/20 | 6/37/115/115  | -       |
| 14  | CLA  | M     | 102  | -    | 1/1/7/20  | 0/2/72/115    | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | A     | 804  | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 14  | CLA  | a     | 802  | -    | 1/1/15/20 | 15/37/115/115 | -       |
| 15  | PQN  | b     | 843  | -    | -         | 1/23/43/43    | 0/2/2/2 |
| 14  | CLA  | 1     | 1639 | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 14  | CLA  | A     | 831  | -    | 1/1/15/20 | 7/37/115/115  | -       |
| 17  | BCR  | 8     | 1306 | -    | -         | 15/29/63/63   | 0/2/2/2 |
| 17  | BCR  | l     | 202  | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 17  | BCR  | m     | 102  | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 14  | CLA  | A     | 818  | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 14  | CLA  | 1     | 1628 | 21   | 1/1/15/20 | 9/37/115/115  | -       |
| 14  | CLA  | F     | 201  | 21   | 1/1/13/20 | 6/29/107/115  | -       |
| 14  | CLA  | a     | 821  | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 14  | CLA  | A     | 826  | 21   | 1/1/15/20 | 13/37/115/115 | -       |
| 14  | CLA  | 2     | 838  | -    | 1/1/14/20 | 5/31/109/115  | -       |
| 14  | CLA  | B     | 836  | 21   | 1/1/11/20 | 3/13/91/115   | -       |
| 14  | CLA  | a     | 827  | 21   | 1/1/15/20 | 9/37/115/115  | -       |
| 14  | CLA  | 2     | 803  | -    | 1/1/15/20 | 18/37/115/115 | -       |
| 14  | CLA  | A     | 810  | 1    | 1/1/15/20 | 12/37/115/115 | -       |
| 14  | CLA  | a     | 826  | 21   | 1/1/15/20 | 13/37/115/115 | -       |
| 14  | CLA  | x     | 1701 | 12   | 1/1/11/20 | 7/13/91/115   | -       |
| 17  | BCR  | 0     | 201  | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 14  | CLA  | 2     | 824  | -    | 1/1/11/20 | 5/13/91/115   | -       |
| 17  | BCR  | 1     | 1649 | -    | -         | 15/29/63/63   | 0/2/2/2 |
| 17  | BCR  | 0     | 208  | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 14  | CLA  | 1     | 1605 | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 14  | CLA  | B     | 827  | -    | 1/1/15/20 | 15/37/115/115 | -       |
| 14  | CLA  | A     | 809  | 1    | 1/1/15/20 | 11/37/115/115 | -       |
| 14  | CLA  | B     | 829  | -    | 1/1/15/20 | 7/37/115/115  | -       |
| 17  | BCR  | a     | 850  | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 14  | CLA  | A     | 825  | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 14  | CLA  | A     | 829  | -    | 1/1/15/20 | 14/37/115/115 | -       |
| 14  | CLA  | 9     | 103  | 21   | 1/1/13/20 | 9/29/107/115  | -       |
| 14  | CLA  | b     | 803  | -    | 1/1/15/20 | 18/37/115/115 | -       |
| 14  | CLA  | 2     | 833  | -    | 1/1/15/20 | 16/37/115/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | 2     | 827  | -    | 1/1/15/20 | 6/37/115/115  | -       |
| 14  | CLA  | a     | 834  | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 17  | BCR  | a     | 852  | -    | -         | 11/18/35/63   | 0/1/1/2 |
| 18  | LHG  | M     | 101  | -    | -         | 27/53/53/53   | -       |
| 14  | CLA  | b     | 822  | -    | 1/1/11/20 | 5/13/91/115   | -       |
| 14  | CLA  | 2     | 818  | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 14  | CLA  | B     | 839  | -    | -         | 2/16/94/115   | -       |
| 17  | BCR  | A     | 856  | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 14  | CLA  | a     | 836  | -    | 1/1/15/20 | 6/37/115/115  | -       |
| 17  | BCR  | b     | 844  | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 16  | SF4  | c     | 102  | 3    | -         | -             | 0/6/5/5 |
| 17  | BCR  | B     | 843  | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 16  | SF4  | c     | 101  | 3    | -         | -             | 0/6/5/5 |
| 14  | CLA  | 2     | 822  | -    | 1/1/11/20 | 5/13/91/115   | -       |
| 14  | CLA  | K     | 103  | 21   | 1/1/13/20 | 9/29/107/115  | -       |
| 14  | CLA  | B     | 810  | 2    | 1/1/15/20 | 15/37/115/115 | -       |
| 17  | BCR  | F     | 202  | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 16  | SF4  | C     | 101  | 3    | -         | -             | 0/6/5/5 |
| 14  | CLA  | b     | 811  | 2    | 1/1/15/20 | 15/37/115/115 | -       |
| 14  | CLA  | A     | 828  | -    | 1/1/15/20 | 7/37/115/115  | -       |
| 14  | CLA  | a     | 815  | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 14  | CLA  | A     | 844  | 18   | 1/1/11/20 | 5/13/91/115   | -       |
| 14  | CLA  | b     | 835  | -    | 1/1/15/20 | 9/37/115/115  | -       |
| 14  | CLA  | B     | 816  | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 14  | CLA  | 2     | 809  | -    | 1/1/15/20 | 8/37/115/115  | -       |
| 14  | CLA  | a     | 803  | 21   | 1/1/15/20 | 6/37/115/115  | -       |
| 14  | CLA  | 2     | 807  | -    | 1/1/15/20 | 9/37/115/115  | -       |
| 14  | CLA  | B     | 837  | -    | 1/1/14/20 | 4/31/109/115  | -       |
| 14  | CLA  | 1     | 1632 | -    | 1/1/15/20 | 7/37/115/115  | -       |
| 14  | CLA  | a     | 822  | 21   | 1/1/15/20 | 12/37/115/115 | -       |
| 14  | CLA  | z     | 102  | 12   | 1/1/11/20 | 7/13/91/115   | -       |
| 14  | CLA  | 1     | 1611 | 1    | 1/1/15/20 | 12/37/115/115 | -       |
| 14  | CLA  | b     | 805  | -    | 1/1/15/20 | 17/37/115/115 | -       |
| 14  | CLA  | B     | 838  | -    | 1/1/15/20 | 9/37/115/115  | -       |
| 14  | CLA  | A     | 814  | -    | 1/1/15/20 | 15/37/115/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | f     | 201  | 21   | 1/1/13/20 | 6/29/107/115  | -       |
| 14  | CLA  | 1     | 1643 | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 17  | BCR  | M     | 103  | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 14  | CLA  | B     | 805  | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 14  | CLA  | a     | 807  | -    | 1/1/15/20 | 15/37/115/115 | -       |
| 14  | CLA  | B     | 822  | 21   | 1/1/13/20 | 5/25/103/115  | -       |
| 17  | BCR  | a     | 847  | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 14  | CLA  | a     | 833  | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 14  | CLA  | B     | 807  | -    | 1/1/15/20 | 6/37/115/115  | -       |
| 14  | CLA  | 2     | 808  | -    | 1/1/15/20 | 6/37/115/115  | -       |
| 14  | CLA  | B     | 814  | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 14  | CLA  | B     | 809  | 2    | 1/1/15/20 | 11/37/115/115 | -       |
| 14  | CLA  | B     | 833  | -    | 1/1/15/20 | 11/37/115/115 | -       |
| 17  | BCR  | B     | 851  | -    | -         | 15/29/63/63   | 0/2/2/2 |
| 17  | BCR  | f     | 204  | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 14  | CLA  | B     | 830  | -    | 1/1/13/20 | 13/25/103/115 | -       |
| 16  | SF4  | 1     | 1647 | 2,1  | -         | -             | 0/6/5/5 |
| 14  | CLA  | b     | 819  | -    | 1/1/15/20 | 17/37/115/115 | -       |
| 14  | CLA  | b     | 809  | -    | 1/1/15/20 | 8/37/115/115  | -       |
| 14  | CLA  | B     | 806  | -    | 1/1/15/20 | 9/37/115/115  | -       |
| 17  | BCR  | 1     | 1648 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 14  | CLA  | 8     | 1303 | -    | 1/1/8/20  | 0/2/76/115    | -       |
| 14  | CLA  | A     | 830  | -    | 1/1/15/20 | 15/37/115/115 | -       |
| 14  | CLA  | 1     | 1613 | 14   | 1/1/15/20 | 13/37/115/115 | -       |
| 14  | CLA  | 2     | 815  | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 14  | CLA  | A     | 839  | -    | 1/1/15/20 | 20/37/115/115 | -       |
| 14  | CLA  | 1     | 1612 | -    | 1/1/11/20 | 8/18/96/115   | -       |
| 14  | CLA  | A     | 821  | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 14  | CLA  | A     | 840  | -    | 1/1/15/20 | 17/37/115/115 | -       |
| 14  | CLA  | 1     | 1622 | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 14  | CLA  | F     | 203  | 21   | 1/1/11/20 | 2/13/91/115   | -       |
| 14  | CLA  | b     | 830  | -    | 1/1/15/20 | 7/37/115/115  | -       |
| 14  | CLA  | A     | 808  | -    | 1/1/12/20 | 4/21/99/115   | -       |
| 14  | CLA  | 0     | 207  | 21   | 1/1/15/20 | 11/37/115/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 17  | BCR  | 9     | 102  | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 13  | CL0  | a     | 801  | -    | 3/3/20/25 | 10/37/135/135 | -       |
| 14  | CLA  | B     | 828  | -    | 1/1/15/20 | 11/37/115/115 | -       |
| 14  | CLA  | 1     | 1610 | 1    | 1/1/15/20 | 11/37/115/115 | -       |
| 17  | BCR  | 2     | 845  | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 14  | CLA  | a     | 824  | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 14  | CLA  | 2     | 816  | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 14  | CLA  | A     | 816  | -    | 1/1/15/20 | 19/37/115/115 | -       |
| 17  | BCR  | j     | 1304 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 14  | CLA  | 2     | 802  | 21   | 1/1/15/20 | 18/37/115/115 | -       |
| 17  | BCR  | L     | 201  | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 14  | CLA  | A     | 832  | -    | 1/1/14/20 | 6/31/109/115  | -       |
| 15  | PQN  | a     | 845  | -    | -         | 1/23/43/43    | 0/2/2/2 |
| 17  | BCR  | B     | 846  | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 14  | CLA  | A     | 803  | 21   | 1/1/15/20 | 6/37/115/115  | -       |
| 17  | BCR  | A     | 851  | -    | -         | 18/29/63/63   | 0/2/2/2 |
| 14  | CLA  | b     | 813  | -    | 1/1/11/20 | 0/13/91/115   | -       |
| 17  | BCR  | 8     | 1305 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 14  | CLA  | k     | 103  | 21   | 1/1/13/20 | 9/29/107/115  | -       |
| 14  | CLA  | 2     | 806  | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 14  | CLA  | L     | 204  | -    | 1/1/15/20 | 11/37/115/115 | -       |
| 14  | CLA  | 1     | 1637 | -    | 1/1/15/20 | 6/37/115/115  | -       |
| 17  | BCR  | 8     | 1304 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 14  | CLA  | 2     | 813  | -    | 1/1/11/20 | 0/13/91/115   | -       |
| 14  | CLA  | B     | 840  | 21   | 1/1/15/20 | 7/37/115/115  | -       |
| 17  | BCR  | B     | 848  | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 14  | CLA  | J     | 102  | -    | 1/1/8/20  | 0/2/76/115    | -       |
| 14  | CLA  | B     | 817  | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 14  | CLA  | 1     | 1608 | -    | 1/1/15/20 | 15/37/115/115 | -       |
| 17  | BCR  | i     | 101  | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 17  | BCR  | b     | 846  | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 14  | CLA  | A     | 817  | 21   | 1/1/15/20 | 12/37/115/115 | -       |
| 14  | CLA  | 1     | 1614 | -    | 1/1/11/20 | 4/13/91/115   | -       |
| 14  | CLA  | 1     | 1619 | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 14  | CLA  | b     | 812  | -    | 1/1/15/20 | 10/37/115/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | b     | 840  | -    | -         | 2/16/94/115   | -       |
| 14  | CLA  | A     | 834  | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 14  | CLA  | A     | 802  | -    | 1/1/15/20 | 15/37/115/115 | -       |
| 18  | LHG  | a     | 854  | 14   | -         | 13/45/45/53   | -       |
| 17  | BCR  | b     | 852  | -    | -         | 15/29/63/63   | 0/2/2/2 |
| 14  | CLA  | K     | 101  | -    | 1/1/11/20 | 10/15/93/115  | -       |
| 17  | BCR  | b     | 848  | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 14  | CLA  | a     | 839  | -    | 1/1/15/20 | 20/37/115/115 | -       |
| 14  | CLA  | b     | 842  | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 14  | CLA  | 2     | 829  | -    | 1/1/15/20 | 11/37/115/115 | -       |
| 14  | CLA  | 1     | 1609 | -    | 1/1/12/20 | 4/21/99/115   | -       |
| 14  | CLA  | 1     | 1618 | 21   | 1/1/15/20 | 12/37/115/115 | -       |
| 14  | CLA  | A     | 823  | -    | 1/1/11/20 | 8/13/91/115   | -       |
| 14  | CLA  | 1     | 1616 | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 14  | CLA  | A     | 841  | -    | 1/1/15/20 | 14/37/115/115 | -       |
| 14  | CLA  | a     | 831  | -    | 1/1/15/20 | 7/37/115/115  | -       |
| 14  | CLA  | b     | 816  | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 14  | CLA  | l     | 204  | 10   | 1/1/15/20 | 17/37/115/115 | -       |
| 20  | LMG  | 2     | 850  | -    | -         | 27/50/70/70   | 0/1/1/1 |
| 14  | CLA  | A     | 824  | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 14  | CLA  | A     | 815  | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 14  | CLA  | B     | 825  | 21   | 1/1/15/20 | 11/37/115/115 | -       |
| 17  | BCR  | y     | 102  | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 18  | LHG  | A     | 853  | -    | -         | 21/53/53/53   | -       |
| 14  | CLA  | 2     | 828  | -    | 1/1/15/20 | 15/37/115/115 | -       |
| 14  | CLA  | 1     | 1631 | -    | 1/1/15/20 | 15/37/115/115 | -       |
| 18  | LHG  | 1     | 1654 | -    | -         | 21/53/53/53   | -       |
| 14  | CLA  | A     | 836  | -    | 1/1/15/20 | 6/37/115/115  | -       |
| 18  | LHG  | L     | 208  | -    | -         | 27/43/43/53   | -       |
| 14  | CLA  | J     | 101  | -    | 1/1/11/20 | 5/13/91/115   | -       |
| 14  | CLA  | B     | 821  | -    | 1/1/11/20 | 5/13/91/115   | -       |
| 14  | CLA  | 1     | 1620 | -    | 1/1/15/20 | 17/37/115/115 | -       |
| 14  | CLA  | a     | 812  | 14   | 1/1/15/20 | 13/37/115/115 | -       |
| 14  | CLA  | 2     | 811  | 2    | 1/1/15/20 | 15/37/115/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | b     | 837  | 21   | 1/1/11/20 | 3/13/91/115   | -       |
| 14  | CLA  | a     | 820  | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 17  | BCR  | A     | 849  | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 14  | CLA  | j     | 1301 | 21   | 1/1/11/20 | 2/13/91/115   | -       |
| 14  | CLA  | B     | 802  | -    | 1/1/15/20 | 18/37/115/115 | -       |
| 14  | CLA  | 1     | 1634 | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 14  | CLA  | A     | 827  | 21   | 1/1/15/20 | 9/37/115/115  | -       |
| 14  | CLA  | 1     | 1630 | -    | 1/1/15/20 | 14/37/115/115 | -       |
| 14  | CLA  | b     | 804  | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 14  | CLA  | B     | 826  | -    | 1/1/15/20 | 6/37/115/115  | -       |
| 14  | CLA  | A     | 807  | -    | 1/1/15/20 | 15/37/115/115 | -       |
| 14  | CLA  | 2     | 832  | -    | 1/1/11/20 | 10/18/96/115  | -       |
| 14  | CLA  | a     | 811  | -    | 1/1/11/20 | 8/18/96/115   | -       |
| 17  | BCR  | 6     | 204  | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 14  | CLA  | 1     | 1601 | -    | 1/1/7/20  | 0/2/72/115    | -       |
| 16  | SF4  | a     | 846  | 2,1  | -         | -             | 0/6/5/5 |
| 18  | LHG  | 1     | 1655 | 14   | -         | 13/45/45/53   | -       |
| 14  | CLA  | a     | 818  | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 14  | CLA  | B     | 812  | -    | 1/1/11/20 | 0/13/91/115   | -       |
| 14  | CLA  | 2     | 820  | 21   | 1/1/15/20 | 15/37/115/115 | -       |
| 17  | BCR  | 2     | 847  | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 17  | BCR  | 9     | 104  | -    | -         | 4/18/35/63    | 0/1/1/2 |
| 14  | CLA  | A     | 812  | 14   | 1/1/15/20 | 13/37/115/115 | -       |
| 14  | CLA  | 2     | 842  | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 14  | CLA  | b     | 806  | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 14  | CLA  | b     | 814  | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 17  | BCR  | K     | 102  | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 14  | CLA  | B     | 832  | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 14  | CLA  | a     | 837  | 1    | 1/1/11/20 | 5/13/91/115   | -       |
| 14  | CLA  | b     | 826  | 21   | 1/1/15/20 | 11/37/115/115 | -       |
| 17  | BCR  | L     | 207  | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 14  | CLA  | 0     | 206  | -    | 1/1/15/20 | 11/37/115/115 | -       |
| 14  | CLA  | b     | 838  | -    | 1/1/14/20 | 5/31/109/115  | -       |
| 14  | CLA  | B     | 831  | -    | 1/1/11/20 | 10/18/96/115  | -       |
| 17  | BCR  | 2     | 849  | -    | -         | 5/29/63/63    | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | 2     | 834  | -    | 1/1/15/20 | 11/37/115/115 | -       |
| 14  | CLA  | 9     | 101  | -    | 1/1/11/20 | 10/15/93/115  | -       |
| 17  | BCR  | A     | 847  | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 14  | CLA  | b     | 829  | -    | 1/1/15/20 | 11/37/115/115 | -       |
| 14  | CLA  | b     | 817  | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 17  | BCR  | 7     | 101  | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 14  | CLA  | A     | 813  | -    | 1/1/11/20 | 4/13/91/115   | -       |
| 14  | CLA  | B     | 834  | -    | 1/1/15/20 | 9/37/115/115  | -       |
| 17  | BCR  | 2     | 846  | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 14  | CLA  | A     | 822  | 21   | 1/1/15/20 | 12/37/115/115 | -       |
| 17  | BCR  | k     | 104  | -    | -         | 4/18/35/63    | 0/1/1/2 |
| 14  | CLA  | B     | 824  | 2    | 1/1/15/20 | 14/37/115/115 | -       |
| 14  | CLA  | 6     | 203  | -    | 1/1/12/20 | 6/19/97/115   | -       |
| 18  | LHG  | z     | 101  | -    | -         | 18/53/53/53   | -       |
| 14  | CLA  | B     | 841  | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 14  | CLA  | b     | 828  | -    | 1/1/15/20 | 15/37/115/115 | -       |
| 14  | CLA  | j     | 1303 | -    | 1/1/8/20  | 0/2/76/115    | -       |
| 17  | BCR  | 0     | 203  | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 14  | CLA  | a     | 819  | -    | 1/1/15/20 | 17/37/115/115 | -       |
| 17  | BCR  | 1     | 1650 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 14  | CLA  | a     | 840  | -    | 1/1/15/20 | 17/37/115/115 | -       |
| 14  | CLA  | A     | 855  | 21   | 1/1/15/20 | 18/37/115/115 | -       |
| 14  | CLA  | a     | 844  | 18   | 1/1/11/20 | 5/13/91/115   | -       |
| 17  | BCR  | B     | 847  | -    | -         | 11/29/63/63   | 0/2/2/2 |

All (2563) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14  | f     | 203  | CLA  | C4B-NB | 7.82 | 1.42        | 1.35     |
| 14  | A     | 824  | CLA  | C4B-NB | 7.79 | 1.42        | 1.35     |
| 14  | F     | 204  | CLA  | C4B-NB | 7.74 | 1.42        | 1.35     |
| 14  | 1     | 1625 | CLA  | C4B-NB | 7.74 | 1.42        | 1.35     |
| 14  | 6     | 203  | CLA  | C4B-NB | 7.72 | 1.42        | 1.35     |
| 14  | a     | 824  | CLA  | C4B-NB | 7.71 | 1.42        | 1.35     |
| 14  | M     | 102  | CLA  | C4B-NB | 7.69 | 1.42        | 1.35     |
| 14  | b     | 820  | CLA  | C4B-NB | 7.69 | 1.42        | 1.35     |
| 14  | B     | 836  | CLA  | C4B-NB | 7.69 | 1.42        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14  | A     | 857  | CLA  | C4B-NB | 7.69 | 1.42        | 1.35     |
| 14  | z     | 102  | CLA  | C4B-NB | 7.67 | 1.42        | 1.35     |
| 14  | B     | 819  | CLA  | C4B-NB | 7.67 | 1.42        | 1.35     |
| 14  | b     | 837  | CLA  | C4B-NB | 7.66 | 1.42        | 1.35     |
| 14  | 2     | 820  | CLA  | C4B-NB | 7.64 | 1.42        | 1.35     |
| 14  | X     | 1701 | CLA  | C4B-NB | 7.64 | 1.42        | 1.35     |
| 14  | 2     | 837  | CLA  | C4B-NB | 7.64 | 1.42        | 1.35     |
| 14  | 1     | 1601 | CLA  | C4B-NB | 7.63 | 1.42        | 1.35     |
| 14  | b     | 821  | CLA  | C4B-NB | 7.57 | 1.42        | 1.35     |
| 14  | 2     | 840  | CLA  | C4B-NB | 7.56 | 1.41        | 1.35     |
| 14  | B     | 839  | CLA  | C4B-NB | 7.53 | 1.41        | 1.35     |
| 14  | b     | 840  | CLA  | C4B-NB | 7.53 | 1.41        | 1.35     |
| 14  | x     | 1701 | CLA  | C4B-NB | 7.51 | 1.41        | 1.35     |
| 14  | 2     | 828  | CLA  | C4B-NB | 7.51 | 1.41        | 1.35     |
| 14  | B     | 820  | CLA  | C4B-NB | 7.51 | 1.41        | 1.35     |
| 14  | B     | 827  | CLA  | C4B-NB | 7.46 | 1.41        | 1.35     |
| 14  | b     | 813  | CLA  | C4B-NB | 7.45 | 1.41        | 1.35     |
| 14  | 2     | 821  | CLA  | C4B-NB | 7.45 | 1.41        | 1.35     |
| 14  | b     | 833  | CLA  | C4B-NB | 7.44 | 1.41        | 1.35     |
| 14  | B     | 817  | CLA  | C4B-NB | 7.44 | 1.41        | 1.35     |
| 14  | 2     | 813  | CLA  | C4B-NB | 7.43 | 1.41        | 1.35     |
| 14  | F     | 201  | CLA  | C4B-NB | 7.43 | 1.41        | 1.35     |
| 14  | b     | 823  | CLA  | C4B-NB | 7.43 | 1.41        | 1.35     |
| 14  | B     | 832  | CLA  | C4B-NB | 7.42 | 1.41        | 1.35     |
| 14  | b     | 828  | CLA  | C4B-NB | 7.42 | 1.41        | 1.35     |
| 14  | 2     | 833  | CLA  | C4B-NB | 7.41 | 1.41        | 1.35     |
| 14  | B     | 822  | CLA  | C4B-NB | 7.41 | 1.41        | 1.35     |
| 14  | 1     | 1616 | CLA  | C4B-NB | 7.41 | 1.41        | 1.35     |
| 14  | 8     | 1303 | CLA  | C4B-NB | 7.41 | 1.41        | 1.35     |
| 14  | 2     | 823  | CLA  | C4B-NB | 7.40 | 1.41        | 1.35     |
| 14  | J     | 102  | CLA  | C4B-NB | 7.40 | 1.41        | 1.35     |
| 14  | j     | 1303 | CLA  | C4B-NB | 7.40 | 1.41        | 1.35     |
| 14  | b     | 818  | CLA  | C4B-NB | 7.39 | 1.41        | 1.35     |
| 14  | B     | 835  | CLA  | C4B-NB | 7.39 | 1.41        | 1.35     |
| 14  | 1     | 1620 | CLA  | C4B-NB | 7.39 | 1.41        | 1.35     |
| 14  | A     | 817  | CLA  | C4B-NB | 7.39 | 1.41        | 1.35     |
| 14  | a     | 815  | CLA  | C4B-NB | 7.38 | 1.41        | 1.35     |
| 14  | A     | 837  | CLA  | C4B-NB | 7.38 | 1.41        | 1.35     |
| 14  | 6     | 201  | CLA  | C4B-NB | 7.38 | 1.41        | 1.35     |
| 14  | a     | 837  | CLA  | C4B-NB | 7.37 | 1.41        | 1.35     |
| 14  | 8     | 1302 | CLA  | C4B-NB | 7.37 | 1.41        | 1.35     |
| 14  | 0     | 205  | CLA  | C4B-NB | 7.37 | 1.41        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14  | F     | 203  | CLA  | C4B-NB | 7.37 | 1.41        | 1.35     |
| 14  | 8     | 1301 | CLA  | C4B-NB | 7.37 | 1.41        | 1.35     |
| 14  | A     | 819  | CLA  | C4B-NB | 7.35 | 1.41        | 1.35     |
| 14  | a     | 803  | CLA  | C4B-NB | 7.35 | 1.41        | 1.35     |
| 14  | 2     | 836  | CLA  | C4B-NB | 7.34 | 1.41        | 1.35     |
| 14  | 1     | 1604 | CLA  | C4B-NB | 7.34 | 1.41        | 1.35     |
| 14  | a     | 819  | CLA  | C4B-NB | 7.34 | 1.41        | 1.35     |
| 14  | j     | 1301 | CLA  | C4B-NB | 7.33 | 1.41        | 1.35     |
| 14  | l     | 204  | CLA  | C4B-NB | 7.32 | 1.41        | 1.35     |
| 14  | j     | 1302 | CLA  | C4B-NB | 7.32 | 1.41        | 1.35     |
| 14  | k     | 103  | CLA  | C4B-NB | 7.32 | 1.41        | 1.35     |
| 14  | f     | 201  | CLA  | C4B-NB | 7.32 | 1.41        | 1.35     |
| 14  | a     | 811  | CLA  | C4B-NB | 7.32 | 1.41        | 1.35     |
| 14  | A     | 811  | CLA  | C4B-NB | 7.31 | 1.41        | 1.35     |
| 14  | 2     | 835  | CLA  | C4B-NB | 7.31 | 1.41        | 1.35     |
| 14  | B     | 812  | CLA  | C4B-NB | 7.31 | 1.41        | 1.35     |
| 14  | 2     | 818  | CLA  | C4B-NB | 7.31 | 1.41        | 1.35     |
| 14  | 1     | 1638 | CLA  | C4B-NB | 7.31 | 1.41        | 1.35     |
| 14  | a     | 818  | CLA  | C4B-NB | 7.30 | 1.41        | 1.35     |
| 14  | 1     | 1622 | CLA  | C4B-NB | 7.29 | 1.41        | 1.35     |
| 14  | A     | 815  | CLA  | C4B-NB | 7.29 | 1.41        | 1.35     |
| 14  | A     | 821  | CLA  | C4B-NB | 7.28 | 1.41        | 1.35     |
| 14  | L     | 203  | CLA  | C4B-NB | 7.28 | 1.41        | 1.35     |
| 14  | a     | 817  | CLA  | C4B-NB | 7.28 | 1.41        | 1.35     |
| 14  | 1     | 1612 | CLA  | C4B-NB | 7.28 | 1.41        | 1.35     |
| 14  | b     | 829  | CLA  | C4B-NB | 7.28 | 1.41        | 1.35     |
| 14  | 9     | 103  | CLA  | C4B-NB | 7.28 | 1.41        | 1.35     |
| 14  | b     | 835  | CLA  | C4B-NB | 7.28 | 1.41        | 1.35     |
| 14  | J     | 101  | CLA  | C4B-NB | 7.27 | 1.41        | 1.35     |
| 14  | B     | 825  | CLA  | C4B-NB | 7.27 | 1.41        | 1.35     |
| 14  | B     | 834  | CLA  | C4B-NB | 7.26 | 1.41        | 1.35     |
| 14  | 2     | 829  | CLA  | C4B-NB | 7.25 | 1.41        | 1.35     |
| 14  | A     | 808  | CLA  | C4B-NB | 7.25 | 1.41        | 1.35     |
| 14  | A     | 803  | CLA  | C4B-NB | 7.24 | 1.41        | 1.35     |
| 14  | K     | 103  | CLA  | C4B-NB | 7.24 | 1.41        | 1.35     |
| 14  | b     | 836  | CLA  | C4B-NB | 7.24 | 1.41        | 1.35     |
| 14  | a     | 821  | CLA  | C4B-NB | 7.23 | 1.41        | 1.35     |
| 14  | B     | 828  | CLA  | C4B-NB | 7.23 | 1.41        | 1.35     |
| 14  | 1     | 1618 | CLA  | C4B-NB | 7.23 | 1.41        | 1.35     |
| 14  | K     | 101  | CLA  | C4B-NB | 7.22 | 1.41        | 1.35     |
| 14  | B     | 837  | CLA  | C4B-NB | 7.22 | 1.41        | 1.35     |
| 14  | B     | 823  | CLA  | C4B-NB | 7.21 | 1.41        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14  | 2     | 826  | CLA  | C4B-NB | 7.21 | 1.41        | 1.35     |
| 14  | b     | 838  | CLA  | C4B-NB | 7.20 | 1.41        | 1.35     |
| 14  | b     | 826  | CLA  | C4B-NB | 7.20 | 1.41        | 1.35     |
| 14  | 1     | 1614 | CLA  | C4B-NB | 7.19 | 1.41        | 1.35     |
| 14  | 2     | 838  | CLA  | C4B-NB | 7.19 | 1.41        | 1.35     |
| 14  | a     | 812  | CLA  | C4B-NB | 7.19 | 1.41        | 1.35     |
| 14  | 1     | 1609 | CLA  | C4B-NB | 7.18 | 1.41        | 1.35     |
| 14  | A     | 813  | CLA  | C4B-NB | 7.18 | 1.41        | 1.35     |
| 14  | k     | 101  | CLA  | C4B-NB | 7.18 | 1.41        | 1.35     |
| 14  | A     | 818  | CLA  | C4B-NB | 7.17 | 1.41        | 1.35     |
| 14  | B     | 833  | CLA  | C4B-NB | 7.16 | 1.41        | 1.35     |
| 14  | 1     | 1644 | CLA  | C4B-NB | 7.16 | 1.41        | 1.35     |
| 14  | 1     | 1619 | CLA  | C4B-NB | 7.16 | 1.41        | 1.35     |
| 14  | 1     | 1613 | CLA  | C4B-NB | 7.16 | 1.41        | 1.35     |
| 14  | a     | 843  | CLA  | C4B-NB | 7.15 | 1.41        | 1.35     |
| 14  | a     | 808  | CLA  | C4B-NB | 7.15 | 1.41        | 1.35     |
| 14  | 9     | 101  | CLA  | C4B-NB | 7.15 | 1.41        | 1.35     |
| 14  | A     | 812  | CLA  | C4B-NB | 7.14 | 1.41        | 1.35     |
| 14  | 2     | 824  | CLA  | C4B-NB | 7.14 | 1.41        | 1.35     |
| 14  | b     | 824  | CLA  | C4B-NB | 7.14 | 1.41        | 1.35     |
| 14  | a     | 814  | CLA  | C4B-NB | 7.13 | 1.41        | 1.35     |
| 14  | a     | 816  | CLA  | C4B-NB | 7.13 | 1.41        | 1.35     |
| 14  | A     | 816  | CLA  | C4B-NB | 7.12 | 1.41        | 1.35     |
| 14  | 1     | 1615 | CLA  | C4B-NB | 7.11 | 1.41        | 1.35     |
| 14  | a     | 840  | CLA  | C4B-NB | 7.11 | 1.41        | 1.35     |
| 14  | a     | 813  | CLA  | C4B-NB | 7.10 | 1.41        | 1.35     |
| 14  | B     | 821  | CLA  | C4B-NB | 7.10 | 1.41        | 1.35     |
| 14  | 1     | 1623 | CLA  | C4B-NB | 7.10 | 1.41        | 1.35     |
| 14  | b     | 822  | CLA  | C4B-NB | 7.09 | 1.41        | 1.35     |
| 14  | A     | 814  | CLA  | C4B-NB | 7.09 | 1.41        | 1.35     |
| 14  | b     | 817  | CLA  | C4B-NB | 7.09 | 1.41        | 1.35     |
| 14  | 1     | 1643 | CLA  | C4B-NB | 7.07 | 1.41        | 1.35     |
| 14  | 1     | 1617 | CLA  | C4B-NB | 7.07 | 1.41        | 1.35     |
| 14  | a     | 831  | CLA  | C4B-NB | 7.07 | 1.41        | 1.35     |
| 14  | 2     | 817  | CLA  | C4B-NB | 7.07 | 1.41        | 1.35     |
| 14  | 1     | 1641 | CLA  | C4B-NB | 7.07 | 1.41        | 1.35     |
| 14  | 1     | 1624 | CLA  | C4B-NB | 7.06 | 1.41        | 1.35     |
| 14  | A     | 840  | CLA  | C4B-NB | 7.06 | 1.41        | 1.35     |
| 14  | 2     | 834  | CLA  | C4B-NB | 7.06 | 1.41        | 1.35     |
| 14  | 2     | 822  | CLA  | C4B-NB | 7.06 | 1.41        | 1.35     |
| 14  | a     | 828  | CLA  | C4B-NB | 7.06 | 1.41        | 1.35     |
| 14  | A     | 843  | CLA  | C4B-NB | 7.05 | 1.41        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14  | A     | 823  | CLA  | C4B-NB | 7.05 | 1.41        | 1.35     |
| 14  | a     | 842  | CLA  | C4B-NB | 7.04 | 1.41        | 1.35     |
| 14  | A     | 831  | CLA  | C4B-NB | 7.04 | 1.41        | 1.35     |
| 14  | B     | 816  | CLA  | C4B-NB | 7.03 | 1.41        | 1.35     |
| 14  | b     | 834  | CLA  | C4B-NB | 7.02 | 1.41        | 1.35     |
| 14  | 1     | 1611 | CLA  | C4B-NB | 7.02 | 1.41        | 1.35     |
| 14  | 2     | 805  | CLA  | C4B-NB | 7.01 | 1.41        | 1.35     |
| 14  | A     | 810  | CLA  | C4B-NB | 7.00 | 1.41        | 1.35     |
| 14  | 1     | 1629 | CLA  | C4B-NB | 7.00 | 1.41        | 1.35     |
| 14  | 2     | 816  | CLA  | C4B-NB | 7.00 | 1.41        | 1.35     |
| 14  | a     | 829  | CLA  | C4B-NB | 7.00 | 1.41        | 1.35     |
| 14  | A     | 822  | CLA  | C4B-NB | 6.99 | 1.41        | 1.35     |
| 14  | b     | 805  | CLA  | C4B-NB | 6.99 | 1.41        | 1.35     |
| 14  | 1     | 1606 | CLA  | C4B-NB | 6.98 | 1.41        | 1.35     |
| 14  | 1     | 1610 | CLA  | C4B-NB | 6.98 | 1.41        | 1.35     |
| 14  | 1     | 1632 | CLA  | C4B-NB | 6.98 | 1.41        | 1.35     |
| 14  | A     | 809  | CLA  | C4B-NB | 6.98 | 1.41        | 1.35     |
| 14  | a     | 805  | CLA  | C4B-NB | 6.98 | 1.41        | 1.35     |
| 14  | a     | 809  | CLA  | C4B-NB | 6.97 | 1.41        | 1.35     |
| 14  | a     | 822  | CLA  | C4B-NB | 6.97 | 1.41        | 1.35     |
| 14  | a     | 823  | CLA  | C4B-NB | 6.96 | 1.41        | 1.35     |
| 14  | A     | 805  | CLA  | C4B-NB | 6.96 | 1.41        | 1.35     |
| 14  | A     | 842  | CLA  | C4B-NB | 6.95 | 1.41        | 1.35     |
| 14  | B     | 815  | CLA  | C4B-NB | 6.95 | 1.41        | 1.35     |
| 14  | a     | 810  | CLA  | C4B-NB | 6.95 | 1.41        | 1.35     |
| 14  | B     | 804  | CLA  | C4B-NB | 6.94 | 1.41        | 1.35     |
| 14  | A     | 828  | CLA  | C4B-NB | 6.93 | 1.41        | 1.35     |
| 14  | B     | 831  | CLA  | C4B-NB | 6.93 | 1.41        | 1.35     |
| 14  | b     | 812  | CLA  | C4B-NB | 6.93 | 1.41        | 1.35     |
| 14  | 1     | 1630 | CLA  | C4B-NB | 6.93 | 1.41        | 1.35     |
| 14  | a     | 836  | CLA  | C4B-NB | 6.93 | 1.41        | 1.35     |
| 14  | a     | 841  | CLA  | C4B-NB | 6.92 | 1.41        | 1.35     |
| 14  | b     | 825  | CLA  | C4B-NB | 6.92 | 1.41        | 1.35     |
| 14  | A     | 829  | CLA  | C4B-NB | 6.91 | 1.41        | 1.35     |
| 14  | 2     | 825  | CLA  | C4B-NB | 6.91 | 1.41        | 1.35     |
| 14  | b     | 816  | CLA  | C4B-NB | 6.91 | 1.41        | 1.35     |
| 14  | B     | 841  | CLA  | C4B-NB | 6.90 | 1.41        | 1.35     |
| 14  | 2     | 842  | CLA  | C4B-NB | 6.89 | 1.41        | 1.35     |
| 14  | b     | 832  | CLA  | C4B-NB | 6.89 | 1.41        | 1.35     |
| 14  | b     | 842  | CLA  | C4B-NB | 6.87 | 1.41        | 1.35     |
| 14  | 1     | 1637 | CLA  | C4B-NB | 6.87 | 1.41        | 1.35     |
| 14  | 1     | 1642 | CLA  | C4B-NB | 6.86 | 1.41        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14  | 2     | 812  | CLA  | C4B-NB | 6.86 | 1.41        | 1.35     |
| 14  | A     | 836  | CLA  | C4B-NB | 6.86 | 1.41        | 1.35     |
| 14  | b     | 827  | CLA  | C4B-NB | 6.85 | 1.41        | 1.35     |
| 14  | 2     | 815  | CLA  | C4B-NB | 6.84 | 1.41        | 1.35     |
| 14  | B     | 824  | CLA  | C4B-NB | 6.84 | 1.41        | 1.35     |
| 14  | 2     | 832  | CLA  | C4B-NB | 6.84 | 1.41        | 1.35     |
| 14  | 2     | 827  | CLA  | C4B-NB | 6.83 | 1.41        | 1.35     |
| 14  | A     | 841  | CLA  | C4B-NB | 6.83 | 1.41        | 1.35     |
| 14  | b     | 815  | CLA  | C4B-NB | 6.83 | 1.41        | 1.35     |
| 14  | B     | 826  | CLA  | C4B-NB | 6.82 | 1.41        | 1.35     |
| 14  | a     | 826  | CLA  | C4B-NB | 6.82 | 1.41        | 1.35     |
| 14  | B     | 811  | CLA  | C4B-NB | 6.82 | 1.41        | 1.35     |
| 14  | B     | 805  | CLA  | C4B-NB | 6.81 | 1.41        | 1.35     |
| 14  | a     | 844  | CLA  | C4B-NB | 6.81 | 1.41        | 1.35     |
| 14  | 2     | 806  | CLA  | C4B-NB | 6.81 | 1.41        | 1.35     |
| 14  | A     | 826  | CLA  | C4B-NB | 6.80 | 1.41        | 1.35     |
| 14  | B     | 814  | CLA  | C4B-NB | 6.79 | 1.41        | 1.35     |
| 14  | a     | 820  | CLA  | C4B-NB | 6.79 | 1.41        | 1.35     |
| 14  | 2     | 807  | CLA  | C4B-NB | 6.78 | 1.41        | 1.35     |
| 14  | 1     | 1621 | CLA  | C4B-NB | 6.77 | 1.41        | 1.35     |
| 14  | 1     | 1627 | CLA  | C4B-NB | 6.77 | 1.41        | 1.35     |
| 14  | A     | 820  | CLA  | C4B-NB | 6.77 | 1.41        | 1.35     |
| 14  | b     | 806  | CLA  | C4B-NB | 6.76 | 1.41        | 1.35     |
| 14  | 1     | 1645 | CLA  | C4B-NB | 6.76 | 1.41        | 1.35     |
| 14  | 2     | 811  | CLA  | C4B-NB | 6.75 | 1.41        | 1.35     |
| 14  | b     | 811  | CLA  | C4B-NB | 6.75 | 1.41        | 1.35     |
| 14  | b     | 807  | CLA  | C4B-NB | 6.75 | 1.41        | 1.35     |
| 14  | b     | 839  | CLA  | C4B-NB | 6.75 | 1.41        | 1.35     |
| 14  | B     | 818  | CLA  | C4B-NB | 6.74 | 1.41        | 1.35     |
| 14  | A     | 844  | CLA  | C4B-NB | 6.74 | 1.41        | 1.35     |
| 14  | B     | 806  | CLA  | C4B-NB | 6.73 | 1.41        | 1.35     |
| 14  | 2     | 839  | CLA  | C4B-NB | 6.73 | 1.41        | 1.35     |
| 14  | B     | 810  | CLA  | C4B-NB | 6.73 | 1.41        | 1.35     |
| 14  | A     | 825  | CLA  | C4B-NB | 6.73 | 1.41        | 1.35     |
| 14  | A     | 807  | CLA  | C4B-NB | 6.72 | 1.41        | 1.35     |
| 14  | 2     | 819  | CLA  | C4B-NB | 6.72 | 1.41        | 1.35     |
| 14  | b     | 831  | CLA  | C4B-NB | 6.71 | 1.41        | 1.35     |
| 14  | B     | 813  | CLA  | C4B-NB | 6.70 | 1.41        | 1.35     |
| 14  | 2     | 831  | CLA  | C4B-NB | 6.70 | 1.41        | 1.35     |
| 14  | B     | 807  | CLA  | C4B-NB | 6.70 | 1.41        | 1.35     |
| 14  | B     | 838  | CLA  | C4B-NB | 6.69 | 1.41        | 1.35     |
| 14  | a     | 825  | CLA  | C4B-NB | 6.69 | 1.41        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14  | b     | 814  | CLA  | C4B-NB | 6.69 | 1.41        | 1.35     |
| 14  | a     | 807  | CLA  | C4B-NB | 6.69 | 1.41        | 1.35     |
| 14  | 2     | 814  | CLA  | C4B-NB | 6.69 | 1.41        | 1.35     |
| 14  | 2     | 841  | CLA  | C4B-NB | 6.68 | 1.41        | 1.35     |
| 14  | 2     | 808  | CLA  | C4B-NB | 6.68 | 1.41        | 1.35     |
| 14  | B     | 840  | CLA  | C4B-NB | 6.66 | 1.41        | 1.35     |
| 14  | B     | 830  | CLA  | C4B-NB | 6.66 | 1.41        | 1.35     |
| 14  | 1     | 1608 | CLA  | C4B-NB | 6.66 | 1.41        | 1.35     |
| 14  | a     | 802  | CLA  | C4B-NB | 6.65 | 1.41        | 1.35     |
| 14  | b     | 808  | CLA  | C4B-NB | 6.65 | 1.41        | 1.35     |
| 14  | b     | 819  | CLA  | C4B-NB | 6.65 | 1.41        | 1.35     |
| 14  | a     | 834  | CLA  | C4B-NB | 6.65 | 1.41        | 1.35     |
| 14  | 1     | 1639 | CLA  | C4B-NB | 6.65 | 1.41        | 1.35     |
| 14  | 1     | 1603 | CLA  | C4B-NB | 6.64 | 1.41        | 1.35     |
| 14  | A     | 802  | CLA  | C4B-NB | 6.63 | 1.41        | 1.35     |
| 14  | b     | 841  | CLA  | C4B-NB | 6.63 | 1.41        | 1.35     |
| 14  | A     | 827  | CLA  | C4B-NB | 6.63 | 1.41        | 1.35     |
| 14  | B     | 808  | CLA  | C4B-NB | 6.63 | 1.41        | 1.35     |
| 14  | 2     | 809  | CLA  | C4B-NB | 6.62 | 1.41        | 1.35     |
| 14  | 1     | 1626 | CLA  | C4B-NB | 6.62 | 1.41        | 1.35     |
| 14  | A     | 804  | CLA  | C4B-NB | 6.61 | 1.41        | 1.35     |
| 14  | A     | 834  | CLA  | C4B-NB | 6.61 | 1.41        | 1.35     |
| 14  | A     | 855  | CLA  | C4B-NB | 6.61 | 1.41        | 1.35     |
| 14  | a     | 838  | CLA  | C4B-NB | 6.61 | 1.41        | 1.35     |
| 14  | 1     | 1635 | CLA  | C4B-NB | 6.59 | 1.41        | 1.35     |
| 14  | 1     | 1636 | CLA  | C4B-NB | 6.59 | 1.41        | 1.35     |
| 14  | a     | 804  | CLA  | C4B-NB | 6.59 | 1.41        | 1.35     |
| 14  | a     | 835  | CLA  | C4B-NB | 6.58 | 1.41        | 1.35     |
| 13  | 1     | 1602 | CL0  | C4B-NB | 6.57 | 1.41        | 1.35     |
| 14  | b     | 809  | CLA  | C4B-NB | 6.57 | 1.41        | 1.35     |
| 14  | A     | 835  | CLA  | C4B-NB | 6.57 | 1.41        | 1.35     |
| 14  | b     | 802  | CLA  | C4B-NB | 6.56 | 1.41        | 1.35     |
| 14  | 1     | 1605 | CLA  | C4B-NB | 6.56 | 1.41        | 1.35     |
| 14  | a     | 833  | CLA  | C4B-NB | 6.56 | 1.41        | 1.35     |
| 13  | A     | 801  | CL0  | C4B-NB | 6.55 | 1.41        | 1.35     |
| 14  | 1     | 1628 | CLA  | C4B-NB | 6.55 | 1.41        | 1.35     |
| 14  | A     | 838  | CLA  | C4B-NB | 6.54 | 1.41        | 1.35     |
| 14  | A     | 832  | CLA  | C4B-NB | 6.54 | 1.41        | 1.35     |
| 14  | a     | 839  | CLA  | C4B-NB | 6.53 | 1.41        | 1.35     |
| 14  | 1     | 1633 | CLA  | C4B-NB | 6.52 | 1.41        | 1.35     |
| 14  | 2     | 802  | CLA  | C4B-NB | 6.52 | 1.41        | 1.35     |
| 14  | 2     | 810  | CLA  | C4B-NB | 6.52 | 1.41        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 827  | CLA  | C4B-NB  | 6.52  | 1.41        | 1.35     |
| 14  | b     | 810  | CLA  | C4B-NB  | 6.51  | 1.41        | 1.35     |
| 14  | 1     | 1634 | CLA  | C4B-NB  | 6.51  | 1.41        | 1.35     |
| 13  | a     | 801  | CL0  | C4B-NB  | 6.51  | 1.41        | 1.35     |
| 14  | B     | 829  | CLA  | C4B-NB  | 6.50  | 1.41        | 1.35     |
| 14  | 0     | 207  | CLA  | C4B-NB  | 6.49  | 1.41        | 1.35     |
| 14  | a     | 832  | CLA  | C4B-NB  | 6.48  | 1.41        | 1.35     |
| 14  | A     | 833  | CLA  | C4B-NB  | 6.47  | 1.41        | 1.35     |
| 14  | b     | 830  | CLA  | C4B-NB  | 6.47  | 1.41        | 1.35     |
| 14  | A     | 806  | CLA  | C4B-NB  | 6.46  | 1.41        | 1.35     |
| 14  | L     | 205  | CLA  | C4B-NB  | 6.46  | 1.41        | 1.35     |
| 14  | 2     | 830  | CLA  | C4B-NB  | 6.43  | 1.40        | 1.35     |
| 14  | l     | 206  | CLA  | C4B-NB  | 6.42  | 1.40        | 1.35     |
| 14  | 1     | 1640 | CLA  | C4B-NB  | 6.42  | 1.40        | 1.35     |
| 14  | a     | 806  | CLA  | C4B-NB  | 6.40  | 1.40        | 1.35     |
| 14  | B     | 809  | CLA  | C4B-NB  | 6.40  | 1.40        | 1.35     |
| 14  | 1     | 1607 | CLA  | C4B-NB  | 6.38  | 1.40        | 1.35     |
| 14  | A     | 839  | CLA  | C4B-NB  | 6.36  | 1.40        | 1.35     |
| 14  | 2     | 803  | CLA  | C4B-NB  | 6.33  | 1.40        | 1.35     |
| 14  | a     | 830  | CLA  | C4B-NB  | 6.24  | 1.40        | 1.35     |
| 14  | B     | 802  | CLA  | C4B-NB  | 6.23  | 1.40        | 1.35     |
| 14  | 0     | 206  | CLA  | C4B-NB  | 6.21  | 1.40        | 1.35     |
| 14  | l     | 205  | CLA  | C4B-NB  | 6.21  | 1.40        | 1.35     |
| 14  | b     | 803  | CLA  | C4B-NB  | 6.21  | 1.40        | 1.35     |
| 14  | A     | 830  | CLA  | C4B-NB  | 6.20  | 1.40        | 1.35     |
| 14  | L     | 204  | CLA  | C4B-NB  | 6.19  | 1.40        | 1.35     |
| 14  | 1     | 1631 | CLA  | C4B-NB  | 6.19  | 1.40        | 1.35     |
| 14  | B     | 803  | CLA  | C4B-NB  | 6.08  | 1.40        | 1.35     |
| 14  | b     | 804  | CLA  | C4B-NB  | 6.04  | 1.40        | 1.35     |
| 14  | 2     | 804  | CLA  | C4B-NB  | 6.02  | 1.40        | 1.35     |
| 17  | B     | 845  | BCR  | C30-C25 | -4.08 | 1.48        | 1.53     |
| 17  | 1     | 1651 | BCR  | C30-C25 | -4.06 | 1.48        | 1.53     |
| 17  | a     | 850  | BCR  | C30-C25 | -4.02 | 1.48        | 1.53     |
| 17  | b     | 846  | BCR  | C30-C25 | -4.01 | 1.48        | 1.53     |
| 17  | 2     | 844  | BCR  | C1-C6   | -4.01 | 1.48        | 1.53     |
| 17  | B     | 848  | BCR  | C1-C6   | -4.00 | 1.48        | 1.53     |
| 14  | J     | 102  | CLA  | C1D-ND  | 3.99  | 1.42        | 1.37     |
| 14  | j     | 1303 | CLA  | C1D-ND  | 3.99  | 1.42        | 1.37     |
| 17  | 2     | 846  | BCR  | C30-C25 | -3.99 | 1.48        | 1.53     |
| 17  | 1     | 1650 | BCR  | C1-C6   | -3.99 | 1.48        | 1.53     |
| 17  | 2     | 849  | BCR  | C1-C6   | -3.98 | 1.48        | 1.53     |
| 17  | B     | 843  | BCR  | C1-C6   | -3.98 | 1.48        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | 2     | 848  | BCR  | C30-C25 | -3.97 | 1.48        | 1.53     |
| 17  | A     | 850  | BCR  | C30-C25 | -3.96 | 1.48        | 1.53     |
| 17  | A     | 856  | BCR  | C1-C6   | -3.96 | 1.48        | 1.53     |
| 17  | b     | 849  | BCR  | C1-C6   | -3.95 | 1.48        | 1.53     |
| 17  | b     | 844  | BCR  | C1-C6   | -3.95 | 1.48        | 1.53     |
| 17  | j     | 1305 | BCR  | C1-C6   | -3.94 | 1.48        | 1.53     |
| 17  | A     | 849  | BCR  | C1-C6   | -3.94 | 1.48        | 1.53     |
| 17  | 8     | 1305 | BCR  | C1-C6   | -3.93 | 1.48        | 1.53     |
| 17  | b     | 848  | BCR  | C30-C25 | -3.93 | 1.48        | 1.53     |
| 17  | B     | 847  | BCR  | C30-C25 | -3.92 | 1.48        | 1.53     |
| 14  | 8     | 1303 | CLA  | C1D-ND  | 3.91  | 1.42        | 1.37     |
| 17  | a     | 849  | BCR  | C1-C6   | -3.91 | 1.48        | 1.53     |
| 17  | m     | 102  | BCR  | C1-C6   | -3.91 | 1.48        | 1.53     |
| 17  | b     | 848  | BCR  | C1-C6   | -3.90 | 1.48        | 1.53     |
| 17  | 7     | 101  | BCR  | C1-C6   | -3.90 | 1.48        | 1.53     |
| 17  | L     | 201  | BCR  | C1-C6   | -3.89 | 1.48        | 1.53     |
| 17  | I     | 101  | BCR  | C1-C6   | -3.89 | 1.48        | 1.53     |
| 17  | M     | 103  | BCR  | C1-C6   | -3.88 | 1.48        | 1.53     |
| 17  | 2     | 849  | BCR  | C30-C25 | -3.88 | 1.48        | 1.53     |
| 14  | J     | 101  | CLA  | C1D-ND  | 3.88  | 1.42        | 1.37     |
| 14  | 8     | 1302 | CLA  | C1D-ND  | 3.87  | 1.42        | 1.37     |
| 14  | K     | 103  | CLA  | C1D-ND  | 3.87  | 1.42        | 1.37     |
| 17  | 0     | 203  | BCR  | C1-C6   | -3.87 | 1.48        | 1.53     |
| 14  | k     | 103  | CLA  | C1D-ND  | 3.86  | 1.42        | 1.37     |
| 17  | 0     | 203  | BCR  | C30-C25 | -3.86 | 1.48        | 1.53     |
| 17  | 1     | 1652 | BCR  | C1-C6   | -3.85 | 1.48        | 1.53     |
| 17  | i     | 101  | BCR  | C1-C6   | -3.85 | 1.48        | 1.53     |
| 17  | l     | 202  | BCR  | C30-C25 | -3.85 | 1.48        | 1.53     |
| 17  | F     | 202  | BCR  | C30-C25 | -3.85 | 1.48        | 1.53     |
| 17  | b     | 849  | BCR  | C30-C25 | -3.85 | 1.48        | 1.53     |
| 14  | j     | 1302 | CLA  | C1D-ND  | 3.85  | 1.42        | 1.37     |
| 14  | a     | 816  | CLA  | C1D-ND  | 3.84  | 1.42        | 1.37     |
| 17  | L     | 201  | BCR  | C30-C25 | -3.84 | 1.48        | 1.53     |
| 17  | A     | 851  | BCR  | C1-C6   | -3.84 | 1.48        | 1.53     |
| 17  | a     | 851  | BCR  | C1-C6   | -3.84 | 1.48        | 1.53     |
| 17  | l     | 202  | BCR  | C1-C6   | -3.84 | 1.48        | 1.53     |
| 17  | y     | 102  | BCR  | C1-C6   | -3.84 | 1.48        | 1.53     |
| 17  | 6     | 202  | BCR  | C30-C25 | -3.83 | 1.48        | 1.53     |
| 14  | 9     | 103  | CLA  | C1D-ND  | 3.83  | 1.42        | 1.37     |
| 17  | 2     | 848  | BCR  | C1-C6   | -3.83 | 1.48        | 1.53     |
| 17  | f     | 202  | BCR  | C30-C25 | -3.83 | 1.48        | 1.53     |
| 17  | a     | 848  | BCR  | C30-C25 | -3.83 | 1.48        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | 1     | 1649 | BCR  | C30-C25 | -3.83 | 1.48        | 1.53     |
| 14  | 1     | 1618 | CLA  | C1D-ND  | 3.83  | 1.42        | 1.37     |
| 14  | l     | 205  | CLA  | C4D-ND  | -3.83 | 1.32        | 1.37     |
| 14  | 0     | 206  | CLA  | C4D-ND  | -3.83 | 1.32        | 1.37     |
| 14  | 6     | 203  | CLA  | C1D-ND  | 3.82  | 1.42        | 1.37     |
| 14  | B     | 819  | CLA  | C1D-ND  | 3.82  | 1.42        | 1.37     |
| 14  | a     | 817  | CLA  | C1D-ND  | 3.82  | 1.42        | 1.37     |
| 14  | 1     | 1617 | CLA  | C1D-ND  | 3.82  | 1.42        | 1.37     |
| 14  | A     | 816  | CLA  | C1D-ND  | 3.82  | 1.42        | 1.37     |
| 14  | a     | 824  | CLA  | C1D-ND  | 3.82  | 1.42        | 1.37     |
| 14  | a     | 821  | CLA  | C1D-ND  | 3.82  | 1.42        | 1.37     |
| 14  | b     | 822  | CLA  | C1D-ND  | 3.81  | 1.42        | 1.37     |
| 14  | A     | 817  | CLA  | C1D-ND  | 3.81  | 1.42        | 1.37     |
| 14  | L     | 204  | CLA  | C4D-ND  | -3.80 | 1.32        | 1.37     |
| 14  | f     | 203  | CLA  | C1D-ND  | 3.80  | 1.42        | 1.37     |
| 14  | 1     | 1622 | CLA  | C1D-ND  | 3.80  | 1.42        | 1.37     |
| 17  | B     | 847  | BCR  | C1-C6   | -3.80 | 1.48        | 1.53     |
| 14  | A     | 824  | CLA  | C1D-ND  | 3.79  | 1.42        | 1.37     |
| 14  | B     | 821  | CLA  | C1D-ND  | 3.79  | 1.42        | 1.37     |
| 17  | B     | 851  | BCR  | C1-C6   | -3.78 | 1.48        | 1.53     |
| 14  | A     | 821  | CLA  | C1D-ND  | 3.78  | 1.42        | 1.37     |
| 17  | B     | 848  | BCR  | C30-C25 | -3.77 | 1.48        | 1.53     |
| 14  | 1     | 1625 | CLA  | C1D-ND  | 3.77  | 1.42        | 1.37     |
| 14  | 2     | 820  | CLA  | C1D-ND  | 3.76  | 1.42        | 1.37     |
| 14  | F     | 204  | CLA  | C1D-ND  | 3.76  | 1.42        | 1.37     |
| 14  | A     | 815  | CLA  | C1D-ND  | 3.76  | 1.42        | 1.37     |
| 17  | b     | 852  | BCR  | C1-C6   | -3.75 | 1.48        | 1.53     |
| 17  | 8     | 1306 | BCR  | C1-C6   | -3.75 | 1.48        | 1.53     |
| 17  | B     | 845  | BCR  | C1-C6   | -3.74 | 1.48        | 1.53     |
| 14  | 2     | 822  | CLA  | C1D-ND  | 3.74  | 1.42        | 1.37     |
| 17  | 2     | 846  | BCR  | C1-C6   | -3.74 | 1.48        | 1.53     |
| 14  | 1     | 1616 | CLA  | C1D-ND  | 3.73  | 1.42        | 1.37     |
| 17  | A     | 848  | BCR  | C30-C25 | -3.72 | 1.48        | 1.53     |
| 17  | b     | 846  | BCR  | C1-C6   | -3.71 | 1.48        | 1.53     |
| 14  | 1     | 1601 | CLA  | C1D-ND  | 3.70  | 1.42        | 1.37     |
| 14  | a     | 815  | CLA  | C1D-ND  | 3.70  | 1.42        | 1.37     |
| 14  | 1     | 1624 | CLA  | C1D-ND  | 3.69  | 1.42        | 1.37     |
| 14  | b     | 820  | CLA  | C1D-ND  | 3.69  | 1.42        | 1.37     |
| 14  | 2     | 831  | CLA  | C1D-ND  | 3.68  | 1.42        | 1.37     |
| 14  | 2     | 840  | CLA  | C1D-ND  | 3.68  | 1.42        | 1.37     |
| 14  | M     | 102  | CLA  | C1D-ND  | 3.68  | 1.42        | 1.37     |
| 14  | A     | 857  | CLA  | C1D-ND  | 3.67  | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 831  | CLA  | C1D-ND  | 3.67  | 1.42        | 1.37     |
| 14  | B     | 824  | CLA  | C1D-ND  | 3.67  | 1.42        | 1.37     |
| 14  | A     | 831  | CLA  | CMB-C2B | -3.66 | 1.44        | 1.51     |
| 14  | k     | 101  | CLA  | C1D-ND  | 3.66  | 1.42        | 1.37     |
| 14  | l     | 1632 | CLA  | CMB-C2B | -3.66 | 1.44        | 1.51     |
| 14  | B     | 817  | CLA  | C1D-ND  | 3.65  | 1.42        | 1.37     |
| 14  | X     | 1701 | CLA  | C1D-ND  | 3.65  | 1.42        | 1.37     |
| 14  | B     | 839  | CLA  | C1D-ND  | 3.65  | 1.42        | 1.37     |
| 14  | 2     | 827  | CLA  | C1D-ND  | 3.65  | 1.42        | 1.37     |
| 14  | B     | 830  | CLA  | C1D-ND  | 3.65  | 1.42        | 1.37     |
| 14  | K     | 101  | CLA  | C1D-ND  | 3.65  | 1.42        | 1.37     |
| 14  | b     | 818  | CLA  | C1D-ND  | 3.64  | 1.42        | 1.37     |
| 14  | a     | 831  | CLA  | CMB-C2B | -3.64 | 1.44        | 1.51     |
| 17  | l     | 1651 | BCR  | C1-C6   | -3.64 | 1.48        | 1.53     |
| 14  | a     | 823  | CLA  | C1D-ND  | 3.64  | 1.42        | 1.37     |
| 17  | A     | 850  | BCR  | C1-C6   | -3.63 | 1.48        | 1.53     |
| 17  | f     | 204  | BCR  | C1-C6   | -3.63 | 1.48        | 1.53     |
| 14  | a     | 810  | CLA  | C1D-ND  | 3.63  | 1.42        | 1.37     |
| 14  | x     | 1701 | CLA  | C1D-ND  | 3.63  | 1.42        | 1.37     |
| 14  | l     | 1612 | CLA  | C1D-ND  | 3.62  | 1.42        | 1.37     |
| 14  | 9     | 101  | CLA  | C1D-ND  | 3.62  | 1.42        | 1.37     |
| 17  | B     | 846  | BCR  | C30-C25 | -3.62 | 1.48        | 1.53     |
| 17  | F     | 205  | BCR  | C1-C6   | -3.62 | 1.48        | 1.53     |
| 14  | 2     | 813  | CLA  | C1D-ND  | 3.62  | 1.42        | 1.37     |
| 14  | 2     | 818  | CLA  | C1D-ND  | 3.62  | 1.42        | 1.37     |
| 14  | A     | 823  | CLA  | C1D-ND  | 3.62  | 1.42        | 1.37     |
| 14  | B     | 836  | CLA  | C1D-ND  | 3.61  | 1.42        | 1.37     |
| 14  | b     | 840  | CLA  | C1D-ND  | 3.61  | 1.42        | 1.37     |
| 14  | a     | 820  | CLA  | C1D-ND  | 3.61  | 1.42        | 1.37     |
| 14  | 2     | 812  | CLA  | C1D-ND  | 3.61  | 1.42        | 1.37     |
| 14  | l     | 1611 | CLA  | C1D-ND  | 3.60  | 1.42        | 1.37     |
| 14  | b     | 827  | CLA  | C1D-ND  | 3.60  | 1.42        | 1.37     |
| 17  | f     | 202  | BCR  | C1-C6   | -3.60 | 1.48        | 1.53     |
| 14  | B     | 826  | CLA  | C1D-ND  | 3.60  | 1.42        | 1.37     |
| 17  | F     | 202  | BCR  | C1-C6   | -3.60 | 1.48        | 1.53     |
| 14  | b     | 825  | CLA  | C1D-ND  | 3.59  | 1.42        | 1.37     |
| 14  | l     | 1645 | CLA  | C1D-ND  | 3.59  | 1.42        | 1.37     |
| 17  | a     | 850  | BCR  | C1-C6   | -3.59 | 1.48        | 1.53     |
| 14  | b     | 812  | CLA  | C1D-ND  | 3.59  | 1.42        | 1.37     |
| 17  | b     | 847  | BCR  | C30-C25 | -3.59 | 1.48        | 1.53     |
| 17  | 2     | 847  | BCR  | C30-C25 | -3.59 | 1.48        | 1.53     |
| 14  | b     | 837  | CLA  | C1D-ND  | 3.59  | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 844  | CLA  | C1D-ND  | 3.59  | 1.42        | 1.37     |
| 14  | A     | 814  | CLA  | C1D-ND  | 3.58  | 1.42        | 1.37     |
| 14  | A     | 820  | CLA  | C1D-ND  | 3.58  | 1.42        | 1.37     |
| 14  | B     | 812  | CLA  | C1D-ND  | 3.58  | 1.42        | 1.37     |
| 14  | b     | 813  | CLA  | C1D-ND  | 3.58  | 1.42        | 1.37     |
| 14  | b     | 821  | CLA  | C1D-ND  | 3.58  | 1.42        | 1.37     |
| 14  | j     | 1301 | CLA  | C1D-ND  | 3.58  | 1.42        | 1.37     |
| 17  | 6     | 204  | BCR  | C1-C6   | -3.58 | 1.48        | 1.53     |
| 14  | B     | 816  | CLA  | C1D-ND  | 3.57  | 1.42        | 1.37     |
| 14  | 2     | 817  | CLA  | C1D-ND  | 3.57  | 1.42        | 1.37     |
| 14  | B     | 820  | CLA  | C1D-ND  | 3.57  | 1.42        | 1.37     |
| 17  | 6     | 202  | BCR  | C1-C6   | -3.57 | 1.48        | 1.53     |
| 14  | 2     | 825  | CLA  | C1D-ND  | 3.56  | 1.42        | 1.37     |
| 14  | F     | 203  | CLA  | C1D-ND  | 3.56  | 1.42        | 1.37     |
| 14  | z     | 102  | CLA  | C1D-ND  | 3.56  | 1.42        | 1.37     |
| 14  | A     | 813  | CLA  | C1D-ND  | 3.55  | 1.42        | 1.37     |
| 14  | a     | 814  | CLA  | C1D-ND  | 3.55  | 1.42        | 1.37     |
| 14  | 1     | 1615 | CLA  | C1D-ND  | 3.55  | 1.42        | 1.37     |
| 14  | 2     | 837  | CLA  | C1D-ND  | 3.55  | 1.42        | 1.37     |
| 17  | k     | 102  | BCR  | C1-C6   | -3.55 | 1.48        | 1.53     |
| 14  | B     | 813  | CLA  | C1D-ND  | 3.54  | 1.42        | 1.37     |
| 14  | a     | 813  | CLA  | C1D-ND  | 3.54  | 1.42        | 1.37     |
| 14  | A     | 810  | CLA  | C1D-ND  | 3.54  | 1.42        | 1.37     |
| 14  | a     | 811  | CLA  | C1D-ND  | 3.54  | 1.42        | 1.37     |
| 14  | B     | 811  | CLA  | C1D-ND  | 3.53  | 1.42        | 1.37     |
| 14  | a     | 837  | CLA  | C1D-ND  | 3.53  | 1.42        | 1.37     |
| 14  | 2     | 824  | CLA  | C1D-ND  | 3.53  | 1.42        | 1.37     |
| 14  | a     | 844  | CLA  | C1D-ND  | 3.53  | 1.42        | 1.37     |
| 14  | 1     | 1628 | CLA  | C4D-ND  | -3.53 | 1.32        | 1.37     |
| 14  | 1     | 1621 | CLA  | C1D-ND  | 3.53  | 1.42        | 1.37     |
| 14  | b     | 817  | CLA  | C1D-ND  | 3.53  | 1.42        | 1.37     |
| 17  | K     | 102  | BCR  | C1-C6   | -3.52 | 1.48        | 1.53     |
| 14  | A     | 811  | CLA  | C1D-ND  | 3.52  | 1.42        | 1.37     |
| 17  | 9     | 102  | BCR  | C1-C6   | -3.51 | 1.48        | 1.53     |
| 17  | B     | 851  | BCR  | C30-C25 | -3.50 | 1.49        | 1.53     |
| 14  | 2     | 814  | CLA  | C1D-ND  | 3.50  | 1.42        | 1.37     |
| 14  | A     | 837  | CLA  | C1D-ND  | 3.50  | 1.42        | 1.37     |
| 14  | b     | 814  | CLA  | C1D-ND  | 3.50  | 1.42        | 1.37     |
| 14  | A     | 827  | CLA  | C4D-ND  | -3.49 | 1.32        | 1.37     |
| 14  | 8     | 1301 | CLA  | C1D-ND  | 3.49  | 1.42        | 1.37     |
| 14  | A     | 818  | CLA  | C1D-ND  | 3.49  | 1.42        | 1.37     |
| 14  | 1     | 1614 | CLA  | C1D-ND  | 3.49  | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 822  | CLA  | C1D-ND  | 3.49  | 1.42        | 1.37     |
| 14  | B     | 823  | CLA  | C1D-ND  | 3.49  | 1.42        | 1.37     |
| 14  | 2     | 821  | CLA  | C1D-ND  | 3.49  | 1.42        | 1.37     |
| 17  | K     | 104  | BCR  | C1-C6   | -3.48 | 1.49        | 1.53     |
| 17  | b     | 845  | BCR  | C1-C6   | -3.48 | 1.49        | 1.53     |
| 14  | B     | 831  | CLA  | C1D-ND  | 3.48  | 1.42        | 1.37     |
| 14  | a     | 827  | CLA  | C4D-ND  | -3.47 | 1.32        | 1.37     |
| 14  | 1     | 1634 | CLA  | C4D-ND  | -3.47 | 1.32        | 1.37     |
| 17  | i     | 101  | BCR  | C30-C25 | -3.47 | 1.49        | 1.53     |
| 14  | a     | 833  | CLA  | C4D-ND  | -3.47 | 1.32        | 1.37     |
| 14  | b     | 824  | CLA  | C1D-ND  | 3.47  | 1.42        | 1.37     |
| 14  | 2     | 823  | CLA  | C1D-ND  | 3.47  | 1.42        | 1.37     |
| 14  | b     | 839  | CLA  | C1D-ND  | 3.47  | 1.42        | 1.37     |
| 14  | B     | 835  | CLA  | C1D-ND  | 3.46  | 1.42        | 1.37     |
| 14  | 1     | 1638 | CLA  | C1D-ND  | 3.46  | 1.42        | 1.37     |
| 14  | 2     | 836  | CLA  | C1D-ND  | 3.46  | 1.42        | 1.37     |
| 14  | a     | 828  | CLA  | C4D-ND  | -3.46 | 1.32        | 1.37     |
| 17  | 8     | 1306 | BCR  | C30-C25 | -3.46 | 1.49        | 1.53     |
| 14  | b     | 808  | CLA  | C1D-ND  | 3.46  | 1.42        | 1.37     |
| 14  | 2     | 804  | CLA  | C4D-ND  | -3.46 | 1.32        | 1.37     |
| 14  | 1     | 1630 | CLA  | C1D-ND  | 3.46  | 1.42        | 1.37     |
| 14  | b     | 823  | CLA  | C1D-ND  | 3.46  | 1.42        | 1.37     |
| 14  | b     | 832  | CLA  | C1D-ND  | 3.45  | 1.42        | 1.37     |
| 14  | b     | 836  | CLA  | C1D-ND  | 3.45  | 1.42        | 1.37     |
| 14  | A     | 822  | CLA  | C1D-ND  | 3.45  | 1.42        | 1.37     |
| 14  | b     | 835  | CLA  | C1D-ND  | 3.45  | 1.42        | 1.37     |
| 14  | A     | 806  | CLA  | C4D-ND  | -3.45 | 1.33        | 1.37     |
| 17  | 7     | 101  | BCR  | C30-C25 | -3.45 | 1.49        | 1.53     |
| 17  | 9     | 102  | BCR  | C30-C25 | -3.45 | 1.49        | 1.53     |
| 14  | A     | 804  | CLA  | C1D-ND  | 3.45  | 1.42        | 1.37     |
| 14  | 1     | 1619 | CLA  | C1D-ND  | 3.44  | 1.42        | 1.37     |
| 17  | 9     | 104  | BCR  | C1-C6   | -3.44 | 1.49        | 1.53     |
| 14  | A     | 832  | CLA  | C4D-ND  | -3.44 | 1.33        | 1.37     |
| 14  | b     | 828  | CLA  | C4D-ND  | -3.44 | 1.33        | 1.37     |
| 17  | b     | 852  | BCR  | C30-C25 | -3.44 | 1.49        | 1.53     |
| 14  | a     | 829  | CLA  | C1D-ND  | 3.44  | 1.42        | 1.37     |
| 14  | A     | 833  | CLA  | C4D-ND  | -3.44 | 1.33        | 1.37     |
| 14  | 1     | 1623 | CLA  | C1D-ND  | 3.44  | 1.42        | 1.37     |
| 14  | 1     | 1609 | CLA  | C1D-ND  | 3.44  | 1.42        | 1.37     |
| 17  | B     | 844  | BCR  | C1-C6   | -3.44 | 1.49        | 1.53     |
| 14  | A     | 829  | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 14  | 2     | 832  | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | 0     | 205  | CLA  | C4D-ND  | -3.43 | 1.33        | 1.37     |
| 14  | 1     | 1629 | CLA  | C4D-ND  | -3.43 | 1.33        | 1.37     |
| 14  | 2     | 808  | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 17  | A     | 852  | BCR  | C1-C6   | -3.43 | 1.49        | 1.53     |
| 14  | B     | 814  | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 14  | 2     | 815  | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 14  | b     | 815  | CLA  | C1D-ND  | 3.42  | 1.42        | 1.37     |
| 14  | B     | 818  | CLA  | C4D-ND  | -3.42 | 1.33        | 1.37     |
| 14  | 1     | 1605 | CLA  | C1D-ND  | 3.42  | 1.42        | 1.37     |
| 14  | a     | 822  | CLA  | C1D-ND  | 3.42  | 1.42        | 1.37     |
| 14  | 2     | 842  | CLA  | C4D-ND  | -3.42 | 1.33        | 1.37     |
| 14  | a     | 802  | CLA  | C4D-ND  | -3.41 | 1.33        | 1.37     |
| 14  | a     | 806  | CLA  | C4D-ND  | -3.41 | 1.33        | 1.37     |
| 14  | b     | 804  | CLA  | C4D-ND  | -3.41 | 1.33        | 1.37     |
| 17  | y     | 102  | BCR  | C30-C25 | -3.41 | 1.49        | 1.53     |
| 14  | A     | 808  | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 14  | a     | 839  | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 14  | B     | 841  | CLA  | C4D-ND  | -3.41 | 1.33        | 1.37     |
| 17  | k     | 104  | BCR  | C1-C6   | -3.41 | 1.49        | 1.53     |
| 14  | B     | 840  | CLA  | C4D-ND  | -3.41 | 1.33        | 1.37     |
| 14  | b     | 816  | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 14  | 2     | 819  | CLA  | C4D-ND  | -3.41 | 1.33        | 1.37     |
| 14  | A     | 819  | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 17  | 1     | 1653 | BCR  | C1-C6   | -3.40 | 1.49        | 1.53     |
| 14  | B     | 805  | CLA  | C4D-ND  | -3.40 | 1.33        | 1.37     |
| 17  | K     | 102  | BCR  | C30-C25 | -3.40 | 1.49        | 1.53     |
| 17  | a     | 852  | BCR  | C1-C6   | -3.40 | 1.49        | 1.53     |
| 14  | a     | 818  | CLA  | C1D-ND  | 3.40  | 1.42        | 1.37     |
| 14  | a     | 819  | CLA  | C1D-ND  | 3.40  | 1.42        | 1.37     |
| 14  | A     | 828  | CLA  | C4D-ND  | -3.40 | 1.33        | 1.37     |
| 14  | 1     | 1640 | CLA  | C1D-ND  | 3.40  | 1.42        | 1.37     |
| 14  | a     | 808  | CLA  | C1D-ND  | 3.40  | 1.42        | 1.37     |
| 17  | m     | 102  | BCR  | C30-C25 | -3.40 | 1.49        | 1.53     |
| 14  | A     | 802  | CLA  | C4D-ND  | -3.40 | 1.33        | 1.37     |
| 14  | 1     | 1637 | CLA  | C1D-ND  | 3.40  | 1.42        | 1.37     |
| 14  | 2     | 816  | CLA  | C1D-ND  | 3.40  | 1.42        | 1.37     |
| 14  | B     | 827  | CLA  | C4D-ND  | -3.40 | 1.33        | 1.37     |
| 14  | 1     | 1607 | CLA  | C4D-ND  | -3.40 | 1.33        | 1.37     |
| 14  | 2     | 841  | CLA  | C4D-ND  | -3.40 | 1.33        | 1.37     |
| 17  | 2     | 845  | BCR  | C1-C6   | -3.40 | 1.49        | 1.53     |
| 14  | B     | 834  | CLA  | C1D-ND  | 3.40  | 1.42        | 1.37     |
| 14  | B     | 832  | CLA  | C1D-ND  | 3.39  | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 838  | CLA  | C1D-ND  | 3.39  | 1.42        | 1.37     |
| 14  | b     | 841  | CLA  | C4D-ND  | -3.39 | 1.33        | 1.37     |
| 14  | 1     | 1644 | CLA  | C4D-ND  | -3.39 | 1.33        | 1.37     |
| 14  | B     | 803  | CLA  | C4D-ND  | -3.39 | 1.33        | 1.37     |
| 17  | F     | 205  | BCR  | C30-C25 | -3.39 | 1.49        | 1.53     |
| 17  | I     | 101  | BCR  | C30-C25 | -3.39 | 1.49        | 1.53     |
| 14  | B     | 815  | CLA  | C1D-ND  | 3.39  | 1.42        | 1.37     |
| 17  | 0     | 209  | BCR  | C1-C6   | -3.39 | 1.49        | 1.53     |
| 14  | a     | 812  | CLA  | C1D-ND  | 3.39  | 1.42        | 1.37     |
| 14  | a     | 842  | CLA  | C4D-ND  | -3.39 | 1.33        | 1.37     |
| 14  | a     | 821  | CLA  | CHC-C1C | 3.39  | 1.43        | 1.35     |
| 14  | a     | 825  | CLA  | C4D-ND  | -3.38 | 1.33        | 1.37     |
| 14  | A     | 812  | CLA  | C1D-ND  | 3.38  | 1.41        | 1.37     |
| 14  | L     | 205  | CLA  | C4D-ND  | -3.38 | 1.33        | 1.37     |
| 14  | b     | 806  | CLA  | C4D-ND  | -3.38 | 1.33        | 1.37     |
| 17  | f     | 204  | BCR  | C30-C25 | -3.38 | 1.49        | 1.53     |
| 14  | A     | 839  | CLA  | C1D-ND  | 3.38  | 1.41        | 1.37     |
| 14  | B     | 807  | CLA  | C1D-ND  | 3.38  | 1.41        | 1.37     |
| 14  | A     | 842  | CLA  | C4D-ND  | -3.38 | 1.33        | 1.37     |
| 14  | 2     | 839  | CLA  | C1D-ND  | 3.38  | 1.41        | 1.37     |
| 14  | 2     | 835  | CLA  | C1D-ND  | 3.38  | 1.41        | 1.37     |
| 14  | b     | 805  | CLA  | C1D-ND  | 3.38  | 1.41        | 1.37     |
| 17  | L     | 207  | BCR  | C1-C6   | -3.38 | 1.49        | 1.53     |
| 17  | 0     | 201  | BCR  | C1-C6   | -3.38 | 1.49        | 1.53     |
| 14  | 1     | 1620 | CLA  | C1D-ND  | 3.38  | 1.41        | 1.37     |
| 14  | 1     | 1622 | CLA  | CHC-C1C | 3.38  | 1.43        | 1.35     |
| 14  | a     | 836  | CLA  | C1D-ND  | 3.37  | 1.41        | 1.37     |
| 14  | b     | 819  | CLA  | C4D-ND  | -3.37 | 1.33        | 1.37     |
| 17  | 6     | 204  | BCR  | C30-C25 | -3.37 | 1.49        | 1.53     |
| 14  | 2     | 807  | CLA  | C4D-ND  | -3.37 | 1.33        | 1.37     |
| 14  | l     | 204  | CLA  | C4D-ND  | -3.37 | 1.33        | 1.37     |
| 17  | A     | 856  | BCR  | C30-C25 | -3.37 | 1.49        | 1.53     |
| 14  | a     | 841  | CLA  | C1D-ND  | 3.37  | 1.41        | 1.37     |
| 14  | 2     | 805  | CLA  | C1D-ND  | 3.37  | 1.41        | 1.37     |
| 17  | k     | 102  | BCR  | C30-C25 | -3.37 | 1.49        | 1.53     |
| 17  | 8     | 1305 | BCR  | C30-C25 | -3.37 | 1.49        | 1.53     |
| 14  | l     | 206  | CLA  | C1D-ND  | 3.37  | 1.41        | 1.37     |
| 14  | 1     | 1643 | CLA  | C4D-ND  | -3.36 | 1.33        | 1.37     |
| 14  | a     | 832  | CLA  | C4D-ND  | -3.36 | 1.33        | 1.37     |
| 14  | 2     | 828  | CLA  | C4D-ND  | -3.36 | 1.33        | 1.37     |
| 17  | B     | 846  | BCR  | C1-C6   | -3.36 | 1.49        | 1.53     |
| 14  | 1     | 1613 | CLA  | C1D-ND  | 3.36  | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 821  | CLA  | CHC-C1C | 3.36  | 1.43        | 1.35     |
| 14  | A     | 803  | CLA  | C4D-ND  | -3.36 | 1.33        | 1.37     |
| 14  | l     | 206  | CLA  | C4D-ND  | -3.36 | 1.33        | 1.37     |
| 17  | A     | 849  | BCR  | C30-C25 | -3.36 | 1.49        | 1.53     |
| 17  | b     | 845  | BCR  | C30-C25 | -3.36 | 1.49        | 1.53     |
| 14  | A     | 836  | CLA  | C1D-ND  | 3.36  | 1.41        | 1.37     |
| 14  | B     | 825  | CLA  | C4D-ND  | -3.36 | 1.33        | 1.37     |
| 14  | 1     | 1633 | CLA  | C4D-ND  | -3.36 | 1.33        | 1.37     |
| 14  | 0     | 207  | CLA  | C4D-ND  | -3.36 | 1.33        | 1.37     |
| 17  | j     | 1305 | BCR  | C30-C25 | -3.35 | 1.49        | 1.53     |
| 14  | a     | 826  | CLA  | C1D-ND  | 3.35  | 1.41        | 1.37     |
| 17  | A     | 847  | BCR  | C30-C25 | -3.35 | 1.49        | 1.53     |
| 14  | A     | 834  | CLA  | C4D-ND  | -3.35 | 1.33        | 1.37     |
| 17  | a     | 847  | BCR  | C30-C25 | -3.35 | 1.49        | 1.53     |
| 14  | B     | 806  | CLA  | C4D-ND  | -3.35 | 1.33        | 1.37     |
| 17  | M     | 103  | BCR  | C30-C25 | -3.35 | 1.49        | 1.53     |
| 14  | b     | 842  | CLA  | C4D-ND  | -3.35 | 1.33        | 1.37     |
| 14  | A     | 826  | CLA  | C1D-ND  | 3.35  | 1.41        | 1.37     |
| 14  | 2     | 806  | CLA  | C4D-ND  | -3.35 | 1.33        | 1.37     |
| 14  | A     | 843  | CLA  | C4D-ND  | -3.35 | 1.33        | 1.37     |
| 14  | F     | 201  | CLA  | C1D-ND  | 3.35  | 1.41        | 1.37     |
| 14  | A     | 825  | CLA  | C1D-ND  | 3.34  | 1.41        | 1.37     |
| 17  | a     | 849  | BCR  | C30-C25 | -3.34 | 1.49        | 1.53     |
| 14  | 2     | 826  | CLA  | C4D-ND  | -3.34 | 1.33        | 1.37     |
| 14  | 1     | 1615 | CLA  | C4D-ND  | -3.34 | 1.33        | 1.37     |
| 17  | 1     | 1648 | BCR  | C30-C25 | -3.34 | 1.49        | 1.53     |
| 14  | L     | 203  | CLA  | C4D-ND  | -3.34 | 1.33        | 1.37     |
| 14  | B     | 806  | CLA  | C1D-ND  | 3.34  | 1.41        | 1.37     |
| 17  | B     | 844  | BCR  | C30-C25 | -3.34 | 1.49        | 1.53     |
| 14  | 1     | 1603 | CLA  | C4D-ND  | -3.33 | 1.33        | 1.37     |
| 14  | 1     | 1627 | CLA  | C1D-ND  | 3.33  | 1.41        | 1.37     |
| 14  | b     | 826  | CLA  | C4D-ND  | -3.33 | 1.33        | 1.37     |
| 17  | 2     | 847  | BCR  | C1-C6   | -3.33 | 1.49        | 1.53     |
| 14  | L     | 205  | CLA  | C1D-ND  | 3.33  | 1.41        | 1.37     |
| 14  | 2     | 803  | CLA  | C4D-ND  | -3.33 | 1.33        | 1.37     |
| 14  | a     | 804  | CLA  | C1D-ND  | 3.33  | 1.41        | 1.37     |
| 14  | 2     | 833  | CLA  | C1D-ND  | 3.33  | 1.41        | 1.37     |
| 14  | 1     | 1626 | CLA  | C1D-ND  | 3.33  | 1.41        | 1.37     |
| 14  | 1     | 1642 | CLA  | C1D-ND  | 3.33  | 1.41        | 1.37     |
| 17  | b     | 847  | BCR  | C1-C6   | -3.33 | 1.49        | 1.53     |
| 17  | 2     | 845  | BCR  | C30-C25 | -3.33 | 1.49        | 1.53     |
| 17  | J     | 103  | BCR  | C1-C6   | -3.33 | 1.49        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 833  | CLA  | C1D-ND  | 3.33  | 1.41        | 1.37     |
| 14  | A     | 825  | CLA  | C4D-ND  | -3.32 | 1.33        | 1.37     |
| 17  | A     | 848  | BCR  | C1-C6   | -3.32 | 1.49        | 1.53     |
| 14  | 2     | 839  | CLA  | C4D-ND  | -3.32 | 1.33        | 1.37     |
| 17  | A     | 847  | BCR  | C1-C6   | -3.32 | 1.49        | 1.53     |
| 14  | b     | 803  | CLA  | C4D-ND  | -3.32 | 1.33        | 1.37     |
| 17  | 1     | 1649 | BCR  | C1-C6   | -3.32 | 1.49        | 1.53     |
| 14  | a     | 814  | CLA  | C4D-ND  | -3.31 | 1.33        | 1.37     |
| 17  | j     | 1304 | BCR  | C1-C6   | -3.31 | 1.49        | 1.53     |
| 14  | a     | 828  | CLA  | C1D-ND  | 3.31  | 1.41        | 1.37     |
| 14  | B     | 838  | CLA  | C4D-ND  | -3.31 | 1.33        | 1.37     |
| 14  | 6     | 201  | CLA  | C1D-ND  | 3.31  | 1.41        | 1.37     |
| 14  | 0     | 207  | CLA  | C1D-ND  | 3.31  | 1.41        | 1.37     |
| 14  | b     | 834  | CLA  | C4D-ND  | -3.31 | 1.33        | 1.37     |
| 14  | A     | 814  | CLA  | C4D-ND  | -3.31 | 1.33        | 1.37     |
| 14  | b     | 827  | CLA  | C4D-ND  | -3.31 | 1.33        | 1.37     |
| 14  | 1     | 1635 | CLA  | C4D-ND  | -3.30 | 1.33        | 1.37     |
| 17  | a     | 848  | BCR  | C1-C6   | -3.30 | 1.49        | 1.53     |
| 14  | B     | 826  | CLA  | C4D-ND  | -3.30 | 1.33        | 1.37     |
| 14  | 2     | 808  | CLA  | C4D-ND  | -3.30 | 1.33        | 1.37     |
| 14  | B     | 807  | CLA  | C4D-ND  | -3.30 | 1.33        | 1.37     |
| 14  | A     | 830  | CLA  | C4D-ND  | -3.30 | 1.33        | 1.37     |
| 14  | B     | 829  | CLA  | C1D-ND  | 3.30  | 1.41        | 1.37     |
| 14  | A     | 806  | CLA  | C1D-ND  | 3.30  | 1.41        | 1.37     |
| 14  | a     | 805  | CLA  | C1D-ND  | 3.30  | 1.41        | 1.37     |
| 14  | f     | 201  | CLA  | C1D-ND  | 3.30  | 1.41        | 1.37     |
| 14  | a     | 843  | CLA  | C4D-ND  | -3.30 | 1.33        | 1.37     |
| 17  | 1     | 1650 | BCR  | C30-C25 | -3.30 | 1.49        | 1.53     |
| 14  | b     | 830  | CLA  | C1D-ND  | 3.30  | 1.41        | 1.37     |
| 14  | 1     | 1606 | CLA  | C1D-ND  | 3.30  | 1.41        | 1.37     |
| 14  | a     | 834  | CLA  | C4D-ND  | -3.29 | 1.33        | 1.37     |
| 14  | B     | 818  | CLA  | C1D-ND  | 3.29  | 1.41        | 1.37     |
| 14  | 1     | 1626 | CLA  | C4D-ND  | -3.29 | 1.33        | 1.37     |
| 14  | 1     | 1637 | CLA  | C4D-ND  | -3.29 | 1.33        | 1.37     |
| 14  | 1     | 1604 | CLA  | C4D-ND  | -3.29 | 1.33        | 1.37     |
| 14  | A     | 841  | CLA  | C1D-ND  | 3.29  | 1.41        | 1.37     |
| 17  | a     | 847  | BCR  | C1-C6   | -3.29 | 1.49        | 1.53     |
| 14  | b     | 807  | CLA  | C1D-ND  | 3.29  | 1.41        | 1.37     |
| 14  | 1     | 1629 | CLA  | C1D-ND  | 3.29  | 1.41        | 1.37     |
| 14  | a     | 836  | CLA  | C4D-ND  | -3.29 | 1.33        | 1.37     |
| 14  | z     | 102  | CLA  | CHC-C1C | 3.28  | 1.43        | 1.35     |
| 14  | 2     | 827  | CLA  | C4D-ND  | -3.28 | 1.33        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 803  | CLA  | C4D-ND  | -3.28 | 1.33        | 1.37     |
| 17  | 8     | 1304 | BCR  | C1-C6   | -3.28 | 1.49        | 1.53     |
| 14  | x     | 1701 | CLA  | CHC-C1C | 3.28  | 1.43        | 1.35     |
| 14  | A     | 836  | CLA  | C4D-ND  | -3.28 | 1.33        | 1.37     |
| 14  | b     | 839  | CLA  | C4D-ND  | -3.27 | 1.33        | 1.37     |
| 14  | 2     | 834  | CLA  | C4D-ND  | -3.27 | 1.33        | 1.37     |
| 14  | B     | 837  | CLA  | C1D-ND  | 3.27  | 1.41        | 1.37     |
| 14  | b     | 826  | CLA  | C1D-ND  | 3.27  | 1.41        | 1.37     |
| 14  | a     | 825  | CLA  | C1D-ND  | 3.27  | 1.41        | 1.37     |
| 14  | 2     | 819  | CLA  | C1D-ND  | 3.27  | 1.41        | 1.37     |
| 13  | 1     | 1602 | CL0  | C4D-ND  | -3.27 | 1.33        | 1.37     |
| 14  | f     | 201  | CLA  | C4D-ND  | -3.27 | 1.33        | 1.37     |
| 14  | a     | 809  | CLA  | C1D-ND  | 3.27  | 1.41        | 1.37     |
| 14  | X     | 1701 | CLA  | CHC-C1C | 3.27  | 1.43        | 1.35     |
| 14  | b     | 819  | CLA  | C1D-ND  | 3.27  | 1.41        | 1.37     |
| 14  | B     | 804  | CLA  | C1D-ND  | 3.26  | 1.41        | 1.37     |
| 14  | B     | 825  | CLA  | C1D-ND  | 3.26  | 1.41        | 1.37     |
| 14  | 2     | 830  | CLA  | C1D-ND  | 3.26  | 1.41        | 1.37     |
| 14  | A     | 828  | CLA  | C1D-ND  | 3.26  | 1.41        | 1.37     |
| 14  | 2     | 807  | CLA  | C1D-ND  | 3.26  | 1.41        | 1.37     |
| 14  | 1     | 1639 | CLA  | C1D-ND  | 3.26  | 1.41        | 1.37     |
| 14  | b     | 806  | CLA  | C1D-ND  | 3.26  | 1.41        | 1.37     |
| 14  | b     | 809  | CLA  | C4D-ND  | -3.26 | 1.33        | 1.37     |
| 14  | b     | 807  | CLA  | C4D-ND  | -3.26 | 1.33        | 1.37     |
| 14  | b     | 834  | CLA  | C1D-ND  | 3.26  | 1.41        | 1.37     |
| 14  | 2     | 838  | CLA  | C1D-ND  | 3.26  | 1.41        | 1.37     |
| 14  | a     | 835  | CLA  | C4D-ND  | -3.26 | 1.33        | 1.37     |
| 14  | 1     | 1608 | CLA  | C4D-ND  | -3.25 | 1.33        | 1.37     |
| 14  | b     | 838  | CLA  | C1D-ND  | 3.25  | 1.41        | 1.37     |
| 14  | 2     | 826  | CLA  | C1D-ND  | 3.25  | 1.41        | 1.37     |
| 17  | 1     | 1648 | BCR  | C1-C6   | -3.25 | 1.49        | 1.53     |
| 13  | A     | 801  | CL0  | C4D-ND  | -3.24 | 1.33        | 1.37     |
| 14  | B     | 833  | CLA  | C1D-ND  | 3.24  | 1.41        | 1.37     |
| 14  | A     | 807  | CLA  | C4D-ND  | -3.24 | 1.33        | 1.37     |
| 14  | B     | 802  | CLA  | C4D-ND  | -3.24 | 1.33        | 1.37     |
| 14  | a     | 806  | CLA  | C1D-ND  | 3.24  | 1.41        | 1.37     |
| 14  | F     | 203  | CLA  | C4D-ND  | -3.24 | 1.33        | 1.37     |
| 14  | 2     | 814  | CLA  | C4D-ND  | -3.24 | 1.33        | 1.37     |
| 14  | 2     | 816  | CLA  | C4D-ND  | -3.24 | 1.33        | 1.37     |
| 14  | B     | 830  | CLA  | C4D-ND  | -3.24 | 1.33        | 1.37     |
| 14  | A     | 838  | CLA  | C1D-ND  | 3.24  | 1.41        | 1.37     |
| 14  | 0     | 205  | CLA  | C1D-ND  | 3.24  | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | 2     | 831  | CLA  | C4D-ND  | -3.23 | 1.33        | 1.37     |
| 17  | 8     | 1304 | BCR  | C30-C25 | -3.23 | 1.49        | 1.53     |
| 14  | B     | 833  | CLA  | C4D-ND  | -3.23 | 1.33        | 1.37     |
| 14  | A     | 805  | CLA  | C1D-ND  | 3.23  | 1.41        | 1.37     |
| 14  | a     | 812  | CLA  | C4D-ND  | -3.23 | 1.33        | 1.37     |
| 17  | j     | 1304 | BCR  | C30-C25 | -3.23 | 1.49        | 1.53     |
| 14  | B     | 805  | CLA  | C1D-ND  | 3.23  | 1.41        | 1.37     |
| 14  | B     | 809  | CLA  | C4D-ND  | -3.23 | 1.33        | 1.37     |
| 17  | l     | 207  | BCR  | C1-C6   | -3.23 | 1.49        | 1.53     |
| 17  | 0     | 208  | BCR  | C1-C6   | -3.23 | 1.49        | 1.53     |
| 14  | B     | 813  | CLA  | C4D-ND  | -3.23 | 1.33        | 1.37     |
| 14  | A     | 840  | CLA  | C4D-ND  | -3.23 | 1.33        | 1.37     |
| 14  | 1     | 1640 | CLA  | C4D-ND  | -3.22 | 1.33        | 1.37     |
| 14  | 2     | 806  | CLA  | C1D-ND  | 3.22  | 1.41        | 1.37     |
| 14  | a     | 829  | CLA  | C4D-ND  | -3.22 | 1.33        | 1.37     |
| 14  | a     | 839  | CLA  | C4D-ND  | -3.22 | 1.33        | 1.37     |
| 14  | 2     | 809  | CLA  | C4D-ND  | -3.22 | 1.33        | 1.37     |
| 14  | A     | 809  | CLA  | C1D-ND  | 3.22  | 1.41        | 1.37     |
| 14  | 8     | 1301 | CLA  | C4D-ND  | -3.22 | 1.33        | 1.37     |
| 14  | b     | 838  | CLA  | C4D-ND  | -3.21 | 1.33        | 1.37     |
| 14  | j     | 1301 | CLA  | C4D-ND  | -3.21 | 1.33        | 1.37     |
| 14  | 1     | 1636 | CLA  | C4D-ND  | -3.21 | 1.33        | 1.37     |
| 14  | 1     | 1631 | CLA  | C4D-ND  | -3.21 | 1.33        | 1.37     |
| 14  | A     | 816  | CLA  | CHC-C1C | 3.21  | 1.43        | 1.35     |
| 14  | l     | 204  | CLA  | C1D-ND  | 3.21  | 1.41        | 1.37     |
| 14  | b     | 808  | CLA  | C4D-ND  | -3.21 | 1.33        | 1.37     |
| 14  | A     | 839  | CLA  | C4D-ND  | -3.21 | 1.33        | 1.37     |
| 14  | b     | 832  | CLA  | C4D-ND  | -3.21 | 1.33        | 1.37     |
| 14  | a     | 840  | CLA  | C4D-ND  | -3.21 | 1.33        | 1.37     |
| 14  | 1     | 1630 | CLA  | C4D-ND  | -3.21 | 1.33        | 1.37     |
| 14  | A     | 855  | CLA  | C4D-ND  | -3.21 | 1.33        | 1.37     |
| 17  | J     | 103  | BCR  | C30-C25 | -3.20 | 1.49        | 1.53     |
| 14  | B     | 810  | CLA  | C1D-ND  | 3.20  | 1.41        | 1.37     |
| 14  | 1     | 1620 | CLA  | C4D-ND  | -3.20 | 1.33        | 1.37     |
| 14  | B     | 808  | CLA  | C4D-ND  | -3.20 | 1.33        | 1.37     |
| 14  | a     | 807  | CLA  | C4D-ND  | -3.20 | 1.33        | 1.37     |
| 14  | a     | 816  | CLA  | CHC-C1C | 3.20  | 1.43        | 1.35     |
| 14  | 1     | 1607 | CLA  | C1D-ND  | 3.20  | 1.41        | 1.37     |
| 14  | a     | 832  | CLA  | CMB-C2B | -3.20 | 1.45        | 1.51     |
| 14  | A     | 835  | CLA  | C1D-ND  | 3.20  | 1.41        | 1.37     |
| 14  | 2     | 834  | CLA  | C1D-ND  | 3.20  | 1.41        | 1.37     |
| 14  | A     | 822  | CLA  | C4D-ND  | -3.20 | 1.33        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | 2     | 810  | CLA  | C4D-ND  | -3.19 | 1.33        | 1.37     |
| 14  | A     | 835  | CLA  | C4D-ND  | -3.19 | 1.33        | 1.37     |
| 14  | a     | 842  | CLA  | C1D-ND  | 3.19  | 1.41        | 1.37     |
| 14  | a     | 830  | CLA  | C4D-ND  | -3.19 | 1.33        | 1.37     |
| 14  | b     | 810  | CLA  | CMB-C2B | -3.19 | 1.45        | 1.51     |
| 13  | a     | 801  | CL0  | C4D-ND  | -3.19 | 1.33        | 1.37     |
| 14  | B     | 809  | CLA  | CMB-C2B | -3.19 | 1.45        | 1.51     |
| 14  | 2     | 810  | CLA  | CMB-C2B | -3.19 | 1.45        | 1.51     |
| 14  | F     | 201  | CLA  | C4D-ND  | -3.19 | 1.33        | 1.37     |
| 14  | 1     | 1608 | CLA  | C1D-ND  | 3.19  | 1.41        | 1.37     |
| 17  | L     | 206  | BCR  | C1-C6   | -3.19 | 1.49        | 1.53     |
| 14  | b     | 811  | CLA  | C1D-ND  | 3.19  | 1.41        | 1.37     |
| 14  | 2     | 832  | CLA  | C4D-ND  | -3.19 | 1.33        | 1.37     |
| 14  | 6     | 201  | CLA  | C4D-ND  | -3.19 | 1.33        | 1.37     |
| 14  | 1     | 1610 | CLA  | C1D-ND  | 3.18  | 1.41        | 1.37     |
| 14  | A     | 855  | CLA  | C1D-ND  | 3.18  | 1.41        | 1.37     |
| 14  | a     | 838  | CLA  | C1D-ND  | 3.18  | 1.41        | 1.37     |
| 14  | 2     | 829  | CLA  | C1D-ND  | 3.18  | 1.41        | 1.37     |
| 17  | 1     | 1652 | BCR  | C30-C25 | -3.18 | 1.49        | 1.53     |
| 17  | 0     | 209  | BCR  | C30-C25 | -3.18 | 1.49        | 1.53     |
| 14  | B     | 815  | CLA  | C4D-ND  | -3.18 | 1.33        | 1.37     |
| 14  | 1     | 1612 | CLA  | CHC-C1C | 3.18  | 1.43        | 1.35     |
| 14  | 2     | 809  | CLA  | C1D-ND  | 3.18  | 1.41        | 1.37     |
| 14  | b     | 810  | CLA  | C4D-ND  | -3.17 | 1.33        | 1.37     |
| 14  | 1     | 1639 | CLA  | C4D-ND  | -3.17 | 1.33        | 1.37     |
| 14  | 2     | 840  | CLA  | C4D-ND  | -3.17 | 1.33        | 1.37     |
| 14  | 1     | 1617 | CLA  | CHC-C1C | 3.17  | 1.43        | 1.35     |
| 14  | b     | 814  | CLA  | C4D-ND  | -3.17 | 1.33        | 1.37     |
| 14  | B     | 828  | CLA  | C1D-ND  | 3.17  | 1.41        | 1.37     |
| 14  | B     | 839  | CLA  | C4D-ND  | -3.17 | 1.33        | 1.37     |
| 14  | a     | 831  | CLA  | C4D-ND  | -3.17 | 1.33        | 1.37     |
| 14  | B     | 837  | CLA  | C4D-ND  | -3.17 | 1.33        | 1.37     |
| 14  | l     | 204  | CLA  | CHC-C1C | 3.17  | 1.43        | 1.35     |
| 14  | A     | 811  | CLA  | CHC-C1C | 3.17  | 1.43        | 1.35     |
| 14  | B     | 822  | CLA  | CHC-C1C | 3.17  | 1.43        | 1.35     |
| 14  | A     | 829  | CLA  | C4D-ND  | -3.16 | 1.33        | 1.37     |
| 14  | 2     | 838  | CLA  | C4D-ND  | -3.16 | 1.33        | 1.37     |
| 14  | A     | 834  | CLA  | C1D-ND  | 3.16  | 1.41        | 1.37     |
| 14  | 2     | 823  | CLA  | CHC-C1C | 3.16  | 1.43        | 1.35     |
| 14  | 2     | 802  | CLA  | C4D-ND  | -3.16 | 1.33        | 1.37     |
| 14  | 8     | 1303 | CLA  | CHC-C1C | 3.16  | 1.43        | 1.35     |
| 14  | B     | 831  | CLA  | C4D-ND  | -3.16 | 1.33        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 819  | CLA  | C4D-ND  | -3.16 | 1.33        | 1.37     |
| 14  | 1     | 1633 | CLA  | CMB-C2B | -3.16 | 1.45        | 1.51     |
| 14  | b     | 840  | CLA  | C4D-ND  | -3.15 | 1.33        | 1.37     |
| 14  | 1     | 1632 | CLA  | C4D-ND  | -3.15 | 1.33        | 1.37     |
| 14  | A     | 832  | CLA  | CMB-C2B | -3.15 | 1.45        | 1.51     |
| 17  | a     | 851  | BCR  | C30-C25 | -3.15 | 1.49        | 1.53     |
| 14  | b     | 816  | CLA  | C4D-ND  | -3.15 | 1.33        | 1.37     |
| 14  | 1     | 1613 | CLA  | C4D-ND  | -3.15 | 1.33        | 1.37     |
| 14  | B     | 808  | CLA  | C1D-ND  | 3.15  | 1.41        | 1.37     |
| 14  | A     | 838  | CLA  | C4D-ND  | -3.15 | 1.33        | 1.37     |
| 14  | a     | 807  | CLA  | C1D-ND  | 3.15  | 1.41        | 1.37     |
| 14  | a     | 840  | CLA  | C1D-ND  | 3.15  | 1.41        | 1.37     |
| 14  | 0     | 205  | CLA  | CHC-C1C | 3.15  | 1.43        | 1.35     |
| 14  | a     | 810  | CLA  | C4D-ND  | -3.15 | 1.33        | 1.37     |
| 14  | a     | 808  | CLA  | C4D-ND  | -3.15 | 1.33        | 1.37     |
| 14  | A     | 831  | CLA  | C4D-ND  | -3.15 | 1.33        | 1.37     |
| 14  | 2     | 805  | CLA  | C4D-ND  | -3.15 | 1.33        | 1.37     |
| 14  | A     | 819  | CLA  | C4D-ND  | -3.15 | 1.33        | 1.37     |
| 14  | 1     | 1641 | CLA  | C4D-ND  | -3.14 | 1.33        | 1.37     |
| 14  | A     | 807  | CLA  | C1D-ND  | 3.14  | 1.41        | 1.37     |
| 14  | A     | 842  | CLA  | C1D-ND  | 3.14  | 1.41        | 1.37     |
| 14  | b     | 841  | CLA  | C1D-ND  | 3.14  | 1.41        | 1.37     |
| 14  | 2     | 824  | CLA  | CHC-C1C | 3.14  | 1.43        | 1.35     |
| 14  | 2     | 811  | CLA  | C1D-ND  | 3.14  | 1.41        | 1.37     |
| 14  | 1     | 1623 | CLA  | C4D-ND  | -3.14 | 1.33        | 1.37     |
| 14  | 1     | 1635 | CLA  | C1D-ND  | 3.14  | 1.41        | 1.37     |
| 14  | 1     | 1643 | CLA  | C1D-ND  | 3.14  | 1.41        | 1.37     |
| 14  | b     | 805  | CLA  | C4D-ND  | -3.14 | 1.33        | 1.37     |
| 14  | a     | 822  | CLA  | C4D-ND  | -3.14 | 1.33        | 1.37     |
| 14  | b     | 823  | CLA  | CHC-C1C | 3.14  | 1.43        | 1.35     |
| 14  | A     | 840  | CLA  | C1D-ND  | 3.14  | 1.41        | 1.37     |
| 14  | a     | 811  | CLA  | C4D-ND  | -3.14 | 1.33        | 1.37     |
| 14  | a     | 826  | CLA  | C4D-ND  | -3.14 | 1.33        | 1.37     |
| 14  | 1     | 1636 | CLA  | C1D-ND  | 3.14  | 1.41        | 1.37     |
| 14  | B     | 810  | CLA  | C4D-ND  | -3.14 | 1.33        | 1.37     |
| 14  | 2     | 833  | CLA  | C4D-ND  | -3.14 | 1.33        | 1.37     |
| 14  | L     | 203  | CLA  | C1D-ND  | 3.14  | 1.41        | 1.37     |
| 14  | a     | 813  | CLA  | C4D-ND  | -3.14 | 1.33        | 1.37     |
| 14  | b     | 802  | CLA  | C4D-ND  | -3.14 | 1.33        | 1.37     |
| 14  | j     | 1303 | CLA  | CHC-C1C | 3.14  | 1.43        | 1.35     |
| 14  | b     | 829  | CLA  | C1D-ND  | 3.14  | 1.41        | 1.37     |
| 14  | a     | 803  | CLA  | C1D-ND  | 3.13  | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 829  | CLA  | C4D-ND  | -3.13 | 1.33        | 1.37     |
| 14  | b     | 809  | CLA  | C1D-ND  | 3.13  | 1.41        | 1.37     |
| 14  | 2     | 811  | CLA  | C4D-ND  | -3.13 | 1.33        | 1.37     |
| 14  | J     | 102  | CLA  | CHC-C1C | 3.13  | 1.43        | 1.35     |
| 14  | A     | 804  | CLA  | C4D-ND  | -3.13 | 1.33        | 1.37     |
| 14  | B     | 804  | CLA  | C4D-ND  | -3.13 | 1.33        | 1.37     |
| 14  | b     | 831  | CLA  | C4D-ND  | -3.13 | 1.33        | 1.37     |
| 14  | A     | 812  | CLA  | C4D-ND  | -3.13 | 1.33        | 1.37     |
| 14  | L     | 203  | CLA  | CHC-C1C | 3.13  | 1.43        | 1.35     |
| 14  | 1     | 1605 | CLA  | C4D-ND  | -3.13 | 1.33        | 1.37     |
| 17  | A     | 851  | BCR  | C30-C25 | -3.13 | 1.49        | 1.53     |
| 13  | A     | 801  | CL0  | C1D-ND  | 3.13  | 1.41        | 1.37     |
| 14  | A     | 826  | CLA  | C4D-ND  | -3.13 | 1.33        | 1.37     |
| 14  | B     | 839  | CLA  | CHC-C1C | 3.13  | 1.43        | 1.35     |
| 14  | a     | 811  | CLA  | CHC-C1C | 3.12  | 1.43        | 1.35     |
| 14  | b     | 840  | CLA  | CHC-C1C | 3.12  | 1.43        | 1.35     |
| 14  | 1     | 1609 | CLA  | C4D-ND  | -3.12 | 1.33        | 1.37     |
| 14  | B     | 828  | CLA  | C4D-ND  | -3.12 | 1.33        | 1.37     |
| 14  | b     | 810  | CLA  | C1D-ND  | 3.12  | 1.41        | 1.37     |
| 14  | 8     | 1301 | CLA  | CHC-C1C | 3.12  | 1.43        | 1.35     |
| 17  | 0     | 201  | BCR  | C30-C25 | -3.12 | 1.49        | 1.53     |
| 14  | a     | 835  | CLA  | C1D-ND  | 3.12  | 1.41        | 1.37     |
| 14  | a     | 834  | CLA  | C1D-ND  | 3.12  | 1.41        | 1.37     |
| 14  | F     | 203  | CLA  | CHC-C1C | 3.12  | 1.43        | 1.35     |
| 17  | L     | 207  | BCR  | C30-C25 | -3.12 | 1.49        | 1.53     |
| 14  | b     | 824  | CLA  | CHC-C1C | 3.12  | 1.43        | 1.35     |
| 14  | B     | 832  | CLA  | C4D-ND  | -3.12 | 1.33        | 1.37     |
| 14  | 1     | 1624 | CLA  | C4D-ND  | -3.11 | 1.33        | 1.37     |
| 13  | 1     | 1602 | CL0  | C1D-ND  | 3.11  | 1.41        | 1.37     |
| 14  | A     | 823  | CLA  | C4D-ND  | -3.11 | 1.33        | 1.37     |
| 14  | b     | 829  | CLA  | CMB-C2B | -3.11 | 1.45        | 1.51     |
| 14  | k     | 103  | CLA  | CHC-C1C | 3.11  | 1.42        | 1.35     |
| 14  | A     | 810  | CLA  | C4D-ND  | -3.11 | 1.33        | 1.37     |
| 14  | B     | 823  | CLA  | CHC-C1C | 3.11  | 1.42        | 1.35     |
| 14  | a     | 838  | CLA  | C4D-ND  | -3.11 | 1.33        | 1.37     |
| 14  | 1     | 1611 | CLA  | C4D-ND  | -3.11 | 1.33        | 1.37     |
| 14  | F     | 201  | CLA  | CHC-C1C | 3.11  | 1.42        | 1.35     |
| 14  | 1     | 1619 | CLA  | CHC-C1C | 3.11  | 1.42        | 1.35     |
| 14  | 1     | 1645 | CLA  | C4D-ND  | -3.11 | 1.33        | 1.37     |
| 14  | B     | 820  | CLA  | C4D-ND  | -3.11 | 1.33        | 1.37     |
| 13  | a     | 801  | CL0  | C1D-ND  | 3.10  | 1.41        | 1.37     |
| 14  | B     | 840  | CLA  | C1D-ND  | 3.10  | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 802  | CLA  | C1D-ND  | 3.10  | 1.41        | 1.37     |
| 14  | 2     | 802  | CLA  | C1D-ND  | 3.10  | 1.41        | 1.37     |
| 14  | A     | 803  | CLA  | C1D-ND  | 3.10  | 1.41        | 1.37     |
| 14  | A     | 802  | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 14  | j     | 1301 | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 14  | B     | 820  | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 14  | 9     | 103  | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 14  | f     | 201  | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 14  | 1     | 1618 | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 14  | 2     | 815  | CLA  | C4D-ND  | -3.10 | 1.33        | 1.37     |
| 14  | 2     | 803  | CLA  | C1D-ND  | 3.10  | 1.41        | 1.37     |
| 14  | 2     | 829  | CLA  | C4D-ND  | -3.10 | 1.33        | 1.37     |
| 14  | K     | 103  | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 14  | B     | 828  | CLA  | CMB-C2B | -3.10 | 1.45        | 1.51     |
| 14  | 1     | 1612 | CLA  | C4D-ND  | -3.10 | 1.33        | 1.37     |
| 14  | 2     | 810  | CLA  | C1D-ND  | 3.10  | 1.41        | 1.37     |
| 14  | 2     | 821  | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 14  | A     | 808  | CLA  | C4D-ND  | -3.10 | 1.33        | 1.37     |
| 14  | A     | 817  | CLA  | CHC-C1C | 3.09  | 1.42        | 1.35     |
| 14  | 1     | 1610 | CLA  | C4D-ND  | -3.09 | 1.33        | 1.37     |
| 14  | A     | 813  | CLA  | C4D-ND  | -3.09 | 1.33        | 1.37     |
| 14  | 2     | 840  | CLA  | CHC-C1C | 3.09  | 1.42        | 1.35     |
| 14  | b     | 821  | CLA  | CHC-C1C | 3.09  | 1.42        | 1.35     |
| 14  | A     | 818  | CLA  | CHC-C1C | 3.09  | 1.42        | 1.35     |
| 14  | 1     | 1627 | CLA  | C4D-ND  | -3.09 | 1.33        | 1.37     |
| 14  | B     | 829  | CLA  | C4D-ND  | -3.09 | 1.33        | 1.37     |
| 14  | 2     | 829  | CLA  | CMB-C2B | -3.09 | 1.45        | 1.51     |
| 17  | b     | 844  | BCR  | C30-C25 | -3.09 | 1.49        | 1.53     |
| 14  | 1     | 1604 | CLA  | C1D-ND  | 3.09  | 1.41        | 1.37     |
| 14  | a     | 815  | CLA  | C4D-ND  | -3.09 | 1.33        | 1.37     |
| 14  | k     | 101  | CLA  | C4D-ND  | -3.09 | 1.33        | 1.37     |
| 14  | B     | 814  | CLA  | C4D-ND  | -3.09 | 1.33        | 1.37     |
| 14  | A     | 816  | CLA  | C4D-ND  | -3.09 | 1.33        | 1.37     |
| 14  | 1     | 1616 | CLA  | C4D-ND  | -3.09 | 1.33        | 1.37     |
| 14  | a     | 817  | CLA  | CHC-C1C | 3.09  | 1.42        | 1.35     |
| 14  | 6     | 201  | CLA  | CHC-C1C | 3.09  | 1.42        | 1.35     |
| 14  | b     | 811  | CLA  | C4D-ND  | -3.09 | 1.33        | 1.37     |
| 14  | 2     | 830  | CLA  | C4D-ND  | -3.09 | 1.33        | 1.37     |
| 14  | A     | 815  | CLA  | C4D-ND  | -3.09 | 1.33        | 1.37     |
| 14  | a     | 809  | CLA  | C4D-ND  | -3.08 | 1.33        | 1.37     |
| 14  | 1     | 1641 | CLA  | C1D-ND  | 3.08  | 1.41        | 1.37     |
| 14  | b     | 821  | CLA  | C4D-ND  | -3.08 | 1.33        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | 1     | 1614 | CLA  | C4D-ND  | -3.08 | 1.33        | 1.37     |
| 17  | 2     | 844  | BCR  | C30-C25 | -3.08 | 1.49        | 1.53     |
| 14  | A     | 837  | CLA  | CHC-C1C | 3.08  | 1.42        | 1.35     |
| 14  | 2     | 841  | CLA  | C1D-ND  | 3.08  | 1.41        | 1.37     |
| 14  | A     | 805  | CLA  | C4D-ND  | -3.08 | 1.33        | 1.37     |
| 14  | a     | 818  | CLA  | CHC-C1C | 3.08  | 1.42        | 1.35     |
| 14  | 1     | 1638 | CLA  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 14  | B     | 835  | CLA  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 14  | K     | 101  | CLA  | C4D-ND  | -3.07 | 1.33        | 1.37     |
| 14  | a     | 844  | CLA  | C4D-ND  | -3.07 | 1.33        | 1.37     |
| 14  | j     | 1302 | CLA  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 14  | a     | 823  | CLA  | C4D-ND  | -3.07 | 1.33        | 1.37     |
| 14  | b     | 838  | CLA  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 17  | B     | 843  | BCR  | C30-C25 | -3.07 | 1.49        | 1.53     |
| 14  | b     | 836  | CLA  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 14  | a     | 802  | CLA  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 14  | B     | 822  | CLA  | C4D-ND  | -3.07 | 1.33        | 1.37     |
| 14  | b     | 828  | CLA  | C1D-ND  | 3.07  | 1.41        | 1.37     |
| 14  | A     | 844  | CLA  | C4D-ND  | -3.07 | 1.33        | 1.37     |
| 14  | b     | 830  | CLA  | C4D-ND  | -3.07 | 1.33        | 1.37     |
| 14  | B     | 835  | CLA  | C4D-ND  | -3.07 | 1.33        | 1.37     |
| 14  | 1     | 1603 | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 14  | A     | 828  | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 14  | b     | 830  | CLA  | CMB-C2B | -3.06 | 1.45        | 1.51     |
| 14  | 1     | 1638 | CLA  | C4D-ND  | -3.06 | 1.33        | 1.37     |
| 14  | 1     | 1606 | CLA  | C4D-ND  | -3.06 | 1.33        | 1.37     |
| 14  | 9     | 101  | CLA  | C4D-ND  | -3.06 | 1.33        | 1.37     |
| 14  | 1     | 1617 | CLA  | C4D-ND  | -3.06 | 1.33        | 1.37     |
| 14  | 2     | 805  | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 14  | 1     | 1634 | CLA  | C1D-ND  | 3.06  | 1.41        | 1.37     |
| 14  | 2     | 836  | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 14  | a     | 804  | CLA  | C4D-ND  | -3.06 | 1.33        | 1.37     |
| 14  | a     | 816  | CLA  | C4D-ND  | -3.06 | 1.33        | 1.37     |
| 14  | A     | 809  | CLA  | C4D-ND  | -3.06 | 1.33        | 1.37     |
| 14  | A     | 837  | CLA  | C4D-ND  | -3.06 | 1.33        | 1.37     |
| 14  | B     | 827  | CLA  | C1D-ND  | 3.06  | 1.41        | 1.37     |
| 14  | 1     | 1632 | CLA  | C1D-ND  | 3.06  | 1.41        | 1.37     |
| 14  | b     | 825  | CLA  | C4D-ND  | -3.06 | 1.33        | 1.37     |
| 14  | 1     | 1616 | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 14  | B     | 802  | CLA  | C1D-ND  | 3.06  | 1.41        | 1.37     |
| 14  | b     | 803  | CLA  | C1D-ND  | 3.06  | 1.41        | 1.37     |
| 14  | 2     | 828  | CLA  | C1D-ND  | 3.06  | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 841  | CLA  | C4D-ND  | -3.06 | 1.33        | 1.37     |
| 14  | A     | 811  | CLA  | C4D-ND  | -3.06 | 1.33        | 1.37     |
| 14  | a     | 837  | CLA  | C4D-ND  | -3.06 | 1.33        | 1.37     |
| 14  | B     | 813  | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 14  | a     | 828  | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 14  | B     | 829  | CLA  | CMB-C2B | -3.06 | 1.45        | 1.51     |
| 14  | 8     | 1302 | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 14  | b     | 820  | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 14  | 2     | 838  | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 14  | A     | 813  | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 14  | B     | 827  | CLA  | CHC-C1C | 3.05  | 1.42        | 1.35     |
| 14  | b     | 812  | CLA  | C4D-ND  | -3.05 | 1.33        | 1.37     |
| 14  | b     | 835  | CLA  | CHC-C1C | 3.05  | 1.42        | 1.35     |
| 14  | B     | 812  | CLA  | C4D-ND  | -3.05 | 1.33        | 1.37     |
| 14  | B     | 837  | CLA  | CHC-C1C | 3.05  | 1.42        | 1.35     |
| 14  | b     | 842  | CLA  | C1D-ND  | 3.05  | 1.41        | 1.37     |
| 14  | 2     | 835  | CLA  | CHC-C1C | 3.05  | 1.42        | 1.35     |
| 14  | a     | 837  | CLA  | CHC-C1C | 3.05  | 1.42        | 1.35     |
| 14  | b     | 837  | CLA  | C4D-ND  | -3.05 | 1.33        | 1.37     |
| 14  | 2     | 828  | CLA  | CHC-C1C | 3.05  | 1.42        | 1.35     |
| 14  | A     | 841  | CLA  | C4D-ND  | -3.05 | 1.33        | 1.37     |
| 14  | B     | 809  | CLA  | C1D-ND  | 3.05  | 1.41        | 1.37     |
| 14  | a     | 805  | CLA  | C4D-ND  | -3.04 | 1.33        | 1.37     |
| 14  | B     | 819  | CLA  | C4D-ND  | -3.04 | 1.33        | 1.37     |
| 14  | 2     | 815  | CLA  | CHC-C1C | 3.04  | 1.42        | 1.35     |
| 14  | A     | 815  | CLA  | CHC-C1C | 3.04  | 1.42        | 1.35     |
| 14  | 2     | 820  | CLA  | CHC-C1C | 3.04  | 1.42        | 1.35     |
| 14  | b     | 814  | CLA  | CHC-C1C | 3.04  | 1.42        | 1.35     |
| 14  | b     | 815  | CLA  | CHC-C1C | 3.04  | 1.42        | 1.35     |
| 14  | b     | 823  | CLA  | C4D-ND  | -3.04 | 1.33        | 1.37     |
| 14  | a     | 813  | CLA  | CHC-C1C | 3.04  | 1.42        | 1.35     |
| 14  | b     | 805  | CLA  | CHC-C1C | 3.04  | 1.42        | 1.35     |
| 14  | b     | 815  | CLA  | C4D-ND  | -3.04 | 1.33        | 1.37     |
| 14  | k     | 103  | CLA  | C4D-ND  | -3.04 | 1.33        | 1.37     |
| 14  | 2     | 821  | CLA  | C4D-ND  | -3.04 | 1.33        | 1.37     |
| 14  | J     | 101  | CLA  | CHC-C1C | 3.04  | 1.42        | 1.35     |
| 14  | 1     | 1609 | CLA  | CHC-C1C | 3.04  | 1.42        | 1.35     |
| 14  | 2     | 842  | CLA  | C1D-ND  | 3.04  | 1.41        | 1.37     |
| 14  | A     | 832  | CLA  | C1D-ND  | 3.04  | 1.41        | 1.37     |
| 14  | B     | 824  | CLA  | C4D-ND  | -3.04 | 1.33        | 1.37     |
| 14  | B     | 841  | CLA  | C1D-ND  | 3.03  | 1.41        | 1.37     |
| 14  | a     | 815  | CLA  | CHC-C1C | 3.03  | 1.42        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | 1     | 1614 | CLA  | CHC-C1C | 3.03  | 1.42        | 1.35     |
| 14  | 2     | 830  | CLA  | CMB-C2B | -3.03 | 1.45        | 1.51     |
| 14  | 1     | 1626 | CLA  | CHC-C1C | 3.03  | 1.42        | 1.35     |
| 14  | B     | 817  | CLA  | C4D-ND  | -3.03 | 1.33        | 1.37     |
| 14  | K     | 103  | CLA  | C4D-ND  | -3.03 | 1.33        | 1.37     |
| 14  | 1     | 1633 | CLA  | C1D-ND  | 3.03  | 1.41        | 1.37     |
| 14  | b     | 820  | CLA  | C4D-ND  | -3.03 | 1.33        | 1.37     |
| 14  | a     | 825  | CLA  | CHC-C1C | 3.03  | 1.42        | 1.35     |
| 14  | 1     | 1642 | CLA  | C4D-ND  | -3.03 | 1.33        | 1.37     |
| 14  | b     | 833  | CLA  | C4D-ND  | -3.03 | 1.33        | 1.37     |
| 14  | 2     | 818  | CLA  | C4D-ND  | -3.03 | 1.33        | 1.37     |
| 14  | b     | 826  | CLA  | CHC-C1C | 3.03  | 1.42        | 1.35     |
| 14  | b     | 828  | CLA  | CHC-C1C | 3.03  | 1.42        | 1.35     |
| 14  | B     | 825  | CLA  | CHC-C1C | 3.03  | 1.42        | 1.35     |
| 14  | 2     | 812  | CLA  | C4D-ND  | -3.03 | 1.33        | 1.37     |
| 14  | A     | 803  | CLA  | CHC-C1C | 3.03  | 1.42        | 1.35     |
| 14  | 2     | 813  | CLA  | C4D-ND  | -3.03 | 1.33        | 1.37     |
| 14  | 1     | 1629 | CLA  | CHC-C1C | 3.02  | 1.42        | 1.35     |
| 14  | B     | 811  | CLA  | C4D-ND  | -3.02 | 1.33        | 1.37     |
| 14  | 2     | 820  | CLA  | C4D-ND  | -3.02 | 1.33        | 1.37     |
| 14  | a     | 809  | CLA  | CHC-C1C | 3.02  | 1.42        | 1.35     |
| 14  | 2     | 826  | CLA  | CHC-C1C | 3.02  | 1.42        | 1.35     |
| 14  | A     | 825  | CLA  | CHC-C1C | 3.02  | 1.42        | 1.35     |
| 14  | A     | 840  | CLA  | CHC-C1C | 3.02  | 1.42        | 1.35     |
| 14  | B     | 834  | CLA  | CHC-C1C | 3.02  | 1.42        | 1.35     |
| 14  | a     | 822  | CLA  | CHC-C1C | 3.02  | 1.42        | 1.35     |
| 14  | 2     | 814  | CLA  | CHC-C1C | 3.02  | 1.42        | 1.35     |
| 14  | B     | 833  | CLA  | CHC-C1C | 3.02  | 1.42        | 1.35     |
| 14  | b     | 825  | CLA  | CHC-C1C | 3.02  | 1.42        | 1.35     |
| 14  | A     | 823  | CLA  | CHC-C1C | 3.02  | 1.42        | 1.35     |
| 14  | B     | 836  | CLA  | C4D-ND  | -3.02 | 1.33        | 1.37     |
| 14  | B     | 804  | CLA  | CHC-C1C | 3.02  | 1.42        | 1.35     |
| 14  | B     | 819  | CLA  | CHC-C1C | 3.02  | 1.42        | 1.35     |
| 14  | 1     | 1604 | CLA  | CHC-C1C | 3.02  | 1.42        | 1.35     |
| 14  | A     | 842  | CLA  | CHC-C1C | 3.01  | 1.42        | 1.35     |
| 14  | 2     | 837  | CLA  | C4D-ND  | -3.01 | 1.33        | 1.37     |
| 14  | A     | 834  | CLA  | CHC-C1C | 3.01  | 1.42        | 1.35     |
| 14  | 1     | 1624 | CLA  | CHC-C1C | 3.01  | 1.42        | 1.35     |
| 14  | B     | 814  | CLA  | CHC-C1C | 3.01  | 1.42        | 1.35     |
| 14  | A     | 822  | CLA  | CHC-C1C | 3.01  | 1.42        | 1.35     |
| 14  | b     | 818  | CLA  | C4D-ND  | -3.01 | 1.33        | 1.37     |
| 14  | b     | 834  | CLA  | CHC-C1C | 3.01  | 1.42        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 824  | CLA  | CHC-C1C | 3.01  | 1.42        | 1.35     |
| 14  | 1     | 1623 | CLA  | CHC-C1C | 3.01  | 1.42        | 1.35     |
| 14  | b     | 804  | CLA  | C1D-ND  | 3.01  | 1.41        | 1.37     |
| 14  | 2     | 834  | CLA  | CHC-C1C | 3.01  | 1.42        | 1.35     |
| 14  | b     | 827  | CLA  | CHC-C1C | 3.01  | 1.42        | 1.35     |
| 14  | 9     | 103  | CLA  | C4D-ND  | -3.00 | 1.33        | 1.37     |
| 14  | B     | 826  | CLA  | CHC-C1C | 3.00  | 1.42        | 1.35     |
| 14  | 1     | 1641 | CLA  | CHC-C1C | 3.00  | 1.42        | 1.35     |
| 14  | a     | 834  | CLA  | CHC-C1C | 3.00  | 1.42        | 1.35     |
| 14  | a     | 840  | CLA  | CHC-C1C | 3.00  | 1.42        | 1.35     |
| 14  | 2     | 825  | CLA  | CHC-C1C | 3.00  | 1.42        | 1.35     |
| 14  | B     | 828  | CLA  | CHC-C1C | 3.00  | 1.42        | 1.35     |
| 14  | a     | 823  | CLA  | CHC-C1C | 3.00  | 1.42        | 1.35     |
| 14  | 1     | 1635 | CLA  | CHC-C1C | 3.00  | 1.42        | 1.35     |
| 14  | A     | 808  | CLA  | CHC-C1C | 3.00  | 1.42        | 1.35     |
| 14  | b     | 822  | CLA  | CHC-C1C | 2.99  | 1.42        | 1.35     |
| 14  | a     | 843  | CLA  | CMB-C2B | -2.99 | 1.45        | 1.51     |
| 14  | 1     | 1606 | CLA  | CHC-C1C | 2.99  | 1.42        | 1.35     |
| 14  | A     | 805  | CLA  | CHC-C1C | 2.99  | 1.42        | 1.35     |
| 14  | 2     | 827  | CLA  | CHC-C1C | 2.99  | 1.42        | 1.35     |
| 14  | 2     | 825  | CLA  | C4D-ND  | -2.99 | 1.33        | 1.37     |
| 14  | a     | 831  | CLA  | C1D-ND  | 2.99  | 1.41        | 1.37     |
| 14  | a     | 805  | CLA  | CHC-C1C | 2.99  | 1.42        | 1.35     |
| 14  | a     | 814  | CLA  | CHC-C1C | 2.99  | 1.42        | 1.35     |
| 14  | a     | 833  | CLA  | C1D-ND  | 2.99  | 1.41        | 1.37     |
| 14  | a     | 808  | CLA  | CHC-C1C | 2.99  | 1.42        | 1.35     |
| 14  | a     | 842  | CLA  | CHC-C1C | 2.99  | 1.42        | 1.35     |
| 14  | 2     | 836  | CLA  | C4D-ND  | -2.99 | 1.33        | 1.37     |
| 14  | A     | 820  | CLA  | C4D-ND  | -2.99 | 1.33        | 1.37     |
| 14  | 2     | 823  | CLA  | C4D-ND  | -2.99 | 1.33        | 1.37     |
| 14  | B     | 821  | CLA  | CHC-C1C | 2.99  | 1.42        | 1.35     |
| 14  | 1     | 1644 | CLA  | CMB-C2B | -2.98 | 1.45        | 1.51     |
| 14  | 1     | 1610 | CLA  | CHC-C1C | 2.98  | 1.42        | 1.35     |
| 14  | A     | 830  | CLA  | C1D-ND  | 2.98  | 1.41        | 1.37     |
| 14  | 1     | 1645 | CLA  | CHC-C1C | 2.98  | 1.42        | 1.35     |
| 14  | a     | 820  | CLA  | C4D-ND  | -2.98 | 1.33        | 1.37     |
| 14  | a     | 803  | CLA  | CHC-C1C | 2.98  | 1.42        | 1.35     |
| 14  | 6     | 203  | CLA  | C4D-ND  | -2.98 | 1.33        | 1.37     |
| 14  | A     | 833  | CLA  | C1D-ND  | 2.98  | 1.41        | 1.37     |
| 14  | a     | 836  | CLA  | CMB-C2B | -2.98 | 1.45        | 1.51     |
| 14  | b     | 836  | CLA  | C4D-ND  | -2.98 | 1.33        | 1.37     |
| 14  | B     | 831  | CLA  | CHC-C1C | 2.98  | 1.42        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 832  | CLA  | C1D-ND  | 2.98  | 1.41        | 1.37     |
| 14  | F     | 204  | CLA  | C4D-ND  | -2.98 | 1.33        | 1.37     |
| 14  | B     | 819  | CLA  | CMB-C2B | -2.98 | 1.45        | 1.51     |
| 14  | 2     | 832  | CLA  | CHC-C1C | 2.97  | 1.42        | 1.35     |
| 14  | b     | 817  | CLA  | C4D-ND  | -2.97 | 1.33        | 1.37     |
| 14  | 1     | 1637 | CLA  | CMB-C2B | -2.97 | 1.45        | 1.51     |
| 14  | a     | 844  | CLA  | CHC-C1C | 2.97  | 1.42        | 1.35     |
| 14  | 2     | 804  | CLA  | C1D-ND  | 2.97  | 1.41        | 1.37     |
| 14  | a     | 830  | CLA  | C1D-ND  | 2.97  | 1.41        | 1.37     |
| 14  | 1     | 1644 | CLA  | CMD-C2D | -2.97 | 1.44        | 1.50     |
| 14  | b     | 829  | CLA  | CHC-C1C | 2.96  | 1.42        | 1.35     |
| 14  | A     | 843  | CLA  | CMB-C2B | -2.96 | 1.45        | 1.51     |
| 14  | a     | 833  | CLA  | CHC-C1C | 2.96  | 1.42        | 1.35     |
| 14  | b     | 818  | CLA  | CMB-C2B | -2.96 | 1.45        | 1.51     |
| 14  | A     | 836  | CLA  | CMB-C2B | -2.96 | 1.45        | 1.51     |
| 14  | 6     | 203  | CLA  | CHC-C1C | 2.96  | 1.42        | 1.35     |
| 14  | A     | 809  | CLA  | CHC-C1C | 2.96  | 1.42        | 1.35     |
| 14  | f     | 203  | CLA  | C4D-ND  | -2.96 | 1.33        | 1.37     |
| 14  | k     | 101  | CLA  | CHC-C1C | 2.96  | 1.42        | 1.35     |
| 14  | 1     | 1620 | CLA  | CHC-C1C | 2.96  | 1.42        | 1.35     |
| 14  | 2     | 817  | CLA  | C4D-ND  | -2.96 | 1.33        | 1.37     |
| 14  | A     | 831  | CLA  | C1D-ND  | 2.96  | 1.41        | 1.37     |
| 14  | 1     | 1642 | CLA  | CHC-C1C | 2.96  | 1.42        | 1.35     |
| 14  | 1     | 1643 | CLA  | CHC-C1C | 2.96  | 1.42        | 1.35     |
| 14  | 2     | 803  | CLA  | CMB-C2B | -2.96 | 1.45        | 1.51     |
| 14  | A     | 812  | CLA  | CHC-C1C | 2.96  | 1.42        | 1.35     |
| 14  | a     | 843  | CLA  | CMD-C2D | -2.96 | 1.44        | 1.50     |
| 14  | 2     | 822  | CLA  | CHC-C1C | 2.96  | 1.42        | 1.35     |
| 14  | b     | 820  | CLA  | CMB-C2B | -2.96 | 1.45        | 1.51     |
| 14  | A     | 833  | CLA  | CHC-C1C | 2.96  | 1.42        | 1.35     |
| 14  | 1     | 1628 | CLA  | CHC-C1C | 2.96  | 1.42        | 1.35     |
| 14  | 1     | 1615 | CLA  | CHC-C1C | 2.96  | 1.42        | 1.35     |
| 14  | b     | 839  | CLA  | CMB-C2B | -2.96 | 1.45        | 1.51     |
| 14  | J     | 101  | CLA  | C4D-ND  | -2.96 | 1.33        | 1.37     |
| 14  | 2     | 829  | CLA  | CHC-C1C | 2.96  | 1.42        | 1.35     |
| 14  | 1     | 1621 | CLA  | C4D-ND  | -2.95 | 1.33        | 1.37     |
| 20  | B     | 849  | LMG  | O7-C8   | -2.95 | 1.39        | 1.46     |
| 14  | X     | 1701 | CLA  | C4D-ND  | -2.95 | 1.33        | 1.37     |
| 14  | a     | 827  | CLA  | CHC-C1C | 2.95  | 1.42        | 1.35     |
| 14  | 1     | 1634 | CLA  | CHC-C1C | 2.95  | 1.42        | 1.35     |
| 14  | A     | 844  | CLA  | CHC-C1C | 2.95  | 1.42        | 1.35     |
| 14  | b     | 832  | CLA  | CHC-C1C | 2.95  | 1.42        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 810  | CLA  | CHC-C1C | 2.95  | 1.42        | 1.35     |
| 14  | B     | 817  | CLA  | CMB-C2B | -2.95 | 1.45        | 1.51     |
| 14  | A     | 819  | CLA  | CHC-C1C | 2.95  | 1.42        | 1.35     |
| 14  | b     | 813  | CLA  | C4D-ND  | -2.95 | 1.33        | 1.37     |
| 14  | a     | 829  | CLA  | CHC-C1C | 2.95  | 1.42        | 1.35     |
| 14  | A     | 814  | CLA  | CHC-C1C | 2.95  | 1.42        | 1.35     |
| 14  | 1     | 1630 | CLA  | CHC-C1C | 2.95  | 1.42        | 1.35     |
| 14  | 2     | 824  | CLA  | C4D-ND  | -2.94 | 1.33        | 1.37     |
| 14  | f     | 203  | CLA  | CHC-C1C | 2.94  | 1.42        | 1.35     |
| 14  | 9     | 101  | CLA  | CHC-C1C | 2.94  | 1.42        | 1.35     |
| 14  | 2     | 837  | CLA  | CHC-C1C | 2.94  | 1.42        | 1.35     |
| 13  | a     | 801  | CL0  | CMB-C2B | -2.94 | 1.45        | 1.51     |
| 14  | b     | 803  | CLA  | CMB-C2B | -2.94 | 1.45        | 1.51     |
| 14  | B     | 816  | CLA  | C4D-ND  | -2.94 | 1.33        | 1.37     |
| 14  | 2     | 839  | CLA  | CMB-C2B | -2.94 | 1.45        | 1.51     |
| 14  | 2     | 820  | CLA  | CMB-C2B | -2.94 | 1.45        | 1.51     |
| 14  | A     | 824  | CLA  | CHC-C1C | 2.94  | 1.42        | 1.35     |
| 14  | A     | 827  | CLA  | CHC-C1C | 2.94  | 1.42        | 1.35     |
| 14  | 2     | 816  | CLA  | CHC-C1C | 2.94  | 1.42        | 1.35     |
| 14  | a     | 820  | CLA  | CHC-C1C | 2.94  | 1.42        | 1.35     |
| 14  | K     | 101  | CLA  | CHC-C1C | 2.94  | 1.42        | 1.35     |
| 20  | 2     | 850  | LMG  | O7-C8   | -2.94 | 1.39        | 1.46     |
| 14  | a     | 810  | CLA  | CHC-C1C | 2.93  | 1.42        | 1.35     |
| 20  | b     | 850  | LMG  | O7-C8   | -2.93 | 1.39        | 1.46     |
| 13  | A     | 801  | CL0  | CMB-C2B | -2.93 | 1.45        | 1.51     |
| 14  | A     | 843  | CLA  | CMD-C2D | -2.93 | 1.44        | 1.50     |
| 14  | A     | 829  | CLA  | CHC-C1C | 2.93  | 1.42        | 1.35     |
| 14  | 1     | 1634 | CLA  | CMB-C2B | -2.93 | 1.45        | 1.51     |
| 14  | 1     | 1631 | CLA  | C1D-ND  | 2.93  | 1.41        | 1.37     |
| 14  | a     | 812  | CLA  | CHC-C1C | 2.93  | 1.42        | 1.35     |
| 14  | a     | 841  | CLA  | CHC-C1C | 2.93  | 1.42        | 1.35     |
| 14  | a     | 824  | CLA  | C4D-ND  | -2.93 | 1.33        | 1.37     |
| 14  | 1     | 1611 | CLA  | CHC-C1C | 2.93  | 1.42        | 1.35     |
| 14  | B     | 837  | CLA  | CMB-C2B | -2.93 | 1.45        | 1.51     |
| 14  | F     | 204  | CLA  | CHC-C1C | 2.93  | 1.42        | 1.35     |
| 14  | B     | 838  | CLA  | CMB-C2B | -2.93 | 1.45        | 1.51     |
| 14  | B     | 802  | CLA  | CMB-C2B | -2.93 | 1.45        | 1.51     |
| 14  | 1     | 1613 | CLA  | CHC-C1C | 2.93  | 1.42        | 1.35     |
| 14  | b     | 837  | CLA  | CHC-C1C | 2.93  | 1.42        | 1.35     |
| 14  | A     | 841  | CLA  | CHC-C1C | 2.93  | 1.42        | 1.35     |
| 14  | a     | 819  | CLA  | CHC-C1C | 2.93  | 1.42        | 1.35     |
| 14  | a     | 824  | CLA  | CHC-C1C | 2.93  | 1.42        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | 2     | 838  | CLA  | CMB-C2B | -2.93 | 1.45        | 1.51     |
| 14  | 1     | 1621 | CLA  | CHC-C1C | 2.93  | 1.42        | 1.35     |
| 14  | L     | 204  | CLA  | C1D-ND  | 2.92  | 1.41        | 1.37     |
| 14  | A     | 820  | CLA  | CHC-C1C | 2.92  | 1.42        | 1.35     |
| 14  | B     | 804  | CLA  | CMB-C2B | -2.92 | 1.45        | 1.51     |
| 14  | b     | 805  | CLA  | CMB-C2B | -2.92 | 1.45        | 1.51     |
| 14  | 1     | 1628 | CLA  | CMB-C2B | -2.92 | 1.45        | 1.51     |
| 14  | A     | 827  | CLA  | CMB-C2B | -2.92 | 1.45        | 1.51     |
| 14  | 0     | 206  | CLA  | CMB-C2B | -2.92 | 1.45        | 1.51     |
| 14  | 2     | 805  | CLA  | CMB-C2B | -2.92 | 1.45        | 1.51     |
| 14  | 2     | 831  | CLA  | CHC-C1C | 2.92  | 1.42        | 1.35     |
| 14  | B     | 821  | CLA  | C4D-ND  | -2.92 | 1.33        | 1.37     |
| 14  | 2     | 818  | CLA  | CMB-C2B | -2.92 | 1.45        | 1.51     |
| 14  | b     | 813  | CLA  | CHC-C1C | 2.92  | 1.42        | 1.35     |
| 14  | 1     | 1625 | CLA  | CHC-C1C | 2.92  | 1.42        | 1.35     |
| 14  | l     | 206  | CLA  | CMB-C2B | -2.92 | 1.45        | 1.51     |
| 14  | a     | 827  | CLA  | CMB-C2B | -2.92 | 1.45        | 1.51     |
| 14  | A     | 821  | CLA  | C4D-ND  | -2.92 | 1.33        | 1.37     |
| 14  | A     | 833  | CLA  | CMB-C2B | -2.92 | 1.45        | 1.51     |
| 14  | 1     | 1601 | CLA  | C4D-ND  | -2.92 | 1.33        | 1.37     |
| 14  | 1     | 1601 | CLA  | CHC-C1C | 2.91  | 1.42        | 1.35     |
| 14  | b     | 824  | CLA  | C4D-ND  | -2.91 | 1.33        | 1.37     |
| 13  | 1     | 1602 | CL0  | CMB-C2B | -2.91 | 1.45        | 1.51     |
| 14  | 2     | 833  | CLA  | CHC-C1C | 2.91  | 1.42        | 1.35     |
| 14  | A     | 827  | CLA  | C1D-ND  | 2.91  | 1.41        | 1.37     |
| 14  | 1     | 1622 | CLA  | C4D-ND  | -2.91 | 1.33        | 1.37     |
| 14  | j     | 1302 | CLA  | C4D-ND  | -2.91 | 1.33        | 1.37     |
| 14  | B     | 823  | CLA  | C4D-ND  | -2.91 | 1.33        | 1.37     |
| 14  | b     | 831  | CLA  | CHC-C1C | 2.91  | 1.42        | 1.35     |
| 14  | 8     | 1302 | CLA  | C4D-ND  | -2.91 | 1.33        | 1.37     |
| 14  | B     | 836  | CLA  | CHC-C1C | 2.90  | 1.42        | 1.35     |
| 14  | B     | 803  | CLA  | C1D-ND  | 2.90  | 1.41        | 1.37     |
| 14  | b     | 833  | CLA  | CHC-C1C | 2.90  | 1.42        | 1.35     |
| 14  | l     | 205  | CLA  | CMB-C2B | -2.90 | 1.45        | 1.51     |
| 14  | b     | 819  | CLA  | CHC-C1C | 2.90  | 1.42        | 1.35     |
| 14  | L     | 204  | CLA  | CMB-C2B | -2.90 | 1.45        | 1.51     |
| 14  | B     | 832  | CLA  | CHC-C1C | 2.90  | 1.42        | 1.35     |
| 14  | A     | 857  | CLA  | C4D-ND  | -2.90 | 1.33        | 1.37     |
| 14  | 1     | 1619 | CLA  | C4D-ND  | -2.90 | 1.33        | 1.37     |
| 14  | B     | 830  | CLA  | CHC-C1C | 2.90  | 1.42        | 1.35     |
| 14  | 2     | 813  | CLA  | CHC-C1C | 2.90  | 1.42        | 1.35     |
| 14  | 2     | 812  | CLA  | CHC-C1C | 2.90  | 1.42        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | 1     | 1625 | CLA  | C4D-ND  | -2.90 | 1.33        | 1.37     |
| 14  | b     | 816  | CLA  | CHC-C1C | 2.90  | 1.42        | 1.35     |
| 14  | b     | 806  | CLA  | CMB-C2B | -2.90 | 1.45        | 1.51     |
| 14  | A     | 818  | CLA  | C4D-ND  | -2.90 | 1.33        | 1.37     |
| 14  | A     | 824  | CLA  | C4D-ND  | -2.90 | 1.33        | 1.37     |
| 14  | x     | 1701 | CLA  | C4D-ND  | -2.89 | 1.33        | 1.37     |
| 14  | a     | 827  | CLA  | C1D-ND  | 2.89  | 1.41        | 1.37     |
| 14  | A     | 857  | CLA  | CHC-C1C | 2.89  | 1.42        | 1.35     |
| 14  | M     | 102  | CLA  | CHC-C1C | 2.89  | 1.42        | 1.35     |
| 14  | a     | 843  | CLA  | C1D-ND  | 2.89  | 1.41        | 1.37     |
| 14  | 1     | 1623 | CLA  | CMB-C2B | -2.89 | 1.45        | 1.51     |
| 14  | b     | 835  | CLA  | C4D-ND  | -2.89 | 1.33        | 1.37     |
| 14  | B     | 812  | CLA  | CHC-C1C | 2.89  | 1.42        | 1.35     |
| 14  | b     | 822  | CLA  | C4D-ND  | -2.89 | 1.33        | 1.37     |
| 14  | 2     | 841  | CLA  | CHC-C1C | 2.89  | 1.42        | 1.35     |
| 14  | A     | 803  | CLA  | CMB-C2B | -2.89 | 1.45        | 1.51     |
| 14  | b     | 841  | CLA  | CHC-C1C | 2.89  | 1.42        | 1.35     |
| 14  | 2     | 819  | CLA  | CHC-C1C | 2.89  | 1.42        | 1.35     |
| 14  | 1     | 1628 | CLA  | C1D-ND  | 2.88  | 1.41        | 1.37     |
| 14  | B     | 811  | CLA  | CHC-C1C | 2.88  | 1.42        | 1.35     |
| 14  | A     | 826  | CLA  | CHC-C1C | 2.88  | 1.42        | 1.35     |
| 18  | A     | 853  | LHG  | O7-C5   | -2.88 | 1.39        | 1.46     |
| 14  | B     | 815  | CLA  | CHC-C1C | 2.88  | 1.42        | 1.35     |
| 14  | a     | 822  | CLA  | CMB-C2B | -2.88 | 1.45        | 1.51     |
| 14  | 0     | 207  | CLA  | CMB-C2B | -2.88 | 1.45        | 1.51     |
| 14  | A     | 802  | CLA  | C1D-ND  | 2.88  | 1.41        | 1.37     |
| 14  | a     | 818  | CLA  | C4D-ND  | -2.88 | 1.33        | 1.37     |
| 14  | B     | 840  | CLA  | CMB-C2B | -2.88 | 1.45        | 1.51     |
| 14  | b     | 812  | CLA  | CHC-C1C | 2.88  | 1.42        | 1.35     |
| 14  | b     | 817  | CLA  | CHC-C1C | 2.87  | 1.42        | 1.35     |
| 14  | 1     | 1604 | CLA  | C3B-C2B | -2.87 | 1.36        | 1.40     |
| 14  | 2     | 802  | CLA  | CHC-C1C | 2.87  | 1.42        | 1.35     |
| 14  | B     | 840  | CLA  | CHC-C1C | 2.87  | 1.42        | 1.35     |
| 14  | b     | 841  | CLA  | CMB-C2B | -2.87 | 1.45        | 1.51     |
| 14  | 1     | 1627 | CLA  | CHC-C1C | 2.87  | 1.42        | 1.35     |
| 14  | z     | 102  | CLA  | C4D-ND  | -2.87 | 1.33        | 1.37     |
| 14  | b     | 838  | CLA  | CMB-C2B | -2.87 | 1.45        | 1.51     |
| 14  | 2     | 809  | CLA  | CHC-C1C | 2.87  | 1.42        | 1.35     |
| 14  | A     | 822  | CLA  | CMB-C2B | -2.87 | 1.45        | 1.51     |
| 14  | a     | 833  | CLA  | CMB-C2B | -2.87 | 1.45        | 1.51     |
| 14  | 1     | 1604 | CLA  | CMB-C2B | -2.87 | 1.45        | 1.51     |
| 14  | 1     | 1640 | CLA  | CMB-C2B | -2.87 | 1.45        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 803  | CLA  | CMB-C2B | -2.87 | 1.45        | 1.51     |
| 14  | L     | 205  | CLA  | CMB-C2B | -2.87 | 1.45        | 1.51     |
| 14  | b     | 807  | CLA  | CHC-C1C | 2.87  | 1.42        | 1.35     |
| 14  | M     | 102  | CLA  | C4D-ND  | -2.86 | 1.33        | 1.37     |
| 14  | 2     | 806  | CLA  | CMB-C2B | -2.86 | 1.45        | 1.51     |
| 14  | B     | 806  | CLA  | CHC-C1C | 2.86  | 1.42        | 1.35     |
| 14  | 1     | 1603 | CLA  | C1D-ND  | 2.86  | 1.41        | 1.37     |
| 14  | 2     | 822  | CLA  | C4D-ND  | -2.86 | 1.33        | 1.37     |
| 14  | B     | 818  | CLA  | CHC-C1C | 2.86  | 1.42        | 1.35     |
| 14  | a     | 821  | CLA  | C4D-ND  | -2.86 | 1.33        | 1.37     |
| 14  | a     | 826  | CLA  | CHC-C1C | 2.86  | 1.42        | 1.35     |
| 14  | A     | 855  | CLA  | CHC-C1C | 2.86  | 1.42        | 1.35     |
| 14  | a     | 802  | CLA  | C1D-ND  | 2.86  | 1.41        | 1.37     |
| 14  | 1     | 1610 | CLA  | CMB-C2B | -2.86 | 1.45        | 1.51     |
| 14  | B     | 841  | CLA  | CHC-C1C | 2.86  | 1.42        | 1.35     |
| 14  | B     | 805  | CLA  | CMB-C2B | -2.86 | 1.45        | 1.51     |
| 14  | b     | 809  | CLA  | CHC-C1C | 2.85  | 1.42        | 1.35     |
| 14  | 2     | 807  | CLA  | CHC-C1C | 2.85  | 1.42        | 1.35     |
| 14  | B     | 838  | CLA  | CHC-C1C | 2.85  | 1.42        | 1.35     |
| 14  | a     | 809  | CLA  | CMB-C2B | -2.85 | 1.45        | 1.51     |
| 14  | 1     | 1607 | CLA  | CMB-C2B | -2.85 | 1.45        | 1.51     |
| 14  | B     | 808  | CLA  | CHC-C1C | 2.85  | 1.42        | 1.35     |
| 14  | a     | 837  | CLA  | CMB-C2B | -2.85 | 1.45        | 1.51     |
| 18  | 1     | 1654 | LHG  | O7-C5   | -2.85 | 1.39        | 1.46     |
| 14  | b     | 842  | CLA  | CHC-C1C | 2.85  | 1.42        | 1.35     |
| 14  | 0     | 206  | CLA  | C1D-ND  | 2.85  | 1.41        | 1.37     |
| 14  | 2     | 842  | CLA  | CHC-C1C | 2.84  | 1.42        | 1.35     |
| 14  | j     | 1303 | CLA  | C4D-ND  | -2.84 | 1.33        | 1.37     |
| 14  | A     | 809  | CLA  | CMB-C2B | -2.84 | 1.45        | 1.51     |
| 14  | b     | 835  | CLA  | CMB-C2B | -2.84 | 1.45        | 1.51     |
| 18  | a     | 853  | LHG  | O7-C5   | -2.84 | 1.39        | 1.46     |
| 14  | 2     | 841  | CLA  | CMD-C2D | -2.84 | 1.44        | 1.50     |
| 14  | 1     | 1638 | CLA  | CMB-C2B | -2.84 | 1.45        | 1.51     |
| 14  | 2     | 817  | CLA  | CHC-C1C | 2.84  | 1.42        | 1.35     |
| 14  | b     | 839  | CLA  | CHC-C1C | 2.84  | 1.42        | 1.35     |
| 14  | L     | 204  | CLA  | CHC-C1C | 2.84  | 1.42        | 1.35     |
| 14  | a     | 839  | CLA  | CMB-C2B | -2.84 | 1.45        | 1.51     |
| 14  | a     | 806  | CLA  | CMB-C2B | -2.84 | 1.45        | 1.51     |
| 14  | 2     | 842  | CLA  | CMB-C2B | -2.84 | 1.45        | 1.51     |
| 14  | 2     | 835  | CLA  | C4D-ND  | -2.84 | 1.33        | 1.37     |
| 14  | l     | 205  | CLA  | CHC-C1C | 2.84  | 1.42        | 1.35     |
| 14  | l     | 205  | CLA  | C1D-ND  | 2.84  | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 816  | CLA  | CHC-C1C | 2.84  | 1.42        | 1.35     |
| 14  | B     | 841  | CLA  | CMB-C2B | -2.84 | 1.45        | 1.51     |
| 14  | A     | 839  | CLA  | CMB-C2B | -2.83 | 1.45        | 1.51     |
| 14  | A     | 806  | CLA  | CMB-C2B | -2.83 | 1.45        | 1.51     |
| 14  | 2     | 841  | CLA  | CMB-C2B | -2.83 | 1.45        | 1.51     |
| 14  | 2     | 831  | CLA  | CMB-C2B | -2.83 | 1.45        | 1.51     |
| 14  | A     | 803  | CLA  | C3B-C2B | -2.83 | 1.36        | 1.40     |
| 14  | b     | 818  | CLA  | CHC-C1C | 2.83  | 1.42        | 1.35     |
| 14  | b     | 802  | CLA  | CHC-C1C | 2.83  | 1.42        | 1.35     |
| 14  | b     | 826  | CLA  | CMB-C2B | -2.82 | 1.45        | 1.51     |
| 14  | L     | 205  | CLA  | CHC-C1C | 2.82  | 1.42        | 1.35     |
| 14  | b     | 831  | CLA  | CMB-C2B | -2.82 | 1.45        | 1.51     |
| 14  | 2     | 835  | CLA  | CMB-C2B | -2.82 | 1.45        | 1.51     |
| 14  | A     | 843  | CLA  | C1D-ND  | 2.82  | 1.41        | 1.37     |
| 14  | 0     | 206  | CLA  | CHC-C1C | 2.82  | 1.42        | 1.35     |
| 14  | B     | 834  | CLA  | C4D-ND  | -2.82 | 1.33        | 1.37     |
| 14  | 0     | 207  | CLA  | CHC-C1C | 2.82  | 1.42        | 1.35     |
| 14  | B     | 840  | CLA  | CMD-C2D | -2.82 | 1.44        | 1.50     |
| 14  | A     | 842  | CLA  | CMB-C2B | -2.82 | 1.45        | 1.51     |
| 14  | B     | 830  | CLA  | CMB-C2B | -2.82 | 1.45        | 1.51     |
| 14  | 1     | 1631 | CLA  | CHC-C1C | 2.82  | 1.42        | 1.35     |
| 14  | 1     | 1633 | CLA  | CHC-C1C | 2.82  | 1.42        | 1.35     |
| 14  | 2     | 839  | CLA  | CHC-C1C | 2.81  | 1.42        | 1.35     |
| 14  | A     | 832  | CLA  | CHC-C1C | 2.81  | 1.42        | 1.35     |
| 14  | a     | 835  | CLA  | CHC-C1C | 2.81  | 1.42        | 1.35     |
| 14  | A     | 837  | CLA  | CMB-C2B | -2.81 | 1.45        | 1.51     |
| 14  | 2     | 818  | CLA  | CHC-C1C | 2.81  | 1.42        | 1.35     |
| 14  | A     | 830  | CLA  | CHC-C1C | 2.81  | 1.42        | 1.35     |
| 14  | A     | 835  | CLA  | CHC-C1C | 2.80  | 1.42        | 1.35     |
| 14  | a     | 806  | CLA  | CHC-C1C | 2.80  | 1.42        | 1.35     |
| 14  | 8     | 1303 | CLA  | C4D-ND  | -2.80 | 1.33        | 1.37     |
| 14  | J     | 102  | CLA  | C4D-ND  | -2.80 | 1.33        | 1.37     |
| 14  | 1     | 1618 | CLA  | C4D-ND  | -2.80 | 1.33        | 1.37     |
| 14  | b     | 842  | CLA  | CMB-C2B | -2.80 | 1.45        | 1.51     |
| 14  | a     | 842  | CLA  | CMB-C2B | -2.80 | 1.45        | 1.51     |
| 14  | 2     | 807  | CLA  | CMB-C2B | -2.80 | 1.45        | 1.51     |
| 14  | a     | 832  | CLA  | CHC-C1C | 2.80  | 1.42        | 1.35     |
| 14  | B     | 811  | CLA  | CMB-C2B | -2.80 | 1.45        | 1.51     |
| 14  | 1     | 1636 | CLA  | CHC-C1C | 2.80  | 1.42        | 1.35     |
| 14  | B     | 817  | CLA  | CHC-C1C | 2.80  | 1.42        | 1.35     |
| 14  | a     | 830  | CLA  | CHC-C1C | 2.80  | 1.42        | 1.35     |
| 14  | B     | 834  | CLA  | CMB-C2B | -2.80 | 1.45        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | l     | 206  | CLA  | CHC-C1C | 2.80  | 1.42        | 1.35     |
| 14  | 1     | 1631 | CLA  | CMD-C2D | -2.79 | 1.44        | 1.50     |
| 14  | B     | 806  | CLA  | CMB-C2B | -2.79 | 1.45        | 1.51     |
| 14  | 1     | 1643 | CLA  | CMB-C2B | -2.79 | 1.45        | 1.51     |
| 14  | 1     | 1637 | CLA  | CHC-C1C | 2.79  | 1.42        | 1.35     |
| 14  | 1     | 1644 | CLA  | C1D-ND  | 2.79  | 1.41        | 1.37     |
| 14  | a     | 830  | CLA  | CMD-C2D | -2.79 | 1.44        | 1.50     |
| 14  | A     | 843  | CLA  | CHC-C1C | 2.78  | 1.42        | 1.35     |
| 14  | 1     | 1644 | CLA  | CHC-C1C | 2.78  | 1.42        | 1.35     |
| 14  | 2     | 812  | CLA  | CMB-C2B | -2.78 | 1.45        | 1.51     |
| 14  | b     | 841  | CLA  | CMD-C2D | -2.78 | 1.44        | 1.50     |
| 14  | 2     | 803  | CLA  | CHC-C1C | 2.78  | 1.42        | 1.35     |
| 14  | 2     | 808  | CLA  | CHC-C1C | 2.78  | 1.42        | 1.35     |
| 14  | B     | 825  | CLA  | CMB-C2B | -2.78 | 1.45        | 1.51     |
| 14  | A     | 810  | CLA  | CMB-C2B | -2.78 | 1.45        | 1.51     |
| 14  | a     | 838  | CLA  | CHC-C1C | 2.78  | 1.42        | 1.35     |
| 14  | a     | 817  | CLA  | C4D-ND  | -2.78 | 1.33        | 1.37     |
| 14  | A     | 806  | CLA  | CHC-C1C | 2.78  | 1.42        | 1.35     |
| 14  | B     | 807  | CLA  | CHC-C1C | 2.77  | 1.42        | 1.35     |
| 14  | A     | 817  | CLA  | C4D-ND  | -2.77 | 1.33        | 1.37     |
| 14  | 1     | 1639 | CLA  | CHC-C1C | 2.77  | 1.42        | 1.35     |
| 14  | 1     | 1611 | CLA  | CMB-C2B | -2.77 | 1.45        | 1.51     |
| 14  | A     | 836  | CLA  | CHC-C1C | 2.77  | 1.42        | 1.35     |
| 14  | 1     | 1607 | CLA  | CHC-C1C | 2.77  | 1.42        | 1.35     |
| 14  | A     | 838  | CLA  | CHC-C1C | 2.77  | 1.42        | 1.35     |
| 14  | A     | 807  | CLA  | CHC-C1C | 2.76  | 1.42        | 1.35     |
| 14  | a     | 803  | CLA  | C3B-C2B | -2.76 | 1.36        | 1.40     |
| 14  | a     | 810  | CLA  | CMB-C2B | -2.76 | 1.45        | 1.51     |
| 14  | a     | 802  | CLA  | CMD-C2D | -2.76 | 1.44        | 1.50     |
| 14  | A     | 826  | CLA  | CMB-C2B | -2.76 | 1.45        | 1.51     |
| 14  | 2     | 823  | CLA  | CMB-C2B | -2.76 | 1.45        | 1.51     |
| 14  | b     | 804  | CLA  | CHC-C1C | 2.76  | 1.42        | 1.35     |
| 17  | 0     | 208  | BCR  | C30-C25 | -2.76 | 1.50        | 1.53     |
| 14  | B     | 805  | CLA  | CHC-C1C | 2.76  | 1.42        | 1.35     |
| 14  | a     | 807  | CLA  | CHC-C1C | 2.76  | 1.42        | 1.35     |
| 14  | a     | 826  | CLA  | CMB-C2B | -2.76 | 1.45        | 1.51     |
| 14  | 1     | 1608 | CLA  | CHC-C1C | 2.75  | 1.42        | 1.35     |
| 14  | B     | 803  | CLA  | CHC-C1C | 2.75  | 1.42        | 1.35     |
| 14  | b     | 808  | CLA  | CHC-C1C | 2.75  | 1.42        | 1.35     |
| 14  | b     | 812  | CLA  | CMB-C2B | -2.75 | 1.45        | 1.51     |
| 14  | b     | 837  | CLA  | CMB-C2B | -2.75 | 1.45        | 1.51     |
| 14  | 2     | 826  | CLA  | CMB-C2B | -2.75 | 1.45        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 819  | CLA  | CMB-C2B | -2.75 | 1.45        | 1.51     |
| 14  | 1     | 1641 | CLA  | CMB-C2B | -2.75 | 1.45        | 1.51     |
| 17  | L     | 206  | BCR  | C30-C25 | -2.74 | 1.50        | 1.53     |
| 14  | a     | 843  | CLA  | CHC-C1C | 2.74  | 1.42        | 1.35     |
| 14  | b     | 807  | CLA  | CMB-C2B | -2.74 | 1.45        | 1.51     |
| 14  | 2     | 837  | CLA  | CMB-C2B | -2.74 | 1.45        | 1.51     |
| 14  | b     | 823  | CLA  | CMB-C2B | -2.74 | 1.45        | 1.51     |
| 14  | 1     | 1620 | CLA  | CMB-C2B | -2.74 | 1.45        | 1.51     |
| 14  | a     | 807  | CLA  | CMB-C2B | -2.74 | 1.45        | 1.51     |
| 14  | a     | 841  | CLA  | CMB-C2B | -2.74 | 1.45        | 1.51     |
| 14  | A     | 807  | CLA  | CMB-C2B | -2.74 | 1.46        | 1.51     |
| 14  | A     | 830  | CLA  | CMD-C2D | -2.73 | 1.45        | 1.50     |
| 14  | B     | 802  | CLA  | CHC-C1C | 2.73  | 1.42        | 1.35     |
| 14  | L     | 203  | CLA  | CMB-C2B | -2.73 | 1.46        | 1.51     |
| 14  | 1     | 1627 | CLA  | CMB-C2B | -2.73 | 1.46        | 1.51     |
| 14  | B     | 836  | CLA  | CMB-C2B | -2.73 | 1.46        | 1.51     |
| 14  | A     | 820  | CLA  | CMB-C2B | -2.73 | 1.46        | 1.51     |
| 14  | A     | 840  | CLA  | CMB-C2B | -2.73 | 1.46        | 1.51     |
| 14  | a     | 804  | CLA  | CMB-C2B | -2.73 | 1.46        | 1.51     |
| 14  | a     | 836  | CLA  | CHC-C1C | 2.73  | 1.42        | 1.35     |
| 14  | B     | 822  | CLA  | CMB-C2B | -2.73 | 1.46        | 1.51     |
| 14  | 1     | 1608 | CLA  | CMB-C2B | -2.72 | 1.46        | 1.51     |
| 14  | b     | 803  | CLA  | CHC-C1C | 2.72  | 1.41        | 1.35     |
| 14  | 2     | 804  | CLA  | CHC-C1C | 2.72  | 1.41        | 1.35     |
| 14  | a     | 840  | CLA  | CMB-C2B | -2.72 | 1.46        | 1.51     |
| 14  | 2     | 806  | CLA  | CHC-C1C | 2.72  | 1.41        | 1.35     |
| 14  | a     | 802  | CLA  | CMB-C2B | -2.72 | 1.46        | 1.51     |
| 14  | A     | 802  | CLA  | CMB-C2B | -2.72 | 1.46        | 1.51     |
| 14  | b     | 806  | CLA  | CHC-C1C | 2.72  | 1.41        | 1.35     |
| 14  | 2     | 840  | CLA  | C3B-C2B | -2.72 | 1.36        | 1.40     |
| 14  | B     | 807  | CLA  | CMB-C2B | -2.71 | 1.46        | 1.51     |
| 14  | A     | 802  | CLA  | CMD-C2D | -2.71 | 1.45        | 1.50     |
| 14  | B     | 839  | CLA  | CMB-C2B | -2.71 | 1.46        | 1.51     |
| 14  | 2     | 829  | CLA  | CMD-C2D | -2.71 | 1.45        | 1.50     |
| 14  | a     | 824  | CLA  | CMB-C2B | -2.71 | 1.46        | 1.51     |
| 14  | b     | 840  | CLA  | CMB-C2B | -2.71 | 1.46        | 1.51     |
| 14  | 1     | 1632 | CLA  | CHC-C1C | 2.71  | 1.41        | 1.35     |
| 14  | 1     | 1603 | CLA  | CMD-C2D | -2.71 | 1.45        | 1.50     |
| 14  | b     | 808  | CLA  | CMB-C2B | -2.71 | 1.46        | 1.51     |
| 14  | 2     | 808  | CLA  | CMB-C2B | -2.71 | 1.46        | 1.51     |
| 14  | B     | 839  | CLA  | C3B-C2B | -2.71 | 1.36        | 1.40     |
| 14  | 1     | 204  | CLA  | CMB-C2B | -2.71 | 1.46        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 828  | CLA  | CMB-C2B | -2.70 | 1.46        | 1.51     |
| 14  | A     | 813  | CLA  | CMB-C2B | -2.70 | 1.46        | 1.51     |
| 14  | A     | 841  | CLA  | CMB-C2B | -2.70 | 1.46        | 1.51     |
| 14  | 1     | 1603 | CLA  | CMB-C2B | -2.70 | 1.46        | 1.51     |
| 14  | B     | 833  | CLA  | CMB-C2B | -2.70 | 1.46        | 1.51     |
| 14  | 0     | 205  | CLA  | CMB-C2B | -2.70 | 1.46        | 1.51     |
| 14  | 1     | 1640 | CLA  | CHC-C1C | 2.70  | 1.41        | 1.35     |
| 14  | 1     | 1621 | CLA  | CMB-C2B | -2.70 | 1.46        | 1.51     |
| 14  | 1     | 1605 | CLA  | CMB-C2B | -2.69 | 1.46        | 1.51     |
| 14  | A     | 804  | CLA  | CMB-C2B | -2.69 | 1.46        | 1.51     |
| 14  | A     | 831  | CLA  | C3B-C2B | -2.69 | 1.36        | 1.40     |
| 14  | A     | 855  | CLA  | CMB-C2B | -2.69 | 1.46        | 1.51     |
| 17  | l     | 207  | BCR  | C30-C25 | -2.69 | 1.50        | 1.53     |
| 14  | b     | 829  | CLA  | CMD-C2D | -2.69 | 1.45        | 1.50     |
| 20  | b     | 850  | LMG  | O1-C7   | -2.69 | 1.38        | 1.43     |
| 14  | A     | 815  | CLA  | CMB-C2B | -2.69 | 1.46        | 1.51     |
| 14  | a     | 820  | CLA  | CMB-C2B | -2.69 | 1.46        | 1.51     |
| 14  | 1     | 1632 | CLA  | C3B-C2B | -2.69 | 1.36        | 1.40     |
| 14  | a     | 831  | CLA  | CHC-C1C | 2.69  | 1.41        | 1.35     |
| 14  | a     | 815  | CLA  | CMB-C2B | -2.68 | 1.46        | 1.51     |
| 14  | 1     | 1636 | CLA  | CMB-C2B | -2.68 | 1.46        | 1.51     |
| 14  | B     | 828  | CLA  | CMD-C2D | -2.68 | 1.45        | 1.50     |
| 14  | A     | 831  | CLA  | CHC-C1C | 2.68  | 1.41        | 1.35     |
| 14  | 1     | 1616 | CLA  | CMB-C2B | -2.68 | 1.46        | 1.51     |
| 14  | A     | 819  | CLA  | CMB-C2B | -2.68 | 1.46        | 1.51     |
| 14  | 1     | 1642 | CLA  | CMB-C2B | -2.68 | 1.46        | 1.51     |
| 14  | 2     | 834  | CLA  | CMB-C2B | -2.68 | 1.46        | 1.51     |
| 14  | a     | 835  | CLA  | CMB-C2B | -2.68 | 1.46        | 1.51     |
| 14  | b     | 832  | CLA  | CMB-C2B | -2.68 | 1.46        | 1.51     |
| 14  | 1     | 1625 | CLA  | CMB-C2B | -2.68 | 1.46        | 1.51     |
| 14  | b     | 834  | CLA  | CMB-C2B | -2.68 | 1.46        | 1.51     |
| 14  | 1     | 1626 | CLA  | CMB-C2B | -2.67 | 1.46        | 1.51     |
| 14  | 2     | 811  | CLA  | CHC-C1C | 2.67  | 1.41        | 1.35     |
| 14  | b     | 814  | CLA  | CMB-C2B | -2.67 | 1.46        | 1.51     |
| 14  | B     | 835  | CLA  | CMB-C2B | -2.67 | 1.46        | 1.51     |
| 14  | 2     | 840  | CLA  | CMB-C2B | -2.67 | 1.46        | 1.51     |
| 20  | 2     | 850  | LMG  | O1-C7   | -2.67 | 1.38        | 1.43     |
| 14  | b     | 802  | CLA  | CMB-C2B | -2.67 | 1.46        | 1.51     |
| 14  | B     | 832  | CLA  | CMB-C2B | -2.67 | 1.46        | 1.51     |
| 14  | a     | 813  | CLA  | CMB-C2B | -2.67 | 1.46        | 1.51     |
| 14  | b     | 840  | CLA  | C3B-C2B | -2.67 | 1.36        | 1.40     |
| 20  | B     | 849  | LMG  | O1-C7   | -2.67 | 1.38        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 844  | CLA  | CMB-C2B | -2.67 | 1.46        | 1.51     |
| 14  | a     | 825  | CLA  | CMB-C2B | -2.67 | 1.46        | 1.51     |
| 14  | 2     | 832  | CLA  | CMB-C2B | -2.67 | 1.46        | 1.51     |
| 14  | A     | 835  | CLA  | CMB-C2B | -2.66 | 1.46        | 1.51     |
| 14  | b     | 810  | CLA  | CHC-C1C | 2.66  | 1.41        | 1.35     |
| 14  | A     | 834  | CLA  | CMB-C2B | -2.66 | 1.46        | 1.51     |
| 14  | B     | 813  | CLA  | CMB-C2B | -2.66 | 1.46        | 1.51     |
| 14  | B     | 831  | CLA  | CMB-C2B | -2.66 | 1.46        | 1.51     |
| 14  | 2     | 836  | CLA  | CMB-C2B | -2.66 | 1.46        | 1.51     |
| 14  | B     | 809  | CLA  | CHC-C1C | 2.66  | 1.41        | 1.35     |
| 14  | f     | 201  | CLA  | CMB-C2B | -2.66 | 1.46        | 1.51     |
| 14  | b     | 811  | CLA  | CHC-C1C | 2.66  | 1.41        | 1.35     |
| 14  | B     | 810  | CLA  | CHC-C1C | 2.65  | 1.41        | 1.35     |
| 14  | A     | 839  | CLA  | CHC-C1C | 2.65  | 1.41        | 1.35     |
| 14  | B     | 827  | CLA  | CMB-C2B | -2.65 | 1.46        | 1.51     |
| 14  | A     | 804  | CLA  | CHC-C1C | 2.65  | 1.41        | 1.35     |
| 14  | 1     | 1645 | CLA  | CMB-C2B | -2.65 | 1.46        | 1.51     |
| 14  | 2     | 804  | CLA  | CMB-C2B | -2.65 | 1.46        | 1.51     |
| 14  | A     | 824  | CLA  | CMB-C2B | -2.65 | 1.46        | 1.51     |
| 14  | b     | 833  | CLA  | CMB-C2B | -2.65 | 1.46        | 1.51     |
| 14  | a     | 844  | CLA  | CMB-C2B | -2.65 | 1.46        | 1.51     |
| 14  | B     | 812  | CLA  | CMB-C2B | -2.65 | 1.46        | 1.51     |
| 14  | a     | 812  | CLA  | CMB-C2B | -2.65 | 1.46        | 1.51     |
| 14  | a     | 839  | CLA  | CHC-C1C | 2.65  | 1.41        | 1.35     |
| 14  | b     | 811  | CLA  | CMB-C2B | -2.65 | 1.46        | 1.51     |
| 14  | F     | 201  | CLA  | CMB-C2B | -2.65 | 1.46        | 1.51     |
| 14  | 2     | 810  | CLA  | CHC-C1C | 2.65  | 1.41        | 1.35     |
| 14  | B     | 803  | CLA  | CMB-C2B | -2.64 | 1.46        | 1.51     |
| 14  | b     | 836  | CLA  | CMB-C2B | -2.64 | 1.46        | 1.51     |
| 14  | 2     | 828  | CLA  | CMB-C2B | -2.64 | 1.46        | 1.51     |
| 14  | A     | 840  | CLA  | CMD-C2D | -2.64 | 1.45        | 1.50     |
| 14  | 1     | 1635 | CLA  | CMB-C2B | -2.64 | 1.46        | 1.51     |
| 14  | 2     | 802  | CLA  | CMB-C2B | -2.64 | 1.46        | 1.51     |
| 14  | B     | 808  | CLA  | CMC-C2C | -2.64 | 1.45        | 1.50     |
| 14  | 6     | 201  | CLA  | CMB-C2B | -2.64 | 1.46        | 1.51     |
| 14  | b     | 804  | CLA  | CMB-C2B | -2.64 | 1.46        | 1.51     |
| 14  | b     | 819  | CLA  | CMB-C2B | -2.64 | 1.46        | 1.51     |
| 14  | 2     | 833  | CLA  | CMB-C2B | -2.64 | 1.46        | 1.51     |
| 14  | 1     | 1614 | CLA  | CMB-C2B | -2.64 | 1.46        | 1.51     |
| 14  | a     | 831  | CLA  | C3B-C2B | -2.64 | 1.36        | 1.40     |
| 14  | 1     | 1613 | CLA  | CMB-C2B | -2.64 | 1.46        | 1.51     |
| 14  | 2     | 816  | CLA  | CMB-C2B | -2.64 | 1.46        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | 1     | 1605 | CLA  | CHC-C1C | 2.64  | 1.41        | 1.35     |
| 14  | 2     | 809  | CLA  | CMC-C2C | -2.64 | 1.45        | 1.50     |
| 14  | b     | 817  | CLA  | CMB-C2B | -2.63 | 1.46        | 1.51     |
| 14  | A     | 825  | CLA  | CMB-C2B | -2.63 | 1.46        | 1.51     |
| 14  | a     | 804  | CLA  | CHC-C1C | 2.63  | 1.41        | 1.35     |
| 14  | B     | 810  | CLA  | CMB-C2B | -2.63 | 1.46        | 1.51     |
| 14  | B     | 815  | CLA  | CMB-C2B | -2.63 | 1.46        | 1.51     |
| 14  | 2     | 814  | CLA  | CMB-C2B | -2.63 | 1.46        | 1.51     |
| 14  | B     | 816  | CLA  | CMB-C2B | -2.63 | 1.46        | 1.51     |
| 14  | 2     | 817  | CLA  | CMB-C2B | -2.63 | 1.46        | 1.51     |
| 14  | a     | 838  | CLA  | CMB-C2B | -2.63 | 1.46        | 1.51     |
| 14  | 1     | 1629 | CLA  | CMB-C2B | -2.62 | 1.46        | 1.51     |
| 14  | A     | 828  | CLA  | CMB-C2B | -2.62 | 1.46        | 1.51     |
| 14  | a     | 834  | CLA  | CMB-C2B | -2.62 | 1.46        | 1.51     |
| 14  | 2     | 819  | CLA  | CMB-C2B | -2.62 | 1.46        | 1.51     |
| 14  | B     | 820  | CLA  | CMB-C2B | -2.62 | 1.46        | 1.51     |
| 14  | a     | 828  | CLA  | CMB-C2B | -2.62 | 1.46        | 1.51     |
| 14  | 2     | 811  | CLA  | CMB-C2B | -2.62 | 1.46        | 1.51     |
| 14  | b     | 809  | CLA  | CMC-C2C | -2.62 | 1.45        | 1.50     |
| 14  | a     | 814  | CLA  | CMB-C2B | -2.62 | 1.46        | 1.51     |
| 14  | 1     | 1615 | CLA  | CMB-C2B | -2.61 | 1.46        | 1.51     |
| 13  | 1     | 1602 | CL0  | CHC-C1C | 2.61  | 1.41        | 1.35     |
| 14  | B     | 808  | CLA  | CMB-C2B | -2.61 | 1.46        | 1.51     |
| 14  | A     | 812  | CLA  | CMB-C2B | -2.61 | 1.46        | 1.51     |
| 14  | B     | 810  | CLA  | CMC-C2C | -2.60 | 1.45        | 1.50     |
| 14  | 2     | 821  | CLA  | CMB-C2B | -2.60 | 1.46        | 1.51     |
| 14  | A     | 808  | CLA  | CMB-C2B | -2.60 | 1.46        | 1.51     |
| 14  | 1     | 1606 | CLA  | CMB-C2B | -2.60 | 1.46        | 1.51     |
| 14  | 2     | 811  | CLA  | CMC-C2C | -2.60 | 1.45        | 1.50     |
| 14  | b     | 821  | CLA  | CMB-C2B | -2.60 | 1.46        | 1.51     |
| 14  | B     | 807  | CLA  | CMD-C2D | -2.60 | 1.45        | 1.50     |
| 14  | b     | 816  | CLA  | CMB-C2B | -2.60 | 1.46        | 1.51     |
| 14  | 1     | 1641 | CLA  | CMD-C2D | -2.59 | 1.45        | 1.50     |
| 14  | 2     | 824  | CLA  | CMB-C2B | -2.59 | 1.46        | 1.51     |
| 13  | a     | 801  | CL0  | CHC-C1C | 2.59  | 1.41        | 1.35     |
| 14  | b     | 804  | CLA  | CMD-C2D | -2.59 | 1.45        | 1.50     |
| 14  | 2     | 808  | CLA  | CMD-C2D | -2.59 | 1.45        | 1.50     |
| 14  | A     | 838  | CLA  | CMB-C2B | -2.59 | 1.46        | 1.51     |
| 14  | k     | 101  | CLA  | CMB-C2B | -2.59 | 1.46        | 1.51     |
| 14  | 1     | 1639 | CLA  | CMB-C2B | -2.59 | 1.46        | 1.51     |
| 14  | 2     | 813  | CLA  | CMB-C2B | -2.59 | 1.46        | 1.51     |
| 14  | A     | 831  | CLA  | CMD-C2D | -2.59 | 1.45        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | 1     | 1632 | CLA  | CMD-C2D | -2.59 | 1.45        | 1.50     |
| 14  | A     | 814  | CLA  | CMB-C2B | -2.59 | 1.46        | 1.51     |
| 14  | a     | 805  | CLA  | CMB-C2B | -2.59 | 1.46        | 1.51     |
| 13  | A     | 801  | CL0  | CHC-C1C | 2.59  | 1.41        | 1.35     |
| 14  | B     | 824  | CLA  | CMB-C2B | -2.59 | 1.46        | 1.51     |
| 14  | b     | 813  | CLA  | CMB-C2B | -2.59 | 1.46        | 1.51     |
| 14  | a     | 840  | CLA  | CMD-C2D | -2.58 | 1.45        | 1.50     |
| 14  | b     | 809  | CLA  | CMB-C2B | -2.58 | 1.46        | 1.51     |
| 14  | a     | 831  | CLA  | CMD-C2D | -2.58 | 1.45        | 1.50     |
| 14  | b     | 811  | CLA  | CMC-C2C | -2.58 | 1.45        | 1.50     |
| 14  | 1     | 1633 | CLA  | CMD-C2D | -2.58 | 1.45        | 1.50     |
| 14  | A     | 805  | CLA  | CMB-C2B | -2.58 | 1.46        | 1.51     |
| 14  | 2     | 827  | CLA  | CMB-C2B | -2.58 | 1.46        | 1.51     |
| 14  | B     | 803  | CLA  | CMD-C2D | -2.58 | 1.45        | 1.50     |
| 14  | b     | 827  | CLA  | CMB-C2B | -2.58 | 1.46        | 1.51     |
| 14  | l     | 205  | CLA  | C3B-C2B | -2.57 | 1.36        | 1.40     |
| 14  | 2     | 834  | CLA  | CMC-C2C | -2.57 | 1.45        | 1.50     |
| 14  | 2     | 809  | CLA  | CMB-C2B | -2.57 | 1.46        | 1.51     |
| 14  | b     | 824  | CLA  | CMB-C2B | -2.57 | 1.46        | 1.51     |
| 14  | 9     | 101  | CLA  | CMB-C2B | -2.56 | 1.46        | 1.51     |
| 14  | 1     | 1644 | CLA  | CMC-C2C | -2.56 | 1.45        | 1.50     |
| 14  | a     | 808  | CLA  | CMB-C2B | -2.56 | 1.46        | 1.51     |
| 14  | B     | 818  | CLA  | CMB-C2B | -2.56 | 1.46        | 1.51     |
| 14  | a     | 830  | CLA  | CMB-C2B | -2.56 | 1.46        | 1.51     |
| 14  | 1     | 1631 | CLA  | CMB-C2B | -2.56 | 1.46        | 1.51     |
| 14  | A     | 843  | CLA  | CMC-C2C | -2.56 | 1.45        | 1.50     |
| 14  | b     | 834  | CLA  | CMC-C2C | -2.56 | 1.45        | 1.50     |
| 14  | B     | 823  | CLA  | CMB-C2B | -2.56 | 1.46        | 1.51     |
| 14  | A     | 832  | CLA  | CMD-C2D | -2.56 | 1.45        | 1.50     |
| 14  | a     | 832  | CLA  | CMD-C2D | -2.55 | 1.45        | 1.50     |
| 14  | 1     | 1624 | CLA  | CMB-C2B | -2.55 | 1.46        | 1.51     |
| 14  | 1     | 1640 | CLA  | CMD-C2D | -2.55 | 1.45        | 1.50     |
| 14  | a     | 839  | CLA  | CMD-C2D | -2.55 | 1.45        | 1.50     |
| 14  | F     | 203  | CLA  | CMB-C2B | -2.55 | 1.46        | 1.51     |
| 14  | A     | 830  | CLA  | CMB-C2B | -2.55 | 1.46        | 1.51     |
| 14  | 2     | 804  | CLA  | CMD-C2D | -2.55 | 1.45        | 1.50     |
| 14  | 2     | 825  | CLA  | CMB-C2B | -2.55 | 1.46        | 1.51     |
| 14  | K     | 101  | CLA  | CMB-C2B | -2.55 | 1.46        | 1.51     |
| 14  | a     | 823  | CLA  | CMB-C2B | -2.55 | 1.46        | 1.51     |
| 14  | b     | 808  | CLA  | CMD-C2D | -2.55 | 1.45        | 1.50     |
| 14  | B     | 826  | CLA  | CMB-C2B | -2.55 | 1.46        | 1.51     |
| 14  | B     | 828  | CLA  | C3B-C2B | -2.55 | 1.36        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | 1     | 1630 | CLA  | CMC-C2C | -2.54 | 1.45        | 1.50     |
| 13  | A     | 801  | CL0  | CMD-C2D | -2.54 | 1.45        | 1.50     |
| 14  | A     | 829  | CLA  | CMC-C2C | -2.54 | 1.45        | 1.50     |
| 13  | 1     | 1602 | CL0  | CMD-C2D | -2.54 | 1.45        | 1.50     |
| 13  | a     | 801  | CL0  | CMD-C2D | -2.54 | 1.45        | 1.50     |
| 14  | b     | 830  | CLA  | CMD-C2D | -2.54 | 1.45        | 1.50     |
| 14  | 2     | 805  | CLA  | CMD-C2D | -2.54 | 1.45        | 1.50     |
| 14  | 2     | 810  | CLA  | CMC-C2C | -2.53 | 1.45        | 1.50     |
| 14  | B     | 833  | CLA  | CMC-C2C | -2.53 | 1.45        | 1.50     |
| 14  | A     | 823  | CLA  | CMB-C2B | -2.53 | 1.46        | 1.51     |
| 14  | b     | 825  | CLA  | CMB-C2B | -2.53 | 1.46        | 1.51     |
| 14  | 2     | 811  | CLA  | CMD-C2D | -2.53 | 1.45        | 1.50     |
| 14  | 1     | 1609 | CLA  | CMB-C2B | -2.53 | 1.46        | 1.51     |
| 14  | B     | 841  | CLA  | CMD-C2D | -2.53 | 1.45        | 1.50     |
| 14  | B     | 810  | CLA  | CMD-C2D | -2.53 | 1.45        | 1.50     |
| 14  | a     | 843  | CLA  | CMC-C2C | -2.53 | 1.45        | 1.50     |
| 18  | y     | 101  | LHG  | O7-C5   | -2.53 | 1.40        | 1.46     |
| 14  | b     | 810  | CLA  | CMC-C2C | -2.53 | 1.45        | 1.50     |
| 14  | 2     | 830  | CLA  | CMD-C2D | -2.52 | 1.45        | 1.50     |
| 14  | A     | 839  | CLA  | CMD-C2D | -2.52 | 1.45        | 1.50     |
| 14  | b     | 805  | CLA  | CMD-C2D | -2.52 | 1.45        | 1.50     |
| 14  | j     | 1301 | CLA  | CMB-C2B | -2.52 | 1.46        | 1.51     |
| 14  | B     | 829  | CLA  | CMD-C2D | -2.52 | 1.45        | 1.50     |
| 14  | 2     | 842  | CLA  | CMD-C2D | -2.52 | 1.45        | 1.50     |
| 14  | B     | 802  | CLA  | CMD-C2D | -2.52 | 1.45        | 1.50     |
| 14  | j     | 1302 | CLA  | CMB-C2B | -2.52 | 1.46        | 1.51     |
| 18  | m     | 101  | LHG  | O7-C5   | -2.52 | 1.40        | 1.46     |
| 14  | b     | 803  | CLA  | CMD-C2D | -2.52 | 1.45        | 1.50     |
| 14  | a     | 829  | CLA  | CMC-C2C | -2.52 | 1.45        | 1.50     |
| 14  | J     | 101  | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 14  | 8     | 1302 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 14  | 0     | 206  | CLA  | CMD-C2D | -2.51 | 1.45        | 1.50     |
| 14  | b     | 842  | CLA  | C3B-C2B | -2.51 | 1.36        | 1.40     |
| 14  | b     | 842  | CLA  | CMD-C2D | -2.51 | 1.45        | 1.50     |
| 14  | 2     | 829  | CLA  | C3B-C2B | -2.51 | 1.36        | 1.40     |
| 14  | B     | 804  | CLA  | CMD-C2D | -2.51 | 1.45        | 1.50     |
| 14  | L     | 204  | CLA  | CMD-C2D | -2.51 | 1.45        | 1.50     |
| 14  | b     | 831  | CLA  | C3B-C2B | -2.51 | 1.36        | 1.40     |
| 14  | B     | 830  | CLA  | C3B-C2B | -2.51 | 1.36        | 1.40     |
| 14  | 1     | 1641 | CLA  | C3B-C2B | -2.50 | 1.36        | 1.40     |
| 14  | b     | 815  | CLA  | CMD-C2D | -2.50 | 1.45        | 1.50     |
| 14  | 8     | 1301 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 821  | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 14  | 2     | 803  | CLA  | CMD-C2D | -2.50 | 1.45        | 1.50     |
| 18  | M     | 101  | LHG  | O7-C5   | -2.50 | 1.40        | 1.46     |
| 14  | L     | 204  | CLA  | C3B-C2B | -2.50 | 1.36        | 1.40     |
| 14  | 2     | 815  | CLA  | CMD-C2D | -2.49 | 1.45        | 1.50     |
| 14  | B     | 841  | CLA  | C3B-C2B | -2.49 | 1.36        | 1.40     |
| 14  | A     | 840  | CLA  | C3B-C2B | -2.49 | 1.36        | 1.40     |
| 14  | a     | 842  | CLA  | CMD-C2D | -2.49 | 1.45        | 1.50     |
| 14  | B     | 814  | CLA  | CMD-C2D | -2.49 | 1.45        | 1.50     |
| 14  | M     | 102  | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 14  | A     | 857  | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 14  | l     | 205  | CLA  | CMD-C2D | -2.49 | 1.45        | 1.50     |
| 14  | 2     | 831  | CLA  | C3B-C2B | -2.49 | 1.36        | 1.40     |
| 14  | B     | 809  | CLA  | CMC-C2C | -2.49 | 1.45        | 1.50     |
| 14  | b     | 811  | CLA  | CMD-C2D | -2.49 | 1.45        | 1.50     |
| 14  | f     | 203  | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 14  | 1     | 1637 | CLA  | CMC-C2C | -2.48 | 1.45        | 1.50     |
| 14  | a     | 806  | CLA  | CMD-C2D | -2.48 | 1.45        | 1.50     |
| 14  | a     | 803  | CLA  | CMD-C2D | -2.48 | 1.45        | 1.50     |
| 14  | A     | 842  | CLA  | CMC-C2C | -2.48 | 1.45        | 1.50     |
| 14  | b     | 829  | CLA  | C3B-C2B | -2.48 | 1.36        | 1.40     |
| 14  | L     | 203  | CLA  | C3B-C2B | -2.48 | 1.36        | 1.40     |
| 14  | 1     | 1604 | CLA  | CMD-C2D | -2.48 | 1.45        | 1.50     |
| 14  | 1     | 1643 | CLA  | CMC-C2C | -2.47 | 1.45        | 1.50     |
| 14  | A     | 836  | CLA  | CMC-C2C | -2.47 | 1.45        | 1.50     |
| 14  | a     | 840  | CLA  | C3B-C2B | -2.47 | 1.36        | 1.40     |
| 14  | 0     | 206  | CLA  | C3B-C2B | -2.47 | 1.36        | 1.40     |
| 14  | 0     | 206  | CLA  | C3B-CAB | -2.47 | 1.42        | 1.47     |
| 14  | A     | 842  | CLA  | CMD-C2D | -2.47 | 1.45        | 1.50     |
| 14  | L     | 204  | CLA  | C3B-CAB | -2.47 | 1.42        | 1.47     |
| 14  | A     | 841  | CLA  | CMD-C2D | -2.47 | 1.45        | 1.50     |
| 14  | 1     | 1601 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 14  | A     | 817  | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 14  | A     | 806  | CLA  | CMD-C2D | -2.47 | 1.45        | 1.50     |
| 14  | F     | 204  | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 14  | 1     | 1618 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 14  | a     | 842  | CLA  | CMC-C2C | -2.47 | 1.45        | 1.50     |
| 14  | b     | 802  | CLA  | CMC-C2C | -2.47 | 1.45        | 1.50     |
| 14  | a     | 803  | CLA  | CMC-C2C | -2.46 | 1.45        | 1.50     |
| 14  | a     | 836  | CLA  | CMC-C2C | -2.46 | 1.45        | 1.50     |
| 14  | A     | 803  | CLA  | CMD-C2D | -2.46 | 1.45        | 1.50     |
| 14  | b     | 810  | CLA  | CMD-C2D | -2.46 | 1.45        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 841  | CLA  | CMD-C2D | -2.46 | 1.45        | 1.50     |
| 14  | a     | 829  | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 14  | 1     | 1630 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 14  | 1     | 1633 | CLA  | C3B-C2B | -2.46 | 1.37        | 1.40     |
| 14  | 2     | 822  | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 14  | 0     | 205  | CLA  | C3B-C2B | -2.46 | 1.37        | 1.40     |
| 14  | a     | 807  | CLA  | CMD-C2D | -2.46 | 1.45        | 1.50     |
| 14  | 1     | 1603 | CLA  | CMC-C2C | -2.46 | 1.45        | 1.50     |
| 14  | a     | 832  | CLA  | C3B-C2B | -2.46 | 1.37        | 1.40     |
| 14  | 2     | 842  | CLA  | C3B-C2B | -2.46 | 1.37        | 1.40     |
| 14  | a     | 817  | CLA  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 14  | 2     | 815  | CLA  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 14  | L     | 205  | CLA  | CMD-C2D | -2.45 | 1.45        | 1.50     |
| 14  | b     | 838  | CLA  | C3B-C2B | -2.45 | 1.37        | 1.40     |
| 14  | A     | 807  | CLA  | CMD-C2D | -2.45 | 1.45        | 1.50     |
| 14  | b     | 805  | CLA  | CMC-C2C | -2.45 | 1.45        | 1.50     |
| 14  | 2     | 802  | CLA  | CMC-C2C | -2.45 | 1.45        | 1.50     |
| 14  | A     | 802  | CLA  | CMC-C2C | -2.45 | 1.45        | 1.50     |
| 14  | A     | 855  | CLA  | CMC-C2C | -2.45 | 1.45        | 1.50     |
| 14  | z     | 102  | CLA  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 14  | 1     | 1607 | CLA  | CMD-C2D | -2.45 | 1.45        | 1.50     |
| 14  | A     | 803  | CLA  | CMC-C2C | -2.45 | 1.45        | 1.50     |
| 14  | b     | 822  | CLA  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 14  | 1     | 1604 | CLA  | CMC-C2C | -2.45 | 1.45        | 1.50     |
| 14  | 1     | 1643 | CLA  | CMD-C2D | -2.45 | 1.45        | 1.50     |
| 14  | B     | 814  | CLA  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 14  | A     | 829  | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 14  | l     | 206  | CLA  | CMD-C2D | -2.44 | 1.45        | 1.50     |
| 14  | b     | 815  | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 14  | B     | 837  | CLA  | C3B-C2B | -2.44 | 1.37        | 1.40     |
| 14  | 1     | 1612 | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 14  | 2     | 805  | CLA  | CMC-C2C | -2.44 | 1.45        | 1.50     |
| 14  | 1     | 1619 | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 14  | 1     | 1642 | CLA  | CMD-C2D | -2.44 | 1.45        | 1.50     |
| 14  | X     | 1701 | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 14  | 0     | 207  | CLA  | CMD-C2D | -2.44 | 1.45        | 1.50     |
| 14  | 6     | 203  | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 14  | 1     | 1608 | CLA  | CMD-C2D | -2.44 | 1.45        | 1.50     |
| 18  | 1     | 1655 | LHG  | O7-C5   | -2.44 | 1.40        | 1.46     |
| 14  | a     | 811  | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 14  | l     | 205  | CLA  | CMC-C2C | -2.43 | 1.45        | 1.50     |
| 14  | 6     | 201  | CLA  | CMD-C2D | -2.43 | 1.45        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | 1     | 1634 | CLA  | CMD-C2D | -2.43 | 1.45        | 1.50     |
| 14  | b     | 820  | CLA  | C3B-C2B | -2.43 | 1.37        | 1.40     |
| 18  | A     | 854  | LHG  | O7-C5   | -2.43 | 1.40        | 1.46     |
| 14  | 2     | 838  | CLA  | C3B-C2B | -2.43 | 1.37        | 1.40     |
| 14  | a     | 835  | CLA  | C3B-C2B | -2.43 | 1.37        | 1.40     |
| 14  | A     | 826  | CLA  | CMD-C2D | -2.43 | 1.45        | 1.50     |
| 14  | J     | 102  | CLA  | CMB-C2B | -2.43 | 1.46        | 1.51     |
| 14  | l     | 205  | CLA  | C3B-CAB | -2.43 | 1.43        | 1.47     |
| 18  | a     | 854  | LHG  | O7-C5   | -2.43 | 1.40        | 1.46     |
| 14  | k     | 103  | CLA  | CMB-C2B | -2.43 | 1.46        | 1.51     |
| 14  | K     | 103  | CLA  | CMB-C2B | -2.43 | 1.46        | 1.51     |
| 14  | B     | 804  | CLA  | CMC-C2C | -2.43 | 1.45        | 1.50     |
| 14  | a     | 802  | CLA  | CMC-C2C | -2.43 | 1.45        | 1.50     |
| 14  | A     | 818  | CLA  | CMB-C2B | -2.43 | 1.46        | 1.51     |
| 14  | B     | 809  | CLA  | CMD-C2D | -2.43 | 1.45        | 1.50     |
| 14  | F     | 201  | CLA  | CMD-C2D | -2.43 | 1.45        | 1.50     |
| 14  | a     | 818  | CLA  | CMB-C2B | -2.43 | 1.46        | 1.51     |
| 14  | 2     | 826  | CLA  | CMD-C2D | -2.42 | 1.45        | 1.50     |
| 14  | 2     | 831  | CLA  | C3B-CAB | -2.42 | 1.43        | 1.47     |
| 14  | 8     | 1303 | CLA  | CMB-C2B | -2.42 | 1.46        | 1.51     |
| 14  | 2     | 820  | CLA  | C3B-C2B | -2.42 | 1.37        | 1.40     |
| 14  | 1     | 1639 | CLA  | CMD-C2D | -2.42 | 1.45        | 1.50     |
| 14  | A     | 836  | CLA  | C3B-C2B | -2.42 | 1.37        | 1.40     |
| 14  | A     | 811  | CLA  | CMB-C2B | -2.42 | 1.46        | 1.51     |
| 14  | b     | 826  | CLA  | CMD-C2D | -2.42 | 1.45        | 1.50     |
| 14  | b     | 808  | CLA  | C3B-C2B | -2.42 | 1.37        | 1.40     |
| 14  | 1     | 1627 | CLA  | CMD-C2D | -2.41 | 1.45        | 1.50     |
| 14  | x     | 1701 | CLA  | CMB-C2B | -2.41 | 1.46        | 1.51     |
| 14  | l     | 204  | CLA  | C3B-C2B | -2.41 | 1.37        | 1.40     |
| 14  | L     | 204  | CLA  | CMC-C2C | -2.41 | 1.45        | 1.50     |
| 14  | j     | 1303 | CLA  | CMB-C2B | -2.41 | 1.46        | 1.51     |
| 14  | 2     | 806  | CLA  | CMC-C2C | -2.41 | 1.45        | 1.50     |
| 14  | 2     | 810  | CLA  | CMD-C2D | -2.41 | 1.45        | 1.50     |
| 14  | 9     | 103  | CLA  | CMB-C2B | -2.41 | 1.46        | 1.51     |
| 14  | 1     | 1635 | CLA  | CMD-C2D | -2.41 | 1.45        | 1.50     |
| 14  | A     | 838  | CLA  | CMD-C2D | -2.41 | 1.45        | 1.50     |
| 14  | a     | 826  | CLA  | CMD-C2D | -2.41 | 1.45        | 1.50     |
| 14  | b     | 806  | CLA  | CMC-C2C | -2.40 | 1.45        | 1.50     |
| 14  | a     | 838  | CLA  | CMD-C2D | -2.40 | 1.45        | 1.50     |
| 14  | B     | 804  | CLA  | C3B-C2B | -2.40 | 1.37        | 1.40     |
| 14  | B     | 826  | CLA  | CMD-C2D | -2.40 | 1.45        | 1.50     |
| 14  | b     | 803  | CLA  | CMC-C2C | -2.40 | 1.45        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 805  | CLA  | CMC-C2C | -2.40 | 1.45        | 1.50     |
| 14  | B     | 841  | CLA  | CMC-C2C | -2.40 | 1.45        | 1.50     |
| 14  | a     | 827  | CLA  | CMD-C2D | -2.40 | 1.45        | 1.50     |
| 14  | a     | 833  | CLA  | CMD-C2D | -2.40 | 1.45        | 1.50     |
| 14  | a     | 843  | CLA  | C3B-C2B | -2.40 | 1.37        | 1.40     |
| 14  | a     | 834  | CLA  | CMD-C2D | -2.40 | 1.45        | 1.50     |
| 14  | b     | 827  | CLA  | CMD-C2D | -2.40 | 1.45        | 1.50     |
| 14  | 0     | 206  | CLA  | CMC-C2C | -2.40 | 1.45        | 1.50     |
| 14  | A     | 832  | CLA  | C3B-C2B | -2.40 | 1.37        | 1.40     |
| 14  | a     | 820  | CLA  | CMD-C2D | -2.40 | 1.45        | 1.50     |
| 14  | B     | 806  | CLA  | CMD-C2D | -2.39 | 1.45        | 1.50     |
| 14  | B     | 825  | CLA  | CMD-C2D | -2.39 | 1.45        | 1.50     |
| 14  | 1     | 1636 | CLA  | CMD-C2D | -2.39 | 1.45        | 1.50     |
| 14  | B     | 819  | CLA  | C3B-C2B | -2.39 | 1.37        | 1.40     |
| 14  | 2     | 808  | CLA  | C3B-C2B | -2.39 | 1.37        | 1.40     |
| 14  | f     | 201  | CLA  | CMD-C2D | -2.39 | 1.45        | 1.50     |
| 14  | A     | 843  | CLA  | C3B-C2B | -2.39 | 1.37        | 1.40     |
| 14  | 2     | 838  | CLA  | CMD-C2D | -2.39 | 1.45        | 1.50     |
| 14  | A     | 818  | CLA  | CMD-C2D | -2.39 | 1.45        | 1.50     |
| 14  | A     | 833  | CLA  | CMD-C2D | -2.39 | 1.45        | 1.50     |
| 14  | b     | 810  | CLA  | C3B-C2B | -2.39 | 1.37        | 1.40     |
| 14  | a     | 829  | CLA  | CMD-C2D | -2.39 | 1.45        | 1.50     |
| 14  | 1     | 1628 | CLA  | CMD-C2D | -2.39 | 1.45        | 1.50     |
| 14  | A     | 835  | CLA  | CMD-C2D | -2.39 | 1.45        | 1.50     |
| 14  | b     | 834  | CLA  | CMD-C2D | -2.39 | 1.45        | 1.50     |
| 14  | A     | 827  | CLA  | CMD-C2D | -2.39 | 1.45        | 1.50     |
| 14  | a     | 828  | CLA  | CMD-C2D | -2.38 | 1.45        | 1.50     |
| 14  | 2     | 827  | CLA  | CMD-C2D | -2.38 | 1.45        | 1.50     |
| 14  | 1     | 1637 | CLA  | C3B-C2B | -2.38 | 1.37        | 1.40     |
| 14  | b     | 807  | CLA  | CMD-C2D | -2.38 | 1.45        | 1.50     |
| 14  | b     | 831  | CLA  | C3B-CAB | -2.38 | 1.43        | 1.47     |
| 14  | A     | 828  | CLA  | CMD-C2D | -2.38 | 1.45        | 1.50     |
| 14  | b     | 828  | CLA  | CMC-C2C | -2.38 | 1.45        | 1.50     |
| 14  | A     | 832  | CLA  | C3B-CAB | -2.38 | 1.43        | 1.47     |
| 14  | 2     | 834  | CLA  | CMD-C2D | -2.38 | 1.45        | 1.50     |
| 14  | A     | 813  | CLA  | CMD-C2D | -2.38 | 1.45        | 1.50     |
| 14  | B     | 802  | CLA  | CMC-C2C | -2.38 | 1.45        | 1.50     |
| 14  | a     | 836  | CLA  | C3B-C2B | -2.37 | 1.37        | 1.40     |
| 14  | 2     | 805  | CLA  | C3B-C2B | -2.37 | 1.37        | 1.40     |
| 14  | 2     | 826  | CLA  | C3B-C2B | -2.37 | 1.37        | 1.40     |
| 14  | 1     | 1617 | CLA  | CMB-C2B | -2.37 | 1.46        | 1.51     |
| 14  | B     | 830  | CLA  | C3B-CAB | -2.37 | 1.43        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | 1     | 1621 | CLA  | CMD-C2D | -2.37 | 1.45        | 1.50     |
| 14  | a     | 813  | CLA  | CMD-C2D | -2.37 | 1.45        | 1.50     |
| 14  | b     | 805  | CLA  | C3B-C2B | -2.37 | 1.37        | 1.40     |
| 14  | 2     | 807  | CLA  | CMD-C2D | -2.37 | 1.45        | 1.50     |
| 14  | b     | 842  | CLA  | CMC-C2C | -2.37 | 1.45        | 1.50     |
| 14  | B     | 833  | CLA  | CMD-C2D | -2.36 | 1.45        | 1.50     |
| 14  | 2     | 823  | CLA  | CMD-C2D | -2.36 | 1.45        | 1.50     |
| 14  | B     | 809  | CLA  | C3B-C2B | -2.36 | 1.37        | 1.40     |
| 14  | a     | 824  | CLA  | C3B-C2B | -2.36 | 1.37        | 1.40     |
| 14  | A     | 820  | CLA  | CMD-C2D | -2.36 | 1.45        | 1.50     |
| 14  | B     | 807  | CLA  | C3B-C2B | -2.36 | 1.37        | 1.40     |
| 14  | b     | 808  | CLA  | C3B-CAB | -2.36 | 1.43        | 1.47     |
| 14  | A     | 834  | CLA  | CMD-C2D | -2.36 | 1.45        | 1.50     |
| 14  | 2     | 808  | CLA  | C3B-CAB | -2.36 | 1.43        | 1.47     |
| 14  | A     | 839  | CLA  | C3B-CAB | -2.36 | 1.43        | 1.47     |
| 14  | B     | 837  | CLA  | CMD-C2D | -2.36 | 1.45        | 1.50     |
| 14  | 1     | 1614 | CLA  | CMD-C2D | -2.36 | 1.45        | 1.50     |
| 14  | 2     | 842  | CLA  | CMC-C2C | -2.36 | 1.45        | 1.50     |
| 14  | A     | 822  | CLA  | CMD-C2D | -2.36 | 1.45        | 1.50     |
| 14  | B     | 834  | CLA  | CMD-C2D | -2.36 | 1.45        | 1.50     |
| 14  | 2     | 803  | CLA  | CMC-C2C | -2.35 | 1.45        | 1.50     |
| 14  | B     | 827  | CLA  | CMC-C2C | -2.35 | 1.45        | 1.50     |
| 14  | B     | 802  | CLA  | C3B-CAB | -2.35 | 1.43        | 1.47     |
| 14  | A     | 829  | CLA  | CMD-C2D | -2.35 | 1.45        | 1.50     |
| 14  | 1     | 1630 | CLA  | CMD-C2D | -2.35 | 1.45        | 1.50     |
| 14  | a     | 822  | CLA  | CMD-C2D | -2.35 | 1.45        | 1.50     |
| 14  | B     | 818  | CLA  | CMD-C2D | -2.35 | 1.45        | 1.50     |
| 14  | a     | 816  | CLA  | CMB-C2B | -2.35 | 1.46        | 1.51     |
| 14  | a     | 832  | CLA  | C3B-CAB | -2.35 | 1.43        | 1.47     |
| 14  | B     | 822  | CLA  | CMD-C2D | -2.35 | 1.45        | 1.50     |
| 14  | l     | 204  | CLA  | CMD-C2D | -2.35 | 1.45        | 1.50     |
| 14  | 1     | 1619 | CLA  | CMD-C2D | -2.35 | 1.45        | 1.50     |
| 14  | a     | 818  | CLA  | CMD-C2D | -2.35 | 1.45        | 1.50     |
| 14  | b     | 838  | CLA  | CMD-C2D | -2.35 | 1.45        | 1.50     |
| 14  | 2     | 804  | CLA  | CMC-C2C | -2.35 | 1.45        | 1.50     |
| 14  | 1     | 1636 | CLA  | C3B-C2B | -2.34 | 1.37        | 1.40     |
| 14  | A     | 857  | CLA  | CMD-C2D | -2.34 | 1.45        | 1.50     |
| 14  | L     | 203  | CLA  | CMD-C2D | -2.34 | 1.45        | 1.50     |
| 14  | b     | 804  | CLA  | CMC-C2C | -2.34 | 1.45        | 1.50     |
| 14  | B     | 807  | CLA  | C3B-CAB | -2.34 | 1.43        | 1.47     |
| 14  | 2     | 810  | CLA  | C3B-C2B | -2.34 | 1.37        | 1.40     |
| 14  | A     | 809  | CLA  | CMD-C2D | -2.34 | 1.45        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | 2     | 826  | CLA  | CMC-C2C | -2.34 | 1.45        | 1.50     |
| 14  | 2     | 828  | CLA  | CMC-C2C | -2.34 | 1.45        | 1.50     |
| 14  | 2     | 841  | CLA  | C3B-C2B | -2.34 | 1.37        | 1.40     |
| 14  | 1     | 1611 | CLA  | CMD-C2D | -2.34 | 1.45        | 1.50     |
| 14  | b     | 819  | CLA  | CMD-C2D | -2.34 | 1.45        | 1.50     |
| 14  | b     | 823  | CLA  | CMD-C2D | -2.34 | 1.45        | 1.50     |
| 14  | a     | 835  | CLA  | CMD-C2D | -2.34 | 1.45        | 1.50     |
| 14  | 1     | 1629 | CLA  | CMD-C2D | -2.33 | 1.45        | 1.50     |
| 14  | A     | 824  | CLA  | C3B-C2B | -2.33 | 1.37        | 1.40     |
| 14  | A     | 820  | CLA  | CMC-C2C | -2.33 | 1.45        | 1.50     |
| 14  | 2     | 828  | CLA  | CMD-C2D | -2.33 | 1.45        | 1.50     |
| 14  | 1     | 1615 | CLA  | CMC-C2C | -2.33 | 1.45        | 1.50     |
| 14  | b     | 803  | CLA  | C3B-CAB | -2.33 | 1.43        | 1.47     |
| 14  | a     | 804  | CLA  | CMD-C2D | -2.33 | 1.45        | 1.50     |
| 14  | B     | 838  | CLA  | CMD-C2D | -2.32 | 1.45        | 1.50     |
| 14  | b     | 835  | CLA  | CMD-C2D | -2.32 | 1.45        | 1.50     |
| 14  | B     | 827  | CLA  | CMD-C2D | -2.32 | 1.45        | 1.50     |
| 14  | a     | 820  | CLA  | CMC-C2C | -2.32 | 1.45        | 1.50     |
| 14  | 2     | 840  | CLA  | CMD-C2D | -2.32 | 1.45        | 1.50     |
| 14  | A     | 804  | CLA  | CMD-C2D | -2.32 | 1.45        | 1.50     |
| 14  | 2     | 839  | CLA  | CMD-C2D | -2.32 | 1.45        | 1.50     |
| 14  | 1     | 1625 | CLA  | C3B-C2B | -2.32 | 1.37        | 1.40     |
| 14  | b     | 826  | CLA  | CMC-C2C | -2.32 | 1.45        | 1.50     |
| 14  | 2     | 819  | CLA  | CMD-C2D | -2.32 | 1.45        | 1.50     |
| 14  | a     | 809  | CLA  | CMD-C2D | -2.32 | 1.45        | 1.50     |
| 14  | 1     | 1644 | CLA  | C3B-C2B | -2.32 | 1.37        | 1.40     |
| 14  | b     | 839  | CLA  | CMD-C2D | -2.32 | 1.45        | 1.50     |
| 14  | M     | 102  | CLA  | CMD-C2D | -2.32 | 1.45        | 1.50     |
| 14  | 0     | 205  | CLA  | CMD-C2D | -2.32 | 1.45        | 1.50     |
| 14  | 2     | 835  | CLA  | CMD-C2D | -2.32 | 1.45        | 1.50     |
| 14  | a     | 810  | CLA  | CMD-C2D | -2.31 | 1.45        | 1.50     |
| 14  | B     | 825  | CLA  | C3B-C2B | -2.31 | 1.37        | 1.40     |
| 14  | 1     | 1621 | CLA  | CMC-C2C | -2.31 | 1.45        | 1.50     |
| 14  | A     | 816  | CLA  | CMB-C2B | -2.31 | 1.46        | 1.51     |
| 14  | 1     | 1610 | CLA  | CMD-C2D | -2.31 | 1.45        | 1.50     |
| 14  | 2     | 803  | CLA  | C3B-CAB | -2.31 | 1.43        | 1.47     |
| 14  | b     | 840  | CLA  | CMD-C2D | -2.31 | 1.45        | 1.50     |
| 14  | B     | 839  | CLA  | CMD-C2D | -2.31 | 1.45        | 1.50     |
| 14  | 1     | 1633 | CLA  | C3B-CAB | -2.31 | 1.43        | 1.47     |
| 14  | B     | 825  | CLA  | CMC-C2C | -2.31 | 1.45        | 1.50     |
| 17  | b     | 849  | BCR  | C38-C26 | -2.31 | 1.47        | 1.50     |
| 14  | A     | 814  | CLA  | CMC-C2C | -2.31 | 1.45        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | 1     | 1623 | CLA  | CMD-C2D | -2.30 | 1.45        | 1.50     |
| 14  | 2     | 833  | CLA  | CMD-C2D | -2.30 | 1.45        | 1.50     |
| 14  | A     | 831  | CLA  | CMC-C2C | -2.30 | 1.45        | 1.50     |
| 14  | a     | 814  | CLA  | CMC-C2C | -2.30 | 1.45        | 1.50     |
| 20  | b     | 850  | LMG  | O6-C5   | -2.30 | 1.38        | 1.44     |
| 17  | B     | 848  | BCR  | C38-C26 | -2.30 | 1.47        | 1.50     |
| 14  | B     | 803  | CLA  | CMC-C2C | -2.30 | 1.45        | 1.50     |
| 20  | B     | 849  | LMG  | O8-C9   | -2.30 | 1.39        | 1.45     |
| 14  | B     | 817  | CLA  | C3B-C2B | -2.30 | 1.37        | 1.40     |
| 14  | 1     | 1640 | CLA  | C3B-CAB | -2.30 | 1.43        | 1.47     |
| 20  | b     | 850  | LMG  | O8-C9   | -2.29 | 1.39        | 1.45     |
| 14  | 1     | 1613 | CLA  | CMD-C2D | -2.29 | 1.45        | 1.50     |
| 14  | a     | 825  | CLA  | CMD-C2D | -2.29 | 1.45        | 1.50     |
| 14  | A     | 835  | CLA  | C3B-C2B | -2.29 | 1.37        | 1.40     |
| 14  | a     | 839  | CLA  | C3B-CAB | -2.29 | 1.43        | 1.47     |
| 14  | 1     | 1632 | CLA  | CMC-C2C | -2.29 | 1.45        | 1.50     |
| 14  | a     | 830  | CLA  | C3B-CAB | -2.29 | 1.43        | 1.47     |
| 14  | A     | 810  | CLA  | CMD-C2D | -2.29 | 1.45        | 1.50     |
| 14  | b     | 836  | CLA  | CMD-C2D | -2.29 | 1.45        | 1.50     |
| 14  | 1     | 1605 | CLA  | CMD-C2D | -2.29 | 1.45        | 1.50     |
| 14  | B     | 815  | CLA  | CMD-C2D | -2.29 | 1.45        | 1.50     |
| 14  | 1     | 1601 | CLA  | CMD-C2D | -2.29 | 1.45        | 1.50     |
| 14  | 2     | 833  | CLA  | C3B-C2B | -2.29 | 1.37        | 1.40     |
| 14  | j     | 1301 | CLA  | CMD-C2D | -2.29 | 1.46        | 1.50     |
| 14  | A     | 823  | CLA  | CMD-C2D | -2.28 | 1.46        | 1.50     |
| 14  | b     | 830  | CLA  | CHC-C1C | 2.28  | 1.40        | 1.35     |
| 14  | B     | 832  | CLA  | CMD-C2D | -2.28 | 1.46        | 1.50     |
| 20  | B     | 849  | LMG  | O6-C5   | -2.28 | 1.38        | 1.44     |
| 14  | b     | 826  | CLA  | C3B-C2B | -2.28 | 1.37        | 1.40     |
| 14  | 1     | 1620 | CLA  | CMD-C2D | -2.28 | 1.46        | 1.50     |
| 20  | 2     | 850  | LMG  | O6-C5   | -2.28 | 1.38        | 1.44     |
| 20  | 2     | 850  | LMG  | O8-C9   | -2.28 | 1.40        | 1.45     |
| 14  | b     | 828  | CLA  | CMD-C2D | -2.28 | 1.46        | 1.50     |
| 14  | 1     | 1626 | CLA  | CMD-C2D | -2.27 | 1.46        | 1.50     |
| 14  | 2     | 825  | CLA  | CMC-C2C | -2.27 | 1.46        | 1.50     |
| 14  | 2     | 838  | CLA  | CMC-C2C | -2.27 | 1.46        | 1.50     |
| 14  | A     | 812  | CLA  | CMD-C2D | -2.27 | 1.46        | 1.50     |
| 14  | a     | 833  | CLA  | C3B-CAB | -2.27 | 1.43        | 1.47     |
| 14  | B     | 832  | CLA  | C3B-C2B | -2.27 | 1.37        | 1.40     |
| 14  | j     | 1301 | CLA  | CMC-C2C | -2.27 | 1.46        | 1.50     |
| 14  | a     | 819  | CLA  | CMD-C2D | -2.27 | 1.46        | 1.50     |
| 14  | l     | 204  | CLA  | CMC-C2C | -2.27 | 1.46        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 832  | CLA  | CMD-C2D | -2.27 | 1.46        | 1.50     |
| 14  | k     | 101  | CLA  | CMD-C2D | -2.27 | 1.46        | 1.50     |
| 14  | a     | 831  | CLA  | CMC-C2C | -2.27 | 1.46        | 1.50     |
| 14  | 2     | 816  | CLA  | CMD-C2D | -2.27 | 1.46        | 1.50     |
| 14  | b     | 833  | CLA  | C3B-C2B | -2.27 | 1.37        | 1.40     |
| 14  | B     | 837  | CLA  | CMC-C2C | -2.27 | 1.46        | 1.50     |
| 14  | 1     | 1631 | CLA  | C3B-CAB | -2.26 | 1.43        | 1.47     |
| 14  | b     | 838  | CLA  | CMC-C2C | -2.26 | 1.46        | 1.50     |
| 14  | 1     | 1607 | CLA  | CMC-C2C | -2.26 | 1.46        | 1.50     |
| 14  | A     | 825  | CLA  | CMD-C2D | -2.26 | 1.46        | 1.50     |
| 14  | 8     | 1301 | CLA  | CMC-C2C | -2.26 | 1.46        | 1.50     |
| 14  | B     | 829  | CLA  | CHC-C1C | 2.26  | 1.40        | 1.35     |
| 14  | A     | 819  | CLA  | CMD-C2D | -2.26 | 1.46        | 1.50     |
| 14  | a     | 812  | CLA  | CMD-C2D | -2.26 | 1.46        | 1.50     |
| 14  | b     | 806  | CLA  | CMD-C2D | -2.26 | 1.46        | 1.50     |
| 14  | B     | 840  | CLA  | C3B-CAB | -2.26 | 1.43        | 1.47     |
| 14  | b     | 816  | CLA  | CMD-C2D | -2.26 | 1.46        | 1.50     |
| 14  | B     | 805  | CLA  | CMD-C2D | -2.26 | 1.46        | 1.50     |
| 14  | 2     | 832  | CLA  | CMD-C2D | -2.26 | 1.46        | 1.50     |
| 14  | 2     | 806  | CLA  | CMD-C2D | -2.26 | 1.46        | 1.50     |
| 14  | 2     | 836  | CLA  | CMD-C2D | -2.26 | 1.46        | 1.50     |
| 14  | A     | 827  | CLA  | C3B-CAB | -2.26 | 1.43        | 1.47     |
| 14  | 1     | 1624 | CLA  | CMD-C2D | -2.26 | 1.46        | 1.50     |
| 14  | 0     | 207  | CLA  | CMC-C2C | -2.26 | 1.46        | 1.50     |
| 14  | B     | 824  | CLA  | CMC-C2C | -2.26 | 1.46        | 1.50     |
| 14  | b     | 814  | CLA  | CMD-C2D | -2.25 | 1.46        | 1.50     |
| 14  | 0     | 205  | CLA  | CMC-C2C | -2.25 | 1.46        | 1.50     |
| 14  | b     | 841  | CLA  | C3B-C2B | -2.25 | 1.37        | 1.40     |
| 14  | 1     | 1634 | CLA  | C3B-CAB | -2.25 | 1.43        | 1.47     |
| 14  | A     | 833  | CLA  | CMC-C2C | -2.25 | 1.46        | 1.50     |
| 14  | B     | 813  | CLA  | CMD-C2D | -2.25 | 1.46        | 1.50     |
| 14  | B     | 835  | CLA  | CMD-C2D | -2.25 | 1.46        | 1.50     |
| 14  | a     | 824  | CLA  | CMD-C2D | -2.25 | 1.46        | 1.50     |
| 14  | A     | 824  | CLA  | CMD-C2D | -2.25 | 1.46        | 1.50     |
| 14  | b     | 833  | CLA  | CMD-C2D | -2.25 | 1.46        | 1.50     |
| 14  | B     | 831  | CLA  | CMD-C2D | -2.25 | 1.46        | 1.50     |
| 14  | 8     | 1301 | CLA  | CMD-C2D | -2.25 | 1.46        | 1.50     |
| 14  | B     | 840  | CLA  | C3B-C2B | -2.25 | 1.37        | 1.40     |
| 14  | A     | 836  | CLA  | C3B-CAB | -2.25 | 1.43        | 1.47     |
| 14  | B     | 829  | CLA  | CMC-C2C | -2.25 | 1.46        | 1.50     |
| 14  | a     | 805  | CLA  | CMD-C2D | -2.25 | 1.46        | 1.50     |
| 14  | a     | 834  | CLA  | CMC-C2C | -2.25 | 1.46        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | 2     | 849  | BCR  | C38-C26 | -2.25 | 1.47        | 1.50     |
| 14  | a     | 827  | CLA  | C3B-CAB | -2.25 | 1.43        | 1.47     |
| 14  | 2     | 830  | CLA  | CMC-C2C | -2.25 | 1.46        | 1.50     |
| 14  | K     | 101  | CLA  | CMD-C2D | -2.24 | 1.46        | 1.50     |
| 14  | 1     | 1625 | CLA  | CMD-C2D | -2.24 | 1.46        | 1.50     |
| 14  | 9     | 101  | CLA  | CMD-C2D | -2.24 | 1.46        | 1.50     |
| 14  | 1     | 1637 | CLA  | C3B-CAB | -2.24 | 1.43        | 1.47     |
| 14  | 1     | 1606 | CLA  | CMD-C2D | -2.24 | 1.46        | 1.50     |
| 14  | b     | 841  | CLA  | C3B-CAB | -2.24 | 1.43        | 1.47     |
| 14  | 2     | 830  | CLA  | CHC-C1C | 2.24  | 1.40        | 1.35     |
| 14  | b     | 840  | CLA  | C3B-CAB | -2.24 | 1.43        | 1.47     |
| 14  | A     | 830  | CLA  | C3B-CAB | -2.24 | 1.43        | 1.47     |
| 14  | 2     | 818  | CLA  | C3B-C2B | -2.24 | 1.37        | 1.40     |
| 14  | F     | 203  | CLA  | CMC-C2C | -2.24 | 1.46        | 1.50     |
| 14  | a     | 806  | CLA  | CMC-C2C | -2.24 | 1.46        | 1.50     |
| 14  | 1     | 1635 | CLA  | CMC-C2C | -2.24 | 1.46        | 1.50     |
| 14  | 2     | 814  | CLA  | CMD-C2D | -2.24 | 1.46        | 1.50     |
| 14  | l     | 206  | CLA  | CMC-C2C | -2.24 | 1.46        | 1.50     |
| 14  | 1     | 1641 | CLA  | CMC-C2C | -2.24 | 1.46        | 1.50     |
| 14  | a     | 823  | CLA  | CMD-C2D | -2.23 | 1.46        | 1.50     |
| 14  | b     | 825  | CLA  | CMC-C2C | -2.23 | 1.46        | 1.50     |
| 14  | b     | 830  | CLA  | CMC-C2C | -2.23 | 1.46        | 1.50     |
| 14  | a     | 830  | CLA  | MG-ND   | -2.23 | 2.01        | 2.05     |
| 14  | B     | 808  | CLA  | CMD-C2D | -2.23 | 1.46        | 1.50     |
| 14  | b     | 818  | CLA  | C3B-C2B | -2.23 | 1.37        | 1.40     |
| 14  | L     | 203  | CLA  | CMC-C2C | -2.23 | 1.46        | 1.50     |
| 14  | A     | 834  | CLA  | CMC-C2C | -2.23 | 1.46        | 1.50     |
| 14  | F     | 203  | CLA  | CMD-C2D | -2.23 | 1.46        | 1.50     |
| 14  | 1     | 1609 | CLA  | CMC-C2C | -2.23 | 1.46        | 1.50     |
| 14  | A     | 805  | CLA  | CMD-C2D | -2.23 | 1.46        | 1.50     |
| 14  | A     | 840  | CLA  | CMC-C2C | -2.23 | 1.46        | 1.50     |
| 14  | A     | 830  | CLA  | MG-ND   | -2.23 | 2.01        | 2.05     |
| 14  | 2     | 821  | CLA  | CMD-C2D | -2.23 | 1.46        | 1.50     |
| 14  | 1     | 1628 | CLA  | C3B-CAB | -2.23 | 1.43        | 1.47     |
| 14  | A     | 833  | CLA  | C3B-CAB | -2.23 | 1.43        | 1.47     |
| 14  | b     | 821  | CLA  | CMD-C2D | -2.23 | 1.46        | 1.50     |
| 14  | a     | 836  | CLA  | C3B-CAB | -2.23 | 1.43        | 1.47     |
| 14  | L     | 205  | CLA  | CMC-C2C | -2.22 | 1.46        | 1.50     |
| 14  | 2     | 841  | CLA  | C3B-CAB | -2.22 | 1.43        | 1.47     |
| 14  | 1     | 1631 | CLA  | MG-ND   | -2.22 | 2.01        | 2.05     |
| 14  | B     | 820  | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 14  | 1     | 1628 | CLA  | C3B-C2B | -2.22 | 1.37        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 826  | CLA  | C3B-CAB | -2.22 | 1.43        | 1.47     |
| 14  | 2     | 820  | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 17  | B     | 845  | BCR  | C38-C26 | -2.22 | 1.47        | 1.50     |
| 14  | A     | 806  | CLA  | CMC-C2C | -2.22 | 1.46        | 1.50     |
| 14  | a     | 808  | CLA  | CMC-C2C | -2.22 | 1.46        | 1.50     |
| 14  | b     | 802  | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 17  | 2     | 846  | BCR  | C38-C26 | -2.22 | 1.47        | 1.50     |
| 14  | 2     | 802  | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 14  | B     | 819  | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 17  | l     | 202  | BCR  | C33-C5  | -2.21 | 1.47        | 1.50     |
| 14  | b     | 809  | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |
| 17  | 0     | 203  | BCR  | C33-C5  | -2.21 | 1.47        | 1.50     |
| 14  | 1     | 1634 | CLA  | CMC-C2C | -2.21 | 1.46        | 1.50     |
| 14  | B     | 806  | CLA  | CMC-C2C | -2.21 | 1.46        | 1.50     |
| 14  | b     | 841  | CLA  | CMC-C2C | -2.21 | 1.46        | 1.50     |
| 17  | B     | 848  | BCR  | C33-C5  | -2.21 | 1.47        | 1.50     |
| 13  | 1     | 1602 | CL0  | C3B-C2B | -2.21 | 1.37        | 1.40     |
| 14  | B     | 804  | CLA  | C3B-CAB | -2.21 | 1.43        | 1.47     |
| 13  | A     | 801  | CL0  | C3B-C2B | -2.21 | 1.37        | 1.40     |
| 14  | 2     | 809  | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |
| 14  | B     | 839  | CLA  | C3B-CAB | -2.20 | 1.43        | 1.47     |
| 14  | a     | 839  | CLA  | C3B-C2B | -2.20 | 1.37        | 1.40     |
| 14  | a     | 833  | CLA  | CMC-C2C | -2.20 | 1.46        | 1.50     |
| 14  | A     | 808  | CLA  | CMC-C2C | -2.20 | 1.46        | 1.50     |
| 14  | b     | 820  | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 14  | B     | 825  | CLA  | C3B-CAB | -2.20 | 1.43        | 1.47     |
| 13  | a     | 801  | CL0  | C3B-C2B | -2.20 | 1.37        | 1.40     |
| 14  | X     | 1701 | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 14  | A     | 825  | CLA  | C3B-CAB | -2.20 | 1.43        | 1.47     |
| 17  | b     | 846  | BCR  | C38-C26 | -2.20 | 1.47        | 1.50     |
| 14  | A     | 855  | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 14  | B     | 813  | CLA  | CMC-C2C | -2.20 | 1.46        | 1.50     |
| 14  | 2     | 805  | CLA  | C3B-CAB | -2.20 | 1.43        | 1.47     |
| 14  | b     | 807  | CLA  | CMC-C2C | -2.20 | 1.46        | 1.50     |
| 14  | b     | 808  | CLA  | CMC-C2C | -2.20 | 1.46        | 1.50     |
| 14  | a     | 840  | CLA  | CMC-C2C | -2.20 | 1.46        | 1.50     |
| 14  | 2     | 812  | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 14  | b     | 817  | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 14  | 1     | 1626 | CLA  | C3B-CAB | -2.20 | 1.43        | 1.47     |
| 14  | B     | 803  | CLA  | C3B-CAB | -2.20 | 1.43        | 1.47     |
| 14  | A     | 839  | CLA  | C3B-C2B | -2.20 | 1.37        | 1.40     |
| 14  | B     | 816  | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | 2     | 836  | CLA  | C3B-C2B | -2.19 | 1.37        | 1.40     |
| 14  | 2     | 814  | CLA  | CMC-C2C | -2.19 | 1.46        | 1.50     |
| 14  | a     | 825  | CLA  | C3B-CAB | -2.19 | 1.43        | 1.47     |
| 17  | b     | 849  | BCR  | C33-C5  | -2.19 | 1.47        | 1.50     |
| 17  | 7     | 101  | BCR  | C38-C26 | -2.19 | 1.47        | 1.50     |
| 14  | A     | 840  | CLA  | C3B-CAB | -2.19 | 1.43        | 1.47     |
| 14  | 2     | 804  | CLA  | C3B-CAB | -2.19 | 1.43        | 1.47     |
| 14  | B     | 836  | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 17  | 2     | 849  | BCR  | C33-C5  | -2.19 | 1.47        | 1.50     |
| 14  | 2     | 840  | CLA  | C3B-CAB | -2.19 | 1.43        | 1.47     |
| 14  | B     | 817  | CLA  | CMC-C2C | -2.19 | 1.46        | 1.50     |
| 14  | 1     | 1641 | CLA  | C3B-CAB | -2.19 | 1.43        | 1.47     |
| 17  | 1     | 1649 | BCR  | C38-C26 | -2.19 | 1.47        | 1.50     |
| 14  | a     | 824  | CLA  | CMC-C2C | -2.19 | 1.46        | 1.50     |
| 14  | a     | 814  | CLA  | C3B-C2B | -2.19 | 1.37        | 1.40     |
| 14  | 1     | 1640 | CLA  | C3B-C2B | -2.19 | 1.37        | 1.40     |
| 14  | 2     | 825  | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 14  | b     | 814  | CLA  | CMC-C2C | -2.19 | 1.46        | 1.50     |
| 14  | a     | 840  | CLA  | C3B-CAB | -2.18 | 1.43        | 1.47     |
| 14  | B     | 807  | CLA  | CMC-C2C | -2.18 | 1.46        | 1.50     |
| 14  | 2     | 818  | CLA  | CMC-C2C | -2.18 | 1.46        | 1.50     |
| 14  | 1     | 1622 | CLA  | CMB-C2B | -2.18 | 1.47        | 1.51     |
| 14  | a     | 825  | CLA  | CMC-C2C | -2.18 | 1.46        | 1.50     |
| 14  | 2     | 813  | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 14  | B     | 811  | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 14  | a     | 811  | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 14  | A     | 812  | CLA  | CMC-C2C | -2.18 | 1.46        | 1.50     |
| 14  | a     | 806  | CLA  | C3B-CAB | -2.18 | 1.43        | 1.47     |
| 14  | 1     | 1612 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 14  | a     | 821  | CLA  | CMB-C2B | -2.18 | 1.47        | 1.51     |
| 14  | 2     | 841  | CLA  | CMC-C2C | -2.18 | 1.46        | 1.50     |
| 14  | 2     | 831  | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 14  | B     | 829  | CLA  | C4B-CHC | -2.18 | 1.34        | 1.41     |
| 14  | b     | 825  | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 14  | a     | 843  | CLA  | MG-ND   | -2.18 | 2.01        | 2.05     |
| 14  | A     | 828  | CLA  | CMC-C2C | -2.18 | 1.46        | 1.50     |
| 14  | 1     | 1625 | CLA  | CMC-C2C | -2.18 | 1.46        | 1.50     |
| 14  | 1     | 1636 | CLA  | CMC-C2C | -2.18 | 1.46        | 1.50     |
| 14  | A     | 811  | CLA  | C3B-C2B | -2.18 | 1.37        | 1.40     |
| 14  | b     | 805  | CLA  | C3B-CAB | -2.18 | 1.43        | 1.47     |
| 17  | M     | 103  | BCR  | C33-C5  | -2.17 | 1.47        | 1.50     |
| 14  | L     | 203  | CLA  | C3B-CAB | -2.17 | 1.43        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | l     | 204  | CLA  | C3B-CAB | -2.17 | 1.43        | 1.47     |
| 14  | A     | 825  | CLA  | CMC-C2C | -2.17 | 1.46        | 1.50     |
| 14  | b     | 812  | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 14  | 2     | 826  | CLA  | C3B-CAB | -2.17 | 1.43        | 1.47     |
| 14  | a     | 835  | CLA  | CMC-C2C | -2.17 | 1.46        | 1.50     |
| 14  | A     | 827  | CLA  | C3B-C2B | -2.17 | 1.37        | 1.40     |
| 14  | b     | 830  | CLA  | C4B-CHC | -2.17 | 1.35        | 1.41     |
| 14  | A     | 835  | CLA  | CMC-C2C | -2.17 | 1.46        | 1.50     |
| 14  | 2     | 808  | CLA  | CMC-C2C | -2.17 | 1.46        | 1.50     |
| 17  | L     | 206  | BCR  | C38-C26 | -2.17 | 1.47        | 1.50     |
| 14  | b     | 813  | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 14  | b     | 831  | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 14  | 1     | 1620 | CLA  | CMC-C2C | -2.17 | 1.46        | 1.50     |
| 14  | j     | 1303 | CLA  | CBD-CAD | 2.17  | 1.56        | 1.51     |
| 14  | a     | 827  | CLA  | C3B-C2B | -2.17 | 1.37        | 1.40     |
| 14  | b     | 836  | CLA  | C3B-C2B | -2.17 | 1.37        | 1.40     |
| 14  | A     | 819  | CLA  | CMC-C2C | -2.17 | 1.46        | 1.50     |
| 14  | 2     | 807  | CLA  | CMC-C2C | -2.17 | 1.46        | 1.50     |
| 14  | b     | 804  | CLA  | C3B-CAB | -2.17 | 1.43        | 1.47     |
| 14  | A     | 833  | CLA  | C3B-C2B | -2.17 | 1.37        | 1.40     |
| 14  | b     | 828  | CLA  | C3B-C2B | -2.17 | 1.37        | 1.40     |
| 14  | a     | 808  | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 17  | l     | 207  | BCR  | C38-C26 | -2.17 | 1.47        | 1.50     |
| 14  | x     | 1701 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 14  | 1     | 1613 | CLA  | CMC-C2C | -2.17 | 1.46        | 1.50     |
| 14  | z     | 102  | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 14  | A     | 839  | CLA  | CMC-C2C | -2.16 | 1.46        | 1.50     |
| 14  | A     | 832  | CLA  | CMC-C2C | -2.16 | 1.46        | 1.50     |
| 14  | B     | 824  | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 14  | 1     | 1637 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 14  | A     | 804  | CLA  | CMC-C2C | -2.16 | 1.46        | 1.50     |
| 14  | 1     | 1640 | CLA  | CMC-C2C | -2.16 | 1.46        | 1.50     |
| 14  | B     | 835  | CLA  | C3B-C2B | -2.16 | 1.37        | 1.40     |
| 14  | a     | 812  | CLA  | CMC-C2C | -2.16 | 1.46        | 1.50     |
| 14  | a     | 819  | CLA  | CMC-C2C | -2.16 | 1.46        | 1.50     |
| 14  | 1     | 1629 | CLA  | CMC-C2C | -2.16 | 1.46        | 1.50     |
| 14  | 1     | 1645 | CLA  | CMC-C2C | -2.16 | 1.46        | 1.50     |
| 14  | 1     | 1626 | CLA  | CMC-C2C | -2.16 | 1.46        | 1.50     |
| 14  | 2     | 817  | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 14  | 1     | 1615 | CLA  | C3B-CAB | -2.16 | 1.43        | 1.47     |
| 14  | A     | 806  | CLA  | C3B-C2B | -2.16 | 1.37        | 1.40     |
| 14  | 1     | 1612 | CLA  | C3B-C2B | -2.16 | 1.37        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 833  | CLA  | MG-ND   | -2.16 | 2.01        | 2.05     |
| 14  | 8     | 1303 | CLA  | CBD-CAD | 2.16  | 1.56        | 1.51     |
| 14  | 2     | 819  | CLA  | CMC-C2C | -2.16 | 1.46        | 1.50     |
| 14  | a     | 844  | CLA  | CMC-C2C | -2.16 | 1.46        | 1.50     |
| 17  | F     | 202  | BCR  | C38-C26 | -2.16 | 1.47        | 1.50     |
| 13  | a     | 801  | CL0  | MG-ND   | -2.16 | 2.01        | 2.05     |
| 14  | 1     | 1607 | CLA  | C3B-CAB | -2.16 | 1.43        | 1.47     |
| 14  | 1     | 1605 | CLA  | CMC-C2C | -2.16 | 1.46        | 1.50     |
| 14  | A     | 811  | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 14  | a     | 807  | CLA  | CMC-C2C | -2.15 | 1.46        | 1.50     |
| 14  | B     | 840  | CLA  | CMC-C2C | -2.15 | 1.46        | 1.50     |
| 18  | y     | 101  | LHG  | P-O6    | 2.15  | 1.68        | 1.59     |
| 14  | B     | 827  | CLA  | C3B-C2B | -2.15 | 1.37        | 1.40     |
| 14  | A     | 836  | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 14  | a     | 836  | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 14  | B     | 830  | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 14  | 2     | 830  | CLA  | C4B-CHC | -2.15 | 1.35        | 1.41     |
| 17  | L     | 201  | BCR  | C33-C5  | -2.15 | 1.47        | 1.50     |
| 14  | B     | 818  | CLA  | CMC-C2C | -2.15 | 1.46        | 1.50     |
| 14  | a     | 810  | CLA  | CMC-C2C | -2.15 | 1.46        | 1.50     |
| 14  | a     | 804  | CLA  | CMC-C2C | -2.15 | 1.46        | 1.50     |
| 14  | b     | 824  | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 14  | a     | 828  | CLA  | CMC-C2C | -2.15 | 1.46        | 1.50     |
| 14  | a     | 841  | CLA  | CMC-C2C | -2.15 | 1.46        | 1.50     |
| 14  | A     | 806  | CLA  | C3B-CAB | -2.15 | 1.43        | 1.47     |
| 14  | a     | 811  | CLA  | C3B-C2B | -2.15 | 1.37        | 1.40     |
| 14  | A     | 841  | CLA  | CMC-C2C | -2.15 | 1.46        | 1.50     |
| 14  | 8     | 1303 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 14  | J     | 102  | CLA  | CBD-CAD | 2.15  | 1.56        | 1.51     |
| 14  | b     | 836  | CLA  | C3B-CAB | -2.15 | 1.43        | 1.47     |
| 14  | 1     | 1632 | CLA  | MG-ND   | -2.15 | 2.01        | 2.05     |
| 14  | B     | 812  | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 14  | A     | 821  | CLA  | CMB-C2B | -2.14 | 1.47        | 1.51     |
| 14  | 1     | 1642 | CLA  | CMC-C2C | -2.14 | 1.46        | 1.50     |
| 14  | b     | 809  | CLA  | C3B-C2B | -2.14 | 1.37        | 1.40     |
| 14  | A     | 813  | CLA  | CMC-C2C | -2.14 | 1.46        | 1.50     |
| 14  | j     | 1303 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 14  | 0     | 205  | CLA  | C3B-CAB | -2.14 | 1.43        | 1.47     |
| 14  | 2     | 827  | CLA  | CMC-C2C | -2.14 | 1.46        | 1.50     |
| 14  | 0     | 207  | CLA  | C3B-CAB | -2.14 | 1.43        | 1.47     |
| 14  | b     | 818  | CLA  | CMC-C2C | -2.14 | 1.46        | 1.50     |
| 18  | M     | 101  | LHG  | P-O6    | 2.14  | 1.68        | 1.59     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | i     | 101  | BCR  | C38-C26 | -2.14 | 1.47        | 1.50     |
| 14  | 2     | 829  | CLA  | CMC-C2C | -2.14 | 1.46        | 1.50     |
| 14  | A     | 814  | CLA  | C3B-CAB | -2.14 | 1.43        | 1.47     |
| 14  | a     | 837  | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 17  | f     | 202  | BCR  | C38-C26 | -2.14 | 1.47        | 1.50     |
| 14  | a     | 839  | CLA  | CMC-C2C | -2.14 | 1.46        | 1.50     |
| 18  | m     | 101  | LHG  | P-O6    | 2.14  | 1.67        | 1.59     |
| 14  | B     | 812  | CLA  | CMC-C2C | -2.13 | 1.46        | 1.50     |
| 14  | 2     | 837  | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 17  | l     | 202  | BCR  | C38-C26 | -2.13 | 1.47        | 1.50     |
| 14  | B     | 821  | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 14  | 2     | 830  | CLA  | CAC-C3C | -2.13 | 1.45        | 1.51     |
| 14  | A     | 810  | CLA  | CMC-C2C | -2.13 | 1.46        | 1.50     |
| 14  | b     | 837  | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 14  | 1     | 1614 | CLA  | CMC-C2C | -2.13 | 1.46        | 1.50     |
| 17  | y     | 102  | BCR  | C33-C5  | -2.13 | 1.47        | 1.50     |
| 14  | b     | 818  | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 14  | A     | 805  | CLA  | CMC-C2C | -2.13 | 1.46        | 1.50     |
| 14  | 2     | 828  | CLA  | C3B-C2B | -2.13 | 1.37        | 1.40     |
| 13  | A     | 801  | CL0  | CMC-C2C | -2.13 | 1.46        | 1.50     |
| 14  | 1     | 1609 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 14  | B     | 835  | CLA  | C3B-CAB | -2.13 | 1.43        | 1.47     |
| 14  | A     | 830  | CLA  | CMC-C2C | -2.13 | 1.46        | 1.50     |
| 14  | b     | 813  | CLA  | CMC-C2C | -2.13 | 1.46        | 1.50     |
| 14  | L     | 205  | CLA  | C3B-CAB | -2.13 | 1.43        | 1.47     |
| 14  | A     | 824  | CLA  | CMC-C2C | -2.13 | 1.46        | 1.50     |
| 14  | A     | 843  | CLA  | MG-ND   | -2.13 | 2.01        | 2.05     |
| 14  | 2     | 842  | CLA  | C3B-CAB | -2.13 | 1.43        | 1.47     |
| 14  | L     | 204  | CLA  | MG-ND   | -2.13 | 2.01        | 2.05     |
| 14  | l     | 206  | CLA  | C3B-CAB | -2.13 | 1.43        | 1.47     |
| 14  | b     | 833  | CLA  | CMC-C2C | -2.13 | 1.46        | 1.50     |
| 14  | 1     | 1611 | CLA  | CMC-C2C | -2.13 | 1.46        | 1.50     |
| 14  | 2     | 836  | CLA  | CMC-C2C | -2.13 | 1.46        | 1.50     |
| 17  | I     | 101  | BCR  | C38-C26 | -2.13 | 1.47        | 1.50     |
| 17  | 6     | 202  | BCR  | C38-C26 | -2.13 | 1.47        | 1.50     |
| 14  | a     | 831  | CLA  | MG-ND   | -2.13 | 2.01        | 2.05     |
| 14  | 2     | 809  | CLA  | C3B-C2B | -2.13 | 1.37        | 1.40     |
| 14  | b     | 842  | CLA  | C3B-CAB | -2.13 | 1.43        | 1.47     |
| 14  | A     | 817  | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 14  | a     | 832  | CLA  | CMC-C2C | -2.13 | 1.46        | 1.50     |
| 14  | B     | 829  | CLA  | CAC-C3C | -2.13 | 1.45        | 1.51     |
| 14  | A     | 832  | CLA  | MG-ND   | -2.13 | 2.01        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 822  | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 17  | 2     | 848  | BCR  | C38-C26 | -2.12 | 1.47        | 1.50     |
| 14  | A     | 808  | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 14  | B     | 826  | CLA  | C3B-CAB | -2.12 | 1.43        | 1.47     |
| 14  | A     | 827  | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 14  | 1     | 1633 | CLA  | MG-ND   | -2.12 | 2.01        | 2.05     |
| 14  | b     | 830  | CLA  | CAC-C3C | -2.12 | 1.45        | 1.51     |
| 14  | 2     | 836  | CLA  | C3B-CAB | -2.12 | 1.43        | 1.47     |
| 14  | 2     | 818  | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 14  | J     | 102  | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 14  | B     | 826  | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 14  | A     | 844  | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 14  | b     | 803  | CLA  | MG-ND   | -2.12 | 2.01        | 2.05     |
| 14  | 1     | 1609 | CLA  | C3B-C2B | -2.12 | 1.37        | 1.40     |
| 14  | B     | 828  | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 14  | 1     | 1606 | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 17  | A     | 848  | BCR  | C38-C26 | -2.12 | 1.47        | 1.50     |
| 14  | b     | 804  | CLA  | C3B-C2B | -2.12 | 1.37        | 1.40     |
| 14  | B     | 817  | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 14  | a     | 833  | CLA  | C3B-C2B | -2.12 | 1.37        | 1.40     |
| 14  | A     | 837  | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 14  | 1     | 1618 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 14  | B     | 838  | CLA  | C3B-CAB | -2.11 | 1.43        | 1.47     |
| 14  | 2     | 839  | CLA  | C3B-CAB | -2.11 | 1.43        | 1.47     |
| 14  | b     | 819  | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 14  | 1     | 1608 | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 14  | A     | 831  | CLA  | MG-ND   | -2.11 | 2.01        | 2.05     |
| 17  | b     | 845  | BCR  | C38-C26 | -2.11 | 1.47        | 1.50     |
| 17  | b     | 848  | BCR  | C38-C26 | -2.11 | 1.47        | 1.50     |
| 14  | B     | 803  | CLA  | C3B-C2B | -2.11 | 1.37        | 1.40     |
| 14  | 1     | 1607 | CLA  | C3B-C2B | -2.11 | 1.37        | 1.40     |
| 17  | B     | 844  | BCR  | C38-C26 | -2.11 | 1.47        | 1.50     |
| 17  | m     | 102  | BCR  | C33-C5  | -2.11 | 1.47        | 1.50     |
| 14  | a     | 832  | CLA  | MG-ND   | -2.11 | 2.01        | 2.05     |
| 14  | A     | 826  | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 14  | B     | 823  | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 14  | 0     | 207  | CLA  | C3B-C2B | -2.11 | 1.37        | 1.40     |
| 14  | a     | 830  | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 14  | B     | 802  | CLA  | MG-ND   | -2.11 | 2.01        | 2.05     |
| 14  | 0     | 207  | CLA  | MG-ND   | -2.11 | 2.01        | 2.05     |
| 14  | A     | 814  | CLA  | C3B-C2B | -2.11 | 1.37        | 1.40     |
| 14  | b     | 807  | CLA  | C3B-CAB | -2.11 | 1.43        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | 1     | 1634 | CLA  | MG-ND   | -2.11 | 2.01        | 2.05     |
| 14  | 1     | 1644 | CLA  | MG-ND   | -2.11 | 2.01        | 2.05     |
| 14  | A     | 835  | CLA  | C3B-CAB | -2.11 | 1.43        | 1.47     |
| 14  | b     | 814  | CLA  | C3B-CAB | -2.11 | 1.43        | 1.47     |
| 14  | 2     | 827  | CLA  | C3B-CAB | -2.11 | 1.43        | 1.47     |
| 14  | A     | 844  | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 14  | b     | 836  | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 14  | A     | 815  | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 14  | 1     | 1636 | CLA  | C3B-CAB | -2.11 | 1.43        | 1.47     |
| 14  | 2     | 834  | CLA  | C3B-CAB | -2.11 | 1.43        | 1.47     |
| 14  | b     | 816  | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 14  | 2     | 833  | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 13  | A     | 801  | CL0  | MG-ND   | -2.11 | 2.01        | 2.05     |
| 14  | B     | 830  | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 14  | 1     | 1628 | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 14  | 2     | 813  | CLA  | C3B-C2B | -2.11 | 1.37        | 1.40     |
| 14  | 2     | 824  | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 14  | a     | 805  | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 14  | 1     | 1612 | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 14  | 9     | 101  | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 17  | L     | 201  | BCR  | C38-C26 | -2.10 | 1.47        | 1.50     |
| 14  | A     | 808  | CLA  | C3B-CAB | -2.10 | 1.43        | 1.47     |
| 14  | b     | 807  | CLA  | C3B-C2B | -2.10 | 1.37        | 1.40     |
| 14  | 2     | 804  | CLA  | C3B-C2B | -2.10 | 1.37        | 1.40     |
| 14  | 2     | 838  | CLA  | C3B-CAB | -2.10 | 1.43        | 1.47     |
| 17  | a     | 850  | BCR  | C38-C26 | -2.10 | 1.47        | 1.50     |
| 17  | 2     | 845  | BCR  | C38-C26 | -2.10 | 1.47        | 1.50     |
| 17  | 0     | 208  | BCR  | C38-C26 | -2.10 | 1.47        | 1.50     |
| 14  | 1     | 1633 | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |
| 14  | 1     | 1638 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 14  | B     | 835  | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |
| 14  | 1     | 1627 | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |
| 17  | B     | 847  | BCR  | C38-C26 | -2.10 | 1.47        | 1.50     |
| 17  | a     | 848  | BCR  | C38-C26 | -2.10 | 1.47        | 1.50     |
| 14  | A     | 837  | CLA  | C3B-C2B | -2.10 | 1.37        | 1.40     |
| 14  | B     | 841  | CLA  | C3B-CAB | -2.10 | 1.43        | 1.47     |
| 14  | 2     | 803  | CLA  | MG-ND   | -2.10 | 2.01        | 2.05     |
| 14  | A     | 821  | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 14  | 1     | 1631 | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |
| 14  | 2     | 822  | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 14  | 1     | 1634 | CLA  | C3B-C2B | -2.10 | 1.37        | 1.40     |
| 14  | B     | 815  | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 826  | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |
| 14  | L     | 205  | CLA  | MG-ND   | -2.10 | 2.01        | 2.05     |
| 14  | 1     | 1627 | CLA  | MG-ND   | -2.10 | 2.01        | 2.05     |
| 14  | a     | 813  | CLA  | C3B-C2B | -2.10 | 1.37        | 1.40     |
| 14  | 1     | 1626 | CLA  | C3B-C2B | -2.10 | 1.37        | 1.40     |
| 14  | B     | 837  | CLA  | C3B-CAB | -2.10 | 1.43        | 1.47     |
| 14  | a     | 835  | CLA  | C3B-CAB | -2.10 | 1.43        | 1.47     |
| 14  | 2     | 807  | CLA  | C3B-CAB | -2.10 | 1.43        | 1.47     |
| 14  | b     | 827  | CLA  | C3B-CAB | -2.10 | 1.43        | 1.47     |
| 17  | 1     | 1651 | BCR  | C38-C26 | -2.10 | 1.47        | 1.50     |
| 17  | 0     | 209  | BCR  | C38-C26 | -2.10 | 1.47        | 1.50     |
| 14  | 1     | 1643 | CLA  | C3B-C2B | -2.09 | 1.37        | 1.40     |
| 14  | a     | 813  | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 14  | 2     | 816  | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 14  | a     | 815  | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 17  | 0     | 203  | BCR  | C38-C26 | -2.09 | 1.47        | 1.50     |
| 14  | a     | 814  | CLA  | C3B-CAB | -2.09 | 1.43        | 1.47     |
| 14  | a     | 841  | CLA  | C3B-CAB | -2.09 | 1.43        | 1.47     |
| 14  | b     | 839  | CLA  | C3B-CAB | -2.09 | 1.43        | 1.47     |
| 14  | b     | 839  | CLA  | C3B-C2B | -2.09 | 1.37        | 1.40     |
| 14  | B     | 832  | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 14  | b     | 829  | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 13  | 1     | 1602 | CL0  | MG-ND   | -2.09 | 2.01        | 2.05     |
| 14  | b     | 837  | CLA  | C3B-C2B | -2.09 | 1.37        | 1.40     |
| 14  | A     | 811  | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 14  | a     | 822  | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 14  | b     | 831  | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 14  | a     | 808  | CLA  | C3B-CAB | -2.09 | 1.43        | 1.47     |
| 14  | 2     | 815  | CLA  | C3B-CAB | -2.09 | 1.43        | 1.47     |
| 14  | b     | 834  | CLA  | C3B-CAB | -2.09 | 1.43        | 1.47     |
| 14  | B     | 839  | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 14  | a     | 827  | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 14  | 1     | 1645 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | a     | 806  | CLA  | C3B-C2B | -2.09 | 1.37        | 1.40     |
| 17  | L     | 207  | BCR  | C38-C26 | -2.09 | 1.47        | 1.50     |
| 14  | K     | 101  | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 14  | B     | 808  | CLA  | C3B-C2B | -2.09 | 1.37        | 1.40     |
| 14  | J     | 102  | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 14  | K     | 103  | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 14  | L     | 205  | CLA  | C3B-C2B | -2.09 | 1.37        | 1.40     |
| 14  | 1     | 1614 | CLA  | C3B-C2B | -2.09 | 1.37        | 1.40     |
| 17  | 0     | 201  | BCR  | C38-C26 | -2.09 | 1.47        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | k     | 101  | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 14  | 2     | 831  | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 14  | B     | 806  | CLA  | C3B-C2B | -2.08 | 1.37        | 1.40     |
| 14  | A     | 807  | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 14  | a     | 808  | CLA  | C3B-C2B | -2.08 | 1.37        | 1.40     |
| 14  | l     | 206  | CLA  | C3B-C2B | -2.08 | 1.37        | 1.40     |
| 14  | 1     | 1615 | CLA  | C3B-C2B | -2.08 | 1.37        | 1.40     |
| 14  | B     | 806  | CLA  | C3B-CAB | -2.08 | 1.43        | 1.47     |
| 14  | 2     | 807  | CLA  | C3B-C2B | -2.08 | 1.37        | 1.40     |
| 14  | 2     | 813  | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 14  | A     | 814  | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | B     | 836  | CLA  | C3B-C2B | -2.08 | 1.37        | 1.40     |
| 14  | l     | 206  | CLA  | MG-ND   | -2.08 | 2.01        | 2.05     |
| 14  | 1     | 1610 | CLA  | C3B-C2B | -2.08 | 1.37        | 1.40     |
| 14  | j     | 1303 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 14  | a     | 816  | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 14  | a     | 817  | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | A     | 809  | CLA  | C3B-C2B | -2.08 | 1.37        | 1.40     |
| 14  | a     | 821  | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | a     | 844  | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | 1     | 1610 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 14  | b     | 830  | CLA  | MG-ND   | -2.08 | 2.01        | 2.05     |
| 14  | a     | 833  | CLA  | MG-ND   | -2.08 | 2.01        | 2.05     |
| 14  | B     | 838  | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 14  | l     | 205  | CLA  | MG-ND   | -2.08 | 2.01        | 2.05     |
| 14  | k     | 103  | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 14  | B     | 813  | CLA  | C3B-CAB | -2.07 | 1.43        | 1.47     |
| 14  | 1     | 1623 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 14  | 1     | 1627 | CLA  | C3B-CAB | -2.07 | 1.43        | 1.47     |
| 14  | 2     | 811  | CLA  | C3B-C2B | -2.07 | 1.37        | 1.40     |
| 14  | a     | 826  | CLA  | MG-ND   | -2.07 | 2.01        | 2.05     |
| 14  | 2     | 811  | CLA  | MG-ND   | -2.07 | 2.01        | 2.05     |
| 13  | 1     | 1602 | CL0  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 14  | 2     | 840  | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 17  | j     | 1304 | BCR  | C38-C26 | -2.07 | 1.47        | 1.50     |
| 14  | A     | 825  | CLA  | C3B-C2B | -2.07 | 1.37        | 1.40     |
| 14  | A     | 841  | CLA  | C3B-CAB | -2.07 | 1.43        | 1.47     |
| 14  | 1     | 1616 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | 0     | 206  | CLA  | MG-ND   | -2.07 | 2.01        | 2.05     |
| 14  | 2     | 837  | CLA  | C3B-C2B | -2.07 | 1.37        | 1.40     |
| 17  | B     | 846  | BCR  | C38-C26 | -2.07 | 1.47        | 1.50     |
| 14  | B     | 829  | CLA  | MG-ND   | -2.07 | 2.01        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | 1     | 1609 | CLA  | C3B-CAB | -2.07 | 1.43        | 1.47     |
| 14  | A     | 819  | CLA  | C3B-C2B | -2.07 | 1.37        | 1.40     |
| 14  | a     | 837  | CLA  | C3B-C2B | -2.07 | 1.37        | 1.40     |
| 14  | B     | 833  | CLA  | C3B-CAB | -2.07 | 1.43        | 1.47     |
| 14  | b     | 832  | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 14  | a     | 809  | CLA  | C3B-C2B | -2.06 | 1.37        | 1.40     |
| 14  | a     | 807  | CLA  | MG-ND   | -2.06 | 2.01        | 2.05     |
| 14  | 1     | 1622 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | A     | 822  | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 14  | b     | 815  | CLA  | C3B-CAB | -2.06 | 1.43        | 1.47     |
| 14  | a     | 842  | CLA  | C3B-C2B | -2.06 | 1.37        | 1.40     |
| 13  | a     | 801  | CL0  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 14  | A     | 826  | CLA  | MG-ND   | -2.06 | 2.01        | 2.05     |
| 14  | B     | 831  | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 14  | 9     | 103  | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 14  | b     | 834  | CLA  | C3B-C2B | -2.06 | 1.37        | 1.40     |
| 14  | 2     | 832  | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 14  | 2     | 814  | CLA  | C3B-CAB | -2.06 | 1.43        | 1.47     |
| 14  | 2     | 803  | CLA  | C3B-C2B | -2.06 | 1.37        | 1.40     |
| 14  | A     | 809  | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 14  | 6     | 201  | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 14  | b     | 804  | CLA  | MG-ND   | -2.06 | 2.01        | 2.05     |
| 17  | 2     | 847  | BCR  | C38-C26 | -2.06 | 1.47        | 1.50     |
| 14  | A     | 815  | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 14  | b     | 827  | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 14  | B     | 810  | CLA  | MG-ND   | -2.06 | 2.01        | 2.05     |
| 18  | B     | 850  | LHG  | O7-C5   | -2.06 | 1.41        | 1.46     |
| 14  | K     | 103  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | a     | 811  | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 14  | b     | 813  | CLA  | C3B-C2B | -2.05 | 1.37        | 1.40     |
| 14  | 8     | 1303 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 14  | A     | 806  | CLA  | MG-ND   | -2.05 | 2.01        | 2.05     |
| 14  | b     | 838  | CLA  | C3B-CAB | -2.05 | 1.43        | 1.47     |
| 14  | 2     | 830  | CLA  | C3B-C2B | -2.05 | 1.37        | 1.40     |
| 14  | a     | 803  | CLA  | C3B-CAB | -2.05 | 1.43        | 1.47     |
| 17  | 8     | 1304 | BCR  | C38-C26 | -2.05 | 1.47        | 1.50     |
| 14  | 2     | 823  | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 14  | M     | 102  | CLA  | CBD-CAD | 2.05  | 1.56        | 1.51     |
| 14  | B     | 821  | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 14  | b     | 821  | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 14  | 2     | 812  | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 14  | b     | 830  | CLA  | C3B-C2B | -2.05 | 1.37        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | 1     | 1642 | CLA  | C3B-CAB | -2.05 | 1.43        | 1.47     |
| 14  | b     | 811  | CLA  | C3B-C2B | -2.05 | 1.37        | 1.40     |
| 14  | B     | 822  | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 17  | 7     | 101  | BCR  | C33-C5  | -2.05 | 1.47        | 1.50     |
| 14  | 1     | 1616 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 14  | a     | 819  | CLA  | C3B-C2B | -2.05 | 1.37        | 1.40     |
| 14  | b     | 803  | CLA  | C3B-C2B | -2.05 | 1.37        | 1.40     |
| 14  | 1     | 1617 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 14  | A     | 811  | CLA  | C3B-CAB | -2.05 | 1.43        | 1.47     |
| 14  | 2     | 810  | CLA  | C4B-CHC | -2.05 | 1.35        | 1.41     |
| 14  | 2     | 804  | CLA  | MG-ND   | -2.05 | 2.01        | 2.05     |
| 14  | A     | 802  | CLA  | MG-ND   | -2.05 | 2.01        | 2.05     |
| 13  | A     | 801  | CL0  | C4B-CHC | -2.05 | 1.35        | 1.41     |
| 14  | A     | 826  | CLA  | C3B-CAB | -2.05 | 1.43        | 1.47     |
| 14  | a     | 814  | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | b     | 840  | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 14  | b     | 811  | CLA  | MG-ND   | -2.04 | 2.01        | 2.05     |
| 14  | a     | 815  | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 17  | A     | 850  | BCR  | C38-C26 | -2.04 | 1.47        | 1.50     |
| 14  | B     | 812  | CLA  | C3B-C2B | -2.04 | 1.37        | 1.40     |
| 14  | 2     | 834  | CLA  | C3B-C2B | -2.04 | 1.37        | 1.40     |
| 14  | 1     | 1601 | CLA  | CBD-CAD | 2.04  | 1.56        | 1.51     |
| 14  | B     | 838  | CLA  | C3B-C2B | -2.04 | 1.37        | 1.40     |
| 14  | 1     | 1638 | CLA  | C3B-C2B | -2.04 | 1.37        | 1.40     |
| 14  | a     | 802  | CLA  | MG-ND   | -2.04 | 2.01        | 2.05     |
| 14  | a     | 817  | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 14  | A     | 857  | CLA  | CBD-CAD | 2.04  | 1.56        | 1.51     |
| 17  | a     | 850  | BCR  | C33-C5  | -2.04 | 1.47        | 1.50     |
| 14  | 1     | 1603 | CLA  | MG-ND   | -2.04 | 2.01        | 2.05     |
| 17  | b     | 847  | BCR  | C38-C26 | -2.04 | 1.47        | 1.50     |
| 14  | 1     | 1607 | CLA  | MG-ND   | -2.04 | 2.01        | 2.05     |
| 14  | B     | 803  | CLA  | C4B-CHC | -2.04 | 1.35        | 1.41     |
| 14  | A     | 803  | CLA  | C3B-CAB | -2.04 | 1.43        | 1.47     |
| 14  | 1     | 1612 | CLA  | C3B-CAB | -2.04 | 1.43        | 1.47     |
| 14  | 2     | 818  | CLA  | C3B-CAB | -2.04 | 1.43        | 1.47     |
| 14  | 2     | 839  | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 14  | A     | 813  | CLA  | C3B-C2B | -2.04 | 1.37        | 1.40     |
| 17  | i     | 101  | BCR  | C33-C5  | -2.04 | 1.47        | 1.50     |
| 14  | B     | 814  | CLA  | C3B-CAB | -2.04 | 1.43        | 1.47     |
| 14  | B     | 820  | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | B     | 823  | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | 2     | 822  | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 826  | CLA  | C3B-CAB | -2.03 | 1.43        | 1.47     |
| 13  | 1     | 1602 | CL0  | C4B-CHC | -2.03 | 1.35        | 1.41     |
| 14  | b     | 810  | CLA  | C4B-CHC | -2.03 | 1.35        | 1.41     |
| 14  | 1     | 1615 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 14  | 2     | 830  | CLA  | MG-ND   | -2.03 | 2.01        | 2.05     |
| 14  | A     | 817  | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | 2     | 839  | CLA  | C3B-C2B | -2.03 | 1.37        | 1.40     |
| 14  | B     | 809  | CLA  | C4B-CHC | -2.03 | 1.35        | 1.41     |
| 14  | b     | 812  | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | 2     | 824  | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | b     | 822  | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | 2     | 830  | CLA  | C3B-CAB | -2.03 | 1.43        | 1.47     |
| 14  | a     | 806  | CLA  | MG-ND   | -2.03 | 2.01        | 2.05     |
| 14  | 2     | 825  | CLA  | C3B-CAB | -2.03 | 1.43        | 1.47     |
| 14  | F     | 201  | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | B     | 829  | CLA  | C3B-C2B | -2.03 | 1.37        | 1.40     |
| 14  | a     | 809  | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | f     | 201  | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | A     | 842  | CLA  | C3B-C2B | -2.03 | 1.37        | 1.40     |
| 14  | b     | 823  | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | b     | 824  | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | b     | 810  | CLA  | C3B-CAB | -2.03 | 1.43        | 1.47     |
| 14  | 1     | 1604 | CLA  | C3B-CAB | -2.03 | 1.43        | 1.47     |
| 14  | B     | 833  | CLA  | C3B-C2B | -2.03 | 1.37        | 1.40     |
| 14  | k     | 103  | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 14  | B     | 829  | CLA  | C3B-CAB | -2.02 | 1.43        | 1.47     |
| 14  | B     | 818  | CLA  | C3B-CAB | -2.02 | 1.43        | 1.47     |
| 14  | A     | 838  | CLA  | MG-ND   | -2.02 | 2.01        | 2.05     |
| 14  | 2     | 821  | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 14  | B     | 817  | CLA  | C3B-CAB | -2.02 | 1.43        | 1.47     |
| 14  | 9     | 103  | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 14  | a     | 838  | CLA  | MG-ND   | -2.02 | 2.01        | 2.05     |
| 14  | a     | 809  | CLA  | C3B-CAB | -2.02 | 1.43        | 1.47     |
| 14  | A     | 816  | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 18  | b     | 851  | LHG  | O7-C5   | -2.02 | 1.41        | 1.46     |
| 14  | B     | 809  | CLA  | C3B-CAB | -2.02 | 1.43        | 1.47     |
| 14  | b     | 804  | CLA  | C4B-CHC | -2.02 | 1.35        | 1.41     |
| 17  | a     | 851  | BCR  | C38-C26 | -2.02 | 1.47        | 1.50     |
| 17  | 1     | 1651 | BCR  | C33-C5  | -2.02 | 1.47        | 1.50     |
| 14  | B     | 819  | CLA  | C3B-CAB | -2.02 | 1.43        | 1.47     |
| 14  | A     | 842  | CLA  | MG-ND   | -2.02 | 2.01        | 2.05     |
| 14  | B     | 802  | CLA  | C3B-C2B | -2.02 | 1.37        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 18  | z     | 101  | LHG  | O7-C5   | -2.01 | 1.41        | 1.46     |
| 18  | A     | 853  | LHG  | O8-C6   | -2.01 | 1.40        | 1.45     |
| 14  | b     | 839  | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 14  | b     | 818  | CLA  | C3B-CAB | -2.01 | 1.43        | 1.47     |
| 14  | 1     | 1616 | CLA  | C3B-C2B | -2.01 | 1.37        | 1.40     |
| 14  | 2     | 810  | CLA  | C3B-CAB | -2.01 | 1.43        | 1.47     |
| 18  | 0     | 202  | LHG  | O7-C5   | -2.01 | 1.41        | 1.46     |
| 17  | J     | 103  | BCR  | C38-C26 | -2.01 | 1.47        | 1.50     |
| 14  | 8     | 1302 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 14  | A     | 831  | CLA  | C3B-CAB | -2.01 | 1.43        | 1.47     |
| 14  | 1     | 1635 | CLA  | C3B-CAB | -2.01 | 1.43        | 1.47     |
| 14  | 2     | 819  | CLA  | C3B-CAB | -2.01 | 1.43        | 1.47     |
| 14  | 2     | 820  | CLA  | C3B-CAB | -2.01 | 1.43        | 1.47     |
| 14  | A     | 815  | CLA  | C3B-C2B | -2.01 | 1.37        | 1.40     |
| 14  | B     | 810  | CLA  | C3B-C2B | -2.01 | 1.37        | 1.40     |
| 13  | a     | 801  | CL0  | C4B-CHC | -2.01 | 1.35        | 1.41     |
| 14  | B     | 811  | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 14  | b     | 830  | CLA  | C3B-CAB | -2.01 | 1.43        | 1.47     |
| 14  | 2     | 815  | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 14  | 1     | 1639 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 17  | A     | 856  | BCR  | C38-C26 | -2.01 | 1.47        | 1.50     |
| 17  | I     | 101  | BCR  | C33-C5  | -2.01 | 1.47        | 1.50     |
| 14  | A     | 807  | CLA  | MG-ND   | -2.01 | 2.01        | 2.05     |
| 14  | 1     | 1639 | CLA  | MG-ND   | -2.01 | 2.01        | 2.05     |
| 14  | 1     | 1624 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 14  | A     | 831  | CLA  | C4B-CHC | -2.01 | 1.35        | 1.41     |
| 14  | A     | 827  | CLA  | MG-ND   | -2.00 | 2.01        | 2.05     |
| 14  | 2     | 802  | CLA  | MG-ND   | -2.00 | 2.01        | 2.05     |
| 14  | 1     | 1618 | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 14  | 1     | 1620 | CLA  | C3B-C2B | -2.00 | 1.37        | 1.40     |
| 14  | a     | 831  | CLA  | C3B-CAB | -2.00 | 1.43        | 1.47     |
| 14  | b     | 815  | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 14  | b     | 810  | CLA  | CAC-C3C | -2.00 | 1.46        | 1.51     |
| 14  | 2     | 810  | CLA  | CAC-C3C | -2.00 | 1.46        | 1.51     |

All (2850) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 14  | B     | 808 | CLA  | C4A-NA-C1A | 8.39 | 110.48      | 106.71   |
| 14  | 2     | 809 | CLA  | C4A-NA-C1A | 8.34 | 110.46      | 106.71   |
| 14  | b     | 809 | CLA  | C4A-NA-C1A | 8.29 | 110.43      | 106.71   |
| 14  | B     | 803 | CLA  | C4A-NA-C1A | 8.28 | 110.43      | 106.71   |

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| Mol | Chain | Res  | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 14  | a     | 835  | CLA  | C4A-NA-C1A | 8.24 | 110.41      | 106.71   |
| 14  | 1     | 1636 | CLA  | C4A-NA-C1A | 8.24 | 110.41      | 106.71   |
| 14  | A     | 835  | CLA  | C4A-NA-C1A | 8.20 | 110.39      | 106.71   |
| 14  | b     | 804  | CLA  | C4A-NA-C1A | 8.17 | 110.38      | 106.71   |
| 14  | 2     | 804  | CLA  | C4A-NA-C1A | 8.10 | 110.35      | 106.71   |
| 14  | B     | 809  | CLA  | C4A-NA-C1A | 8.06 | 110.33      | 106.71   |
| 14  | b     | 810  | CLA  | C4A-NA-C1A | 8.06 | 110.33      | 106.71   |
| 14  | 2     | 810  | CLA  | C4A-NA-C1A | 8.04 | 110.32      | 106.71   |
| 14  | b     | 842  | CLA  | C4A-NA-C1A | 7.94 | 110.28      | 106.71   |
| 14  | B     | 841  | CLA  | C4A-NA-C1A | 7.87 | 110.24      | 106.71   |
| 13  | 1     | 1602 | CL0  | C4A-NA-C1A | 7.87 | 110.24      | 106.71   |
| 14  | 2     | 842  | CLA  | C4A-NA-C1A | 7.81 | 110.22      | 106.71   |
| 13  | A     | 801  | CL0  | C4A-NA-C1A | 7.80 | 110.21      | 106.71   |
| 13  | a     | 801  | CL0  | C4A-NA-C1A | 7.77 | 110.20      | 106.71   |
| 14  | B     | 829  | CLA  | C4A-NA-C1A | 7.75 | 110.19      | 106.71   |
| 14  | b     | 830  | CLA  | C4A-NA-C1A | 7.73 | 110.18      | 106.71   |
| 14  | 2     | 830  | CLA  | C4A-NA-C1A | 7.71 | 110.17      | 106.71   |
| 14  | 2     | 811  | CLA  | C4A-NA-C1A | 7.68 | 110.16      | 106.71   |
| 14  | B     | 810  | CLA  | C4A-NA-C1A | 7.68 | 110.16      | 106.71   |
| 14  | b     | 811  | CLA  | C4A-NA-C1A | 7.62 | 110.13      | 106.71   |
| 14  | 1     | 1632 | CLA  | C4A-NA-C1A | 7.57 | 110.11      | 106.71   |
| 14  | a     | 804  | CLA  | C4A-NA-C1A | 7.56 | 110.10      | 106.71   |
| 14  | A     | 831  | CLA  | C4A-NA-C1A | 7.51 | 110.08      | 106.71   |
| 14  | a     | 829  | CLA  | C4A-NA-C1A | 7.49 | 110.07      | 106.71   |
| 14  | b     | 841  | CLA  | C4A-NA-C1A | 7.48 | 110.07      | 106.71   |
| 14  | 2     | 841  | CLA  | C4A-NA-C1A | 7.47 | 110.06      | 106.71   |
| 14  | A     | 804  | CLA  | C4A-NA-C1A | 7.47 | 110.06      | 106.71   |
| 14  | A     | 841  | CLA  | C4A-NA-C1A | 7.46 | 110.06      | 106.71   |
| 14  | a     | 831  | CLA  | C4A-NA-C1A | 7.46 | 110.06      | 106.71   |
| 14  | 1     | 1630 | CLA  | C4A-NA-C1A | 7.46 | 110.06      | 106.71   |
| 14  | B     | 840  | CLA  | C4A-NA-C1A | 7.45 | 110.06      | 106.71   |
| 14  | A     | 829  | CLA  | C4A-NA-C1A | 7.43 | 110.05      | 106.71   |
| 14  | A     | 843  | CLA  | C4A-NA-C1A | 7.42 | 110.04      | 106.71   |
| 14  | 1     | 1605 | CLA  | C4A-NA-C1A | 7.40 | 110.03      | 106.71   |
| 14  | a     | 843  | CLA  | C4A-NA-C1A | 7.40 | 110.03      | 106.71   |
| 14  | a     | 841  | CLA  | C4A-NA-C1A | 7.39 | 110.03      | 106.71   |
| 14  | 1     | 1644 | CLA  | C4A-NA-C1A | 7.39 | 110.03      | 106.71   |
| 14  | 1     | 1642 | CLA  | C4A-NA-C1A | 7.38 | 110.03      | 106.71   |
| 14  | 1     | 1637 | CLA  | C4A-NA-C1A | 7.36 | 110.02      | 106.71   |
| 14  | a     | 820  | CLA  | C4A-NA-C1A | 7.36 | 110.01      | 106.71   |
| 14  | b     | 834  | CLA  | C4A-NA-C1A | 7.35 | 110.01      | 106.71   |
| 14  | 2     | 806  | CLA  | C4A-NA-C1A | 7.34 | 110.01      | 106.71   |

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| Mol | Chain | Res  | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 14  | A     | 805  | CLA  | C4A-NA-C1A | 7.33 | 110.00      | 106.71   |
| 14  | A     | 836  | CLA  | C4A-NA-C1A | 7.32 | 110.00      | 106.71   |
| 14  | 1     | 1641 | CLA  | C4A-NA-C1A | 7.31 | 109.99      | 106.71   |
| 14  | A     | 820  | CLA  | C4A-NA-C1A | 7.30 | 109.99      | 106.71   |
| 14  | a     | 840  | CLA  | C4A-NA-C1A | 7.30 | 109.99      | 106.71   |
| 14  | B     | 816  | CLA  | C4A-NA-C1A | 7.29 | 109.98      | 106.71   |
| 14  | a     | 836  | CLA  | C4A-NA-C1A | 7.28 | 109.98      | 106.71   |
| 14  | 1     | 1621 | CLA  | C4A-NA-C1A | 7.27 | 109.98      | 106.71   |
| 14  | 1     | 1627 | CLA  | C4A-NA-C1A | 7.27 | 109.97      | 106.71   |
| 14  | 2     | 834  | CLA  | C4A-NA-C1A | 7.27 | 109.97      | 106.71   |
| 14  | B     | 833  | CLA  | C4A-NA-C1A | 7.26 | 109.97      | 106.71   |
| 14  | b     | 806  | CLA  | C4A-NA-C1A | 7.25 | 109.97      | 106.71   |
| 14  | a     | 805  | CLA  | C4A-NA-C1A | 7.25 | 109.96      | 106.71   |
| 14  | b     | 807  | CLA  | C4A-NA-C1A | 7.25 | 109.96      | 106.71   |
| 14  | b     | 825  | CLA  | C4A-NA-C1A | 7.24 | 109.96      | 106.71   |
| 14  | B     | 806  | CLA  | C4A-NA-C1A | 7.23 | 109.96      | 106.71   |
| 14  | A     | 809  | CLA  | C4A-NA-C1A | 7.22 | 109.95      | 106.71   |
| 14  | a     | 809  | CLA  | C4A-NA-C1A | 7.22 | 109.95      | 106.71   |
| 14  | 2     | 817  | CLA  | C4A-NA-C1A | 7.22 | 109.95      | 106.71   |
| 14  | A     | 807  | CLA  | C4A-NA-C1A | 7.22 | 109.95      | 106.71   |
| 14  | a     | 826  | CLA  | C4A-NA-C1A | 7.21 | 109.95      | 106.71   |
| 14  | 1     | 1606 | CLA  | C4A-NA-C1A | 7.21 | 109.95      | 106.71   |
| 14  | 1     | 1610 | CLA  | C4A-NA-C1A | 7.20 | 109.94      | 106.71   |
| 14  | B     | 805  | CLA  | C4A-NA-C1A | 7.19 | 109.94      | 106.71   |
| 14  | b     | 817  | CLA  | C4A-NA-C1A | 7.18 | 109.94      | 106.71   |
| 14  | 2     | 838  | CLA  | C4A-NA-C1A | 7.18 | 109.94      | 106.71   |
| 14  | 2     | 807  | CLA  | C4A-NA-C1A | 7.18 | 109.93      | 106.71   |
| 14  | A     | 840  | CLA  | C4A-NA-C1A | 7.17 | 109.93      | 106.71   |
| 14  | 1     | 1608 | CLA  | C4A-NA-C1A | 7.17 | 109.93      | 106.71   |
| 14  | b     | 838  | CLA  | C4A-NA-C1A | 7.17 | 109.93      | 106.71   |
| 14  | A     | 826  | CLA  | C4A-NA-C1A | 7.16 | 109.93      | 106.71   |
| 14  | B     | 832  | CLA  | C4A-NA-C1A | 7.15 | 109.92      | 106.71   |
| 14  | 2     | 825  | CLA  | C4A-NA-C1A | 7.14 | 109.92      | 106.71   |
| 14  | B     | 837  | CLA  | C4A-NA-C1A | 7.14 | 109.92      | 106.71   |
| 14  | a     | 818  | CLA  | C4A-NA-C1A | 7.13 | 109.91      | 106.71   |
| 14  | 1     | 1631 | CLA  | C4A-NA-C1A | 7.13 | 109.91      | 106.71   |
| 14  | B     | 824  | CLA  | C4A-NA-C1A | 7.12 | 109.91      | 106.71   |
| 14  | 2     | 803  | CLA  | C4A-NA-C1A | 7.12 | 109.91      | 106.71   |
| 14  | 2     | 833  | CLA  | C4A-NA-C1A | 7.12 | 109.91      | 106.71   |
| 14  | 1     | 1619 | CLA  | C4A-NA-C1A | 7.11 | 109.90      | 106.71   |
| 14  | b     | 803  | CLA  | C4A-NA-C1A | 7.10 | 109.90      | 106.71   |
| 14  | 1     | 205  | CLA  | C4A-NA-C1A | 7.08 | 109.89      | 106.71   |

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| Mol | Chain | Res  | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 14  | b     | 833  | CLA  | C4A-NA-C1A | 7.08 | 109.89      | 106.71   |
| 14  | 0     | 206  | CLA  | C4A-NA-C1A | 7.08 | 109.89      | 106.71   |
| 14  | L     | 204  | CLA  | C4A-NA-C1A | 7.07 | 109.89      | 106.71   |
| 14  | A     | 830  | CLA  | C4A-NA-C1A | 7.07 | 109.89      | 106.71   |
| 14  | a     | 807  | CLA  | C4A-NA-C1A | 7.06 | 109.88      | 106.71   |
| 14  | A     | 818  | CLA  | C4A-NA-C1A | 7.05 | 109.88      | 106.71   |
| 14  | a     | 830  | CLA  | C4A-NA-C1A | 7.04 | 109.87      | 106.71   |
| 14  | b     | 805  | CLA  | C4A-NA-C1A | 7.03 | 109.86      | 106.71   |
| 14  | B     | 802  | CLA  | C4A-NA-C1A | 7.02 | 109.86      | 106.71   |
| 14  | B     | 804  | CLA  | C4A-NA-C1A | 7.02 | 109.86      | 106.71   |
| 14  | B     | 830  | CLA  | C4A-NA-C1A | 7.02 | 109.86      | 106.71   |
| 14  | 2     | 831  | CLA  | C4A-NA-C1A | 7.02 | 109.86      | 106.71   |
| 14  | 1     | 1625 | CLA  | C4A-NA-C1A | 7.01 | 109.86      | 106.71   |
| 14  | A     | 810  | CLA  | C4A-NA-C1A | 7.00 | 109.85      | 106.71   |
| 14  | 2     | 815  | CLA  | C4A-NA-C1A | 6.99 | 109.85      | 106.71   |
| 14  | 1     | 1603 | CLA  | C4A-NA-C1A | 6.99 | 109.85      | 106.71   |
| 14  | j     | 1302 | CLA  | C4A-NA-C1A | 6.98 | 109.85      | 106.71   |
| 14  | 2     | 805  | CLA  | C4A-NA-C1A | 6.98 | 109.84      | 106.71   |
| 14  | B     | 821  | CLA  | C4A-NA-C1A | 6.98 | 109.84      | 106.71   |
| 14  | b     | 808  | CLA  | C4A-NA-C1A | 6.97 | 109.84      | 106.71   |
| 14  | a     | 824  | CLA  | C4A-NA-C1A | 6.97 | 109.84      | 106.71   |
| 14  | 1     | 1623 | CLA  | C4A-NA-C1A | 6.97 | 109.84      | 106.71   |
| 14  | A     | 822  | CLA  | C4A-NA-C1A | 6.96 | 109.84      | 106.71   |
| 14  | A     | 838  | CLA  | C4A-NA-C1A | 6.96 | 109.84      | 106.71   |
| 14  | 1     | 1609 | CLA  | C4A-NA-C1A | 6.96 | 109.83      | 106.71   |
| 14  | a     | 834  | CLA  | C4A-NA-C1A | 6.95 | 109.83      | 106.71   |
| 14  | a     | 806  | CLA  | C4A-NA-C1A | 6.94 | 109.83      | 106.71   |
| 14  | b     | 831  | CLA  | C4A-NA-C1A | 6.94 | 109.83      | 106.71   |
| 14  | A     | 808  | CLA  | C4A-NA-C1A | 6.93 | 109.82      | 106.71   |
| 14  | 9     | 101  | CLA  | C4A-NA-C1A | 6.93 | 109.82      | 106.71   |
| 14  | B     | 831  | CLA  | C4A-NA-C1A | 6.93 | 109.82      | 106.71   |
| 14  | b     | 822  | CLA  | C4A-NA-C1A | 6.93 | 109.82      | 106.71   |
| 14  | 1     | 1639 | CLA  | C4A-NA-C1A | 6.93 | 109.82      | 106.71   |
| 14  | J     | 101  | CLA  | C4A-NA-C1A | 6.92 | 109.82      | 106.71   |
| 14  | a     | 822  | CLA  | C4A-NA-C1A | 6.92 | 109.82      | 106.71   |
| 14  | a     | 838  | CLA  | C4A-NA-C1A | 6.92 | 109.82      | 106.71   |
| 14  | 2     | 822  | CLA  | C4A-NA-C1A | 6.91 | 109.81      | 106.71   |
| 14  | B     | 815  | CLA  | C4A-NA-C1A | 6.91 | 109.81      | 106.71   |
| 14  | 2     | 808  | CLA  | C4A-NA-C1A | 6.90 | 109.81      | 106.71   |
| 14  | b     | 815  | CLA  | C4A-NA-C1A | 6.90 | 109.81      | 106.71   |
| 14  | A     | 802  | CLA  | C4A-NA-C1A | 6.90 | 109.81      | 106.71   |
| 14  | 8     | 1302 | CLA  | C4A-NA-C1A | 6.89 | 109.81      | 106.71   |

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| Mol | Chain | Res  | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 14  | 1     | 1607 | CLA  | C4A-NA-C1A | 6.89 | 109.80      | 106.71   |
| 14  | b     | 816  | CLA  | C4A-NA-C1A | 6.89 | 109.80      | 106.71   |
| 14  | 1     | 1635 | CLA  | C4A-NA-C1A | 6.89 | 109.80      | 106.71   |
| 14  | 2     | 812  | CLA  | C4A-NA-C1A | 6.88 | 109.80      | 106.71   |
| 14  | a     | 802  | CLA  | C4A-NA-C1A | 6.88 | 109.80      | 106.71   |
| 14  | B     | 814  | CLA  | C4A-NA-C1A | 6.88 | 109.80      | 106.71   |
| 14  | A     | 824  | CLA  | C4A-NA-C1A | 6.87 | 109.80      | 106.71   |
| 14  | B     | 838  | CLA  | C4A-NA-C1A | 6.87 | 109.79      | 106.71   |
| 14  | 2     | 832  | CLA  | C4A-NA-C1A | 6.86 | 109.79      | 106.71   |
| 14  | B     | 811  | CLA  | C4A-NA-C1A | 6.86 | 109.79      | 106.71   |
| 14  | a     | 844  | CLA  | C4A-NA-C1A | 6.86 | 109.79      | 106.71   |
| 14  | B     | 807  | CLA  | C4A-NA-C1A | 6.85 | 109.78      | 106.71   |
| 14  | a     | 810  | CLA  | C4A-NA-C1A | 6.85 | 109.78      | 106.71   |
| 14  | K     | 101  | CLA  | C4A-NA-C1A | 6.84 | 109.78      | 106.71   |
| 14  | a     | 808  | CLA  | C4A-NA-C1A | 6.84 | 109.78      | 106.71   |
| 14  | 2     | 816  | CLA  | C4A-NA-C1A | 6.83 | 109.78      | 106.71   |
| 14  | 2     | 839  | CLA  | C4A-NA-C1A | 6.83 | 109.78      | 106.71   |
| 14  | k     | 101  | CLA  | C4A-NA-C1A | 6.82 | 109.77      | 106.71   |
| 14  | A     | 834  | CLA  | C4A-NA-C1A | 6.81 | 109.77      | 106.71   |
| 14  | A     | 806  | CLA  | C4A-NA-C1A | 6.81 | 109.77      | 106.71   |
| 14  | A     | 844  | CLA  | C4A-NA-C1A | 6.79 | 109.76      | 106.71   |
| 14  | 1     | 1611 | CLA  | C4A-NA-C1A | 6.79 | 109.76      | 106.71   |
| 14  | b     | 832  | CLA  | C4A-NA-C1A | 6.78 | 109.75      | 106.71   |
| 14  | b     | 812  | CLA  | C4A-NA-C1A | 6.77 | 109.75      | 106.71   |
| 14  | b     | 839  | CLA  | C4A-NA-C1A | 6.75 | 109.74      | 106.71   |
| 14  | 1     | 1618 | CLA  | C4A-NA-C1A | 6.74 | 109.73      | 106.71   |
| 14  | A     | 823  | CLA  | C4A-NA-C1A | 6.73 | 109.73      | 106.71   |
| 14  | a     | 823  | CLA  | C4A-NA-C1A | 6.73 | 109.73      | 106.71   |
| 14  | 1     | 1645 | CLA  | C4A-NA-C1A | 6.72 | 109.72      | 106.71   |
| 14  | A     | 842  | CLA  | C4A-NA-C1A | 6.71 | 109.72      | 106.71   |
| 14  | B     | 834  | CLA  | C4A-NA-C1A | 6.71 | 109.72      | 106.71   |
| 14  | 1     | 1624 | CLA  | C4A-NA-C1A | 6.71 | 109.72      | 106.71   |
| 14  | b     | 837  | CLA  | C4A-NA-C1A | 6.70 | 109.72      | 106.71   |
| 14  | b     | 821  | CLA  | C4A-NA-C1A | 6.70 | 109.72      | 106.71   |
| 14  | 6     | 201  | CLA  | C4A-NA-C1A | 6.70 | 109.72      | 106.71   |
| 14  | B     | 836  | CLA  | C4A-NA-C1A | 6.69 | 109.71      | 106.71   |
| 14  | A     | 815  | CLA  | C4A-NA-C1A | 6.68 | 109.71      | 106.71   |
| 14  | A     | 857  | CLA  | C4A-NA-C1A | 6.68 | 109.71      | 106.71   |
| 14  | A     | 817  | CLA  | C4A-NA-C1A | 6.66 | 109.70      | 106.71   |
| 14  | 1     | 1643 | CLA  | C4A-NA-C1A | 6.66 | 109.70      | 106.71   |
| 14  | 2     | 835  | CLA  | C4A-NA-C1A | 6.66 | 109.70      | 106.71   |
| 14  | a     | 842  | CLA  | C4A-NA-C1A | 6.65 | 109.70      | 106.71   |

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| Mol | Chain | Res  | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 14  | B     | 820  | CLA  | C4A-NA-C1A | 6.65 | 109.69      | 106.71   |
| 14  | a     | 839  | CLA  | C4A-NA-C1A | 6.65 | 109.69      | 106.71   |
| 14  | 1     | 1612 | CLA  | C4A-NA-C1A | 6.65 | 109.69      | 106.71   |
| 14  | a     | 817  | CLA  | C4A-NA-C1A | 6.64 | 109.69      | 106.71   |
| 14  | f     | 201  | CLA  | C4A-NA-C1A | 6.64 | 109.69      | 106.71   |
| 14  | 1     | 1616 | CLA  | C4A-NA-C1A | 6.64 | 109.69      | 106.71   |
| 14  | a     | 812  | CLA  | C4A-NA-C1A | 6.63 | 109.69      | 106.71   |
| 14  | b     | 835  | CLA  | C4A-NA-C1A | 6.62 | 109.68      | 106.71   |
| 14  | A     | 839  | CLA  | C4A-NA-C1A | 6.61 | 109.68      | 106.71   |
| 14  | a     | 811  | CLA  | C4A-NA-C1A | 6.61 | 109.68      | 106.71   |
| 14  | b     | 823  | CLA  | C4A-NA-C1A | 6.61 | 109.68      | 106.71   |
| 14  | M     | 102  | CLA  | C4A-NA-C1A | 6.60 | 109.67      | 106.71   |
| 14  | 1     | 1640 | CLA  | C4A-NA-C1A | 6.60 | 109.67      | 106.71   |
| 14  | 1     | 1633 | CLA  | C4A-NA-C1A | 6.60 | 109.67      | 106.71   |
| 14  | a     | 816  | CLA  | C4A-NA-C1A | 6.59 | 109.67      | 106.71   |
| 14  | a     | 828  | CLA  | C4A-NA-C1A | 6.58 | 109.67      | 106.71   |
| 14  | A     | 825  | CLA  | C4A-NA-C1A | 6.58 | 109.66      | 106.71   |
| 14  | a     | 815  | CLA  | C4A-NA-C1A | 6.58 | 109.66      | 106.71   |
| 14  | F     | 201  | CLA  | C4A-NA-C1A | 6.57 | 109.66      | 106.71   |
| 14  | b     | 813  | CLA  | C4A-NA-C1A | 6.57 | 109.66      | 106.71   |
| 14  | A     | 811  | CLA  | C4A-NA-C1A | 6.57 | 109.66      | 106.71   |
| 14  | B     | 812  | CLA  | C4A-NA-C1A | 6.57 | 109.66      | 106.71   |
| 14  | a     | 832  | CLA  | C4A-NA-C1A | 6.57 | 109.66      | 106.71   |
| 14  | A     | 828  | CLA  | C4A-NA-C1A | 6.56 | 109.66      | 106.71   |
| 14  | 2     | 837  | CLA  | C4A-NA-C1A | 6.56 | 109.66      | 106.71   |
| 14  | B     | 835  | CLA  | C4A-NA-C1A | 6.56 | 109.66      | 106.71   |
| 14  | 2     | 819  | CLA  | C4A-NA-C1A | 6.56 | 109.65      | 106.71   |
| 14  | 2     | 813  | CLA  | C4A-NA-C1A | 6.56 | 109.65      | 106.71   |
| 14  | 1     | 1601 | CLA  | C4A-NA-C1A | 6.55 | 109.65      | 106.71   |
| 14  | a     | 827  | CLA  | C4A-NA-C1A | 6.54 | 109.65      | 106.71   |
| 14  | A     | 827  | CLA  | C4A-NA-C1A | 6.54 | 109.65      | 106.71   |
| 14  | x     | 1701 | CLA  | C4A-NA-C1A | 6.54 | 109.65      | 106.71   |
| 14  | B     | 822  | CLA  | C4A-NA-C1A | 6.53 | 109.64      | 106.71   |
| 14  | 1     | 1613 | CLA  | C4A-NA-C1A | 6.53 | 109.64      | 106.71   |
| 14  | 2     | 836  | CLA  | C4A-NA-C1A | 6.52 | 109.64      | 106.71   |
| 14  | f     | 203  | CLA  | C4A-NA-C1A | 6.52 | 109.64      | 106.71   |
| 14  | 1     | 1629 | CLA  | C4A-NA-C1A | 6.51 | 109.63      | 106.71   |
| 14  | 2     | 821  | CLA  | C4A-NA-C1A | 6.50 | 109.63      | 106.71   |
| 14  | z     | 102  | CLA  | C4A-NA-C1A | 6.50 | 109.63      | 106.71   |
| 14  | B     | 818  | CLA  | C4A-NA-C1A | 6.48 | 109.62      | 106.71   |
| 14  | 1     | 1628 | CLA  | C4A-NA-C1A | 6.48 | 109.62      | 106.71   |
| 14  | b     | 819  | CLA  | C4A-NA-C1A | 6.48 | 109.62      | 106.71   |

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| Mol | Chain | Res  | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 14  | a     | 825  | CLA  | C4A-NA-C1A | 6.47 | 109.62      | 106.71   |
| 14  | A     | 812  | CLA  | C4A-NA-C1A | 6.47 | 109.62      | 106.71   |
| 14  | b     | 836  | CLA  | C4A-NA-C1A | 6.47 | 109.61      | 106.71   |
| 14  | A     | 816  | CLA  | C4A-NA-C1A | 6.46 | 109.61      | 106.71   |
| 14  | L     | 203  | CLA  | C4A-NA-C1A | 6.46 | 109.61      | 106.71   |
| 14  | 1     | 1604 | CLA  | C4A-NA-C1A | 6.45 | 109.61      | 106.71   |
| 14  | A     | 803  | CLA  | C4A-NA-C1A | 6.43 | 109.60      | 106.71   |
| 14  | F     | 204  | CLA  | C4A-NA-C1A | 6.42 | 109.59      | 106.71   |
| 14  | l     | 204  | CLA  | C4A-NA-C1A | 6.42 | 109.59      | 106.71   |
| 14  | A     | 821  | CLA  | C4A-NA-C1A | 6.41 | 109.59      | 106.71   |
| 14  | b     | 826  | CLA  | C4A-NA-C1A | 6.41 | 109.59      | 106.71   |
| 14  | b     | 827  | CLA  | C4A-NA-C1A | 6.41 | 109.59      | 106.71   |
| 14  | 6     | 203  | CLA  | C4A-NA-C1A | 6.41 | 109.59      | 106.71   |
| 14  | k     | 103  | CLA  | C4A-NA-C1A | 6.41 | 109.59      | 106.71   |
| 14  | 1     | 1617 | CLA  | C4A-NA-C1A | 6.40 | 109.58      | 106.71   |
| 14  | A     | 832  | CLA  | C4A-NA-C1A | 6.40 | 109.58      | 106.71   |
| 14  | a     | 803  | CLA  | C4A-NA-C1A | 6.39 | 109.58      | 106.71   |
| 14  | B     | 826  | CLA  | C4A-NA-C1A | 6.39 | 109.58      | 106.71   |
| 14  | 1     | 1622 | CLA  | C4A-NA-C1A | 6.38 | 109.58      | 106.71   |
| 14  | X     | 1701 | CLA  | C4A-NA-C1A | 6.38 | 109.57      | 106.71   |
| 14  | 2     | 823  | CLA  | C4A-NA-C1A | 6.37 | 109.57      | 106.71   |
| 14  | 1     | 1626 | CLA  | C4A-NA-C1A | 6.37 | 109.57      | 106.71   |
| 14  | 2     | 826  | CLA  | C4A-NA-C1A | 6.37 | 109.57      | 106.71   |
| 14  | a     | 821  | CLA  | C4A-NA-C1A | 6.36 | 109.57      | 106.71   |
| 14  | 8     | 1301 | CLA  | C4A-NA-C1A | 6.36 | 109.56      | 106.71   |
| 14  | j     | 1301 | CLA  | C4A-NA-C1A | 6.35 | 109.56      | 106.71   |
| 14  | 1     | 1614 | CLA  | C4A-NA-C1A | 6.35 | 109.56      | 106.71   |
| 14  | 2     | 827  | CLA  | C4A-NA-C1A | 6.34 | 109.56      | 106.71   |
| 14  | B     | 817  | CLA  | C4A-NA-C1A | 6.32 | 109.55      | 106.71   |
| 14  | B     | 825  | CLA  | C4A-NA-C1A | 6.31 | 109.54      | 106.71   |
| 14  | F     | 203  | CLA  | C4A-NA-C1A | 6.31 | 109.54      | 106.71   |
| 14  | b     | 818  | CLA  | C4A-NA-C1A | 6.29 | 109.53      | 106.71   |
| 14  | 0     | 205  | CLA  | C4A-NA-C1A | 6.28 | 109.53      | 106.71   |
| 14  | 9     | 103  | CLA  | C4A-NA-C1A | 6.27 | 109.53      | 106.71   |
| 14  | K     | 103  | CLA  | C4A-NA-C1A | 6.27 | 109.53      | 106.71   |
| 14  | 2     | 814  | CLA  | C4A-NA-C1A | 6.27 | 109.52      | 106.71   |
| 14  | b     | 824  | CLA  | C4A-NA-C1A | 6.25 | 109.52      | 106.71   |
| 14  | a     | 813  | CLA  | C4A-NA-C1A | 6.24 | 109.51      | 106.71   |
| 14  | B     | 823  | CLA  | C4A-NA-C1A | 6.23 | 109.50      | 106.71   |
| 14  | 0     | 207  | CLA  | C4A-NA-C1A | 6.23 | 109.50      | 106.71   |
| 14  | 2     | 818  | CLA  | C4A-NA-C1A | 6.22 | 109.50      | 106.71   |
| 14  | A     | 813  | CLA  | C4A-NA-C1A | 6.21 | 109.50      | 106.71   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | L     | 205  | CLA  | C4A-NA-C1A  | 6.21  | 109.50      | 106.71   |
| 14  | a     | 814  | CLA  | C4A-NA-C1A  | 6.21  | 109.50      | 106.71   |
| 14  | b     | 814  | CLA  | C4A-NA-C1A  | 6.21  | 109.50      | 106.71   |
| 14  | l     | 206  | CLA  | C4A-NA-C1A  | 6.19  | 109.49      | 106.71   |
| 14  | 1     | 1615 | CLA  | C4A-NA-C1A  | 6.19  | 109.49      | 106.71   |
| 14  | A     | 814  | CLA  | C4A-NA-C1A  | 6.19  | 109.49      | 106.71   |
| 14  | J     | 102  | CLA  | C4A-NA-C1A  | 6.19  | 109.49      | 106.71   |
| 14  | 1     | 1634 | CLA  | C4A-NA-C1A  | 6.19  | 109.49      | 106.71   |
| 14  | B     | 819  | CLA  | C4A-NA-C1A  | 6.18  | 109.48      | 106.71   |
| 14  | 2     | 820  | CLA  | C4A-NA-C1A  | 6.18  | 109.48      | 106.71   |
| 14  | 2     | 824  | CLA  | C4A-NA-C1A  | 6.16  | 109.48      | 106.71   |
| 14  | a     | 833  | CLA  | C4A-NA-C1A  | 6.15  | 109.47      | 106.71   |
| 14  | 8     | 1303 | CLA  | C4A-NA-C1A  | 6.15  | 109.47      | 106.71   |
| 14  | b     | 820  | CLA  | C4A-NA-C1A  | 6.14  | 109.47      | 106.71   |
| 14  | j     | 1303 | CLA  | C4A-NA-C1A  | 6.14  | 109.47      | 106.71   |
| 14  | 2     | 829  | CLA  | C4A-NA-C1A  | 6.09  | 109.44      | 106.71   |
| 14  | B     | 813  | CLA  | C4A-NA-C1A  | 6.06  | 109.43      | 106.71   |
| 14  | A     | 833  | CLA  | C4A-NA-C1A  | 6.02  | 109.41      | 106.71   |
| 14  | 1     | 1639 | CLA  | CMB-C2B-C1B | -6.01 | 119.23      | 128.46   |
| 14  | b     | 829  | CLA  | C4A-NA-C1A  | 6.00  | 109.41      | 106.71   |
| 14  | a     | 837  | CLA  | C4A-NA-C1A  | 6.00  | 109.40      | 106.71   |
| 14  | B     | 828  | CLA  | C4A-NA-C1A  | 5.98  | 109.39      | 106.71   |
| 14  | A     | 837  | CLA  | C4A-NA-C1A  | 5.97  | 109.39      | 106.71   |
| 14  | A     | 838  | CLA  | CMB-C2B-C1B | -5.97 | 119.29      | 128.46   |
| 14  | b     | 802  | CLA  | C4A-NA-C1A  | 5.95  | 109.38      | 106.71   |
| 14  | a     | 838  | CLA  | CMB-C2B-C1B | -5.94 | 119.33      | 128.46   |
| 14  | 2     | 802  | CLA  | C4A-NA-C1A  | 5.94  | 109.38      | 106.71   |
| 14  | 1     | 1638 | CLA  | C4A-NA-C1A  | 5.91  | 109.36      | 106.71   |
| 14  | A     | 855  | CLA  | C4A-NA-C1A  | 5.88  | 109.35      | 106.71   |
| 14  | B     | 839  | CLA  | C4A-NA-C1A  | 5.81  | 109.32      | 106.71   |
| 14  | 2     | 828  | CLA  | C4A-NA-C1A  | 5.80  | 109.31      | 106.71   |
| 14  | b     | 840  | CLA  | C4A-NA-C1A  | 5.78  | 109.31      | 106.71   |
| 14  | B     | 827  | CLA  | C4A-NA-C1A  | 5.75  | 109.29      | 106.71   |
| 14  | 2     | 840  | CLA  | C4A-NA-C1A  | 5.73  | 109.28      | 106.71   |
| 14  | 1     | 1608 | CLA  | CMB-C2B-C1B | -5.73 | 119.66      | 128.46   |
| 14  | a     | 821  | CLA  | CMB-C2B-C1B | -5.72 | 119.67      | 128.46   |
| 14  | a     | 807  | CLA  | CMB-C2B-C1B | -5.72 | 119.68      | 128.46   |
| 14  | 1     | 1622 | CLA  | CMB-C2B-C1B | -5.71 | 119.69      | 128.46   |
| 14  | A     | 807  | CLA  | CMB-C2B-C1B | -5.71 | 119.69      | 128.46   |
| 14  | b     | 828  | CLA  | C4A-NA-C1A  | 5.70  | 109.27      | 106.71   |
| 14  | 1     | 1620 | CLA  | C4A-NA-C1A  | 5.69  | 109.27      | 106.71   |
| 14  | A     | 821  | CLA  | CMB-C2B-C1B | -5.69 | 119.71      | 128.46   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 819  | CLA  | C4A-NA-C1A  | 5.64  | 109.24      | 106.71   |
| 14  | A     | 819  | CLA  | C4A-NA-C1A  | 5.63  | 109.23      | 106.71   |
| 14  | B     | 805  | CLA  | CMB-C2B-C1B | -5.55 | 119.94      | 128.46   |
| 14  | 2     | 806  | CLA  | CMB-C2B-C1B | -5.54 | 119.95      | 128.46   |
| 14  | b     | 806  | CLA  | CMB-C2B-C1B | -5.51 | 119.99      | 128.46   |
| 14  | F     | 203  | CLA  | CMB-C2B-C1B | -5.45 | 120.08      | 128.46   |
| 14  | b     | 802  | CLA  | CMB-C2B-C1B | -5.44 | 120.11      | 128.46   |
| 14  | j     | 1301 | CLA  | CMB-C2B-C1B | -5.44 | 120.11      | 128.46   |
| 14  | 2     | 802  | CLA  | CMB-C2B-C1B | -5.44 | 120.11      | 128.46   |
| 14  | 8     | 1301 | CLA  | CMB-C2B-C1B | -5.43 | 120.11      | 128.46   |
| 14  | A     | 855  | CLA  | CMB-C2B-C1B | -5.43 | 120.11      | 128.46   |
| 14  | 1     | 1603 | CLA  | CMB-C2B-C1B | -5.43 | 120.12      | 128.46   |
| 14  | a     | 802  | CLA  | CMB-C2B-C1B | -5.43 | 120.12      | 128.46   |
| 14  | A     | 802  | CLA  | CMB-C2B-C1B | -5.41 | 120.14      | 128.46   |
| 14  | 2     | 822  | CLA  | CMB-C2B-C1B | -5.18 | 120.50      | 128.46   |
| 14  | B     | 821  | CLA  | CMB-C2B-C1B | -5.17 | 120.52      | 128.46   |
| 14  | b     | 822  | CLA  | CMB-C2B-C1B | -5.16 | 120.54      | 128.46   |
| 14  | b     | 812  | CLA  | CMB-C2B-C1B | -5.14 | 120.57      | 128.46   |
| 14  | 2     | 812  | CLA  | CMB-C2B-C1B | -5.13 | 120.59      | 128.46   |
| 14  | B     | 811  | CLA  | CMB-C2B-C1B | -5.11 | 120.61      | 128.46   |
| 14  | b     | 824  | CLA  | CMB-C2B-C1B | -4.99 | 120.79      | 128.46   |
| 14  | A     | 830  | CLA  | CMB-C2B-C1B | -4.96 | 120.84      | 128.46   |
| 14  | 2     | 824  | CLA  | CMB-C2B-C1B | -4.95 | 120.85      | 128.46   |
| 14  | a     | 830  | CLA  | CMB-C2B-C1B | -4.95 | 120.86      | 128.46   |
| 14  | B     | 823  | CLA  | CMB-C2B-C1B | -4.95 | 120.86      | 128.46   |
| 14  | a     | 820  | CLA  | CMB-C2B-C1B | -4.94 | 120.87      | 128.46   |
| 14  | 1     | 1621 | CLA  | CMB-C2B-C1B | -4.94 | 120.87      | 128.46   |
| 14  | 1     | 1639 | CLA  | CMB-C2B-C3B | 4.93  | 133.91      | 124.68   |
| 14  | 1     | 1631 | CLA  | CMB-C2B-C1B | -4.93 | 120.89      | 128.46   |
| 14  | 1     | 1628 | CLA  | CMB-C2B-C1B | -4.92 | 120.91      | 128.46   |
| 14  | a     | 838  | CLA  | CMB-C2B-C3B | 4.91  | 133.87      | 124.68   |
| 14  | A     | 838  | CLA  | CMB-C2B-C3B | 4.91  | 133.87      | 124.68   |
| 14  | A     | 820  | CLA  | CMB-C2B-C1B | -4.90 | 120.93      | 128.46   |
| 14  | A     | 827  | CLA  | CMB-C2B-C1B | -4.90 | 120.93      | 128.46   |
| 14  | a     | 827  | CLA  | CMB-C2B-C1B | -4.89 | 120.94      | 128.46   |
| 14  | a     | 821  | CLA  | CMB-C2B-C3B | 4.88  | 133.80      | 124.68   |
| 14  | 1     | 1622 | CLA  | CMB-C2B-C3B | 4.85  | 133.76      | 124.68   |
| 14  | A     | 821  | CLA  | CMB-C2B-C3B | 4.85  | 133.75      | 124.68   |
| 14  | B     | 827  | CLA  | CMB-C2B-C1B | -4.83 | 121.04      | 128.46   |
| 14  | b     | 828  | CLA  | CMB-C2B-C1B | -4.81 | 121.07      | 128.46   |
| 14  | 2     | 828  | CLA  | CMB-C2B-C1B | -4.81 | 121.07      | 128.46   |
| 14  | B     | 831  | CLA  | CMB-C2B-C1B | -4.64 | 121.33      | 128.46   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 834  | CLA  | CMB-C2B-C1B | -4.63 | 121.34      | 128.46   |
| 14  | 2     | 832  | CLA  | CMB-C2B-C1B | -4.62 | 121.36      | 128.46   |
| 14  | A     | 834  | CLA  | CMB-C2B-C1B | -4.62 | 121.36      | 128.46   |
| 14  | 1     | 1635 | CLA  | CMB-C2B-C1B | -4.62 | 121.37      | 128.46   |
| 14  | L     | 205  | CLA  | CMB-C2B-C1B | -4.61 | 121.37      | 128.46   |
| 14  | A     | 855  | CLA  | CMB-C2B-C3B | 4.60  | 133.29      | 124.68   |
| 14  | l     | 206  | CLA  | CMB-C2B-C1B | -4.60 | 121.39      | 128.46   |
| 14  | A     | 822  | CLA  | CMB-C2B-C1B | -4.60 | 121.40      | 128.46   |
| 14  | b     | 832  | CLA  | CMB-C2B-C1B | -4.59 | 121.40      | 128.46   |
| 14  | 1     | 1623 | CLA  | CMB-C2B-C1B | -4.59 | 121.41      | 128.46   |
| 14  | 0     | 207  | CLA  | CMB-C2B-C1B | -4.59 | 121.41      | 128.46   |
| 14  | b     | 802  | CLA  | CMB-C2B-C3B | 4.59  | 133.27      | 124.68   |
| 14  | a     | 822  | CLA  | CMB-C2B-C1B | -4.58 | 121.43      | 128.46   |
| 14  | a     | 807  | CLA  | CMB-C2B-C3B | 4.58  | 133.24      | 124.68   |
| 14  | 2     | 802  | CLA  | CMB-C2B-C3B | 4.56  | 133.21      | 124.68   |
| 14  | 1     | 1608 | CLA  | CMB-C2B-C3B | 4.55  | 133.19      | 124.68   |
| 14  | A     | 807  | CLA  | CMB-C2B-C3B | 4.53  | 133.16      | 124.68   |
| 14  | A     | 810  | CLA  | CMB-C2B-C1B | -4.51 | 121.53      | 128.46   |
| 14  | a     | 810  | CLA  | CMB-C2B-C1B | -4.51 | 121.54      | 128.46   |
| 14  | 1     | 1645 | CLA  | CMB-C2B-C1B | -4.51 | 121.54      | 128.46   |
| 14  | K     | 103  | CLA  | CMB-C2B-C1B | -4.50 | 121.54      | 128.46   |
| 14  | a     | 844  | CLA  | CMB-C2B-C1B | -4.50 | 121.56      | 128.46   |
| 14  | 9     | 103  | CLA  | CMB-C2B-C1B | -4.49 | 121.56      | 128.46   |
| 14  | A     | 830  | CLA  | CMB-C2B-C3B | 4.49  | 133.07      | 124.68   |
| 14  | A     | 844  | CLA  | CMB-C2B-C1B | -4.48 | 121.58      | 128.46   |
| 14  | 1     | 1611 | CLA  | CMB-C2B-C1B | -4.48 | 121.58      | 128.46   |
| 14  | A     | 825  | CLA  | CMB-C2B-C1B | -4.48 | 121.58      | 128.46   |
| 14  | 1     | 1626 | CLA  | CMB-C2B-C1B | -4.47 | 121.59      | 128.46   |
| 14  | a     | 830  | CLA  | CMB-C2B-C3B | 4.47  | 133.03      | 124.68   |
| 14  | k     | 103  | CLA  | CMB-C2B-C1B | -4.46 | 121.60      | 128.46   |
| 14  | a     | 802  | CLA  | CMB-C2B-C3B | 4.45  | 133.00      | 124.68   |
| 14  | 1     | 1603 | CLA  | CMB-C2B-C3B | 4.45  | 133.00      | 124.68   |
| 14  | 1     | 1631 | CLA  | CMB-C2B-C3B | 4.44  | 132.99      | 124.68   |
| 14  | A     | 802  | CLA  | CMB-C2B-C3B | 4.44  | 132.98      | 124.68   |
| 14  | a     | 829  | CLA  | CMB-C2B-C1B | -4.43 | 121.65      | 128.46   |
| 14  | 1     | 1630 | CLA  | CMB-C2B-C1B | -4.43 | 121.65      | 128.46   |
| 14  | a     | 825  | CLA  | CMB-C2B-C1B | -4.43 | 121.66      | 128.46   |
| 14  | A     | 829  | CLA  | CMB-C2B-C1B | -4.42 | 121.66      | 128.46   |
| 14  | a     | 809  | CLA  | CMB-C2B-C1B | -4.40 | 121.69      | 128.46   |
| 14  | F     | 203  | CLA  | CMB-C2B-C3B | 4.40  | 132.91      | 124.68   |
| 14  | a     | 805  | CLA  | CMB-C2B-C1B | -4.39 | 121.71      | 128.46   |
| 14  | 1     | 1610 | CLA  | CMB-C2B-C1B | -4.39 | 121.72      | 128.46   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 805  | CLA  | CMB-C2B-C3B | 4.39  | 132.89      | 124.68   |
| 14  | 1     | 1605 | CLA  | CMB-C2B-C1B | -4.39 | 121.72      | 128.46   |
| 14  | A     | 809  | CLA  | CMB-C2B-C1B | -4.39 | 121.72      | 128.46   |
| 14  | 1     | 1606 | CLA  | CMB-C2B-C1B | -4.39 | 121.72      | 128.46   |
| 14  | j     | 1301 | CLA  | CMB-C2B-C3B | 4.39  | 132.88      | 124.68   |
| 14  | a     | 833  | CLA  | CMB-C2B-C1B | -4.38 | 121.74      | 128.46   |
| 14  | b     | 806  | CLA  | CMB-C2B-C3B | 4.37  | 132.86      | 124.68   |
| 14  | 8     | 1301 | CLA  | CMB-C2B-C3B | 4.37  | 132.86      | 124.68   |
| 14  | A     | 805  | CLA  | CMB-C2B-C1B | -4.37 | 121.75      | 128.46   |
| 14  | A     | 833  | CLA  | CMB-C2B-C1B | -4.36 | 121.76      | 128.46   |
| 14  | 2     | 806  | CLA  | CMB-C2B-C3B | 4.36  | 132.83      | 124.68   |
| 14  | 1     | 1634 | CLA  | CMB-C2B-C1B | -4.35 | 121.77      | 128.46   |
| 14  | 2     | 819  | CLA  | CMB-C2B-C1B | -4.35 | 121.78      | 128.46   |
| 14  | a     | 804  | CLA  | CMB-C2B-C1B | -4.35 | 121.78      | 128.46   |
| 14  | B     | 818  | CLA  | CMB-C2B-C1B | -4.34 | 121.79      | 128.46   |
| 14  | b     | 819  | CLA  | CMB-C2B-C1B | -4.34 | 121.79      | 128.46   |
| 14  | A     | 804  | CLA  | CMB-C2B-C1B | -4.33 | 121.81      | 128.46   |
| 14  | B     | 822  | CLA  | CMB-C2B-C1B | -4.31 | 121.84      | 128.46   |
| 14  | A     | 826  | CLA  | CMB-C2B-C1B | -4.31 | 121.84      | 128.46   |
| 14  | 1     | 1633 | CLA  | CMB-C2B-C1B | -4.31 | 121.85      | 128.46   |
| 14  | B     | 834  | CLA  | CMB-C2B-C1B | -4.30 | 121.85      | 128.46   |
| 18  | a     | 854  | LHG  | O4-P-O5     | 4.30  | 133.51      | 112.24   |
| 18  | A     | 854  | LHG  | O4-P-O5     | 4.30  | 133.50      | 112.24   |
| 18  | 1     | 1655 | LHG  | O4-P-O5     | 4.30  | 133.49      | 112.24   |
| 18  | A     | 853  | LHG  | O4-P-O5     | 4.29  | 133.46      | 112.24   |
| 14  | b     | 823  | CLA  | CMB-C2B-C1B | -4.29 | 121.87      | 128.46   |
| 14  | 2     | 823  | CLA  | CMB-C2B-C1B | -4.29 | 121.87      | 128.46   |
| 18  | 1     | 1654 | LHG  | O4-P-O5     | 4.29  | 133.45      | 112.24   |
| 14  | A     | 832  | CLA  | CMB-C2B-C1B | -4.29 | 121.87      | 128.46   |
| 14  | a     | 826  | CLA  | CMB-C2B-C1B | -4.29 | 121.87      | 128.46   |
| 18  | a     | 853  | LHG  | O4-P-O5     | 4.28  | 133.41      | 112.24   |
| 14  | a     | 832  | CLA  | CMB-C2B-C1B | -4.28 | 121.89      | 128.46   |
| 14  | 1     | 1627 | CLA  | CMB-C2B-C1B | -4.27 | 121.91      | 128.46   |
| 14  | 2     | 814  | CLA  | CMB-C2B-C1B | -4.26 | 121.92      | 128.46   |
| 14  | 2     | 835  | CLA  | CMB-C2B-C1B | -4.26 | 121.92      | 128.46   |
| 14  | b     | 835  | CLA  | CMB-C2B-C1B | -4.26 | 121.92      | 128.46   |
| 14  | B     | 813  | CLA  | CMB-C2B-C1B | -4.25 | 121.94      | 128.46   |
| 14  | b     | 814  | CLA  | CMB-C2B-C1B | -4.24 | 121.94      | 128.46   |
| 14  | B     | 809  | CLA  | CMB-C2B-C1B | -4.23 | 121.96      | 128.46   |
| 18  | L     | 208  | LHG  | O4-P-O5     | 4.23  | 133.16      | 112.24   |
| 14  | b     | 810  | CLA  | CMB-C2B-C1B | -4.23 | 121.96      | 128.46   |
| 18  | 0     | 202  | LHG  | O4-P-O5     | 4.23  | 133.13      | 112.24   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | l     | 201  | LHG  | O4-P-O5     | 4.22  | 133.12      | 112.24   |
| 14  | 2     | 822  | CLA  | CMB-C2B-C3B | 4.22  | 132.58      | 124.68   |
| 14  | A     | 806  | CLA  | CMB-C2B-C1B | -4.22 | 121.98      | 128.46   |
| 14  | B     | 821  | CLA  | CMB-C2B-C3B | 4.22  | 132.56      | 124.68   |
| 14  | b     | 822  | CLA  | CMB-C2B-C3B | 4.20  | 132.54      | 124.68   |
| 14  | 2     | 810  | CLA  | CMB-C2B-C1B | -4.20 | 122.00      | 128.46   |
| 18  | M     | 101  | LHG  | O4-P-O5     | 4.20  | 133.00      | 112.24   |
| 18  | m     | 101  | LHG  | O4-P-O5     | 4.19  | 132.96      | 112.24   |
| 14  | l     | 1624 | CLA  | CMB-C2B-C1B | -4.19 | 122.03      | 128.46   |
| 18  | y     | 101  | LHG  | O4-P-O5     | 4.19  | 132.95      | 112.24   |
| 14  | a     | 823  | CLA  | CMB-C2B-C1B | -4.19 | 122.03      | 128.46   |
| 14  | l     | 1607 | CLA  | CMB-C2B-C1B | -4.19 | 122.03      | 128.46   |
| 14  | a     | 806  | CLA  | CMB-C2B-C1B | -4.18 | 122.05      | 128.46   |
| 18  | z     | 101  | LHG  | O4-P-O5     | 4.17  | 132.86      | 112.24   |
| 14  | A     | 823  | CLA  | CMB-C2B-C1B | -4.17 | 122.05      | 128.46   |
| 18  | b     | 851  | LHG  | O4-P-O5     | 4.17  | 132.84      | 112.24   |
| 18  | B     | 850  | LHG  | O4-P-O5     | 4.16  | 132.82      | 112.24   |
| 14  | 8     | 1303 | CLA  | CMB-C2B-C1B | -4.16 | 122.07      | 128.46   |
| 14  | J     | 102  | CLA  | CMB-C2B-C1B | -4.14 | 122.10      | 128.46   |
| 14  | j     | 1303 | CLA  | CMB-C2B-C1B | -4.13 | 122.11      | 128.46   |
| 14  | A     | 827  | CLA  | CMB-C2B-C3B | 4.11  | 132.37      | 124.68   |
| 14  | l     | 1628 | CLA  | CMB-C2B-C3B | 4.11  | 132.36      | 124.68   |
| 14  | 2     | 812  | CLA  | CMB-C2B-C3B | 4.11  | 132.36      | 124.68   |
| 14  | B     | 811  | CLA  | CMB-C2B-C3B | 4.10  | 132.35      | 124.68   |
| 14  | b     | 812  | CLA  | CMB-C2B-C3B | 4.10  | 132.35      | 124.68   |
| 14  | a     | 827  | CLA  | CMB-C2B-C3B | 4.10  | 132.35      | 124.68   |
| 14  | A     | 819  | CLA  | CMB-C2B-C1B | -4.08 | 122.20      | 128.46   |
| 14  | a     | 820  | CLA  | CMB-C2B-C3B | 4.08  | 132.30      | 124.68   |
| 14  | a     | 819  | CLA  | CMB-C2B-C1B | -4.07 | 122.21      | 128.46   |
| 14  | l     | 1621 | CLA  | CMB-C2B-C3B | 4.06  | 132.28      | 124.68   |
| 14  | b     | 824  | CLA  | CMB-C2B-C3B | 4.06  | 132.27      | 124.68   |
| 14  | A     | 828  | CLA  | CMB-C2B-C1B | -4.06 | 122.23      | 128.46   |
| 14  | A     | 820  | CLA  | CMB-C2B-C3B | 4.05  | 132.26      | 124.68   |
| 14  | 2     | 824  | CLA  | CMB-C2B-C3B | 4.05  | 132.25      | 124.68   |
| 14  | A     | 816  | CLA  | CMB-C2B-C1B | -4.05 | 122.24      | 128.46   |
| 14  | l     | 1617 | CLA  | CMB-C2B-C1B | -4.04 | 122.25      | 128.46   |
| 14  | F     | 201  | CLA  | CMB-C2B-C1B | -4.04 | 122.25      | 128.46   |
| 14  | a     | 828  | CLA  | CMB-C2B-C1B | -4.04 | 122.25      | 128.46   |
| 14  | A     | 831  | CLA  | CMB-C2B-C1B | -4.04 | 122.25      | 128.46   |
| 14  | a     | 816  | CLA  | CMB-C2B-C1B | -4.04 | 122.26      | 128.46   |
| 14  | B     | 823  | CLA  | CMB-C2B-C3B | 4.03  | 132.23      | 124.68   |
| 14  | f     | 201  | CLA  | CMB-C2B-C1B | -4.03 | 122.26      | 128.46   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | 2     | 817  | CLA  | CMB-C2B-C1B | -4.03 | 122.27      | 128.46   |
| 14  | 1     | 1620 | CLA  | CMB-C2B-C1B | -4.03 | 122.27      | 128.46   |
| 17  | B     | 843  | BCR  | C15-C16-C17 | -4.03 | 115.22      | 123.47   |
| 14  | 6     | 201  | CLA  | CMB-C2B-C1B | -4.03 | 122.27      | 128.46   |
| 17  | 2     | 844  | BCR  | C15-C16-C17 | -4.03 | 115.23      | 123.47   |
| 17  | b     | 844  | BCR  | C15-C16-C17 | -4.02 | 115.23      | 123.47   |
| 14  | 1     | 1629 | CLA  | CMB-C2B-C1B | -4.02 | 122.28      | 128.46   |
| 14  | a     | 831  | CLA  | CMB-C2B-C1B | -4.01 | 122.29      | 128.46   |
| 14  | B     | 816  | CLA  | CMB-C2B-C1B | -4.01 | 122.30      | 128.46   |
| 14  | 1     | 1632 | CLA  | CMB-C2B-C1B | -4.01 | 122.30      | 128.46   |
| 14  | A     | 842  | CLA  | CMB-C2B-C1B | -4.01 | 122.31      | 128.46   |
| 14  | b     | 817  | CLA  | CMB-C2B-C1B | -4.00 | 122.32      | 128.46   |
| 14  | 1     | 1643 | CLA  | CMB-C2B-C1B | -4.00 | 122.32      | 128.46   |
| 14  | z     | 102  | CLA  | CMB-C2B-C1B | -3.99 | 122.33      | 128.46   |
| 14  | a     | 842  | CLA  | CMB-C2B-C1B | -3.99 | 122.34      | 128.46   |
| 14  | a     | 834  | CLA  | CMB-C2B-C3B | 3.98  | 132.13      | 124.68   |
| 14  | X     | 1701 | CLA  | CMB-C2B-C1B | -3.98 | 122.35      | 128.46   |
| 14  | B     | 826  | CLA  | CMB-C2B-C1B | -3.97 | 122.36      | 128.46   |
| 14  | A     | 818  | CLA  | CMB-C2B-C1B | -3.97 | 122.36      | 128.46   |
| 14  | A     | 834  | CLA  | CMB-C2B-C3B | 3.97  | 132.10      | 124.68   |
| 14  | a     | 818  | CLA  | CMB-C2B-C1B | -3.96 | 122.37      | 128.46   |
| 14  | x     | 1701 | CLA  | CMB-C2B-C1B | -3.96 | 122.37      | 128.46   |
| 14  | 1     | 1635 | CLA  | CMB-C2B-C3B | 3.96  | 132.09      | 124.68   |
| 14  | 2     | 827  | CLA  | CMB-C2B-C1B | -3.96 | 122.38      | 128.46   |
| 14  | b     | 826  | CLA  | O2D-CGD-O1D | -3.95 | 116.11      | 123.84   |
| 17  | A     | 847  | BCR  | C2-C1-C6    | 3.95  | 116.57      | 110.48   |
| 14  | 1     | 1619 | CLA  | CMB-C2B-C1B | -3.95 | 122.39      | 128.46   |
| 14  | 2     | 802  | CLA  | C4-C3-C5    | 3.95  | 121.92      | 115.27   |
| 14  | b     | 802  | CLA  | C4-C3-C5    | 3.95  | 121.91      | 115.27   |
| 14  | 2     | 826  | CLA  | O2D-CGD-O1D | -3.94 | 116.12      | 123.84   |
| 14  | A     | 855  | CLA  | C4-C3-C5    | 3.94  | 121.91      | 115.27   |
| 14  | B     | 825  | CLA  | O2D-CGD-O1D | -3.94 | 116.13      | 123.84   |
| 17  | a     | 847  | BCR  | C2-C1-C6    | 3.93  | 116.53      | 110.48   |
| 14  | b     | 827  | CLA  | CMB-C2B-C1B | -3.93 | 122.43      | 128.46   |
| 17  | 1     | 1648 | BCR  | C2-C1-C6    | 3.92  | 116.51      | 110.48   |
| 14  | A     | 815  | CLA  | CMB-C2B-C1B | -3.91 | 122.45      | 128.46   |
| 14  | 1     | 1616 | CLA  | CMB-C2B-C1B | -3.90 | 122.47      | 128.46   |
| 14  | a     | 815  | CLA  | CMB-C2B-C1B | -3.89 | 122.48      | 128.46   |
| 14  | b     | 825  | CLA  | CMB-C2B-C1B | -3.89 | 122.49      | 128.46   |
| 14  | l     | 206  | CLA  | CMB-C2B-C3B | 3.89  | 131.95      | 124.68   |
| 14  | 0     | 206  | CLA  | O2D-CGD-O1D | -3.88 | 116.26      | 123.84   |
| 14  | L     | 205  | CLA  | CMB-C2B-C3B | 3.88  | 131.93      | 124.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | l     | 205  | CLA  | O2D-CGD-O1D | -3.88 | 116.26      | 123.84   |
| 14  | a     | 841  | CLA  | CMB-C2B-C1B | -3.88 | 122.51      | 128.46   |
| 14  | L     | 204  | CLA  | O2D-CGD-O1D | -3.88 | 116.26      | 123.84   |
| 14  | 1     | 1630 | CLA  | CMB-C2B-C3B | 3.87  | 131.92      | 124.68   |
| 14  | 1     | 1642 | CLA  | CMB-C2B-C1B | -3.86 | 122.53      | 128.46   |
| 14  | 2     | 825  | CLA  | CMB-C2B-C1B | -3.86 | 122.53      | 128.46   |
| 14  | 0     | 207  | CLA  | CMB-C2B-C3B | 3.86  | 131.90      | 124.68   |
| 14  | B     | 824  | CLA  | CMB-C2B-C1B | -3.85 | 122.54      | 128.46   |
| 14  | A     | 841  | CLA  | CMB-C2B-C1B | -3.85 | 122.54      | 128.46   |
| 14  | a     | 829  | CLA  | CMB-C2B-C3B | 3.85  | 131.88      | 124.68   |
| 14  | b     | 839  | CLA  | CMB-C2B-C1B | -3.85 | 122.55      | 128.46   |
| 14  | 2     | 839  | CLA  | CMB-C2B-C1B | -3.84 | 122.56      | 128.46   |
| 14  | b     | 828  | CLA  | CMB-C2B-C3B | 3.84  | 131.86      | 124.68   |
| 14  | b     | 816  | CLA  | CMB-C2B-C1B | -3.83 | 122.58      | 128.46   |
| 14  | A     | 829  | CLA  | CMB-C2B-C3B | 3.83  | 131.84      | 124.68   |
| 14  | a     | 839  | CLA  | O2D-CGD-O1D | -3.82 | 116.36      | 123.84   |
| 14  | B     | 838  | CLA  | CMB-C2B-C1B | -3.82 | 122.59      | 128.46   |
| 14  | A     | 839  | CLA  | O2D-CGD-O1D | -3.82 | 116.37      | 123.84   |
| 14  | B     | 831  | CLA  | CMB-C2B-C3B | 3.82  | 131.82      | 124.68   |
| 14  | B     | 827  | CLA  | CMB-C2B-C3B | 3.81  | 131.81      | 124.68   |
| 14  | 2     | 834  | CLA  | CMB-C2B-C1B | -3.80 | 122.62      | 128.46   |
| 14  | 2     | 816  | CLA  | CMB-C2B-C1B | -3.80 | 122.62      | 128.46   |
| 14  | 2     | 832  | CLA  | CMB-C2B-C3B | 3.80  | 131.78      | 124.68   |
| 14  | 1     | 1640 | CLA  | O2D-CGD-O1D | -3.80 | 116.42      | 123.84   |
| 14  | B     | 833  | CLA  | CMB-C2B-C1B | -3.80 | 122.63      | 128.46   |
| 14  | 2     | 828  | CLA  | CMB-C2B-C3B | 3.79  | 131.78      | 124.68   |
| 14  | 2     | 819  | CLA  | CMB-C2B-C3B | 3.79  | 131.77      | 124.68   |
| 14  | B     | 804  | CLA  | CMB-C2B-C1B | -3.79 | 122.64      | 128.46   |
| 14  | b     | 832  | CLA  | CMB-C2B-C3B | 3.78  | 131.75      | 124.68   |
| 14  | 1     | 1626 | CLA  | CMB-C2B-C3B | 3.78  | 131.75      | 124.68   |
| 14  | B     | 815  | CLA  | CMB-C2B-C1B | -3.78 | 122.66      | 128.46   |
| 14  | b     | 819  | CLA  | CMB-C2B-C3B | 3.78  | 131.75      | 124.68   |
| 14  | b     | 805  | CLA  | CMB-C2B-C1B | -3.78 | 122.66      | 128.46   |
| 14  | 1     | 1614 | CLA  | CMB-C2B-C1B | -3.77 | 122.67      | 128.46   |
| 14  | A     | 825  | CLA  | CMB-C2B-C3B | 3.77  | 131.73      | 124.68   |
| 14  | K     | 103  | CLA  | CMB-C2B-C3B | 3.76  | 131.72      | 124.68   |
| 14  | b     | 834  | CLA  | CMB-C2B-C1B | -3.76 | 122.68      | 128.46   |
| 14  | 2     | 805  | CLA  | CMB-C2B-C1B | -3.76 | 122.68      | 128.46   |
| 14  | 9     | 103  | CLA  | CMB-C2B-C3B | 3.76  | 131.71      | 124.68   |
| 14  | B     | 818  | CLA  | CMB-C2B-C3B | 3.75  | 131.70      | 124.68   |
| 14  | k     | 103  | CLA  | CMB-C2B-C3B | 3.75  | 131.70      | 124.68   |
| 14  | a     | 813  | CLA  | CMB-C2B-C1B | -3.75 | 122.70      | 128.46   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 813  | CLA  | CMB-C2B-C1B | -3.75 | 122.71      | 128.46   |
| 14  | 1     | 1645 | CLA  | CMB-C2B-C3B | 3.74  | 131.68      | 124.68   |
| 14  | a     | 825  | CLA  | CMB-C2B-C3B | 3.74  | 131.67      | 124.68   |
| 14  | A     | 844  | CLA  | CMB-C2B-C3B | 3.73  | 131.67      | 124.68   |
| 14  | a     | 844  | CLA  | CMB-C2B-C3B | 3.73  | 131.65      | 124.68   |
| 14  | 2     | 830  | CLA  | CMB-C2B-C1B | -3.72 | 122.74      | 128.46   |
| 14  | 1     | 1606 | CLA  | CMB-C2B-C3B | 3.72  | 131.64      | 124.68   |
| 14  | A     | 837  | CLA  | CMB-C2B-C1B | -3.72 | 122.75      | 128.46   |
| 14  | B     | 829  | CLA  | CMB-C2B-C1B | -3.72 | 122.75      | 128.46   |
| 14  | 1     | 1638 | CLA  | CMB-C2B-C1B | -3.71 | 122.75      | 128.46   |
| 14  | a     | 837  | CLA  | CMB-C2B-C1B | -3.71 | 122.77      | 128.46   |
| 14  | a     | 805  | CLA  | CMB-C2B-C3B | 3.71  | 131.61      | 124.68   |
| 14  | b     | 830  | CLA  | CMB-C2B-C1B | -3.71 | 122.77      | 128.46   |
| 14  | 1     | 1640 | CLA  | CMB-C2B-C1B | -3.69 | 122.80      | 128.46   |
| 14  | A     | 805  | CLA  | CMB-C2B-C3B | 3.68  | 131.56      | 124.68   |
| 17  | l     | 207  | BCR  | C2-C1-C6    | 3.68  | 116.14      | 110.48   |
| 17  | L     | 206  | BCR  | C2-C1-C6    | 3.68  | 116.14      | 110.48   |
| 14  | A     | 839  | CLA  | CMB-C2B-C1B | -3.68 | 122.81      | 128.46   |
| 14  | A     | 812  | CLA  | CMB-C2B-C1B | -3.67 | 122.83      | 128.46   |
| 14  | a     | 812  | CLA  | CMB-C2B-C1B | -3.66 | 122.83      | 128.46   |
| 17  | 0     | 208  | BCR  | C2-C1-C6    | 3.66  | 116.12      | 110.48   |
| 14  | a     | 839  | CLA  | CMB-C2B-C1B | -3.66 | 122.84      | 128.46   |
| 14  | 2     | 815  | CLA  | CMB-C2B-C1B | -3.65 | 122.85      | 128.46   |
| 14  | 1     | 1613 | CLA  | CMB-C2B-C1B | -3.65 | 122.85      | 128.46   |
| 14  | b     | 815  | CLA  | CMB-C2B-C1B | -3.64 | 122.87      | 128.46   |
| 14  | B     | 814  | CLA  | CMB-C2B-C1B | -3.63 | 122.88      | 128.46   |
| 14  | A     | 822  | CLA  | CMB-C2B-C3B | 3.63  | 131.46      | 124.68   |
| 14  | 2     | 841  | CLA  | CMB-C2B-C1B | -3.63 | 122.89      | 128.46   |
| 14  | 1     | 1623 | CLA  | CMB-C2B-C3B | 3.62  | 131.45      | 124.68   |
| 14  | a     | 822  | CLA  | CMB-C2B-C3B | 3.62  | 131.44      | 124.68   |
| 14  | L     | 203  | CLA  | CMB-C2B-C1B | -3.61 | 122.92      | 128.46   |
| 14  | b     | 841  | CLA  | CMB-C2B-C1B | -3.60 | 122.93      | 128.46   |
| 14  | B     | 813  | CLA  | CMB-C2B-C3B | 3.60  | 131.41      | 124.68   |
| 14  | b     | 811  | CLA  | CMB-C2B-C1B | -3.60 | 122.93      | 128.46   |
| 14  | B     | 810  | CLA  | CMB-C2B-C1B | -3.60 | 122.93      | 128.46   |
| 14  | 1     | 1605 | CLA  | CMB-C2B-C3B | 3.60  | 131.41      | 124.68   |
| 14  | 2     | 814  | CLA  | CMB-C2B-C3B | 3.60  | 131.41      | 124.68   |
| 14  | a     | 804  | CLA  | CMB-C2B-C3B | 3.60  | 131.41      | 124.68   |
| 14  | 1     | 1620 | CLA  | C4-C3-C5    | 3.59  | 121.32      | 115.27   |
| 14  | 0     | 205  | CLA  | CMB-C2B-C1B | -3.59 | 122.94      | 128.46   |
| 14  | a     | 819  | CLA  | C4-C3-C5    | 3.59  | 121.30      | 115.27   |
| 14  | l     | 204  | CLA  | CMB-C2B-C1B | -3.58 | 122.95      | 128.46   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 804  | CLA  | CMB-C2B-C3B | 3.58  | 131.38      | 124.68   |
| 14  | a     | 823  | CLA  | CMB-C2B-C3B | 3.58  | 131.38      | 124.68   |
| 14  | L     | 204  | CLA  | CMB-C2B-C1B | -3.58 | 122.96      | 128.46   |
| 14  | A     | 819  | CLA  | C4-C3-C5    | 3.58  | 121.29      | 115.27   |
| 14  | 2     | 811  | CLA  | CMB-C2B-C1B | -3.58 | 122.97      | 128.46   |
| 14  | l     | 205  | CLA  | CMB-C2B-C1B | -3.58 | 122.97      | 128.46   |
| 14  | 0     | 206  | CLA  | CMB-C2B-C1B | -3.58 | 122.97      | 128.46   |
| 14  | b     | 814  | CLA  | CMB-C2B-C3B | 3.57  | 131.36      | 124.68   |
| 14  | A     | 816  | CLA  | CMB-C2B-C3B | 3.57  | 131.35      | 124.68   |
| 14  | B     | 825  | CLA  | CMB-C2B-C1B | -3.57 | 122.98      | 128.46   |
| 14  | A     | 826  | CLA  | CMB-C2B-C3B | 3.57  | 131.35      | 124.68   |
| 14  | 1     | 1611 | CLA  | CMB-C2B-C3B | 3.56  | 131.34      | 124.68   |
| 17  | B     | 851  | BCR  | C7-C8-C9    | -3.56 | 120.85      | 126.23   |
| 14  | A     | 810  | CLA  | CMB-C2B-C3B | 3.56  | 131.34      | 124.68   |
| 14  | a     | 810  | CLA  | CMB-C2B-C3B | 3.56  | 131.34      | 124.68   |
| 14  | 2     | 826  | CLA  | CMB-C2B-C1B | -3.56 | 123.00      | 128.46   |
| 14  | B     | 840  | CLA  | CMB-C2B-C1B | -3.55 | 123.00      | 128.46   |
| 14  | A     | 806  | CLA  | CMB-C2B-C3B | 3.55  | 131.32      | 124.68   |
| 17  | 8     | 1306 | BCR  | C7-C8-C9    | -3.55 | 120.87      | 126.23   |
| 14  | a     | 816  | CLA  | CMB-C2B-C3B | 3.55  | 131.32      | 124.68   |
| 14  | 1     | 1624 | CLA  | CMB-C2B-C3B | 3.55  | 131.32      | 124.68   |
| 14  | 1     | 1610 | CLA  | CMB-C2B-C3B | 3.55  | 131.31      | 124.68   |
| 14  | A     | 823  | CLA  | CMB-C2B-C3B | 3.54  | 131.31      | 124.68   |
| 14  | b     | 826  | CLA  | CMB-C2B-C1B | -3.54 | 123.02      | 128.46   |
| 17  | b     | 852  | BCR  | C7-C8-C9    | -3.54 | 120.88      | 126.23   |
| 14  | 1     | 1617 | CLA  | CMB-C2B-C3B | 3.54  | 131.30      | 124.68   |
| 14  | b     | 820  | CLA  | CMB-C2B-C1B | -3.54 | 123.03      | 128.46   |
| 14  | 1     | 1634 | CLA  | CMB-C2B-C3B | 3.54  | 131.30      | 124.68   |
| 14  | a     | 826  | CLA  | CMB-C2B-C3B | 3.53  | 131.29      | 124.68   |
| 14  | A     | 833  | CLA  | CMB-C2B-C3B | 3.53  | 131.29      | 124.68   |
| 14  | a     | 809  | CLA  | CMB-C2B-C3B | 3.53  | 131.29      | 124.68   |
| 14  | 2     | 820  | CLA  | CMB-C2B-C1B | -3.53 | 123.03      | 128.46   |
| 14  | A     | 809  | CLA  | CMB-C2B-C3B | 3.52  | 131.26      | 124.68   |
| 14  | a     | 806  | CLA  | CMB-C2B-C3B | 3.52  | 131.26      | 124.68   |
| 14  | B     | 819  | CLA  | CMB-C2B-C1B | -3.52 | 123.06      | 128.46   |
| 14  | a     | 833  | CLA  | CMB-C2B-C3B | 3.52  | 131.26      | 124.68   |
| 14  | 1     | 1607 | CLA  | CMB-C2B-C3B | 3.52  | 131.26      | 124.68   |
| 14  | a     | 819  | CLA  | CMB-C2B-C3B | 3.51  | 131.24      | 124.68   |
| 14  | 1     | 1627 | CLA  | CMB-C2B-C3B | 3.50  | 131.23      | 124.68   |
| 14  | b     | 818  | CLA  | C4-C3-C5    | 3.49  | 121.15      | 115.27   |
| 14  | B     | 817  | CLA  | C4-C3-C5    | 3.49  | 121.15      | 115.27   |
| 14  | 8     | 1303 | CLA  | CMB-C2B-C3B | 3.49  | 131.21      | 124.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | 2     | 818  | CLA  | C4-C3-C5    | 3.49  | 121.15      | 115.27   |
| 14  | B     | 803  | CLA  | CMB-C2B-C1B | -3.49 | 123.10      | 128.46   |
| 14  | A     | 855  | CLA  | O2D-CGD-O1D | -3.49 | 117.01      | 123.84   |
| 14  | J     | 102  | CLA  | CMB-C2B-C3B | 3.49  | 131.20      | 124.68   |
| 14  | K     | 101  | CLA  | CMB-C2B-C1B | -3.49 | 123.11      | 128.46   |
| 14  | B     | 829  | CLA  | O2D-CGD-O1D | -3.49 | 117.02      | 123.84   |
| 14  | b     | 802  | CLA  | O2D-CGD-O1D | -3.49 | 117.02      | 123.84   |
| 14  | b     | 807  | CLA  | CMB-C2B-C1B | -3.48 | 123.11      | 128.46   |
| 14  | A     | 819  | CLA  | CMB-C2B-C3B | 3.48  | 131.19      | 124.68   |
| 14  | 1     | 1620 | CLA  | CMB-C2B-C3B | 3.48  | 131.19      | 124.68   |
| 14  | j     | 1303 | CLA  | CMB-C2B-C3B | 3.48  | 131.19      | 124.68   |
| 14  | b     | 804  | CLA  | CMB-C2B-C1B | -3.48 | 123.12      | 128.46   |
| 14  | 2     | 802  | CLA  | O2D-CGD-O1D | -3.48 | 117.04      | 123.84   |
| 14  | 2     | 804  | CLA  | CMB-C2B-C1B | -3.47 | 123.12      | 128.46   |
| 14  | 2     | 830  | CLA  | O2D-CGD-O1D | -3.47 | 117.05      | 123.84   |
| 14  | b     | 830  | CLA  | O2D-CGD-O1D | -3.47 | 117.05      | 123.84   |
| 17  | F     | 205  | BCR  | C35-C13-C14 | -3.47 | 118.06      | 122.92   |
| 17  | M     | 103  | BCR  | C24-C23-C22 | -3.47 | 121.00      | 126.23   |
| 17  | y     | 102  | BCR  | C24-C23-C22 | -3.46 | 121.00      | 126.23   |
| 14  | 9     | 101  | CLA  | CMB-C2B-C1B | -3.46 | 123.14      | 128.46   |
| 14  | b     | 825  | CLA  | CHB-C4A-NA  | 3.46  | 129.30      | 124.51   |
| 14  | F     | 204  | CLA  | CMB-C2B-C1B | -3.46 | 123.15      | 128.46   |
| 17  | 6     | 204  | BCR  | C35-C13-C14 | -3.46 | 118.08      | 122.92   |
| 14  | B     | 828  | CLA  | CMB-C2B-C1B | -3.45 | 123.16      | 128.46   |
| 14  | B     | 824  | CLA  | CHB-C4A-NA  | 3.45  | 129.28      | 124.51   |
| 14  | B     | 806  | CLA  | CMB-C2B-C1B | -3.44 | 123.17      | 128.46   |
| 14  | 1     | 1609 | CLA  | O2D-CGD-O1D | -3.44 | 117.12      | 123.84   |
| 14  | 2     | 825  | CLA  | CHB-C4A-NA  | 3.44  | 129.27      | 124.51   |
| 14  | k     | 101  | CLA  | CMB-C2B-C1B | -3.44 | 123.18      | 128.46   |
| 17  | f     | 204  | BCR  | C35-C13-C14 | -3.43 | 118.11      | 122.92   |
| 17  | m     | 102  | BCR  | C24-C23-C22 | -3.43 | 121.06      | 126.23   |
| 14  | A     | 840  | CLA  | O2D-CGD-O1D | -3.43 | 117.14      | 123.84   |
| 14  | b     | 813  | CLA  | CMB-C2B-C1B | -3.42 | 123.20      | 128.46   |
| 14  | 6     | 203  | CLA  | CMB-C2B-C1B | -3.42 | 123.20      | 128.46   |
| 14  | b     | 829  | CLA  | CMB-C2B-C1B | -3.42 | 123.20      | 128.46   |
| 14  | 2     | 829  | CLA  | CMB-C2B-C1B | -3.42 | 123.20      | 128.46   |
| 14  | f     | 203  | CLA  | CMB-C2B-C1B | -3.42 | 123.20      | 128.46   |
| 14  | 2     | 807  | CLA  | CMB-C2B-C1B | -3.42 | 123.21      | 128.46   |
| 17  | a     | 849  | BCR  | C15-C16-C17 | -3.42 | 116.47      | 123.47   |
| 14  | 2     | 813  | CLA  | CMB-C2B-C1B | -3.41 | 123.22      | 128.46   |
| 14  | B     | 825  | CLA  | C1-C2-C3    | -3.40 | 120.16      | 126.04   |
| 14  | l     | 206  | CLA  | O2D-CGD-O1D | -3.40 | 117.20      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 808  | CLA  | O2D-CGD-O1D | -3.39 | 117.20      | 123.84   |
| 14  | A     | 808  | CLA  | O2D-CGD-O1D | -3.39 | 117.20      | 123.84   |
| 14  | 1     | 1641 | CLA  | O2D-CGD-O1D | -3.39 | 117.21      | 123.84   |
| 14  | B     | 802  | CLA  | CMB-C2B-C1B | -3.39 | 123.25      | 128.46   |
| 14  | 0     | 207  | CLA  | O2D-CGD-O1D | -3.39 | 117.21      | 123.84   |
| 14  | 1     | 1633 | CLA  | CMB-C2B-C3B | 3.39  | 131.02      | 124.68   |
| 14  | b     | 825  | CLA  | CMB-C2B-C3B | 3.39  | 131.01      | 124.68   |
| 14  | a     | 840  | CLA  | O2D-CGD-O1D | -3.39 | 117.22      | 123.84   |
| 14  | B     | 812  | CLA  | CMB-C2B-C1B | -3.38 | 123.26      | 128.46   |
| 14  | A     | 818  | CLA  | CMB-C2B-C3B | 3.38  | 131.01      | 124.68   |
| 14  | X     | 1701 | CLA  | O2D-CGD-O1D | -3.38 | 117.22      | 123.84   |
| 14  | 2     | 826  | CLA  | C1-C2-C3    | -3.38 | 120.19      | 126.04   |
| 17  | 1     | 1650 | BCR  | C15-C16-C17 | -3.38 | 116.55      | 123.47   |
| 14  | x     | 1701 | CLA  | O2D-CGD-O1D | -3.38 | 117.23      | 123.84   |
| 14  | a     | 832  | CLA  | CMB-C2B-C3B | 3.38  | 131.00      | 124.68   |
| 14  | 1     | 1619 | CLA  | CMB-C2B-C3B | 3.38  | 131.00      | 124.68   |
| 17  | A     | 849  | BCR  | C15-C16-C17 | -3.38 | 116.55      | 123.47   |
| 14  | a     | 818  | CLA  | CMB-C2B-C3B | 3.38  | 131.00      | 124.68   |
| 14  | z     | 102  | CLA  | O2D-CGD-O1D | -3.38 | 117.24      | 123.84   |
| 14  | b     | 826  | CLA  | C1-C2-C3    | -3.37 | 120.21      | 126.04   |
| 14  | B     | 824  | CLA  | CMB-C2B-C3B | 3.37  | 130.98      | 124.68   |
| 13  | a     | 801  | CL0  | O2D-CGD-O1D | -3.37 | 117.25      | 123.84   |
| 14  | 2     | 803  | CLA  | CMB-C2B-C1B | -3.37 | 123.29      | 128.46   |
| 14  | A     | 832  | CLA  | CMB-C2B-C3B | 3.37  | 130.97      | 124.68   |
| 14  | 2     | 823  | CLA  | CMB-C2B-C3B | 3.36  | 130.96      | 124.68   |
| 14  | B     | 809  | CLA  | C1-C2-C3    | -3.36 | 120.23      | 126.04   |
| 14  | L     | 205  | CLA  | O2D-CGD-O1D | -3.35 | 117.28      | 123.84   |
| 14  | b     | 803  | CLA  | CMB-C2B-C1B | -3.35 | 123.31      | 128.46   |
| 13  | 1     | 1602 | CL0  | O2D-CGD-O1D | -3.35 | 117.29      | 123.84   |
| 14  | 2     | 812  | CLA  | O2D-CGD-O1D | -3.35 | 117.29      | 123.84   |
| 14  | b     | 808  | CLA  | O2D-CGD-O1D | -3.35 | 117.30      | 123.84   |
| 14  | 1     | 1614 | CLA  | O2D-CGD-O1D | -3.35 | 117.30      | 123.84   |
| 14  | B     | 817  | CLA  | CMB-C2B-C1B | -3.34 | 123.32      | 128.46   |
| 14  | 1     | 1601 | CLA  | CMB-C2B-C1B | -3.34 | 123.33      | 128.46   |
| 14  | A     | 813  | CLA  | O2D-CGD-O1D | -3.34 | 117.30      | 123.84   |
| 14  | B     | 807  | CLA  | O2D-CGD-O1D | -3.34 | 117.31      | 123.84   |
| 14  | b     | 823  | CLA  | CMB-C2B-C3B | 3.34  | 130.93      | 124.68   |
| 14  | 2     | 825  | CLA  | CMB-C2B-C3B | 3.34  | 130.93      | 124.68   |
| 14  | b     | 812  | CLA  | O2D-CGD-O1D | -3.34 | 117.31      | 123.84   |
| 14  | B     | 822  | CLA  | CMB-C2B-C3B | 3.34  | 130.92      | 124.68   |
| 14  | 2     | 827  | CLA  | CMB-C2B-C3B | 3.34  | 130.92      | 124.68   |
| 14  | 2     | 810  | CLA  | C1-C2-C3    | -3.34 | 120.27      | 126.04   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 813  | CLA  | O2D-CGD-O1D | -3.34 | 117.32      | 123.84   |
| 14  | B     | 834  | CLA  | CMB-C2B-C3B | 3.33  | 130.91      | 124.68   |
| 14  | B     | 811  | CLA  | O2D-CGD-O1D | -3.33 | 117.32      | 123.84   |
| 14  | 2     | 808  | CLA  | O2D-CGD-O1D | -3.33 | 117.33      | 123.84   |
| 14  | b     | 810  | CLA  | C1-C2-C3    | -3.33 | 120.29      | 126.04   |
| 13  | A     | 801  | CL0  | O2D-CGD-O1D | -3.32 | 117.34      | 123.84   |
| 14  | 2     | 835  | CLA  | CMB-C2B-C3B | 3.32  | 130.89      | 124.68   |
| 14  | 2     | 818  | CLA  | CMB-C2B-C1B | -3.32 | 123.36      | 128.46   |
| 14  | A     | 857  | CLA  | CMB-C2B-C1B | -3.32 | 123.36      | 128.46   |
| 14  | b     | 835  | CLA  | CMB-C2B-C3B | 3.32  | 130.89      | 124.68   |
| 14  | B     | 826  | CLA  | CMB-C2B-C3B | 3.32  | 130.89      | 124.68   |
| 14  | A     | 830  | CLA  | O2D-CGD-O1D | -3.32 | 117.35      | 123.84   |
| 14  | M     | 102  | CLA  | CMB-C2B-C1B | -3.31 | 123.37      | 128.46   |
| 14  | b     | 827  | CLA  | CMB-C2B-C3B | 3.31  | 130.87      | 124.68   |
| 14  | 2     | 838  | CLA  | O2D-CGD-O1D | -3.31 | 117.38      | 123.84   |
| 14  | A     | 834  | CLA  | C1-C2-C3    | -3.30 | 120.33      | 126.04   |
| 14  | b     | 818  | CLA  | CMB-C2B-C1B | -3.30 | 123.39      | 128.46   |
| 14  | 2     | 821  | CLA  | CMB-C2B-C1B | -3.30 | 123.39      | 128.46   |
| 14  | 1     | 1631 | CLA  | O2D-CGD-O1D | -3.30 | 117.39      | 123.84   |
| 14  | B     | 812  | CLA  | O2D-CGD-O1D | -3.29 | 117.40      | 123.84   |
| 17  | b     | 848  | BCR  | C15-C16-C17 | -3.29 | 116.72      | 123.47   |
| 17  | 2     | 848  | BCR  | C15-C16-C17 | -3.29 | 116.73      | 123.47   |
| 14  | B     | 837  | CLA  | O2D-CGD-O1D | -3.29 | 117.41      | 123.84   |
| 14  | b     | 833  | CLA  | CMB-C2B-C1B | -3.29 | 123.41      | 128.46   |
| 14  | B     | 841  | CLA  | O2D-CGD-O1D | -3.28 | 117.42      | 123.84   |
| 14  | b     | 821  | CLA  | CMB-C2B-C1B | -3.28 | 123.42      | 128.46   |
| 14  | a     | 834  | CLA  | C1-C2-C3    | -3.28 | 120.37      | 126.04   |
| 14  | 1     | 1635 | CLA  | C1-C2-C3    | -3.28 | 120.37      | 126.04   |
| 14  | a     | 830  | CLA  | O2D-CGD-O1D | -3.28 | 117.42      | 123.84   |
| 14  | 2     | 815  | CLA  | CMB-C2B-C3B | 3.28  | 130.81      | 124.68   |
| 14  | 2     | 842  | CLA  | O2D-CGD-O1D | -3.28 | 117.43      | 123.84   |
| 14  | 2     | 813  | CLA  | O2D-CGD-O1D | -3.28 | 117.43      | 123.84   |
| 14  | 6     | 201  | CLA  | CMB-C2B-C3B | 3.27  | 130.80      | 124.68   |
| 14  | 2     | 842  | CLA  | C1-C2-C3    | -3.27 | 120.38      | 126.04   |
| 17  | B     | 847  | BCR  | C15-C16-C17 | -3.27 | 116.77      | 123.47   |
| 14  | 1     | 1642 | CLA  | CMB-C2B-C3B | 3.27  | 130.80      | 124.68   |
| 14  | a     | 829  | CLA  | O2D-CGD-O1D | -3.27 | 117.45      | 123.84   |
| 14  | F     | 201  | CLA  | CMB-C2B-C3B | 3.27  | 130.79      | 124.68   |
| 14  | X     | 1701 | CLA  | CMB-C2B-C3B | 3.27  | 130.79      | 124.68   |
| 14  | B     | 809  | CLA  | CMB-C2B-C3B | 3.27  | 130.79      | 124.68   |
| 14  | B     | 841  | CLA  | C1-C2-C3    | -3.27 | 120.39      | 126.04   |
| 14  | b     | 815  | CLA  | CMB-C2B-C3B | 3.27  | 130.79      | 124.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | f     | 201  | CLA  | CMB-C2B-C3B | 3.27  | 130.79      | 124.68   |
| 14  | B     | 832  | CLA  | CMB-C2B-C1B | -3.26 | 123.45      | 128.46   |
| 14  | 2     | 833  | CLA  | CMB-C2B-C1B | -3.26 | 123.45      | 128.46   |
| 14  | b     | 842  | CLA  | C1-C2-C3    | -3.26 | 120.40      | 126.04   |
| 14  | 1     | 1643 | CLA  | O2D-CGD-O1D | -3.26 | 117.46      | 123.84   |
| 14  | A     | 842  | CLA  | O2D-CGD-O1D | -3.26 | 117.46      | 123.84   |
| 14  | b     | 838  | CLA  | O2D-CGD-O1D | -3.26 | 117.46      | 123.84   |
| 14  | a     | 843  | CLA  | CMB-C2B-C1B | -3.26 | 123.45      | 128.46   |
| 14  | B     | 814  | CLA  | CMB-C2B-C3B | 3.26  | 130.78      | 124.68   |
| 14  | A     | 829  | CLA  | O2D-CGD-O1D | -3.26 | 117.47      | 123.84   |
| 14  | z     | 102  | CLA  | CMB-C2B-C3B | 3.26  | 130.77      | 124.68   |
| 14  | A     | 843  | CLA  | CMB-C2B-C1B | -3.26 | 123.46      | 128.46   |
| 14  | 1     | 1643 | CLA  | C4-C3-C5    | 3.26  | 120.75      | 115.27   |
| 14  | a     | 841  | CLA  | CMB-C2B-C3B | 3.26  | 130.77      | 124.68   |
| 14  | B     | 820  | CLA  | CMB-C2B-C1B | -3.26 | 123.46      | 128.46   |
| 14  | 1     | 1630 | CLA  | O2D-CGD-O1D | -3.25 | 117.47      | 123.84   |
| 14  | b     | 810  | CLA  | CMB-C2B-C3B | 3.25  | 130.77      | 124.68   |
| 14  | b     | 842  | CLA  | O2D-CGD-O1D | -3.25 | 117.48      | 123.84   |
| 14  | A     | 842  | CLA  | C4-C3-C5    | 3.25  | 120.74      | 115.27   |
| 14  | A     | 841  | CLA  | CMB-C2B-C3B | 3.25  | 130.75      | 124.68   |
| 14  | 2     | 834  | CLA  | CMB-C2B-C3B | 3.24  | 130.75      | 124.68   |
| 14  | b     | 813  | CLA  | O2D-CGD-O1D | -3.24 | 117.50      | 123.84   |
| 14  | 1     | 1632 | CLA  | O2D-CGD-O1D | -3.24 | 117.50      | 123.84   |
| 14  | a     | 842  | CLA  | O2D-CGD-O1D | -3.24 | 117.51      | 123.84   |
| 14  | B     | 833  | CLA  | CMB-C2B-C3B | 3.24  | 130.73      | 124.68   |
| 14  | a     | 831  | CLA  | O2D-CGD-O1D | -3.23 | 117.51      | 123.84   |
| 17  | J     | 103  | BCR  | C2-C1-C6    | 3.23  | 115.46      | 110.48   |
| 14  | x     | 1701 | CLA  | CMB-C2B-C3B | 3.23  | 130.72      | 124.68   |
| 14  | 1     | 1644 | CLA  | CMB-C2B-C1B | -3.23 | 123.50      | 128.46   |
| 14  | 2     | 810  | CLA  | CMB-C2B-C3B | 3.23  | 130.72      | 124.68   |
| 14  | b     | 838  | CLA  | CMB-C2B-C1B | -3.23 | 123.50      | 128.46   |
| 14  | B     | 816  | CLA  | CMB-C2B-C3B | 3.23  | 130.72      | 124.68   |
| 14  | B     | 808  | CLA  | O2D-CGD-O1D | -3.23 | 117.53      | 123.84   |
| 17  | 8     | 1304 | BCR  | C2-C1-C6    | 3.22  | 115.44      | 110.48   |
| 14  | 1     | 1618 | CLA  | CMB-C2B-C1B | -3.22 | 123.51      | 128.46   |
| 14  | b     | 836  | CLA  | CMB-C2B-C1B | -3.22 | 123.51      | 128.46   |
| 14  | a     | 828  | CLA  | CMB-C2B-C3B | 3.22  | 130.71      | 124.68   |
| 14  | A     | 828  | CLA  | CMB-C2B-C3B | 3.22  | 130.71      | 124.68   |
| 14  | b     | 817  | CLA  | CMB-C2B-C3B | 3.22  | 130.70      | 124.68   |
| 14  | a     | 842  | CLA  | C4-C3-C5    | 3.22  | 120.69      | 115.27   |
| 14  | A     | 831  | CLA  | O2D-CGD-O1D | -3.22 | 117.55      | 123.84   |
| 14  | B     | 835  | CLA  | CMB-C2B-C1B | -3.21 | 123.53      | 128.46   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | 2     | 838  | CLA  | CMB-C2B-C1B | -3.21 | 123.53      | 128.46   |
| 14  | B     | 837  | CLA  | CMB-C2B-C1B | -3.21 | 123.53      | 128.46   |
| 14  | b     | 833  | CLA  | O2D-CGD-O1D | -3.21 | 117.56      | 123.84   |
| 14  | A     | 817  | CLA  | CMB-C2B-C1B | -3.21 | 123.53      | 128.46   |
| 14  | b     | 809  | CLA  | O2D-CGD-O1D | -3.21 | 117.56      | 123.84   |
| 14  | 2     | 817  | CLA  | CMB-C2B-C3B | 3.21  | 130.68      | 124.68   |
| 14  | 2     | 836  | CLA  | CMB-C2B-C1B | -3.21 | 123.53      | 128.46   |
| 14  | 2     | 809  | CLA  | O2D-CGD-O1D | -3.21 | 117.57      | 123.84   |
| 17  | A     | 848  | BCR  | C37-C22-C21 | -3.21 | 118.43      | 122.92   |
| 14  | 2     | 833  | CLA  | O2D-CGD-O1D | -3.21 | 117.57      | 123.84   |
| 17  | a     | 848  | BCR  | C37-C22-C21 | -3.21 | 118.43      | 122.92   |
| 14  | b     | 834  | CLA  | CMB-C2B-C3B | 3.20  | 130.67      | 124.68   |
| 17  | j     | 1304 | BCR  | C2-C1-C6    | 3.20  | 115.41      | 110.48   |
| 14  | a     | 808  | CLA  | CMB-C2B-C1B | -3.20 | 123.55      | 128.46   |
| 14  | 1     | 1607 | CLA  | C4-C3-C5    | 3.20  | 120.65      | 115.27   |
| 14  | a     | 817  | CLA  | CMB-C2B-C1B | -3.20 | 123.55      | 128.46   |
| 14  | 1     | 1629 | CLA  | CMB-C2B-C3B | 3.20  | 130.66      | 124.68   |
| 14  | B     | 832  | CLA  | O2D-CGD-O1D | -3.20 | 117.59      | 123.84   |
| 14  | 1     | 1621 | CLA  | O2D-CGD-O1D | -3.19 | 117.59      | 123.84   |
| 14  | A     | 820  | CLA  | O2D-CGD-O1D | -3.19 | 117.60      | 123.84   |
| 14  | B     | 809  | CLA  | CHB-C4A-NA  | 3.19  | 128.93      | 124.51   |
| 14  | a     | 820  | CLA  | O2D-CGD-O1D | -3.19 | 117.60      | 123.84   |
| 17  | 1     | 1649 | BCR  | C37-C22-C21 | -3.19 | 118.46      | 122.92   |
| 14  | A     | 806  | CLA  | C4-C3-C5    | 3.18  | 120.62      | 115.27   |
| 14  | 1     | 1609 | CLA  | CMB-C2B-C1B | -3.18 | 123.58      | 128.46   |
| 14  | 2     | 819  | CLA  | O2D-CGD-O1D | -3.18 | 117.63      | 123.84   |
| 14  | a     | 806  | CLA  | C4-C3-C5    | 3.17  | 120.60      | 115.27   |
| 14  | B     | 818  | CLA  | O2D-CGD-O1D | -3.17 | 117.64      | 123.84   |
| 14  | b     | 810  | CLA  | CHB-C4A-NA  | 3.17  | 128.89      | 124.51   |
| 14  | 2     | 810  | CLA  | CHB-C4A-NA  | 3.17  | 128.89      | 124.51   |
| 14  | A     | 805  | CLA  | O2D-CGD-O1D | -3.16 | 117.66      | 123.84   |
| 14  | 1     | 1606 | CLA  | O2D-CGD-O1D | -3.16 | 117.67      | 123.84   |
| 14  | a     | 835  | CLA  | O2D-CGD-O1D | -3.16 | 117.67      | 123.84   |
| 14  | a     | 805  | CLA  | O2D-CGD-O1D | -3.15 | 117.68      | 123.84   |
| 14  | b     | 819  | CLA  | O2D-CGD-O1D | -3.15 | 117.69      | 123.84   |
| 14  | A     | 808  | CLA  | CMB-C2B-C1B | -3.15 | 123.63      | 128.46   |
| 14  | 1     | 1636 | CLA  | O2D-CGD-O1D | -3.14 | 117.69      | 123.84   |
| 14  | 1     | 1616 | CLA  | CMB-C2B-C3B | 3.14  | 130.55      | 124.68   |
| 14  | 1     | 1610 | CLA  | O2D-CGD-O1D | -3.14 | 117.70      | 123.84   |
| 14  | b     | 806  | CLA  | O2D-CGD-O1D | -3.14 | 117.71      | 123.84   |
| 14  | A     | 815  | CLA  | CMB-C2B-C3B | 3.14  | 130.54      | 124.68   |
| 14  | A     | 804  | CLA  | O2D-CGD-O1D | -3.13 | 117.71      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | 1     | 1643 | CLA  | CMB-C2B-C3B | 3.13  | 130.53      | 124.68   |
| 14  | b     | 816  | CLA  | CMB-C2B-C3B | 3.13  | 130.53      | 124.68   |
| 14  | b     | 817  | CLA  | O2D-CGD-O1D | -3.13 | 117.72      | 123.84   |
| 14  | 2     | 816  | CLA  | CMB-C2B-C3B | 3.13  | 130.53      | 124.68   |
| 14  | a     | 809  | CLA  | O2D-CGD-O1D | -3.13 | 117.72      | 123.84   |
| 14  | a     | 815  | CLA  | CMB-C2B-C3B | 3.13  | 130.53      | 124.68   |
| 14  | A     | 835  | CLA  | O2D-CGD-O1D | -3.13 | 117.73      | 123.84   |
| 14  | a     | 842  | CLA  | CMB-C2B-C3B | 3.12  | 130.52      | 124.68   |
| 14  | B     | 805  | CLA  | O2D-CGD-O1D | -3.12 | 117.74      | 123.84   |
| 14  | b     | 835  | CLA  | O2D-CGD-O1D | -3.12 | 117.74      | 123.84   |
| 14  | 2     | 817  | CLA  | O2D-CGD-O1D | -3.11 | 117.75      | 123.84   |
| 14  | B     | 816  | CLA  | O2D-CGD-O1D | -3.11 | 117.76      | 123.84   |
| 14  | 2     | 806  | CLA  | O2D-CGD-O1D | -3.11 | 117.76      | 123.84   |
| 14  | 2     | 835  | CLA  | O2D-CGD-O1D | -3.11 | 117.76      | 123.84   |
| 14  | A     | 842  | CLA  | CMB-C2B-C3B | 3.11  | 130.50      | 124.68   |
| 14  | A     | 809  | CLA  | O2D-CGD-O1D | -3.11 | 117.76      | 123.84   |
| 14  | 1     | 1605 | CLA  | O2D-CGD-O1D | -3.11 | 117.76      | 123.84   |
| 14  | a     | 804  | CLA  | O2D-CGD-O1D | -3.11 | 117.76      | 123.84   |
| 14  | l     | 205  | CLA  | CMB-C2B-C3B | 3.11  | 130.49      | 124.68   |
| 14  | B     | 834  | CLA  | O2D-CGD-O1D | -3.11 | 117.76      | 123.84   |
| 14  | B     | 815  | CLA  | CMB-C2B-C3B | 3.11  | 130.49      | 124.68   |
| 14  | 2     | 826  | CLA  | O2D-CGD-CBD | 3.10  | 116.78      | 111.27   |
| 14  | b     | 826  | CLA  | O2D-CGD-CBD | 3.10  | 116.78      | 111.27   |
| 14  | 0     | 206  | CLA  | CMB-C2B-C3B | 3.10  | 130.48      | 124.68   |
| 14  | B     | 825  | CLA  | O2D-CGD-CBD | 3.10  | 116.77      | 111.27   |
| 14  | L     | 204  | CLA  | CMB-C2B-C3B | 3.10  | 130.47      | 124.68   |
| 14  | a     | 809  | CLA  | CHB-C4A-NA  | 3.10  | 128.79      | 124.51   |
| 14  | 8     | 1302 | CLA  | CMB-C2B-C1B | -3.09 | 123.71      | 128.46   |
| 14  | b     | 831  | CLA  | O2D-CGD-O1D | -3.09 | 117.79      | 123.84   |
| 14  | J     | 101  | CLA  | CMB-C2B-C1B | -3.09 | 123.71      | 128.46   |
| 14  | 2     | 831  | CLA  | O2D-CGD-O1D | -3.09 | 117.79      | 123.84   |
| 14  | 2     | 840  | CLA  | CMB-C2B-C1B | -3.09 | 123.71      | 128.46   |
| 14  | A     | 805  | CLA  | CHB-C4A-NA  | 3.09  | 128.79      | 124.51   |
| 14  | a     | 836  | CLA  | CMB-C2B-C1B | -3.09 | 123.72      | 128.46   |
| 14  | a     | 805  | CLA  | CHB-C4A-NA  | 3.09  | 128.78      | 124.51   |
| 14  | j     | 1302 | CLA  | CMB-C2B-C1B | -3.09 | 123.72      | 128.46   |
| 14  | B     | 839  | CLA  | CMB-C2B-C1B | -3.08 | 123.72      | 128.46   |
| 14  | A     | 809  | CLA  | CHB-C4A-NA  | 3.08  | 128.77      | 124.51   |
| 14  | A     | 836  | CLA  | CMB-C2B-C1B | -3.08 | 123.73      | 128.46   |
| 14  | 1     | 1610 | CLA  | CHB-C4A-NA  | 3.08  | 128.77      | 124.51   |
| 14  | b     | 840  | CLA  | CMB-C2B-C1B | -3.07 | 123.74      | 128.46   |
| 14  | B     | 830  | CLA  | O2D-CGD-O1D | -3.07 | 117.83      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 823  | CLA  | O2D-CGD-O1D | -3.07 | 117.84      | 123.84   |
| 14  | b     | 839  | CLA  | CMB-C2B-C3B | 3.07  | 130.42      | 124.68   |
| 14  | b     | 840  | CLA  | O2D-CGD-O1D | -3.06 | 117.85      | 123.84   |
| 14  | B     | 839  | CLA  | O2D-CGD-O1D | -3.06 | 117.86      | 123.84   |
| 14  | 1     | 1637 | CLA  | CMB-C2B-C1B | -3.06 | 123.76      | 128.46   |
| 14  | 1     | 1640 | CLA  | CMB-C2B-C3B | 3.06  | 130.40      | 124.68   |
| 14  | 2     | 840  | CLA  | O2D-CGD-O1D | -3.05 | 117.87      | 123.84   |
| 14  | A     | 844  | CLA  | O2D-CGD-O1D | -3.05 | 117.87      | 123.84   |
| 14  | 2     | 839  | CLA  | CMB-C2B-C3B | 3.05  | 130.39      | 124.68   |
| 17  | B     | 847  | BCR  | C37-C22-C21 | -3.05 | 118.65      | 122.92   |
| 14  | 1     | 1645 | CLA  | O2D-CGD-O1D | -3.05 | 117.88      | 123.84   |
| 14  | A     | 839  | CLA  | CMB-C2B-C3B | 3.05  | 130.38      | 124.68   |
| 14  | 0     | 205  | CLA  | O2D-CGD-O1D | -3.04 | 117.89      | 123.84   |
| 17  | b     | 848  | BCR  | C37-C22-C21 | -3.04 | 118.66      | 122.92   |
| 17  | 2     | 848  | BCR  | C37-C22-C21 | -3.04 | 118.67      | 122.92   |
| 14  | 2     | 824  | CLA  | O2D-CGD-O1D | -3.04 | 117.89      | 123.84   |
| 14  | 1     | 1606 | CLA  | CHB-C4A-NA  | 3.04  | 128.71      | 124.51   |
| 14  | 1     | 1635 | CLA  | CHB-C4A-NA  | 3.04  | 128.71      | 124.51   |
| 14  | A     | 824  | CLA  | O2D-CGD-O1D | -3.04 | 117.90      | 123.84   |
| 17  | A     | 851  | BCR  | C24-C23-C22 | -3.04 | 121.65      | 126.23   |
| 14  | a     | 834  | CLA  | CHB-C4A-NA  | 3.03  | 128.70      | 124.51   |
| 14  | b     | 811  | CLA  | CHB-C4A-NA  | 3.03  | 128.70      | 124.51   |
| 14  | a     | 814  | CLA  | CMB-C2B-C1B | -3.03 | 123.81      | 128.46   |
| 14  | 1     | 1625 | CLA  | O2D-CGD-O1D | -3.03 | 117.92      | 123.84   |
| 14  | 2     | 822  | CLA  | O2D-CGD-O1D | -3.03 | 117.92      | 123.84   |
| 14  | 1     | 1614 | CLA  | CMB-C2B-C3B | 3.03  | 130.34      | 124.68   |
| 14  | l     | 204  | CLA  | O2D-CGD-O1D | -3.03 | 117.92      | 123.84   |
| 14  | B     | 810  | CLA  | CMB-C2B-C3B | 3.03  | 130.34      | 124.68   |
| 14  | a     | 844  | CLA  | O2D-CGD-O1D | -3.03 | 117.92      | 123.84   |
| 14  | b     | 805  | CLA  | CMB-C2B-C3B | 3.03  | 130.34      | 124.68   |
| 14  | B     | 810  | CLA  | CHB-C4A-NA  | 3.03  | 128.70      | 124.51   |
| 14  | 2     | 805  | CLA  | CMB-C2B-C3B | 3.02  | 130.34      | 124.68   |
| 14  | a     | 824  | CLA  | O2D-CGD-O1D | -3.02 | 117.92      | 123.84   |
| 14  | a     | 839  | CLA  | CMB-C2B-C3B | 3.02  | 130.34      | 124.68   |
| 17  | 1     | 1652 | BCR  | C24-C23-C22 | -3.02 | 121.67      | 126.23   |
| 14  | b     | 824  | CLA  | O2D-CGD-O1D | -3.02 | 117.93      | 123.84   |
| 17  | f     | 204  | BCR  | C2-C1-C6    | 3.02  | 115.13      | 110.48   |
| 14  | 1     | 1625 | CLA  | CMB-C2B-C1B | -3.02 | 123.82      | 128.46   |
| 14  | A     | 813  | CLA  | CMB-C2B-C3B | 3.02  | 130.32      | 124.68   |
| 14  | b     | 808  | CLA  | CMB-C2B-C1B | -3.02 | 123.83      | 128.46   |
| 14  | b     | 811  | CLA  | CMB-C2B-C3B | 3.02  | 130.32      | 124.68   |
| 14  | B     | 804  | CLA  | CMB-C2B-C3B | 3.01  | 130.32      | 124.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 814  | CLA  | CMB-C2B-C1B | -3.01 | 123.83      | 128.46   |
| 14  | 1     | 1615 | CLA  | CMB-C2B-C1B | -3.01 | 123.83      | 128.46   |
| 14  | L     | 203  | CLA  | O2D-CGD-O1D | -3.01 | 117.95      | 123.84   |
| 14  | 2     | 811  | CLA  | CHB-C4A-NA  | 3.01  | 128.67      | 124.51   |
| 14  | b     | 826  | CLA  | CMB-C2B-C3B | 3.01  | 130.30      | 124.68   |
| 14  | 2     | 826  | CLA  | CMB-C2B-C3B | 3.00  | 130.30      | 124.68   |
| 14  | A     | 834  | CLA  | CHB-C4A-NA  | 3.00  | 128.66      | 124.51   |
| 14  | a     | 824  | CLA  | CMB-C2B-C1B | -3.00 | 123.85      | 128.46   |
| 14  | A     | 828  | CLA  | O2D-CGD-O1D | -3.00 | 117.97      | 123.84   |
| 14  | A     | 824  | CLA  | CMB-C2B-C1B | -3.00 | 123.85      | 128.46   |
| 14  | 1     | 1628 | CLA  | O2D-CGD-O1D | -3.00 | 117.97      | 123.84   |
| 17  | 1     | 1651 | BCR  | C15-C16-C17 | -3.00 | 117.33      | 123.47   |
| 14  | A     | 827  | CLA  | O2D-CGD-O1D | -3.00 | 117.97      | 123.84   |
| 14  | a     | 827  | CLA  | O2D-CGD-O1D | -3.00 | 117.97      | 123.84   |
| 14  | B     | 838  | CLA  | CMB-C2B-C3B | 3.00  | 130.29      | 124.68   |
| 14  | a     | 813  | CLA  | CMB-C2B-C3B | 3.00  | 130.29      | 124.68   |
| 17  | a     | 850  | BCR  | C15-C16-C17 | -3.00 | 117.33      | 123.47   |
| 14  | b     | 822  | CLA  | O2D-CGD-O1D | -3.00 | 117.98      | 123.84   |
| 14  | B     | 825  | CLA  | CMB-C2B-C3B | 3.00  | 130.28      | 124.68   |
| 17  | a     | 851  | BCR  | C24-C23-C22 | -2.99 | 121.71      | 126.23   |
| 14  | B     | 821  | CLA  | O2D-CGD-O1D | -2.99 | 117.99      | 123.84   |
| 14  | a     | 843  | CLA  | O2D-CGD-O1D | -2.99 | 117.99      | 123.84   |
| 14  | 2     | 811  | CLA  | CMB-C2B-C3B | 2.99  | 130.27      | 124.68   |
| 14  | f     | 203  | CLA  | O2D-CGD-O1D | -2.99 | 118.00      | 123.84   |
| 14  | B     | 822  | CLA  | O2D-CGD-O1D | -2.98 | 118.00      | 123.84   |
| 14  | b     | 823  | CLA  | O2D-CGD-O1D | -2.98 | 118.00      | 123.84   |
| 14  | 2     | 808  | CLA  | CMB-C2B-C1B | -2.98 | 123.88      | 128.46   |
| 14  | 1     | 1636 | CLA  | CHB-C4A-NA  | 2.98  | 128.64      | 124.51   |
| 17  | A     | 850  | BCR  | C15-C16-C17 | -2.98 | 117.36      | 123.47   |
| 14  | a     | 828  | CLA  | O2D-CGD-O1D | -2.98 | 118.01      | 123.84   |
| 17  | F     | 205  | BCR  | C2-C1-C6    | 2.98  | 115.07      | 110.48   |
| 14  | 2     | 819  | CLA  | C4-C3-C5    | 2.98  | 120.28      | 115.27   |
| 14  | L     | 204  | CLA  | O2D-CGD-CBD | 2.98  | 116.56      | 111.27   |
| 14  | 1     | 1629 | CLA  | O2D-CGD-O1D | -2.98 | 118.02      | 123.84   |
| 14  | b     | 819  | CLA  | C4-C3-C5    | 2.97  | 120.27      | 115.27   |
| 17  | 6     | 204  | BCR  | C2-C1-C6    | 2.97  | 115.06      | 110.48   |
| 14  | A     | 843  | CLA  | O2D-CGD-O1D | -2.97 | 118.02      | 123.84   |
| 14  | A     | 830  | CLA  | CHB-C4A-NA  | 2.97  | 128.62      | 124.51   |
| 14  | b     | 839  | CLA  | O2D-CGD-O1D | -2.97 | 118.03      | 123.84   |
| 14  | F     | 204  | CLA  | O2D-CGD-O1D | -2.97 | 118.03      | 123.84   |
| 14  | 2     | 823  | CLA  | O2D-CGD-O1D | -2.97 | 118.03      | 123.84   |
| 14  | 1     | 1641 | CLA  | CMB-C2B-C1B | -2.97 | 123.90      | 128.46   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 840  | CLA  | CMB-C2B-C1B | -2.97 | 123.90      | 128.46   |
| 14  | A     | 806  | CLA  | O2D-CGD-O1D | -2.97 | 118.03      | 123.84   |
| 14  | 2     | 804  | CLA  | CMB-C2B-C3B | 2.97  | 130.23      | 124.68   |
| 14  | a     | 806  | CLA  | CHB-C4A-NA  | 2.97  | 128.61      | 124.51   |
| 14  | B     | 838  | CLA  | O2D-CGD-O1D | -2.97 | 118.04      | 123.84   |
| 14  | a     | 835  | CLA  | CHB-C4A-NA  | 2.96  | 128.61      | 124.51   |
| 14  | 0     | 206  | CLA  | O2D-CGD-CBD | 2.96  | 116.54      | 111.27   |
| 14  | A     | 819  | CLA  | O2D-CGD-O1D | -2.96 | 118.04      | 123.84   |
| 14  | a     | 806  | CLA  | O2D-CGD-O1D | -2.96 | 118.04      | 123.84   |
| 14  | B     | 818  | CLA  | C4-C3-C5    | 2.96  | 120.26      | 115.27   |
| 14  | B     | 807  | CLA  | CMB-C2B-C1B | -2.96 | 123.91      | 128.46   |
| 14  | b     | 821  | CLA  | O2D-CGD-O1D | -2.96 | 118.05      | 123.84   |
| 14  | 6     | 203  | CLA  | O2D-CGD-O1D | -2.96 | 118.05      | 123.84   |
| 14  | 2     | 832  | CLA  | O2D-CGD-O1D | -2.96 | 118.05      | 123.84   |
| 14  | 2     | 821  | CLA  | O2D-CGD-O1D | -2.96 | 118.06      | 123.84   |
| 14  | A     | 835  | CLA  | CHB-C4A-NA  | 2.95  | 128.60      | 124.51   |
| 14  | a     | 830  | CLA  | CHB-C4A-NA  | 2.95  | 128.60      | 124.51   |
| 17  | a     | 852  | BCR  | C15-C16-C17 | -2.95 | 117.42      | 123.47   |
| 14  | 1     | 1634 | CLA  | O2D-CGD-O1D | -2.95 | 118.06      | 123.84   |
| 14  | 1     | 1644 | CLA  | O2D-CGD-O1D | -2.95 | 118.06      | 123.84   |
| 17  | K     | 102  | BCR  | C7-C8-C9    | -2.95 | 121.77      | 126.23   |
| 14  | B     | 803  | CLA  | CMB-C2B-C3B | 2.95  | 130.20      | 124.68   |
| 14  | b     | 804  | CLA  | CMB-C2B-C3B | 2.95  | 130.20      | 124.68   |
| 14  | b     | 832  | CLA  | O2D-CGD-O1D | -2.95 | 118.07      | 123.84   |
| 14  | b     | 813  | CLA  | CMB-C2B-C3B | 2.95  | 130.19      | 124.68   |
| 14  | 2     | 841  | CLA  | CMB-C2B-C3B | 2.95  | 130.19      | 124.68   |
| 14  | 2     | 820  | CLA  | O2D-CGD-O1D | -2.95 | 118.07      | 123.84   |
| 14  | A     | 840  | CLA  | CMB-C2B-C1B | -2.95 | 123.93      | 128.46   |
| 14  | b     | 820  | CLA  | O2D-CGD-O1D | -2.95 | 118.08      | 123.84   |
| 14  | 1     | 1631 | CLA  | CHB-C4A-NA  | 2.95  | 128.59      | 124.51   |
| 14  | B     | 820  | CLA  | O2D-CGD-O1D | -2.94 | 118.09      | 123.84   |
| 14  | B     | 831  | CLA  | O2D-CGD-O1D | -2.94 | 118.09      | 123.84   |
| 14  | a     | 819  | CLA  | O2D-CGD-O1D | -2.94 | 118.09      | 123.84   |
| 17  | 1     | 1653 | BCR  | C15-C16-C17 | -2.94 | 117.45      | 123.47   |
| 14  | 1     | 1607 | CLA  | CHB-C4A-NA  | 2.94  | 128.58      | 124.51   |
| 14  | A     | 833  | CLA  | O2D-CGD-O1D | -2.94 | 118.09      | 123.84   |
| 17  | A     | 852  | BCR  | C15-C16-C17 | -2.94 | 117.46      | 123.47   |
| 14  | 0     | 205  | CLA  | CMB-C2B-C3B | 2.94  | 130.17      | 124.68   |
| 14  | l     | 205  | CLA  | O2D-CGD-CBD | 2.94  | 116.48      | 111.27   |
| 14  | 1     | 1620 | CLA  | O2D-CGD-O1D | -2.93 | 118.10      | 123.84   |
| 17  | k     | 102  | BCR  | C7-C8-C9    | -2.93 | 121.80      | 126.23   |
| 14  | 2     | 839  | CLA  | O2D-CGD-O1D | -2.93 | 118.10      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | 1     | 1607 | CLA  | O2D-CGD-O1D | -2.93 | 118.11      | 123.84   |
| 14  | 2     | 813  | CLA  | CMB-C2B-C3B | 2.93  | 130.16      | 124.68   |
| 13  | a     | 801  | CL0  | CMB-C2B-C1B | -2.93 | 123.96      | 128.46   |
| 17  | 9     | 102  | BCR  | C7-C8-C9    | -2.93 | 121.81      | 126.23   |
| 17  | L     | 207  | BCR  | C36-C18-C17 | -2.93 | 118.82      | 122.92   |
| 14  | l     | 204  | CLA  | CMB-C2B-C3B | 2.93  | 130.16      | 124.68   |
| 14  | B     | 819  | CLA  | O2D-CGD-O1D | -2.93 | 118.11      | 123.84   |
| 14  | L     | 203  | CLA  | CMB-C2B-C3B | 2.93  | 130.16      | 124.68   |
| 14  | A     | 812  | CLA  | CMB-C2B-C3B | 2.93  | 130.15      | 124.68   |
| 17  | L     | 201  | BCR  | C15-C16-C17 | -2.93 | 117.48      | 123.47   |
| 14  | A     | 806  | CLA  | CHB-C4A-NA  | 2.93  | 128.56      | 124.51   |
| 14  | B     | 828  | CLA  | O2D-CGD-O1D | -2.92 | 118.12      | 123.84   |
| 14  | b     | 829  | CLA  | O2D-CGD-O1D | -2.92 | 118.12      | 123.84   |
| 17  | 0     | 209  | BCR  | C36-C18-C17 | -2.92 | 118.83      | 122.92   |
| 14  | b     | 841  | CLA  | CMB-C2B-C3B | 2.92  | 130.14      | 124.68   |
| 14  | B     | 840  | CLA  | O2D-CGD-O1D | -2.92 | 118.13      | 123.84   |
| 13  | A     | 801  | CL0  | CMB-C2B-C1B | -2.92 | 123.98      | 128.46   |
| 14  | B     | 812  | CLA  | CMB-C2B-C3B | 2.92  | 130.14      | 124.68   |
| 17  | l     | 202  | BCR  | C15-C16-C17 | -2.91 | 117.50      | 123.47   |
| 14  | a     | 812  | CLA  | CMB-C2B-C3B | 2.91  | 130.12      | 124.68   |
| 14  | 1     | 1613 | CLA  | CMB-C2B-C3B | 2.91  | 130.12      | 124.68   |
| 14  | L     | 203  | CLA  | CHB-C4A-NA  | 2.91  | 128.53      | 124.51   |
| 14  | 2     | 841  | CLA  | O2D-CGD-O1D | -2.91 | 118.16      | 123.84   |
| 14  | a     | 833  | CLA  | O2D-CGD-O1D | -2.91 | 118.16      | 123.84   |
| 17  | 0     | 203  | BCR  | C15-C16-C17 | -2.90 | 117.53      | 123.47   |
| 14  | 2     | 826  | CLA  | CAA-C2A-C1A | -2.90 | 102.46      | 111.97   |
| 14  | b     | 830  | CLA  | CMB-C2B-C3B | 2.90  | 130.11      | 124.68   |
| 14  | B     | 824  | CLA  | O2D-CGD-O1D | -2.90 | 118.17      | 123.84   |
| 14  | B     | 840  | CLA  | CMB-C2B-C3B | 2.90  | 130.10      | 124.68   |
| 13  | 1     | 1602 | CL0  | CMB-C2B-C1B | -2.90 | 124.01      | 128.46   |
| 14  | 2     | 816  | CLA  | O2D-CGD-O1D | -2.90 | 118.17      | 123.84   |
| 14  | 2     | 837  | CLA  | O2D-CGD-O1D | -2.90 | 118.17      | 123.84   |
| 14  | B     | 827  | CLA  | O2D-CGD-O1D | -2.89 | 118.18      | 123.84   |
| 18  | y     | 101  | LHG  | O8-C23-C24  | 2.89  | 120.98      | 111.91   |
| 14  | b     | 841  | CLA  | O2D-CGD-O1D | -2.89 | 118.18      | 123.84   |
| 14  | b     | 826  | CLA  | CAA-C2A-C1A | -2.89 | 102.50      | 111.97   |
| 14  | k     | 103  | CLA  | O2D-CGD-O1D | -2.89 | 118.19      | 123.84   |
| 14  | 9     | 103  | CLA  | O2D-CGD-O1D | -2.89 | 118.19      | 123.84   |
| 14  | 2     | 828  | CLA  | O2D-CGD-O1D | -2.89 | 118.19      | 123.84   |
| 14  | 2     | 834  | CLA  | C4-C3-C5    | 2.89  | 120.13      | 115.27   |
| 14  | b     | 834  | CLA  | C4-C3-C5    | 2.89  | 120.13      | 115.27   |
| 17  | 0     | 201  | BCR  | C36-C18-C17 | -2.89 | 118.88      | 122.92   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | 2     | 829  | CLA  | O2D-CGD-O1D | -2.89 | 118.19      | 123.84   |
| 14  | B     | 836  | CLA  | O2D-CGD-O1D | -2.88 | 118.20      | 123.84   |
| 14  | b     | 837  | CLA  | O2D-CGD-O1D | -2.88 | 118.20      | 123.84   |
| 14  | B     | 829  | CLA  | CMB-C2B-C3B | 2.88  | 130.07      | 124.68   |
| 14  | 2     | 815  | CLA  | O2D-CGD-O1D | -2.88 | 118.20      | 123.84   |
| 14  | B     | 825  | CLA  | CAA-C2A-C1A | -2.88 | 102.53      | 111.97   |
| 18  | M     | 101  | LHG  | O8-C23-C24  | 2.88  | 120.95      | 111.91   |
| 14  | b     | 818  | CLA  | CHB-C4A-NA  | 2.88  | 128.49      | 124.51   |
| 14  | B     | 802  | CLA  | CMB-C2B-C3B | 2.88  | 130.06      | 124.68   |
| 14  | 2     | 830  | CLA  | CMB-C2B-C3B | 2.88  | 130.06      | 124.68   |
| 14  | a     | 818  | CLA  | CHB-C4A-NA  | 2.88  | 128.49      | 124.51   |
| 14  | b     | 816  | CLA  | O2D-CGD-O1D | -2.88 | 118.21      | 123.84   |
| 14  | K     | 103  | CLA  | O2D-CGD-O1D | -2.88 | 118.21      | 123.84   |
| 14  | 1     | 1619 | CLA  | CHB-C4A-NA  | 2.88  | 128.49      | 124.51   |
| 14  | B     | 815  | CLA  | O2D-CGD-O1D | -2.88 | 118.21      | 123.84   |
| 14  | A     | 825  | CLA  | C1-C2-C3    | -2.87 | 121.07      | 126.04   |
| 14  | b     | 828  | CLA  | O2D-CGD-O1D | -2.87 | 118.22      | 123.84   |
| 14  | l     | 204  | CLA  | CHB-C4A-NA  | 2.87  | 128.48      | 124.51   |
| 14  | B     | 833  | CLA  | C4-C3-C5    | 2.87  | 120.10      | 115.27   |
| 14  | 2     | 803  | CLA  | CMB-C2B-C3B | 2.87  | 130.05      | 124.68   |
| 14  | b     | 803  | CLA  | CMB-C2B-C3B | 2.87  | 130.04      | 124.68   |
| 14  | B     | 817  | CLA  | CHB-C4A-NA  | 2.87  | 128.48      | 124.51   |
| 14  | b     | 825  | CLA  | O2D-CGD-O1D | -2.87 | 118.23      | 123.84   |
| 18  | m     | 101  | LHG  | O8-C23-C24  | 2.87  | 120.90      | 111.91   |
| 17  | B     | 845  | BCR  | C24-C23-C22 | -2.86 | 121.91      | 126.23   |
| 14  | 2     | 825  | CLA  | O2D-CGD-O1D | -2.86 | 118.24      | 123.84   |
| 14  | b     | 842  | CLA  | CHB-C4A-NA  | 2.86  | 128.47      | 124.51   |
| 17  | b     | 846  | BCR  | C24-C23-C22 | -2.86 | 121.92      | 126.23   |
| 14  | a     | 825  | CLA  | C1-C2-C3    | -2.86 | 121.10      | 126.04   |
| 14  | B     | 835  | CLA  | C1-C2-C3    | -2.86 | 122.13      | 126.75   |
| 17  | 2     | 844  | BCR  | C24-C23-C22 | -2.85 | 121.92      | 126.23   |
| 14  | 2     | 842  | CLA  | CHB-C4A-NA  | 2.85  | 128.46      | 124.51   |
| 17  | 2     | 846  | BCR  | C24-C23-C22 | -2.85 | 121.92      | 126.23   |
| 14  | 2     | 818  | CLA  | CHB-C4A-NA  | 2.85  | 128.46      | 124.51   |
| 14  | 1     | 1604 | CLA  | O2D-CGD-O1D | -2.85 | 118.26      | 123.84   |
| 14  | b     | 815  | CLA  | O2D-CGD-O1D | -2.85 | 118.27      | 123.84   |
| 14  | 1     | 1623 | CLA  | O2D-CGD-O1D | -2.85 | 118.27      | 123.84   |
| 14  | B     | 814  | CLA  | O2D-CGD-O1D | -2.85 | 118.27      | 123.84   |
| 17  | b     | 844  | BCR  | C24-C23-C22 | -2.85 | 121.93      | 126.23   |
| 14  | a     | 826  | CLA  | O2D-CGD-O1D | -2.85 | 118.28      | 123.84   |
| 13  | 1     | 1602 | CL0  | CHB-C4A-NA  | 2.84  | 128.45      | 124.51   |
| 17  | B     | 843  | BCR  | C24-C23-C22 | -2.84 | 121.94      | 126.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | b     | 827  | CLA  | O2D-CGD-O1D | -2.84 | 118.28      | 123.84   |
| 14  | J     | 101  | CLA  | O2D-CGD-O1D | -2.84 | 118.28      | 123.84   |
| 17  | B     | 847  | BCR  | C27-C26-C25 | 2.84  | 126.85      | 122.73   |
| 14  | 1     | 1626 | CLA  | C1-C2-C3    | -2.84 | 121.13      | 126.04   |
| 17  | A     | 847  | BCR  | C15-C16-C17 | -2.84 | 117.66      | 123.47   |
| 14  | 1     | 1627 | CLA  | O2D-CGD-O1D | -2.84 | 118.29      | 123.84   |
| 14  | A     | 802  | CLA  | O2D-CGD-O1D | -2.83 | 118.30      | 123.84   |
| 14  | A     | 822  | CLA  | O2D-CGD-O1D | -2.83 | 118.30      | 123.84   |
| 14  | 8     | 1302 | CLA  | O2D-CGD-O1D | -2.83 | 118.30      | 123.84   |
| 14  | A     | 836  | CLA  | O2D-CGD-O1D | -2.83 | 118.30      | 123.84   |
| 17  | f     | 204  | BCR  | C16-C15-C14 | -2.83 | 117.67      | 123.47   |
| 14  | A     | 826  | CLA  | O2D-CGD-O1D | -2.83 | 118.30      | 123.84   |
| 14  | B     | 826  | CLA  | O2D-CGD-O1D | -2.83 | 118.30      | 123.84   |
| 14  | B     | 841  | CLA  | CHB-C4A-NA  | 2.83  | 128.43      | 124.51   |
| 14  | 1     | 1637 | CLA  | O2D-CGD-O1D | -2.83 | 118.31      | 123.84   |
| 14  | a     | 836  | CLA  | O2D-CGD-O1D | -2.83 | 118.31      | 123.84   |
| 14  | a     | 821  | CLA  | O2D-CGD-O1D | -2.83 | 118.31      | 123.84   |
| 13  | a     | 801  | CL0  | CHB-C4A-NA  | 2.83  | 128.42      | 124.51   |
| 14  | 0     | 205  | CLA  | CHB-C4A-NA  | 2.83  | 128.42      | 124.51   |
| 14  | a     | 840  | CLA  | CHB-C4A-NA  | 2.82  | 128.42      | 124.51   |
| 14  | a     | 802  | CLA  | O2D-CGD-O1D | -2.82 | 118.32      | 123.84   |
| 13  | A     | 801  | CL0  | CHB-C4A-NA  | 2.82  | 128.42      | 124.51   |
| 14  | 1     | 1618 | CLA  | O2D-CGD-O1D | -2.82 | 118.32      | 123.84   |
| 14  | a     | 822  | CLA  | O2D-CGD-O1D | -2.82 | 118.32      | 123.84   |
| 17  | a     | 847  | BCR  | C15-C16-C17 | -2.82 | 117.69      | 123.47   |
| 14  | j     | 1302 | CLA  | O2D-CGD-O1D | -2.82 | 118.32      | 123.84   |
| 17  | F     | 205  | BCR  | C16-C15-C14 | -2.82 | 117.69      | 123.47   |
| 14  | 1     | 1641 | CLA  | CHB-C4A-NA  | 2.82  | 128.41      | 124.51   |
| 14  | b     | 807  | CLA  | CMB-C2B-C3B | 2.82  | 129.95      | 124.68   |
| 17  | 1     | 1648 | BCR  | C15-C16-C17 | -2.82 | 117.70      | 123.47   |
| 14  | 1     | 1622 | CLA  | O2D-CGD-O1D | -2.82 | 118.33      | 123.84   |
| 14  | A     | 807  | CLA  | CHB-C4A-NA  | 2.82  | 128.41      | 124.51   |
| 14  | 2     | 831  | CLA  | CMB-C2B-C1B | -2.82 | 124.13      | 128.46   |
| 14  | 2     | 836  | CLA  | C1-C2-C3    | -2.82 | 122.19      | 126.75   |
| 14  | a     | 837  | CLA  | CMB-C2B-C3B | 2.82  | 129.95      | 124.68   |
| 14  | A     | 818  | CLA  | CHB-C4A-NA  | 2.82  | 128.41      | 124.51   |
| 14  | 2     | 838  | CLA  | CHB-C4A-NA  | 2.82  | 128.41      | 124.51   |
| 14  | a     | 817  | CLA  | O2D-CGD-O1D | -2.82 | 118.33      | 123.84   |
| 14  | b     | 837  | CLA  | CMB-C2B-C1B | -2.82 | 124.14      | 128.46   |
| 14  | A     | 834  | CLA  | O2D-CGD-O1D | -2.81 | 118.33      | 123.84   |
| 17  | 2     | 848  | BCR  | C27-C26-C25 | 2.81  | 126.82      | 122.73   |
| 14  | 2     | 827  | CLA  | O2D-CGD-O1D | -2.81 | 118.34      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 837  | CLA  | CHB-C4A-NA  | 2.81  | 128.40      | 124.51   |
| 14  | a     | 807  | CLA  | CHB-C4A-NA  | 2.81  | 128.40      | 124.51   |
| 14  | 1     | 1608 | CLA  | CHB-C4A-NA  | 2.81  | 128.40      | 124.51   |
| 14  | A     | 837  | CLA  | CMB-C2B-C3B | 2.81  | 129.94      | 124.68   |
| 17  | 0     | 203  | BCR  | C37-C22-C21 | -2.81 | 118.99      | 122.92   |
| 14  | 9     | 101  | CLA  | CMB-C2B-C3B | 2.81  | 129.93      | 124.68   |
| 14  | B     | 810  | CLA  | O2D-CGD-O1D | -2.81 | 118.35      | 123.84   |
| 17  | B     | 851  | BCR  | C15-C16-C17 | -2.81 | 117.72      | 123.47   |
| 14  | A     | 818  | CLA  | O2D-CGD-O1D | -2.81 | 118.35      | 123.84   |
| 14  | A     | 817  | CLA  | O2D-CGD-O1D | -2.81 | 118.35      | 123.84   |
| 14  | A     | 804  | CLA  | CHB-C4A-NA  | 2.81  | 128.39      | 124.51   |
| 14  | a     | 804  | CLA  | CHB-C4A-NA  | 2.80  | 128.39      | 124.51   |
| 14  | b     | 831  | CLA  | CMB-C2B-C1B | -2.80 | 124.16      | 128.46   |
| 14  | a     | 818  | CLA  | O2D-CGD-O1D | -2.80 | 118.36      | 123.84   |
| 14  | A     | 803  | CLA  | O2D-CGD-O1D | -2.80 | 118.36      | 123.84   |
| 17  | 8     | 1306 | BCR  | C15-C16-C17 | -2.80 | 117.73      | 123.47   |
| 14  | 1     | 1603 | CLA  | O2D-CGD-O1D | -2.80 | 118.36      | 123.84   |
| 17  | b     | 848  | BCR  | C27-C26-C25 | 2.80  | 126.80      | 122.73   |
| 14  | b     | 838  | CLA  | CHB-C4A-NA  | 2.80  | 128.38      | 124.51   |
| 14  | B     | 803  | CLA  | O2D-CGD-O1D | -2.80 | 118.36      | 123.84   |
| 14  | a     | 834  | CLA  | O2D-CGD-O1D | -2.80 | 118.37      | 123.84   |
| 14  | 1     | 1612 | CLA  | O2D-CGD-O1D | -2.80 | 118.37      | 123.84   |
| 14  | f     | 203  | CLA  | CMB-C2B-C3B | 2.80  | 129.91      | 124.68   |
| 14  | 1     | 1638 | CLA  | CMB-C2B-C3B | 2.80  | 129.91      | 124.68   |
| 14  | b     | 836  | CLA  | C1-C2-C3    | -2.80 | 122.22      | 126.75   |
| 14  | 2     | 807  | CLA  | CMB-C2B-C3B | 2.80  | 129.91      | 124.68   |
| 14  | A     | 821  | CLA  | O2D-CGD-O1D | -2.80 | 118.37      | 123.84   |
| 14  | a     | 803  | CLA  | O2D-CGD-O1D | -2.80 | 118.37      | 123.84   |
| 14  | B     | 806  | CLA  | CMB-C2B-C3B | 2.79  | 129.91      | 124.68   |
| 17  | 6     | 204  | BCR  | C16-C15-C14 | -2.79 | 117.75      | 123.47   |
| 14  | 2     | 811  | CLA  | O2D-CGD-O1D | -2.79 | 118.38      | 123.84   |
| 17  | L     | 201  | BCR  | C37-C22-C21 | -2.79 | 119.01      | 122.92   |
| 14  | 1     | 1619 | CLA  | O2D-CGD-O1D | -2.79 | 118.38      | 123.84   |
| 14  | k     | 101  | CLA  | CMB-C2B-C3B | 2.79  | 129.90      | 124.68   |
| 14  | 1     | 1621 | CLA  | CHB-C4A-NA  | 2.79  | 128.37      | 124.51   |
| 14  | b     | 811  | CLA  | O2D-CGD-O1D | -2.79 | 118.39      | 123.84   |
| 14  | K     | 101  | CLA  | CMB-C2B-C3B | 2.79  | 129.90      | 124.68   |
| 17  | f     | 202  | BCR  | C15-C16-C17 | -2.79 | 117.76      | 123.47   |
| 14  | B     | 830  | CLA  | CMB-C2B-C1B | -2.79 | 124.18      | 128.46   |
| 14  | F     | 204  | CLA  | CMB-C2B-C3B | 2.79  | 129.89      | 124.68   |
| 14  | A     | 840  | CLA  | CHB-C4A-NA  | 2.79  | 128.37      | 124.51   |
| 17  | b     | 852  | BCR  | C15-C16-C17 | -2.79 | 117.77      | 123.47   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | 2     | 804  | CLA  | O2D-CGD-O1D | -2.79 | 118.39      | 123.84   |
| 14  | b     | 821  | CLA  | CMB-C2B-C3B | 2.78  | 129.89      | 124.68   |
| 14  | 6     | 203  | CLA  | CMB-C2B-C3B | 2.78  | 129.89      | 124.68   |
| 17  | F     | 202  | BCR  | C15-C16-C17 | -2.78 | 117.78      | 123.47   |
| 17  | 6     | 202  | BCR  | C15-C16-C17 | -2.78 | 117.78      | 123.47   |
| 14  | 1     | 1635 | CLA  | O2D-CGD-O1D | -2.78 | 118.41      | 123.84   |
| 14  | 2     | 821  | CLA  | CMB-C2B-C3B | 2.77  | 129.87      | 124.68   |
| 17  | L     | 201  | BCR  | C2-C1-C6    | 2.77  | 114.75      | 110.48   |
| 14  | 1     | 1605 | CLA  | CHB-C4A-NA  | 2.77  | 128.35      | 124.51   |
| 14  | b     | 804  | CLA  | O2D-CGD-O1D | -2.77 | 118.42      | 123.84   |
| 14  | B     | 820  | CLA  | CMB-C2B-C3B | 2.77  | 129.87      | 124.68   |
| 14  | A     | 811  | CLA  | O2D-CGD-O1D | -2.77 | 118.42      | 123.84   |
| 14  | a     | 811  | CLA  | O2D-CGD-O1D | -2.77 | 118.42      | 123.84   |
| 14  | A     | 820  | CLA  | CHB-C4A-NA  | 2.77  | 128.34      | 124.51   |
| 14  | a     | 820  | CLA  | CHB-C4A-NA  | 2.77  | 128.34      | 124.51   |
| 14  | 2     | 807  | CLA  | CHB-C4A-NA  | 2.77  | 128.34      | 124.51   |
| 14  | a     | 814  | CLA  | O2D-CGD-O1D | -2.77 | 118.43      | 123.84   |
| 14  | 2     | 837  | CLA  | CMB-C2B-C1B | -2.77 | 124.21      | 128.46   |
| 14  | A     | 823  | CLA  | O2D-CGD-O1D | -2.77 | 118.43      | 123.84   |
| 14  | b     | 807  | CLA  | CHB-C4A-NA  | 2.77  | 128.34      | 124.51   |
| 17  | l     | 202  | BCR  | C37-C22-C21 | -2.77 | 119.05      | 122.92   |
| 14  | a     | 823  | CLA  | O2D-CGD-O1D | -2.77 | 118.43      | 123.84   |
| 14  | 2     | 814  | CLA  | O2D-CGD-O1D | -2.77 | 118.43      | 123.84   |
| 17  | 0     | 203  | BCR  | C2-C1-C6    | 2.76  | 114.74      | 110.48   |
| 14  | b     | 810  | CLA  | C4-C3-C5    | 2.76  | 119.92      | 115.27   |
| 14  | B     | 836  | CLA  | CMB-C2B-C1B | -2.76 | 124.22      | 128.46   |
| 17  | b     | 847  | BCR  | C27-C26-C25 | 2.76  | 126.74      | 122.73   |
| 14  | B     | 806  | CLA  | CHB-C4A-NA  | 2.75  | 128.32      | 124.51   |
| 17  | 6     | 202  | BCR  | C2-C1-C6    | 2.75  | 114.72      | 110.48   |
| 14  | 1     | 1613 | CLA  | O2D-CGD-O1D | -2.75 | 118.46      | 123.84   |
| 14  | 2     | 836  | CLA  | CHB-C4A-NA  | 2.75  | 128.31      | 124.51   |
| 17  | F     | 202  | BCR  | C2-C1-C6    | 2.75  | 114.71      | 110.48   |
| 17  | f     | 202  | BCR  | C2-C1-C6    | 2.75  | 114.71      | 110.48   |
| 14  | B     | 809  | CLA  | C4-C3-C5    | 2.75  | 119.89      | 115.27   |
| 14  | A     | 803  | CLA  | C1B-CHB-C4A | -2.75 | 124.68      | 130.12   |
| 14  | A     | 814  | CLA  | O2D-CGD-O1D | -2.74 | 118.47      | 123.84   |
| 14  | a     | 819  | CLA  | C1B-CHB-C4A | -2.74 | 124.69      | 130.12   |
| 14  | 1     | 1624 | CLA  | O2D-CGD-O1D | -2.74 | 118.48      | 123.84   |
| 14  | B     | 808  | CLA  | O2A-CGA-O1A | -2.74 | 116.67      | 123.59   |
| 14  | 2     | 809  | CLA  | O2A-CGA-O1A | -2.74 | 116.67      | 123.59   |
| 14  | 1     | 1609 | CLA  | O2D-CGD-CBD | 2.74  | 116.14      | 111.27   |
| 14  | B     | 809  | CLA  | O2D-CGD-O1D | -2.74 | 118.48      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | 1     | 1615 | CLA  | O2D-CGD-O1D | -2.74 | 118.48      | 123.84   |
| 14  | b     | 826  | CLA  | C1B-CHB-C4A | -2.74 | 124.69      | 130.12   |
| 14  | b     | 836  | CLA  | CHB-C4A-NA  | 2.74  | 128.30      | 124.51   |
| 14  | a     | 838  | CLA  | O2A-CGA-O1A | -2.74 | 116.68      | 123.59   |
| 14  | b     | 814  | CLA  | O2D-CGD-O1D | -2.74 | 118.49      | 123.84   |
| 14  | b     | 828  | CLA  | C1B-CHB-C4A | -2.74 | 124.70      | 130.12   |
| 14  | A     | 808  | CLA  | O2D-CGD-CBD | 2.74  | 116.13      | 111.27   |
| 14  | 1     | 1630 | CLA  | C1B-CHB-C4A | -2.74 | 124.70      | 130.12   |
| 14  | 2     | 828  | CLA  | C1B-CHB-C4A | -2.74 | 124.70      | 130.12   |
| 14  | A     | 812  | CLA  | O2D-CGD-O1D | -2.73 | 118.49      | 123.84   |
| 14  | B     | 835  | CLA  | CHB-C4A-NA  | 2.73  | 128.29      | 124.51   |
| 17  | l     | 202  | BCR  | C2-C1-C6    | 2.73  | 114.69      | 110.48   |
| 14  | a     | 817  | CLA  | CMB-C2B-C3B | 2.73  | 129.79      | 124.68   |
| 14  | b     | 809  | CLA  | O2A-CGA-O1A | -2.73 | 116.70      | 123.59   |
| 14  | 1     | 1618 | CLA  | CMB-C2B-C3B | 2.73  | 129.79      | 124.68   |
| 14  | a     | 829  | CLA  | C1B-CHB-C4A | -2.73 | 124.71      | 130.12   |
| 14  | B     | 814  | CLA  | CHB-C4A-NA  | 2.73  | 128.29      | 124.51   |
| 14  | A     | 819  | CLA  | C1B-CHB-C4A | -2.73 | 124.71      | 130.12   |
| 14  | 1     | 1620 | CLA  | C1B-CHB-C4A | -2.73 | 124.71      | 130.12   |
| 17  | B     | 846  | BCR  | C27-C26-C25 | 2.73  | 126.69      | 122.73   |
| 14  | 1     | 1639 | CLA  | O2A-CGA-O1A | -2.73 | 116.71      | 123.59   |
| 14  | A     | 829  | CLA  | C1B-CHB-C4A | -2.73 | 124.72      | 130.12   |
| 14  | 2     | 826  | CLA  | C1B-CHB-C4A | -2.73 | 124.72      | 130.12   |
| 14  | 2     | 810  | CLA  | C4-C3-C5    | 2.73  | 119.86      | 115.27   |
| 14  | b     | 809  | CLA  | CMB-C2B-C1B | -2.73 | 124.28      | 128.46   |
| 14  | 2     | 803  | CLA  | O2D-CGD-O1D | -2.73 | 118.51      | 123.84   |
| 17  | i     | 101  | BCR  | C15-C16-C17 | -2.72 | 117.89      | 123.47   |
| 14  | a     | 803  | CLA  | C1B-CHB-C4A | -2.72 | 124.72      | 130.12   |
| 14  | B     | 813  | CLA  | O2D-CGD-O1D | -2.72 | 118.51      | 123.84   |
| 14  | k     | 101  | CLA  | O2D-CGD-O1D | -2.72 | 118.52      | 123.84   |
| 14  | 9     | 101  | CLA  | O2D-CGD-O1D | -2.72 | 118.52      | 123.84   |
| 14  | a     | 832  | CLA  | O2D-CGD-O1D | -2.72 | 118.52      | 123.84   |
| 14  | b     | 810  | CLA  | O2D-CGD-O1D | -2.72 | 118.52      | 123.84   |
| 14  | 1     | 1624 | CLA  | CHB-C4A-NA  | 2.72  | 128.27      | 124.51   |
| 14  | K     | 101  | CLA  | O2D-CGD-O1D | -2.72 | 118.53      | 123.84   |
| 14  | a     | 812  | CLA  | O2D-CGD-O1D | -2.72 | 118.53      | 123.84   |
| 17  | I     | 101  | BCR  | C15-C16-C17 | -2.72 | 117.91      | 123.47   |
| 17  | 0     | 201  | BCR  | C15-C16-C17 | -2.72 | 117.91      | 123.47   |
| 14  | b     | 808  | CLA  | CMB-C2B-C3B | 2.72  | 129.76      | 124.68   |
| 14  | B     | 827  | CLA  | C1B-CHB-C4A | -2.71 | 124.74      | 130.12   |
| 14  | B     | 807  | CLA  | CMB-C2B-C3B | 2.71  | 129.76      | 124.68   |
| 17  | 7     | 101  | BCR  | C15-C16-C17 | -2.71 | 117.92      | 123.47   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 802  | CLA  | O2D-CGD-O1D | -2.71 | 118.53      | 123.84   |
| 17  | L     | 207  | BCR  | C15-C16-C17 | -2.71 | 117.92      | 123.47   |
| 17  | 2     | 847  | BCR  | C27-C26-C25 | 2.71  | 126.67      | 122.73   |
| 17  | 0     | 209  | BCR  | C15-C16-C17 | -2.71 | 117.92      | 123.47   |
| 14  | a     | 823  | CLA  | CHB-C4A-NA  | 2.71  | 128.26      | 124.51   |
| 14  | A     | 817  | CLA  | CMB-C2B-C3B | 2.71  | 129.75      | 124.68   |
| 14  | b     | 805  | CLA  | CHB-C4A-NA  | 2.71  | 128.26      | 124.51   |
| 14  | 2     | 815  | CLA  | CHB-C4A-NA  | 2.71  | 128.26      | 124.51   |
| 14  | B     | 825  | CLA  | C1B-CHB-C4A | -2.71 | 124.75      | 130.12   |
| 14  | A     | 838  | CLA  | O2A-CGA-O1A | -2.71 | 116.76      | 123.59   |
| 14  | b     | 803  | CLA  | O2D-CGD-O1D | -2.71 | 118.55      | 123.84   |
| 14  | a     | 808  | CLA  | O2D-CGD-CBD | 2.70  | 116.07      | 111.27   |
| 14  | 2     | 809  | CLA  | CMB-C2B-C1B | -2.70 | 124.31      | 128.46   |
| 14  | 2     | 808  | CLA  | CMB-C2B-C3B | 2.70  | 129.74      | 124.68   |
| 14  | b     | 831  | CLA  | CHD-C1D-ND  | -2.70 | 121.97      | 124.45   |
| 17  | 2     | 849  | BCR  | C15-C16-C17 | -2.70 | 117.94      | 123.47   |
| 14  | 1     | 1604 | CLA  | C1B-CHB-C4A | -2.70 | 124.77      | 130.12   |
| 14  | A     | 823  | CLA  | CHB-C4A-NA  | 2.70  | 128.24      | 124.51   |
| 14  | b     | 813  | CLA  | C1B-CHB-C4A | -2.70 | 124.78      | 130.12   |
| 14  | A     | 832  | CLA  | O2D-CGD-O1D | -2.70 | 118.57      | 123.84   |
| 14  | b     | 815  | CLA  | CHB-C4A-NA  | 2.70  | 128.24      | 124.51   |
| 14  | 2     | 810  | CLA  | O2D-CGD-O1D | -2.69 | 118.57      | 123.84   |
| 14  | B     | 808  | CLA  | CMB-C2B-C1B | -2.69 | 124.33      | 128.46   |
| 20  | B     | 849  | LMG  | O6-C1-O1    | -2.69 | 103.60      | 109.97   |
| 14  | B     | 804  | CLA  | CHB-C4A-NA  | 2.69  | 128.23      | 124.51   |
| 14  | A     | 821  | CLA  | CHB-C4A-NA  | 2.69  | 128.23      | 124.51   |
| 14  | 1     | 1642 | CLA  | CHB-C4A-NA  | 2.69  | 128.23      | 124.51   |
| 14  | 2     | 805  | CLA  | O2D-CGD-O1D | -2.69 | 118.58      | 123.84   |
| 14  | a     | 821  | CLA  | CHB-C4A-NA  | 2.69  | 128.23      | 124.51   |
| 14  | b     | 805  | CLA  | O2D-CGD-O1D | -2.69 | 118.58      | 123.84   |
| 20  | 2     | 850  | LMG  | O6-C1-O1    | -2.69 | 103.61      | 109.97   |
| 14  | A     | 841  | CLA  | CHB-C4A-NA  | 2.69  | 128.23      | 124.51   |
| 14  | B     | 803  | CLA  | CHB-C4A-NA  | 2.69  | 128.23      | 124.51   |
| 14  | A     | 840  | CLA  | O2D-CGD-CBD | 2.68  | 116.04      | 111.27   |
| 14  | 2     | 805  | CLA  | CHB-C4A-NA  | 2.68  | 128.22      | 124.51   |
| 17  | B     | 848  | BCR  | C15-C16-C17 | -2.68 | 117.98      | 123.47   |
| 14  | 1     | 1633 | CLA  | O2D-CGD-O1D | -2.68 | 118.59      | 123.84   |
| 14  | b     | 822  | CLA  | CHB-C4A-NA  | 2.68  | 128.22      | 124.51   |
| 14  | B     | 804  | CLA  | O2D-CGD-O1D | -2.68 | 118.60      | 123.84   |
| 17  | b     | 849  | BCR  | C15-C16-C17 | -2.68 | 117.98      | 123.47   |
| 14  | b     | 834  | CLA  | O2D-CGD-O1D | -2.68 | 118.60      | 123.84   |
| 14  | B     | 833  | CLA  | O2D-CGD-O1D | -2.68 | 118.60      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 841  | CLA  | CHB-C4A-NA  | 2.68  | 128.22      | 124.51   |
| 14  | B     | 821  | CLA  | CHB-C4A-NA  | 2.68  | 128.21      | 124.51   |
| 14  | 1     | 1632 | CLA  | CHB-C4A-NA  | 2.68  | 128.21      | 124.51   |
| 17  | 2     | 846  | BCR  | C37-C22-C21 | -2.68 | 119.17      | 122.92   |
| 14  | B     | 835  | CLA  | CMB-C2B-C3B | 2.68  | 129.68      | 124.68   |
| 20  | b     | 850  | LMG  | O6-C1-O1    | -2.68 | 103.64      | 109.97   |
| 14  | 1     | 1622 | CLA  | CHB-C4A-NA  | 2.67  | 128.21      | 124.51   |
| 14  | B     | 812  | CLA  | C1B-CHB-C4A | -2.67 | 124.82      | 130.12   |
| 14  | 2     | 813  | CLA  | C1B-CHB-C4A | -2.67 | 124.83      | 130.12   |
| 14  | 2     | 831  | CLA  | CHD-C1D-ND  | -2.67 | 122.00      | 124.45   |
| 14  | a     | 808  | CLA  | CMB-C2B-C3B | 2.67  | 129.68      | 124.68   |
| 14  | A     | 811  | CLA  | CMB-C2B-C1B | -2.67 | 124.36      | 128.46   |
| 14  | b     | 809  | CLA  | C3A-C2A-C1A | 2.67  | 105.34      | 101.34   |
| 14  | 2     | 836  | CLA  | CMB-C2B-C3B | 2.67  | 129.67      | 124.68   |
| 14  | 2     | 834  | CLA  | O2D-CGD-O1D | -2.67 | 118.62      | 123.84   |
| 17  | K     | 104  | BCR  | C15-C16-C17 | -2.67 | 118.01      | 123.47   |
| 14  | b     | 836  | CLA  | CMB-C2B-C3B | 2.67  | 129.67      | 124.68   |
| 18  | 0     | 202  | LHG  | O8-C23-C24  | 2.66  | 120.27      | 111.91   |
| 17  | 9     | 102  | BCR  | C15-C16-C17 | -2.66 | 118.02      | 123.47   |
| 14  | 2     | 833  | CLA  | CHB-C4A-NA  | 2.66  | 128.19      | 124.51   |
| 14  | 1     | 1621 | CLA  | O2D-CGD-CBD | 2.66  | 116.00      | 111.27   |
| 14  | B     | 832  | CLA  | CHB-C4A-NA  | 2.66  | 128.19      | 124.51   |
| 14  | A     | 831  | CLA  | CHB-C4A-NA  | 2.66  | 128.19      | 124.51   |
| 17  | K     | 102  | BCR  | C15-C16-C17 | -2.66 | 118.03      | 123.47   |
| 14  | 0     | 207  | CLA  | CHB-C4A-NA  | 2.66  | 128.19      | 124.51   |
| 14  | b     | 833  | CLA  | CHB-C4A-NA  | 2.66  | 128.19      | 124.51   |
| 14  | a     | 811  | CLA  | CMB-C2B-C1B | -2.66 | 124.38      | 128.46   |
| 17  | B     | 845  | BCR  | C37-C22-C21 | -2.66 | 119.20      | 122.92   |
| 14  | A     | 808  | CLA  | CMB-C2B-C3B | 2.65  | 129.65      | 124.68   |
| 14  | 1     | 1609 | CLA  | CMB-C2B-C3B | 2.65  | 129.65      | 124.68   |
| 17  | a     | 852  | BCR  | C15-C14-C13 | -2.65 | 123.52      | 127.31   |
| 17  | 9     | 104  | BCR  | C15-C16-C17 | -2.65 | 118.04      | 123.47   |
| 14  | B     | 819  | CLA  | C1B-CHB-C4A | -2.65 | 124.87      | 130.12   |
| 14  | B     | 823  | CLA  | CHB-C4A-NA  | 2.65  | 128.18      | 124.51   |
| 14  | 2     | 822  | CLA  | CHB-C4A-NA  | 2.65  | 128.18      | 124.51   |
| 14  | 2     | 820  | CLA  | C1B-CHB-C4A | -2.65 | 124.87      | 130.12   |
| 17  | k     | 102  | BCR  | C15-C16-C17 | -2.65 | 118.05      | 123.47   |
| 14  | b     | 824  | CLA  | CHB-C4A-NA  | 2.65  | 128.18      | 124.51   |
| 17  | k     | 104  | BCR  | C15-C16-C17 | -2.65 | 118.05      | 123.47   |
| 14  | A     | 820  | CLA  | O2D-CGD-CBD | 2.65  | 115.97      | 111.27   |
| 18  | L     | 208  | LHG  | O8-C23-C24  | 2.65  | 120.22      | 111.91   |
| 18  | A     | 853  | LHG  | C20-C19-C18 | -2.65 | 100.98      | 114.42   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | b     | 846  | BCR  | C37-C22-C21 | -2.65 | 119.21      | 122.92   |
| 14  | 1     | 1641 | CLA  | O2D-CGD-CBD | 2.65  | 115.97      | 111.27   |
| 14  | a     | 840  | CLA  | O2D-CGD-CBD | 2.65  | 115.97      | 111.27   |
| 14  | a     | 831  | CLA  | CHB-C4A-NA  | 2.65  | 128.17      | 124.51   |
| 18  | l     | 201  | LHG  | O8-C23-C24  | 2.64  | 120.21      | 111.91   |
| 14  | l     | 206  | CLA  | CHB-C4A-NA  | 2.64  | 128.16      | 124.51   |
| 18  | a     | 853  | LHG  | C20-C19-C18 | -2.64 | 101.02      | 114.42   |
| 17  | 1     | 1653 | BCR  | C15-C14-C13 | -2.64 | 123.54      | 127.31   |
| 14  | A     | 825  | CLA  | O2D-CGD-O1D | -2.64 | 118.68      | 123.84   |
| 14  | b     | 804  | CLA  | CHB-C4A-NA  | 2.64  | 128.16      | 124.51   |
| 14  | 1     | 1639 | CLA  | CHB-C4A-NA  | 2.64  | 128.16      | 124.51   |
| 14  | B     | 816  | CLA  | CHB-C4A-NA  | 2.64  | 128.16      | 124.51   |
| 14  | A     | 803  | CLA  | CMB-C2B-C1B | -2.64 | 124.41      | 128.46   |
| 14  | 1     | 1632 | CLA  | CMB-C2B-C3B | 2.64  | 129.61      | 124.68   |
| 18  | 1     | 1654 | LHG  | C20-C19-C18 | -2.64 | 101.05      | 114.42   |
| 14  | 2     | 817  | CLA  | CHB-C4A-NA  | 2.64  | 128.16      | 124.51   |
| 14  | b     | 817  | CLA  | CHB-C4A-NA  | 2.63  | 128.16      | 124.51   |
| 14  | 2     | 831  | CLA  | CHB-C4A-NA  | 2.63  | 128.16      | 124.51   |
| 14  | L     | 205  | CLA  | CHB-C4A-NA  | 2.63  | 128.15      | 124.51   |
| 14  | a     | 820  | CLA  | O2D-CGD-CBD | 2.63  | 115.95      | 111.27   |
| 14  | 1     | 1612 | CLA  | CMB-C2B-C1B | -2.63 | 124.42      | 128.46   |
| 14  | a     | 838  | CLA  | CHB-C4A-NA  | 2.63  | 128.15      | 124.51   |
| 14  | 2     | 809  | CLA  | C3A-C2A-C1A | 2.63  | 105.28      | 101.34   |
| 14  | b     | 831  | CLA  | CHB-C4A-NA  | 2.63  | 128.15      | 124.51   |
| 14  | b     | 820  | CLA  | C1B-CHB-C4A | -2.63 | 124.91      | 130.12   |
| 14  | 2     | 809  | CLA  | C1-C2-C3    | -2.63 | 121.50      | 126.04   |
| 14  | a     | 825  | CLA  | O2D-CGD-O1D | -2.63 | 118.70      | 123.84   |
| 14  | 2     | 824  | CLA  | CHB-C4A-NA  | 2.63  | 128.15      | 124.51   |
| 14  | 1     | 1604 | CLA  | CMB-C2B-C1B | -2.63 | 124.43      | 128.46   |
| 14  | A     | 857  | CLA  | CMB-C2B-C3B | 2.63  | 129.59      | 124.68   |
| 14  | 2     | 830  | CLA  | C2D-C1D-ND  | -2.62 | 108.17      | 110.10   |
| 14  | a     | 831  | CLA  | CMB-C2B-C3B | 2.62  | 129.59      | 124.68   |
| 17  | A     | 852  | BCR  | C15-C14-C13 | -2.62 | 123.57      | 127.31   |
| 14  | A     | 838  | CLA  | CHB-C4A-NA  | 2.62  | 128.14      | 124.51   |
| 14  | 1     | 1626 | CLA  | O2D-CGD-O1D | -2.62 | 118.71      | 123.84   |
| 17  | 1     | 1652 | BCR  | C2-C1-C6    | 2.62  | 114.52      | 110.48   |
| 14  | L     | 204  | CLA  | CHB-C4A-NA  | 2.62  | 128.14      | 124.51   |
| 17  | A     | 851  | BCR  | C15-C16-C17 | -2.62 | 118.11      | 123.47   |
| 18  | z     | 101  | LHG  | O8-C23-C24  | 2.62  | 120.13      | 111.91   |
| 17  | A     | 851  | BCR  | C16-C15-C14 | -2.62 | 118.11      | 123.47   |
| 17  | a     | 851  | BCR  | C2-C1-C6    | 2.62  | 114.51      | 110.48   |
| 14  | a     | 841  | CLA  | O2D-CGD-O1D | -2.62 | 118.72      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | B     | 850  | LHG  | O8-C23-C24  | 2.62  | 120.12      | 111.91   |
| 14  | A     | 831  | CLA  | CMB-C2B-C3B | 2.62  | 129.57      | 124.68   |
| 17  | A     | 851  | BCR  | C2-C1-C6    | 2.61  | 114.51      | 110.48   |
| 18  | b     | 851  | LHG  | O8-C23-C24  | 2.61  | 120.11      | 111.91   |
| 14  | 0     | 206  | CLA  | CHB-C4A-NA  | 2.61  | 128.13      | 124.51   |
| 17  | 2     | 846  | BCR  | C27-C26-C25 | 2.61  | 126.53      | 122.73   |
| 14  | B     | 839  | CLA  | C1B-CHB-C4A | -2.61 | 124.95      | 130.12   |
| 14  | 2     | 804  | CLA  | CHB-C4A-NA  | 2.61  | 128.12      | 124.51   |
| 14  | 1     | 1601 | CLA  | CMB-C2B-C3B | 2.61  | 129.56      | 124.68   |
| 14  | a     | 843  | CLA  | CHB-C4A-NA  | 2.61  | 128.12      | 124.51   |
| 14  | 1     | 1644 | CLA  | CHB-C4A-NA  | 2.61  | 128.12      | 124.51   |
| 14  | B     | 817  | CLA  | CMB-C2B-C3B | 2.61  | 129.56      | 124.68   |
| 14  | 1     | 1642 | CLA  | O2D-CGD-O1D | -2.61 | 118.74      | 123.84   |
| 17  | b     | 846  | BCR  | C27-C26-C25 | 2.61  | 126.52      | 122.73   |
| 14  | A     | 815  | CLA  | CHB-C4A-NA  | 2.61  | 128.12      | 124.51   |
| 14  | b     | 808  | CLA  | C1B-CHB-C4A | -2.61 | 124.96      | 130.12   |
| 14  | b     | 821  | CLA  | C1B-CHB-C4A | -2.61 | 124.96      | 130.12   |
| 14  | a     | 838  | CLA  | O2D-CGD-O1D | -2.60 | 118.75      | 123.84   |
| 14  | 1     | 1612 | CLA  | CHB-C4A-NA  | 2.60  | 128.11      | 124.51   |
| 14  | l     | 205  | CLA  | CHB-C4A-NA  | 2.60  | 128.11      | 124.51   |
| 14  | a     | 803  | CLA  | CMB-C2B-C1B | -2.60 | 124.46      | 128.46   |
| 14  | B     | 808  | CLA  | C3A-C2A-C1A | 2.60  | 105.24      | 101.34   |
| 14  | B     | 830  | CLA  | CHB-C4A-NA  | 2.60  | 128.11      | 124.51   |
| 17  | 1     | 1652 | BCR  | C16-C15-C14 | -2.60 | 118.14      | 123.47   |
| 14  | A     | 802  | CLA  | C1-C2-C3    | -2.60 | 121.54      | 126.04   |
| 14  | B     | 827  | CLA  | O2A-CGA-O1A | -2.60 | 117.03      | 123.59   |
| 14  | A     | 827  | CLA  | C1B-CHB-C4A | -2.60 | 124.97      | 130.12   |
| 14  | b     | 826  | CLA  | CHD-C1D-ND  | -2.60 | 122.06      | 124.45   |
| 14  | A     | 807  | CLA  | O1D-CGD-CBD | 2.60  | 129.81      | 124.48   |
| 17  | a     | 851  | BCR  | C16-C15-C14 | -2.60 | 118.15      | 123.47   |
| 14  | 2     | 840  | CLA  | C1B-CHB-C4A | -2.60 | 124.97      | 130.12   |
| 14  | a     | 807  | CLA  | O1D-CGD-CBD | 2.60  | 129.80      | 124.48   |
| 14  | 2     | 828  | CLA  | O2A-CGA-O1A | -2.60 | 117.03      | 123.59   |
| 14  | B     | 817  | CLA  | O2D-CGD-O1D | -2.60 | 118.76      | 123.84   |
| 14  | 1     | 1617 | CLA  | O2D-CGD-O1D | -2.60 | 118.76      | 123.84   |
| 14  | A     | 816  | CLA  | O2D-CGD-O1D | -2.60 | 118.76      | 123.84   |
| 14  | b     | 840  | CLA  | C1B-CHB-C4A | -2.60 | 124.97      | 130.12   |
| 14  | A     | 841  | CLA  | O2D-CGD-O1D | -2.60 | 118.76      | 123.84   |
| 14  | B     | 819  | CLA  | CMB-C2B-C3B | 2.60  | 129.53      | 124.68   |
| 14  | B     | 807  | CLA  | C1B-CHB-C4A | -2.60 | 124.98      | 130.12   |
| 14  | 2     | 819  | CLA  | C1B-CHB-C4A | -2.60 | 124.98      | 130.12   |
| 17  | 2     | 849  | BCR  | C16-C15-C14 | -2.60 | 118.16      | 123.47   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | b     | 809  | CLA  | C1-C2-C3    | -2.59 | 121.56      | 126.04   |
| 14  | 2     | 818  | CLA  | O2D-CGD-O1D | -2.59 | 118.77      | 123.84   |
| 14  | B     | 820  | CLA  | C1B-CHB-C4A | -2.59 | 124.98      | 130.12   |
| 14  | a     | 839  | CLA  | O2D-CGD-CBD | 2.59  | 115.88      | 111.27   |
| 17  | j     | 1305 | BCR  | C15-C16-C17 | -2.59 | 118.16      | 123.47   |
| 17  | 8     | 1305 | BCR  | C15-C16-C17 | -2.59 | 118.16      | 123.47   |
| 14  | A     | 838  | CLA  | O2D-CGD-O1D | -2.59 | 118.77      | 123.84   |
| 17  | A     | 856  | BCR  | C15-C16-C17 | -2.59 | 118.17      | 123.47   |
| 14  | A     | 811  | CLA  | CHB-C4A-NA  | 2.59  | 128.09      | 124.51   |
| 14  | 1     | 1603 | CLA  | C1-C2-C3    | -2.59 | 121.56      | 126.04   |
| 17  | 2     | 846  | BCR  | C15-C16-C17 | -2.59 | 118.17      | 123.47   |
| 14  | A     | 802  | CLA  | CHB-C4A-NA  | 2.59  | 128.09      | 124.51   |
| 14  | A     | 843  | CLA  | CHB-C4A-NA  | 2.59  | 128.09      | 124.51   |
| 14  | 1     | 1623 | CLA  | CHB-C4A-NA  | 2.59  | 128.09      | 124.51   |
| 17  | 1     | 1652 | BCR  | C15-C16-C17 | -2.59 | 118.17      | 123.47   |
| 14  | b     | 828  | CLA  | O2A-CGA-O1A | -2.59 | 117.06      | 123.59   |
| 14  | B     | 830  | CLA  | CHD-C1D-ND  | -2.59 | 122.08      | 124.45   |
| 14  | a     | 811  | CLA  | CHB-C4A-NA  | 2.59  | 128.09      | 124.51   |
| 14  | 1     | 1603 | CLA  | CHB-C4A-NA  | 2.59  | 128.09      | 124.51   |
| 14  | A     | 813  | CLA  | CHB-C4A-NA  | 2.58  | 128.09      | 124.51   |
| 14  | B     | 811  | CLA  | CHB-C4A-NA  | 2.58  | 128.09      | 124.51   |
| 14  | b     | 820  | CLA  | CMB-C2B-C3B | 2.58  | 129.51      | 124.68   |
| 14  | a     | 834  | CLA  | C1B-CHB-C4A | -2.58 | 125.00      | 130.12   |
| 14  | A     | 827  | CLA  | C1-C2-C3    | -2.58 | 121.58      | 126.04   |
| 14  | 1     | 1614 | CLA  | CHB-C4A-NA  | 2.58  | 128.08      | 124.51   |
| 14  | a     | 802  | CLA  | C1-C2-C3    | -2.58 | 121.58      | 126.04   |
| 14  | b     | 819  | CLA  | C1B-CHB-C4A | -2.58 | 125.00      | 130.12   |
| 14  | l     | 205  | CLA  | C1B-CHB-C4A | -2.58 | 125.00      | 130.12   |
| 14  | 2     | 829  | CLA  | C1B-CHB-C4A | -2.58 | 125.00      | 130.12   |
| 14  | 2     | 821  | CLA  | C1B-CHB-C4A | -2.58 | 125.00      | 130.12   |
| 14  | A     | 822  | CLA  | CHB-C4A-NA  | 2.58  | 128.08      | 124.51   |
| 17  | L     | 206  | BCR  | C15-C16-C17 | -2.58 | 118.19      | 123.47   |
| 17  | b     | 849  | BCR  | C16-C15-C14 | -2.58 | 118.19      | 123.47   |
| 14  | 1     | 1628 | CLA  | C1B-CHB-C4A | -2.58 | 125.01      | 130.12   |
| 14  | 2     | 818  | CLA  | CMB-C2B-C3B | 2.58  | 129.50      | 124.68   |
| 14  | 2     | 820  | CLA  | CMB-C2B-C3B | 2.58  | 129.50      | 124.68   |
| 14  | a     | 822  | CLA  | CHB-C4A-NA  | 2.58  | 128.08      | 124.51   |
| 14  | B     | 808  | CLA  | C1-C2-C3    | -2.58 | 121.58      | 126.04   |
| 14  | a     | 839  | CLA  | C1-C2-C3    | -2.58 | 121.58      | 126.04   |
| 14  | a     | 827  | CLA  | C1B-CHB-C4A | -2.58 | 125.01      | 130.12   |
| 14  | A     | 834  | CLA  | C1B-CHB-C4A | -2.58 | 125.01      | 130.12   |
| 17  | a     | 851  | BCR  | C15-C16-C17 | -2.58 | 118.20      | 123.47   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | M     | 102  | CLA  | CMB-C2B-C3B | 2.58  | 129.50      | 124.68   |
| 14  | a     | 815  | CLA  | CHB-C4A-NA  | 2.58  | 128.07      | 124.51   |
| 14  | 2     | 819  | CLA  | CHB-C4A-NA  | 2.58  | 128.07      | 124.51   |
| 14  | 2     | 808  | CLA  | C1B-CHB-C4A | -2.57 | 125.02      | 130.12   |
| 17  | B     | 845  | BCR  | C27-C26-C25 | 2.57  | 126.47      | 122.73   |
| 14  | B     | 818  | CLA  | C1B-CHB-C4A | -2.57 | 125.02      | 130.12   |
| 14  | B     | 829  | CLA  | C2D-C1D-ND  | -2.57 | 108.21      | 110.10   |
| 14  | 1     | 1635 | CLA  | C1B-CHB-C4A | -2.57 | 125.02      | 130.12   |
| 17  | B     | 848  | BCR  | C16-C15-C14 | -2.57 | 118.20      | 123.47   |
| 17  | a     | 847  | BCR  | C27-C26-C25 | 2.57  | 126.47      | 122.73   |
| 14  | 1     | 1616 | CLA  | CHB-C4A-NA  | 2.57  | 128.07      | 124.51   |
| 14  | L     | 204  | CLA  | C1B-CHB-C4A | -2.57 | 125.02      | 130.12   |
| 14  | 1     | 1608 | CLA  | O1D-CGD-CBD | 2.57  | 129.75      | 124.48   |
| 14  | 1     | 1616 | CLA  | O2D-CGD-O1D | -2.57 | 118.81      | 123.84   |
| 14  | a     | 815  | CLA  | O2D-CGD-O1D | -2.57 | 118.81      | 123.84   |
| 17  | A     | 847  | BCR  | C27-C26-C25 | 2.57  | 126.46      | 122.73   |
| 14  | A     | 839  | CLA  | C1-C2-C3    | -2.57 | 121.60      | 126.04   |
| 14  | b     | 818  | CLA  | CMB-C2B-C3B | 2.57  | 129.49      | 124.68   |
| 14  | b     | 818  | CLA  | O2D-CGD-O1D | -2.57 | 118.82      | 123.84   |
| 17  | B     | 845  | BCR  | C15-C16-C17 | -2.57 | 118.22      | 123.47   |
| 14  | a     | 816  | CLA  | O2D-CGD-O1D | -2.57 | 118.82      | 123.84   |
| 14  | A     | 815  | CLA  | O2D-CGD-O1D | -2.57 | 118.82      | 123.84   |
| 14  | 0     | 206  | CLA  | C1B-CHB-C4A | -2.56 | 125.04      | 130.12   |
| 14  | a     | 802  | CLA  | CHB-C4A-NA  | 2.56  | 128.06      | 124.51   |
| 17  | 0     | 208  | BCR  | C15-C16-C17 | -2.56 | 118.22      | 123.47   |
| 14  | 1     | 1640 | CLA  | C1-C2-C3    | -2.56 | 121.61      | 126.04   |
| 17  | 1     | 1648 | BCR  | C27-C26-C25 | 2.56  | 126.45      | 122.73   |
| 17  | b     | 846  | BCR  | C15-C16-C17 | -2.56 | 118.23      | 123.47   |
| 17  | l     | 207  | BCR  | C15-C16-C17 | -2.56 | 118.23      | 123.47   |
| 14  | 1     | 1640 | CLA  | O2D-CGD-CBD | 2.56  | 115.82      | 111.27   |
| 14  | B     | 828  | CLA  | C1B-CHB-C4A | -2.56 | 125.05      | 130.12   |
| 14  | a     | 816  | CLA  | CHB-C4A-NA  | 2.56  | 128.05      | 124.51   |
| 14  | 1     | 1609 | CLA  | CHB-C4A-NA  | 2.55  | 128.04      | 124.51   |
| 14  | 1     | 1628 | CLA  | C1-C2-C3    | -2.55 | 121.62      | 126.04   |
| 14  | b     | 823  | CLA  | C1B-CHB-C4A | -2.55 | 125.06      | 130.12   |
| 17  | A     | 848  | BCR  | C27-C26-C25 | 2.55  | 126.44      | 122.73   |
| 14  | B     | 825  | CLA  | CHD-C1D-ND  | -2.55 | 122.11      | 124.45   |
| 14  | a     | 827  | CLA  | C1-C2-C3    | -2.55 | 121.63      | 126.04   |
| 14  | 2     | 812  | CLA  | CHB-C4A-NA  | 2.55  | 128.04      | 124.51   |
| 17  | 0     | 201  | BCR  | C27-C26-C25 | 2.55  | 126.44      | 122.73   |
| 14  | 1     | 1628 | CLA  | CAA-C2A-C1A | -2.55 | 103.61      | 111.97   |
| 17  | a     | 848  | BCR  | C27-C26-C25 | 2.55  | 126.44      | 122.73   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 839  | CLA  | O2D-CGD-CBD | 2.55  | 115.80      | 111.27   |
| 17  | 0     | 209  | BCR  | C27-C26-C25 | 2.55  | 126.44      | 122.73   |
| 14  | b     | 829  | CLA  | C1B-CHB-C4A | -2.55 | 125.06      | 130.12   |
| 14  | b     | 836  | CLA  | O2D-CGD-O1D | -2.55 | 118.85      | 123.84   |
| 14  | 1     | 1639 | CLA  | O2D-CGD-O1D | -2.55 | 118.85      | 123.84   |
| 14  | 1     | 1623 | CLA  | C1B-CHB-C4A | -2.55 | 125.07      | 130.12   |
| 14  | a     | 808  | CLA  | CHB-C4A-NA  | 2.55  | 128.04      | 124.51   |
| 14  | a     | 827  | CLA  | CAA-C2A-C1A | -2.55 | 103.62      | 111.97   |
| 14  | b     | 833  | CLA  | CMB-C2B-C3B | 2.55  | 129.44      | 124.68   |
| 14  | 2     | 832  | CLA  | CHB-C4A-NA  | 2.55  | 128.03      | 124.51   |
| 14  | j     | 1302 | CLA  | CHB-C4A-NA  | 2.55  | 128.03      | 124.51   |
| 14  | j     | 1302 | CLA  | CMB-C2B-C3B | 2.55  | 129.44      | 124.68   |
| 14  | F     | 204  | CLA  | C1B-CHB-C4A | -2.54 | 125.08      | 130.12   |
| 14  | 1     | 1638 | CLA  | O2D-CGD-O1D | -2.54 | 118.86      | 123.84   |
| 14  | A     | 827  | CLA  | CAA-C2A-C1A | -2.54 | 103.64      | 111.97   |
| 14  | b     | 830  | CLA  | C2D-C1D-ND  | -2.54 | 108.23      | 110.10   |
| 14  | B     | 831  | CLA  | CHB-C4A-NA  | 2.54  | 128.03      | 124.51   |
| 14  | a     | 813  | CLA  | CHB-C4A-NA  | 2.54  | 128.03      | 124.51   |
| 14  | 2     | 811  | CLA  | O2A-CGA-O1A | -2.54 | 117.18      | 123.59   |
| 14  | A     | 810  | CLA  | O2D-CGD-O1D | -2.54 | 118.87      | 123.84   |
| 14  | B     | 810  | CLA  | O2A-CGA-O1A | -2.54 | 117.18      | 123.59   |
| 17  | l     | 207  | BCR  | C7-C8-C9    | -2.54 | 122.40      | 126.23   |
| 14  | b     | 830  | CLA  | O2D-CGD-CBD | 2.54  | 115.78      | 111.27   |
| 14  | J     | 101  | CLA  | CHB-C4A-NA  | 2.54  | 128.02      | 124.51   |
| 14  | A     | 837  | CLA  | O2D-CGD-O1D | -2.54 | 118.88      | 123.84   |
| 14  | A     | 836  | CLA  | C1B-CHB-C4A | -2.54 | 125.09      | 130.12   |
| 14  | 9     | 101  | CLA  | CHB-C4A-NA  | 2.54  | 128.02      | 124.51   |
| 14  | A     | 822  | CLA  | C1B-CHB-C4A | -2.54 | 125.09      | 130.12   |
| 14  | 2     | 833  | CLA  | CMB-C2B-C3B | 2.54  | 129.42      | 124.68   |
| 14  | B     | 832  | CLA  | CMB-C2B-C3B | 2.54  | 129.42      | 124.68   |
| 14  | A     | 808  | CLA  | CHB-C4A-NA  | 2.54  | 128.02      | 124.51   |
| 14  | B     | 835  | CLA  | O2D-CGD-O1D | -2.53 | 118.88      | 123.84   |
| 14  | b     | 812  | CLA  | CHB-C4A-NA  | 2.53  | 128.02      | 124.51   |
| 14  | 2     | 836  | CLA  | O2D-CGD-O1D | -2.53 | 118.88      | 123.84   |
| 14  | 2     | 823  | CLA  | C1B-CHB-C4A | -2.53 | 125.10      | 130.12   |
| 14  | B     | 818  | CLA  | CHB-C4A-NA  | 2.53  | 128.01      | 124.51   |
| 14  | f     | 203  | CLA  | C1B-CHB-C4A | -2.53 | 125.10      | 130.12   |
| 14  | 6     | 203  | CLA  | C1B-CHB-C4A | -2.53 | 125.11      | 130.12   |
| 14  | A     | 836  | CLA  | CHB-C4A-NA  | 2.53  | 128.01      | 124.51   |
| 14  | a     | 837  | CLA  | O2D-CGD-O1D | -2.53 | 118.89      | 123.84   |
| 17  | f     | 202  | BCR  | C27-C26-C25 | 2.53  | 126.40      | 122.73   |
| 14  | b     | 811  | CLA  | O2A-CGA-O1A | -2.53 | 117.21      | 123.59   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | 8     | 1302 | CLA  | CHB-C4A-NA  | 2.53  | 128.01      | 124.51   |
| 17  | F     | 202  | BCR  | C27-C26-C25 | 2.53  | 126.40      | 122.73   |
| 14  | B     | 822  | CLA  | C1B-CHB-C4A | -2.52 | 125.12      | 130.12   |
| 14  | B     | 829  | CLA  | O2D-CGD-CBD | 2.52  | 115.75      | 111.27   |
| 14  | 8     | 1302 | CLA  | CMB-C2B-C3B | 2.52  | 129.40      | 124.68   |
| 14  | b     | 832  | CLA  | CHB-C4A-NA  | 2.52  | 128.00      | 124.51   |
| 14  | 1     | 1625 | CLA  | CHB-C4A-NA  | 2.52  | 128.00      | 124.51   |
| 14  | 2     | 826  | CLA  | CHD-C1D-ND  | -2.52 | 122.14      | 124.45   |
| 14  | A     | 855  | CLA  | C1B-CHB-C4A | -2.52 | 125.12      | 130.12   |
| 14  | b     | 819  | CLA  | CHB-C4A-NA  | 2.52  | 128.00      | 124.51   |
| 14  | B     | 839  | CLA  | CMB-C2B-C3B | 2.52  | 129.39      | 124.68   |
| 17  | 0     | 208  | BCR  | C29-C30-C25 | 2.52  | 114.36      | 110.48   |
| 14  | 2     | 840  | CLA  | CMB-C2B-C3B | 2.52  | 129.39      | 124.68   |
| 17  | L     | 206  | BCR  | C7-C8-C9    | -2.52 | 122.43      | 126.23   |
| 17  | 1     | 1649 | BCR  | C27-C26-C25 | 2.52  | 126.39      | 122.73   |
| 14  | b     | 830  | CLA  | CHB-C4A-NA  | 2.52  | 127.99      | 124.51   |
| 14  | 2     | 835  | CLA  | CHB-C4A-NA  | 2.52  | 127.99      | 124.51   |
| 14  | a     | 822  | CLA  | C1B-CHB-C4A | -2.51 | 125.14      | 130.12   |
| 14  | 2     | 802  | CLA  | C1B-CHB-C4A | -2.51 | 125.14      | 130.12   |
| 14  | 2     | 830  | CLA  | CHB-C4A-NA  | 2.51  | 127.99      | 124.51   |
| 14  | 2     | 817  | CLA  | O2D-CGD-CBD | 2.51  | 115.73      | 111.27   |
| 14  | 2     | 830  | CLA  | O2D-CGD-CBD | 2.51  | 115.73      | 111.27   |
| 14  | 1     | 1637 | CLA  | CHB-C4A-NA  | 2.51  | 127.99      | 124.51   |
| 14  | b     | 840  | CLA  | CMB-C2B-C3B | 2.51  | 129.38      | 124.68   |
| 14  | A     | 832  | CLA  | C1B-CHB-C4A | -2.51 | 125.14      | 130.12   |
| 14  | 1     | 1642 | CLA  | C1B-CHB-C4A | -2.51 | 125.14      | 130.12   |
| 14  | A     | 827  | CLA  | CHB-C4A-NA  | 2.51  | 127.98      | 124.51   |
| 14  | a     | 816  | CLA  | C1B-CHB-C4A | -2.51 | 125.15      | 130.12   |
| 14  | 1     | 1637 | CLA  | C1B-CHB-C4A | -2.51 | 125.15      | 130.12   |
| 17  | L     | 207  | BCR  | C27-C26-C25 | 2.51  | 126.37      | 122.73   |
| 14  | J     | 101  | CLA  | CMB-C2B-C3B | 2.51  | 129.37      | 124.68   |
| 14  | B     | 829  | CLA  | CHB-C4A-NA  | 2.51  | 127.98      | 124.51   |
| 17  | 6     | 202  | BCR  | C27-C26-C25 | 2.51  | 126.37      | 122.73   |
| 14  | 2     | 806  | CLA  | CHB-C4A-NA  | 2.51  | 127.98      | 124.51   |
| 14  | a     | 836  | CLA  | C1B-CHB-C4A | -2.51 | 125.16      | 130.12   |
| 14  | K     | 101  | CLA  | CHB-C4A-NA  | 2.51  | 127.98      | 124.51   |
| 14  | b     | 817  | CLA  | O2D-CGD-CBD | 2.50  | 115.72      | 111.27   |
| 17  | B     | 848  | BCR  | C27-C26-C25 | 2.50  | 126.37      | 122.73   |
| 17  | b     | 849  | BCR  | C27-C26-C25 | 2.50  | 126.36      | 122.73   |
| 17  | 1     | 1649 | BCR  | C15-C14-C13 | -2.50 | 123.74      | 127.31   |
| 14  | b     | 835  | CLA  | CHB-C4A-NA  | 2.50  | 127.97      | 124.51   |
| 14  | b     | 802  | CLA  | C1B-CHB-C4A | -2.50 | 125.16      | 130.12   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | A     | 848  | BCR  | C15-C14-C13 | -2.50 | 123.74      | 127.31   |
| 14  | a     | 809  | CLA  | C1B-CHB-C4A | -2.50 | 125.17      | 130.12   |
| 14  | a     | 836  | CLA  | CHB-C4A-NA  | 2.50  | 127.96      | 124.51   |
| 17  | a     | 848  | BCR  | C15-C14-C13 | -2.50 | 123.75      | 127.31   |
| 14  | B     | 816  | CLA  | O2D-CGD-CBD | 2.49  | 115.70      | 111.27   |
| 14  | B     | 834  | CLA  | CHB-C4A-NA  | 2.49  | 127.96      | 124.51   |
| 14  | a     | 824  | CLA  | CHB-C4A-NA  | 2.49  | 127.96      | 124.51   |
| 14  | 1     | 1610 | CLA  | C1B-CHB-C4A | -2.49 | 125.18      | 130.12   |
| 14  | a     | 810  | CLA  | O2D-CGD-O1D | -2.49 | 118.97      | 123.84   |
| 17  | b     | 847  | BCR  | C38-C26-C25 | -2.49 | 121.73      | 124.53   |
| 14  | A     | 816  | CLA  | CHB-C4A-NA  | 2.49  | 127.95      | 124.51   |
| 17  | 0     | 208  | BCR  | C7-C8-C9    | -2.49 | 122.47      | 126.23   |
| 14  | A     | 814  | CLA  | CMB-C2B-C3B | 2.49  | 129.34      | 124.68   |
| 14  | a     | 814  | CLA  | CMB-C2B-C3B | 2.49  | 129.34      | 124.68   |
| 14  | A     | 841  | CLA  | C1B-CHB-C4A | -2.49 | 125.19      | 130.12   |
| 14  | 1     | 1607 | CLA  | O2A-CGA-O1A | -2.49 | 117.31      | 123.59   |
| 14  | a     | 827  | CLA  | CHB-C4A-NA  | 2.49  | 127.95      | 124.51   |
| 14  | a     | 841  | CLA  | C1B-CHB-C4A | -2.49 | 125.19      | 130.12   |
| 14  | 1     | 1611 | CLA  | O2D-CGD-O1D | -2.49 | 118.98      | 123.84   |
| 14  | k     | 101  | CLA  | CHB-C4A-NA  | 2.48  | 127.95      | 124.51   |
| 14  | a     | 832  | CLA  | C1B-CHB-C4A | -2.48 | 125.20      | 130.12   |
| 14  | 1     | 1615 | CLA  | CMB-C2B-C3B | 2.48  | 129.32      | 124.68   |
| 17  | 2     | 846  | BCR  | C38-C26-C25 | -2.48 | 121.74      | 124.53   |
| 14  | A     | 816  | CLA  | C1B-CHB-C4A | -2.48 | 125.20      | 130.12   |
| 17  | 2     | 849  | BCR  | C27-C26-C25 | 2.48  | 126.33      | 122.73   |
| 14  | A     | 809  | CLA  | C1B-CHB-C4A | -2.48 | 125.20      | 130.12   |
| 14  | 1     | 1633 | CLA  | C1B-CHB-C4A | -2.48 | 125.20      | 130.12   |
| 14  | 0     | 207  | CLA  | C1B-CHB-C4A | -2.48 | 125.20      | 130.12   |
| 14  | a     | 840  | CLA  | CMB-C2B-C3B | 2.48  | 129.32      | 124.68   |
| 14  | b     | 808  | CLA  | CHB-C4A-NA  | 2.48  | 127.94      | 124.51   |
| 14  | b     | 806  | CLA  | CHB-C4A-NA  | 2.48  | 127.94      | 124.51   |
| 14  | 1     | 1617 | CLA  | CHB-C4A-NA  | 2.48  | 127.94      | 124.51   |
| 14  | b     | 827  | CLA  | CHB-C4A-NA  | 2.47  | 127.93      | 124.51   |
| 14  | 2     | 814  | CLA  | C1B-CHB-C4A | -2.47 | 125.22      | 130.12   |
| 14  | B     | 813  | CLA  | C1B-CHB-C4A | -2.47 | 125.22      | 130.12   |
| 17  | 6     | 204  | BCR  | C38-C26-C25 | -2.47 | 121.75      | 124.53   |
| 17  | L     | 206  | BCR  | C29-C30-C25 | 2.47  | 114.28      | 110.48   |
| 18  | A     | 853  | LHG  | O8-C23-C24  | 2.47  | 119.66      | 111.91   |
| 17  | b     | 846  | BCR  | C38-C26-C25 | -2.47 | 121.75      | 124.53   |
| 17  | y     | 102  | BCR  | C27-C26-C25 | 2.47  | 126.32      | 122.73   |
| 14  | 1     | 1641 | CLA  | CMB-C2B-C3B | 2.47  | 129.30      | 124.68   |
| 14  | a     | 817  | CLA  | CHB-C4A-NA  | 2.47  | 127.93      | 124.51   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | 1     | 1628 | CLA  | CHB-C4A-NA  | 2.47  | 127.92      | 124.51   |
| 17  | f     | 202  | BCR  | C38-C26-C25 | -2.47 | 121.76      | 124.53   |
| 14  | x     | 1701 | CLA  | C1B-CHB-C4A | -2.47 | 125.23      | 130.12   |
| 14  | B     | 826  | CLA  | C1-C2-C3    | -2.47 | 121.78      | 126.04   |
| 14  | 1     | 1618 | CLA  | CHB-C4A-NA  | 2.47  | 127.92      | 124.51   |
| 14  | 2     | 820  | CLA  | O2A-CGA-O1A | -2.46 | 117.38      | 123.59   |
| 14  | B     | 805  | CLA  | CHB-C4A-NA  | 2.46  | 127.92      | 124.51   |
| 14  | B     | 803  | CLA  | C1B-CHB-C4A | -2.46 | 125.24      | 130.12   |
| 17  | l     | 207  | BCR  | C29-C30-C25 | 2.46  | 114.27      | 110.48   |
| 17  | m     | 102  | BCR  | C15-C16-C17 | -2.46 | 118.43      | 123.47   |
| 14  | b     | 805  | CLA  | C1B-CHB-C4A | -2.46 | 125.24      | 130.12   |
| 17  | m     | 102  | BCR  | C27-C26-C25 | 2.46  | 126.30      | 122.73   |
| 14  | b     | 814  | CLA  | C1B-CHB-C4A | -2.46 | 125.25      | 130.12   |
| 14  | 1     | 1644 | CLA  | C4-C3-C5    | 2.46  | 119.41      | 115.27   |
| 14  | A     | 825  | CLA  | C1B-CHB-C4A | -2.46 | 125.25      | 130.12   |
| 18  | a     | 853  | LHG  | O8-C23-C24  | 2.46  | 119.61      | 111.91   |
| 14  | A     | 814  | CLA  | C1B-CHB-C4A | -2.46 | 125.25      | 130.12   |
| 14  | A     | 806  | CLA  | O2A-CGA-O1A | -2.46 | 117.39      | 123.59   |
| 14  | B     | 828  | CLA  | CMB-C2B-C3B | 2.46  | 129.27      | 124.68   |
| 14  | 1     | 1615 | CLA  | C1B-CHB-C4A | -2.46 | 125.25      | 130.12   |
| 14  | B     | 817  | CLA  | C1B-CHB-C4A | -2.45 | 125.25      | 130.12   |
| 14  | B     | 804  | CLA  | C1B-CHB-C4A | -2.45 | 125.26      | 130.12   |
| 14  | b     | 818  | CLA  | C1B-CHB-C4A | -2.45 | 125.26      | 130.12   |
| 14  | 1     | 1617 | CLA  | C1B-CHB-C4A | -2.45 | 125.26      | 130.12   |
| 14  | l     | 206  | CLA  | C1B-CHB-C4A | -2.45 | 125.26      | 130.12   |
| 14  | a     | 844  | CLA  | CHB-C4A-NA  | 2.45  | 127.91      | 124.51   |
| 17  | F     | 202  | BCR  | C38-C26-C25 | -2.45 | 121.77      | 124.53   |
| 17  | I     | 101  | BCR  | C27-C26-C25 | 2.45  | 126.29      | 122.73   |
| 14  | b     | 838  | CLA  | CMB-C2B-C3B | 2.45  | 129.27      | 124.68   |
| 14  | A     | 824  | CLA  | CHB-C4A-NA  | 2.45  | 127.90      | 124.51   |
| 14  | A     | 840  | CLA  | CMB-C2B-C3B | 2.45  | 129.27      | 124.68   |
| 14  | L     | 205  | CLA  | C1B-CHB-C4A | -2.45 | 125.26      | 130.12   |
| 14  | a     | 806  | CLA  | O2A-CGA-O1A | -2.45 | 117.41      | 123.59   |
| 14  | 2     | 805  | CLA  | C1B-CHB-C4A | -2.45 | 125.26      | 130.12   |
| 14  | B     | 808  | CLA  | CHB-C4A-NA  | 2.45  | 127.90      | 124.51   |
| 17  | f     | 204  | BCR  | C38-C26-C25 | -2.45 | 121.78      | 124.53   |
| 14  | 1     | 1624 | CLA  | C1B-CHB-C4A | -2.45 | 125.27      | 130.12   |
| 17  | M     | 103  | BCR  | C27-C26-C25 | 2.45  | 126.29      | 122.73   |
| 14  | B     | 809  | CLA  | O1D-CGD-CBD | 2.45  | 129.49      | 124.48   |
| 14  | a     | 814  | CLA  | C1B-CHB-C4A | -2.45 | 125.27      | 130.12   |
| 17  | 0     | 203  | BCR  | C8-C7-C6    | -2.45 | 120.33      | 127.20   |
| 14  | A     | 812  | CLA  | C1B-CHB-C4A | -2.45 | 125.27      | 130.12   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | 1     | 1625 | CLA  | C1B-CHB-C4A | -2.45 | 125.27      | 130.12   |
| 14  | b     | 804  | CLA  | C1B-CHB-C4A | -2.45 | 125.27      | 130.12   |
| 14  | b     | 820  | CLA  | O2A-CGA-O1A | -2.45 | 117.42      | 123.59   |
| 14  | b     | 842  | CLA  | CMB-C2B-C1B | -2.45 | 124.70      | 128.46   |
| 14  | b     | 810  | CLA  | O1D-CGD-CBD | 2.45  | 129.49      | 124.48   |
| 14  | a     | 825  | CLA  | C1B-CHB-C4A | -2.45 | 125.27      | 130.12   |
| 14  | 8     | 1301 | CLA  | C1B-CHB-C4A | -2.44 | 125.28      | 130.12   |
| 14  | B     | 807  | CLA  | CHB-C4A-NA  | 2.44  | 127.89      | 124.51   |
| 17  | L     | 201  | BCR  | C8-C7-C6    | -2.44 | 120.34      | 127.20   |
| 18  | 1     | 1654 | LHG  | O8-C23-C24  | 2.44  | 119.58      | 111.91   |
| 14  | b     | 810  | CLA  | C1B-CHB-C4A | -2.44 | 125.28      | 130.12   |
| 14  | b     | 829  | CLA  | CMB-C2B-C3B | 2.44  | 129.25      | 124.68   |
| 14  | 2     | 825  | CLA  | C2A-C1A-CHA | 2.44  | 128.13      | 123.86   |
| 14  | X     | 1701 | CLA  | C1B-CHB-C4A | -2.44 | 125.28      | 130.12   |
| 14  | a     | 823  | CLA  | C1B-CHB-C4A | -2.44 | 125.28      | 130.12   |
| 17  | B     | 851  | BCR  | C11-C10-C9  | -2.44 | 123.83      | 127.31   |
| 14  | 2     | 829  | CLA  | CMB-C2B-C3B | 2.44  | 129.24      | 124.68   |
| 14  | F     | 203  | CLA  | C1B-CHB-C4A | -2.44 | 125.28      | 130.12   |
| 17  | 2     | 847  | BCR  | C38-C26-C25 | -2.44 | 121.79      | 124.53   |
| 14  | 2     | 808  | CLA  | CHB-C4A-NA  | 2.44  | 127.89      | 124.51   |
| 14  | 2     | 818  | CLA  | C1B-CHB-C4A | -2.44 | 125.28      | 130.12   |
| 14  | 2     | 827  | CLA  | C1-C2-C3    | -2.44 | 121.82      | 126.04   |
| 17  | y     | 102  | BCR  | C15-C16-C17 | -2.44 | 118.48      | 123.47   |
| 14  | 2     | 809  | CLA  | CHB-C4A-NA  | 2.44  | 127.89      | 124.51   |
| 14  | A     | 823  | CLA  | C1B-CHB-C4A | -2.44 | 125.29      | 130.12   |
| 14  | A     | 817  | CLA  | CHB-C4A-NA  | 2.44  | 127.88      | 124.51   |
| 14  | A     | 843  | CLA  | C4-C3-C5    | 2.44  | 119.37      | 115.27   |
| 17  | M     | 103  | BCR  | C15-C16-C17 | -2.44 | 118.48      | 123.47   |
| 14  | 1     | 1622 | CLA  | O2A-CGA-O1A | -2.44 | 117.44      | 123.59   |
| 14  | A     | 802  | CLA  | C1B-CHB-C4A | -2.44 | 125.29      | 130.12   |
| 14  | j     | 1301 | CLA  | C1B-CHB-C4A | -2.44 | 125.29      | 130.12   |
| 14  | a     | 806  | CLA  | C1B-CHB-C4A | -2.44 | 125.29      | 130.12   |
| 14  | 1     | 1626 | CLA  | C1B-CHB-C4A | -2.44 | 125.29      | 130.12   |
| 14  | a     | 818  | CLA  | O2A-CGA-O1A | -2.44 | 117.44      | 123.59   |
| 14  | 1     | 1607 | CLA  | C1B-CHB-C4A | -2.44 | 125.29      | 130.12   |
| 14  | 1     | 1619 | CLA  | O2A-CGA-O1A | -2.43 | 117.45      | 123.59   |
| 14  | B     | 840  | CLA  | CHB-C4A-NA  | 2.43  | 127.88      | 124.51   |
| 14  | 2     | 842  | CLA  | CMB-C2B-C1B | -2.43 | 124.72      | 128.46   |
| 14  | B     | 809  | CLA  | C1B-CHB-C4A | -2.43 | 125.30      | 130.12   |
| 17  | 6     | 202  | BCR  | C38-C26-C25 | -2.43 | 121.80      | 124.53   |
| 14  | 1     | 1645 | CLA  | CHB-C4A-NA  | 2.43  | 127.88      | 124.51   |
| 14  | B     | 841  | CLA  | CMB-C2B-C1B | -2.43 | 124.73      | 128.46   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 824  | CLA  | C2A-C1A-CHA | 2.43  | 128.11      | 123.86   |
| 14  | B     | 837  | CLA  | CMB-C2B-C3B | 2.43  | 129.23      | 124.68   |
| 14  | a     | 835  | CLA  | CMB-C2B-C1B | -2.43 | 124.73      | 128.46   |
| 14  | 2     | 841  | CLA  | CHB-C4A-NA  | 2.43  | 127.87      | 124.51   |
| 17  | y     | 102  | BCR  | C37-C22-C21 | -2.43 | 119.52      | 122.92   |
| 14  | A     | 806  | CLA  | C1B-CHB-C4A | -2.43 | 125.31      | 130.12   |
| 14  | 2     | 838  | CLA  | CMB-C2B-C3B | 2.43  | 129.22      | 124.68   |
| 14  | L     | 203  | CLA  | C1B-CHB-C4A | -2.43 | 125.31      | 130.12   |
| 14  | A     | 821  | CLA  | O2A-CGA-O1A | -2.43 | 117.47      | 123.59   |
| 14  | B     | 819  | CLA  | O2A-CGA-O1A | -2.43 | 117.47      | 123.59   |
| 17  | B     | 845  | BCR  | C38-C26-C25 | -2.43 | 121.80      | 124.53   |
| 14  | 1     | 1613 | CLA  | C1B-CHB-C4A | -2.43 | 125.31      | 130.12   |
| 14  | a     | 821  | CLA  | O2A-CGA-O1A | -2.43 | 117.47      | 123.59   |
| 17  | 8     | 1306 | BCR  | C11-C10-C9  | -2.43 | 123.85      | 127.31   |
| 17  | 7     | 101  | BCR  | C27-C26-C25 | 2.43  | 126.25      | 122.73   |
| 17  | l     | 202  | BCR  | C8-C7-C6    | -2.43 | 120.39      | 127.20   |
| 17  | 9     | 102  | BCR  | C36-C18-C19 | 2.42  | 121.90      | 118.08   |
| 14  | a     | 824  | CLA  | C1B-CHB-C4A | -2.42 | 125.32      | 130.12   |
| 17  | 0     | 208  | BCR  | C24-C23-C22 | -2.42 | 122.57      | 126.23   |
| 14  | A     | 810  | CLA  | CHB-C4A-NA  | 2.42  | 127.86      | 124.51   |
| 14  | k     | 103  | CLA  | CHB-C4A-NA  | 2.42  | 127.86      | 124.51   |
| 17  | B     | 846  | BCR  | C38-C26-C25 | -2.42 | 121.81      | 124.53   |
| 14  | 8     | 1303 | CLA  | C1B-CHB-C4A | -2.42 | 125.32      | 130.12   |
| 14  | b     | 827  | CLA  | C1-C2-C3    | -2.42 | 121.85      | 126.04   |
| 14  | a     | 843  | CLA  | C4-C3-C5    | 2.42  | 119.34      | 115.27   |
| 17  | 6     | 204  | BCR  | C27-C26-C25 | 2.42  | 126.25      | 122.73   |
| 14  | a     | 810  | CLA  | CHB-C4A-NA  | 2.42  | 127.86      | 124.51   |
| 14  | 2     | 804  | CLA  | C1B-CHB-C4A | -2.42 | 125.32      | 130.12   |
| 14  | b     | 831  | CLA  | CMB-C2B-C3B | 2.42  | 129.21      | 124.68   |
| 14  | f     | 201  | CLA  | CHB-C4A-NA  | 2.42  | 127.86      | 124.51   |
| 14  | l     | 204  | CLA  | C1B-CHB-C4A | -2.42 | 125.32      | 130.12   |
| 14  | 1     | 1603 | CLA  | C1B-CHB-C4A | -2.42 | 125.32      | 130.12   |
| 14  | z     | 102  | CLA  | C1B-CHB-C4A | -2.42 | 125.32      | 130.12   |
| 14  | A     | 844  | CLA  | CHB-C4A-NA  | 2.42  | 127.86      | 124.51   |
| 17  | F     | 205  | BCR  | C38-C26-C25 | -2.42 | 121.81      | 124.53   |
| 14  | a     | 842  | CLA  | C1-C2-C3    | -2.42 | 121.86      | 126.04   |
| 14  | A     | 842  | CLA  | C1-C2-C3    | -2.42 | 121.86      | 126.04   |
| 14  | b     | 831  | CLA  | C1B-CHB-C4A | -2.42 | 125.33      | 130.12   |
| 14  | A     | 818  | CLA  | O2A-CGA-O1A | -2.42 | 117.49      | 123.59   |
| 20  | B     | 849  | LMG  | C1-O6-C5    | -2.42 | 108.94      | 113.69   |
| 14  | A     | 815  | CLA  | C1B-CHB-C4A | -2.42 | 125.33      | 130.12   |
| 17  | i     | 101  | BCR  | C27-C26-C25 | 2.42  | 126.24      | 122.73   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 825  | CLA  | CHB-C4A-NA  | 2.42  | 127.85      | 124.51   |
| 14  | B     | 826  | CLA  | CHB-C4A-NA  | 2.42  | 127.85      | 124.51   |
| 14  | A     | 842  | CLA  | C1B-CHB-C4A | -2.41 | 125.33      | 130.12   |
| 14  | 2     | 831  | CLA  | CMB-C2B-C3B | 2.41  | 129.20      | 124.68   |
| 14  | 6     | 201  | CLA  | CHB-C4A-NA  | 2.41  | 127.85      | 124.51   |
| 14  | b     | 841  | CLA  | CHB-C4A-NA  | 2.41  | 127.85      | 124.51   |
| 14  | B     | 830  | CLA  | CMB-C2B-C3B | 2.41  | 129.19      | 124.68   |
| 17  | k     | 102  | BCR  | C36-C18-C19 | 2.41  | 121.88      | 118.08   |
| 14  | B     | 840  | CLA  | C1B-CHB-C4A | -2.41 | 125.34      | 130.12   |
| 20  | 2     | 850  | LMG  | C1-O6-C5    | -2.41 | 108.95      | 113.69   |
| 14  | 1     | 1633 | CLA  | CHB-C4A-NA  | 2.41  | 127.85      | 124.51   |
| 14  | b     | 825  | CLA  | C2A-C1A-CHA | 2.41  | 128.08      | 123.86   |
| 14  | B     | 814  | CLA  | CHD-C1D-ND  | -2.41 | 122.24      | 124.45   |
| 17  | f     | 204  | BCR  | C27-C26-C25 | 2.41  | 126.23      | 122.73   |
| 14  | a     | 842  | CLA  | C1B-CHB-C4A | -2.41 | 125.34      | 130.12   |
| 14  | a     | 802  | CLA  | C1B-CHB-C4A | -2.41 | 125.35      | 130.12   |
| 14  | 9     | 103  | CLA  | CHB-C4A-NA  | 2.41  | 127.84      | 124.51   |
| 14  | 1     | 1636 | CLA  | CMB-C2B-C1B | -2.41 | 124.77      | 128.46   |
| 14  | A     | 840  | CLA  | C1B-CHB-C4A | -2.41 | 125.35      | 130.12   |
| 14  | A     | 824  | CLA  | C1B-CHB-C4A | -2.40 | 125.35      | 130.12   |
| 14  | a     | 836  | CLA  | CMB-C2B-C3B | 2.40  | 129.18      | 124.68   |
| 14  | j     | 1303 | CLA  | C1B-CHB-C4A | -2.40 | 125.36      | 130.12   |
| 14  | 1     | 1643 | CLA  | C1-C2-C3    | -2.40 | 121.89      | 126.04   |
| 14  | a     | 815  | CLA  | C1B-CHB-C4A | -2.40 | 125.36      | 130.12   |
| 14  | 2     | 803  | CLA  | C1B-CHB-C4A | -2.40 | 125.36      | 130.12   |
| 17  | F     | 205  | BCR  | C27-C26-C25 | 2.40  | 126.22      | 122.73   |
| 14  | a     | 836  | CLA  | C4-C3-C5    | 2.40  | 119.31      | 115.27   |
| 14  | 2     | 810  | CLA  | O1D-CGD-CBD | 2.40  | 129.40      | 124.48   |
| 14  | a     | 812  | CLA  | C1B-CHB-C4A | -2.40 | 125.36      | 130.12   |
| 14  | 2     | 841  | CLA  | C1B-CHB-C4A | -2.40 | 125.36      | 130.12   |
| 17  | k     | 102  | BCR  | C38-C26-C25 | -2.40 | 121.83      | 124.53   |
| 14  | B     | 830  | CLA  | C1B-CHB-C4A | -2.40 | 125.36      | 130.12   |
| 14  | A     | 842  | CLA  | CHB-C4A-NA  | 2.40  | 127.83      | 124.51   |
| 14  | 2     | 827  | CLA  | CHB-C4A-NA  | 2.40  | 127.83      | 124.51   |
| 14  | 2     | 810  | CLA  | C1B-CHB-C4A | -2.40 | 125.37      | 130.12   |
| 14  | J     | 102  | CLA  | C1B-CHB-C4A | -2.40 | 125.37      | 130.12   |
| 14  | K     | 103  | CLA  | CHB-C4A-NA  | 2.40  | 127.83      | 124.51   |
| 17  | m     | 102  | BCR  | C37-C22-C21 | -2.40 | 119.56      | 122.92   |
| 14  | 1     | 1643 | CLA  | C1B-CHB-C4A | -2.40 | 125.37      | 130.12   |
| 14  | 0     | 205  | CLA  | C1B-CHB-C4A | -2.40 | 125.37      | 130.12   |
| 14  | a     | 832  | CLA  | CHB-C4A-NA  | 2.40  | 127.83      | 124.51   |
| 17  | L     | 206  | BCR  | C24-C23-C22 | -2.40 | 122.61      | 126.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | K     | 102  | BCR  | C38-C26-C25 | -2.40 | 121.84      | 124.53   |
| 17  | K     | 102  | BCR  | C36-C18-C19 | 2.40  | 121.85      | 118.08   |
| 14  | b     | 841  | CLA  | C1B-CHB-C4A | -2.39 | 125.37      | 130.12   |
| 14  | F     | 201  | CLA  | CHB-C4A-NA  | 2.39  | 127.82      | 124.51   |
| 20  | b     | 850  | LMG  | C1-O6-C5    | -2.39 | 109.00      | 113.69   |
| 14  | b     | 809  | CLA  | CHB-C4A-NA  | 2.39  | 127.82      | 124.51   |
| 14  | l     | 1601 | CLA  | C1B-CHB-C4A | -2.39 | 125.39      | 130.12   |
| 14  | l     | 1641 | CLA  | C1B-CHB-C4A | -2.39 | 125.39      | 130.12   |
| 14  | a     | 825  | CLA  | CHB-C4A-NA  | 2.39  | 127.81      | 124.51   |
| 14  | b     | 815  | CLA  | CHD-C1D-ND  | -2.39 | 122.26      | 124.45   |
| 17  | l     | 207  | BCR  | C24-C23-C22 | -2.39 | 122.63      | 126.23   |
| 14  | 1     | 1637 | CLA  | CMB-C2B-C3B | 2.39  | 129.14      | 124.68   |
| 14  | 1     | 1616 | CLA  | C1B-CHB-C4A | -2.39 | 125.39      | 130.12   |
| 14  | A     | 835  | CLA  | CMB-C2B-C1B | -2.39 | 124.80      | 128.46   |
| 14  | 2     | 831  | CLA  | C1B-CHB-C4A | -2.39 | 125.39      | 130.12   |
| 14  | f     | 201  | CLA  | C1B-CHB-C4A | -2.38 | 125.39      | 130.12   |
| 14  | 2     | 815  | CLA  | CHD-C1D-ND  | -2.38 | 122.26      | 124.45   |
| 14  | A     | 830  | CLA  | C1B-CHB-C4A | -2.38 | 125.40      | 130.12   |
| 14  | A     | 836  | CLA  | CMB-C2B-C3B | 2.38  | 129.13      | 124.68   |
| 14  | j     | 1302 | CLA  | C1B-CHB-C4A | -2.38 | 125.40      | 130.12   |
| 17  | 9     | 102  | BCR  | C38-C26-C25 | -2.38 | 121.86      | 124.53   |
| 14  | 1     | 1611 | CLA  | CHB-C4A-NA  | 2.38  | 127.80      | 124.51   |
| 14  | A     | 857  | CLA  | C1B-CHB-C4A | -2.38 | 125.41      | 130.12   |
| 14  | a     | 840  | CLA  | C1B-CHB-C4A | -2.38 | 125.41      | 130.12   |
| 14  | a     | 844  | CLA  | C1B-CHB-C4A | -2.38 | 125.41      | 130.12   |
| 14  | 1     | 1637 | CLA  | C4-C3-C5    | 2.38  | 119.27      | 115.27   |
| 14  | M     | 102  | CLA  | C1B-CHB-C4A | -2.38 | 125.41      | 130.12   |
| 17  | 2     | 848  | BCR  | C38-C26-C25 | -2.38 | 121.86      | 124.53   |
| 17  | 1     | 1649 | BCR  | C15-C16-C17 | -2.38 | 118.61      | 123.47   |
| 14  | 1     | 1627 | CLA  | CHB-C4A-NA  | 2.38  | 127.80      | 124.51   |
| 17  | b     | 852  | BCR  | C11-C10-C9  | -2.38 | 123.92      | 127.31   |
| 14  | x     | 1701 | CLA  | CHB-C4A-NA  | 2.37  | 127.80      | 124.51   |
| 17  | B     | 847  | BCR  | C38-C26-C25 | -2.37 | 121.86      | 124.53   |
| 17  | A     | 848  | BCR  | C15-C16-C17 | -2.37 | 118.61      | 123.47   |
| 17  | K     | 104  | BCR  | C2-C1-C6    | 2.37  | 114.13      | 110.48   |
| 14  | B     | 802  | CLA  | C1B-CHB-C4A | -2.37 | 125.42      | 130.12   |
| 14  | J     | 101  | CLA  | C1B-CHB-C4A | -2.37 | 125.42      | 130.12   |
| 17  | k     | 104  | BCR  | C2-C1-C6    | 2.37  | 114.13      | 110.48   |
| 14  | 1     | 1632 | CLA  | C1B-CHB-C4A | -2.37 | 125.43      | 130.12   |
| 14  | a     | 826  | CLA  | CHB-C4A-NA  | 2.37  | 127.79      | 124.51   |
| 14  | b     | 834  | CLA  | C1B-CHB-C4A | -2.37 | 125.43      | 130.12   |
| 14  | 1     | 1626 | CLA  | CHB-C4A-NA  | 2.37  | 127.79      | 124.51   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 805  | CLA  | C1B-CHB-C4A | -2.37 | 125.43      | 130.12   |
| 14  | 1     | 1630 | CLA  | CHB-C4A-NA  | 2.37  | 127.78      | 124.51   |
| 14  | B     | 833  | CLA  | C1B-CHB-C4A | -2.37 | 125.43      | 130.12   |
| 14  | A     | 837  | CLA  | C1B-CHB-C4A | -2.36 | 125.44      | 130.12   |
| 17  | M     | 103  | BCR  | C37-C22-C21 | -2.36 | 119.61      | 122.92   |
| 14  | A     | 836  | CLA  | C4-C3-C5    | 2.36  | 119.25      | 115.27   |
| 14  | A     | 805  | CLA  | C1B-CHB-C4A | -2.36 | 125.44      | 130.12   |
| 14  | b     | 827  | CLA  | C1B-CHB-C4A | -2.36 | 125.44      | 130.12   |
| 14  | 6     | 201  | CLA  | C1B-CHB-C4A | -2.36 | 125.44      | 130.12   |
| 14  | B     | 820  | CLA  | CHB-C4A-NA  | 2.36  | 127.78      | 124.51   |
| 14  | 1     | 1634 | CLA  | CHB-C4A-NA  | 2.36  | 127.78      | 124.51   |
| 14  | a     | 834  | CLA  | CHD-C1D-ND  | -2.36 | 122.28      | 124.45   |
| 14  | 2     | 834  | CLA  | C1B-CHB-C4A | -2.36 | 125.44      | 130.12   |
| 14  | b     | 821  | CLA  | CHB-C4A-NA  | 2.36  | 127.77      | 124.51   |
| 14  | J     | 102  | CLA  | CHB-C4A-NA  | 2.36  | 127.77      | 124.51   |
| 14  | b     | 803  | CLA  | C1B-CHB-C4A | -2.36 | 125.45      | 130.12   |
| 14  | b     | 813  | CLA  | CHB-C4A-NA  | 2.36  | 127.77      | 124.51   |
| 17  | 2     | 845  | BCR  | C15-C16-C17 | -2.36 | 118.64      | 123.47   |
| 14  | 8     | 1302 | CLA  | C1B-CHB-C4A | -2.36 | 125.45      | 130.12   |
| 14  | B     | 812  | CLA  | CHB-C4A-NA  | 2.36  | 127.77      | 124.51   |
| 14  | B     | 837  | CLA  | C1B-CHB-C4A | -2.36 | 125.45      | 130.12   |
| 14  | a     | 837  | CLA  | C1B-CHB-C4A | -2.36 | 125.45      | 130.12   |
| 14  | 2     | 802  | CLA  | O2D-CGD-CBD | 2.36  | 115.45      | 111.27   |
| 14  | 2     | 814  | CLA  | CHB-C4A-NA  | 2.35  | 127.77      | 124.51   |
| 17  | a     | 850  | BCR  | C16-C15-C14 | -2.35 | 118.65      | 123.47   |
| 14  | A     | 831  | CLA  | C1B-CHB-C4A | -2.35 | 125.45      | 130.12   |
| 14  | A     | 806  | CLA  | CHD-C1D-ND  | -2.35 | 122.29      | 124.45   |
| 14  | a     | 842  | CLA  | CHB-C4A-NA  | 2.35  | 127.77      | 124.51   |
| 14  | a     | 830  | CLA  | C1B-CHB-C4A | -2.35 | 125.46      | 130.12   |
| 14  | a     | 829  | CLA  | CHB-C4A-NA  | 2.35  | 127.77      | 124.51   |
| 14  | b     | 809  | CLA  | CMB-C2B-C3B | 2.35  | 129.08      | 124.68   |
| 14  | 2     | 809  | CLA  | CMB-C2B-C3B | 2.35  | 129.08      | 124.68   |
| 14  | F     | 201  | CLA  | C1B-CHB-C4A | -2.35 | 125.46      | 130.12   |
| 14  | 1     | 1645 | CLA  | C1B-CHB-C4A | -2.35 | 125.46      | 130.12   |
| 17  | a     | 848  | BCR  | C15-C16-C17 | -2.35 | 118.66      | 123.47   |
| 14  | B     | 823  | CLA  | C1B-CHB-C4A | -2.35 | 125.46      | 130.12   |
| 14  | A     | 832  | CLA  | CHB-C4A-NA  | 2.35  | 127.76      | 124.51   |
| 18  | A     | 854  | LHG  | O8-C23-C24  | 2.35  | 119.28      | 111.91   |
| 14  | a     | 806  | CLA  | CHD-C1D-ND  | -2.35 | 122.29      | 124.45   |
| 14  | A     | 826  | CLA  | CHB-C4A-NA  | 2.35  | 127.76      | 124.51   |
| 14  | 1     | 1631 | CLA  | C1B-CHB-C4A | -2.35 | 125.46      | 130.12   |
| 17  | 9     | 104  | BCR  | C2-C1-C6    | 2.35  | 114.10      | 110.48   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 844  | CLA  | C1B-CHB-C4A | -2.35 | 125.47      | 130.12   |
| 14  | b     | 840  | CLA  | CHD-C1D-ND  | -2.35 | 122.30      | 124.45   |
| 14  | 1     | 1638 | CLA  | C1B-CHB-C4A | -2.35 | 125.47      | 130.12   |
| 14  | B     | 819  | CLA  | C1-O2A-CGA  | 2.35  | 122.60      | 116.44   |
| 14  | b     | 820  | CLA  | C1-O2A-CGA  | 2.35  | 122.60      | 116.44   |
| 14  | 2     | 820  | CLA  | C1-O2A-CGA  | 2.35  | 122.60      | 116.44   |
| 14  | 1     | 1643 | CLA  | CHB-C4A-NA  | 2.35  | 127.76      | 124.51   |
| 14  | a     | 811  | CLA  | O2A-CGA-O1A | -2.35 | 117.67      | 123.59   |
| 14  | 2     | 816  | CLA  | C1B-CHB-C4A | -2.35 | 125.47      | 130.12   |
| 14  | 1     | 1607 | CLA  | CHD-C1D-ND  | -2.35 | 122.30      | 124.45   |
| 17  | 6     | 204  | BCR  | C24-C23-C22 | -2.35 | 122.69      | 126.23   |
| 14  | A     | 811  | CLA  | O2A-CGA-O1A | -2.35 | 117.67      | 123.59   |
| 14  | 2     | 842  | CLA  | CHD-C1D-ND  | -2.35 | 122.30      | 124.45   |
| 14  | B     | 815  | CLA  | C1B-CHB-C4A | -2.35 | 125.47      | 130.12   |
| 14  | A     | 855  | CLA  | O2D-CGD-CBD | 2.35  | 115.44      | 111.27   |
| 17  | F     | 205  | BCR  | C24-C23-C22 | -2.35 | 122.69      | 126.23   |
| 14  | 2     | 838  | CLA  | C1B-CHB-C4A | -2.35 | 125.47      | 130.12   |
| 14  | f     | 201  | CLA  | O2D-CGD-O1D | -2.34 | 119.25      | 123.84   |
| 14  | A     | 834  | CLA  | CHD-C1D-ND  | -2.34 | 122.30      | 124.45   |
| 17  | b     | 845  | BCR  | C15-C16-C17 | -2.34 | 118.67      | 123.47   |
| 17  | 1     | 1651 | BCR  | C16-C15-C14 | -2.34 | 118.67      | 123.47   |
| 14  | 2     | 824  | CLA  | C1B-CHB-C4A | -2.34 | 125.47      | 130.12   |
| 14  | b     | 838  | CLA  | C1B-CHB-C4A | -2.34 | 125.48      | 130.12   |
| 17  | b     | 848  | BCR  | C38-C26-C25 | -2.34 | 121.90      | 124.53   |
| 17  | A     | 850  | BCR  | C16-C15-C14 | -2.34 | 118.67      | 123.47   |
| 14  | a     | 831  | CLA  | C1B-CHB-C4A | -2.34 | 125.48      | 130.12   |
| 14  | b     | 824  | CLA  | C1B-CHB-C4A | -2.34 | 125.48      | 130.12   |
| 14  | 1     | 1612 | CLA  | O2A-CGA-O1A | -2.34 | 117.68      | 123.59   |
| 14  | 2     | 842  | CLA  | C1B-CHB-C4A | -2.34 | 125.48      | 130.12   |
| 14  | j     | 1303 | CLA  | CHB-C4A-NA  | 2.34  | 127.75      | 124.51   |
| 14  | 2     | 840  | CLA  | CHD-C1D-ND  | -2.34 | 122.30      | 124.45   |
| 14  | A     | 813  | CLA  | C1B-CHB-C4A | -2.34 | 125.48      | 130.12   |
| 14  | B     | 805  | CLA  | C1B-CHB-C4A | -2.34 | 125.48      | 130.12   |
| 14  | b     | 816  | CLA  | C1B-CHB-C4A | -2.34 | 125.48      | 130.12   |
| 14  | 2     | 830  | CLA  | C1B-CHB-C4A | -2.34 | 125.48      | 130.12   |
| 14  | b     | 802  | CLA  | O2D-CGD-CBD | 2.34  | 115.42      | 111.27   |
| 14  | B     | 841  | CLA  | CHD-C1D-ND  | -2.34 | 122.31      | 124.45   |
| 14  | 1     | 1614 | CLA  | C1B-CHB-C4A | -2.34 | 125.49      | 130.12   |
| 14  | A     | 829  | CLA  | CHB-C4A-NA  | 2.34  | 127.75      | 124.51   |
| 17  | 1     | 1649 | BCR  | C8-C7-C6    | -2.34 | 120.64      | 127.20   |
| 17  | B     | 844  | BCR  | C15-C16-C17 | -2.34 | 118.69      | 123.47   |
| 14  | 8     | 1303 | CLA  | CHB-C4A-NA  | 2.34  | 127.74      | 124.51   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | b     | 830  | CLA  | C1B-CHB-C4A | -2.34 | 125.49      | 130.12   |
| 14  | 1     | 1635 | CLA  | CHD-C1D-ND  | -2.34 | 122.31      | 124.45   |
| 14  | B     | 811  | CLA  | C1B-CHB-C4A | -2.34 | 125.49      | 130.12   |
| 14  | 6     | 201  | CLA  | O2D-CGD-O1D | -2.34 | 119.27      | 123.84   |
| 17  | A     | 847  | BCR  | C38-C26-C25 | -2.34 | 121.91      | 124.53   |
| 14  | a     | 833  | CLA  | CHB-C4A-NA  | 2.34  | 127.74      | 124.51   |
| 17  | 9     | 102  | BCR  | C24-C23-C22 | -2.34 | 122.71      | 126.23   |
| 14  | 2     | 806  | CLA  | C1B-CHB-C4A | -2.33 | 125.49      | 130.12   |
| 14  | B     | 808  | CLA  | CMB-C2B-C3B | 2.33  | 129.04      | 124.68   |
| 14  | A     | 811  | CLA  | C1B-CHB-C4A | -2.33 | 125.49      | 130.12   |
| 17  | A     | 848  | BCR  | C8-C7-C6    | -2.33 | 120.65      | 127.20   |
| 14  | A     | 820  | CLA  | O2A-CGA-O1A | -2.33 | 117.70      | 123.59   |
| 14  | F     | 204  | CLA  | C1-C2-C3    | -2.33 | 122.98      | 126.75   |
| 18  | a     | 854  | LHG  | O8-C23-C24  | 2.33  | 119.22      | 111.91   |
| 14  | F     | 201  | CLA  | O2D-CGD-O1D | -2.33 | 119.28      | 123.84   |
| 14  | B     | 839  | CLA  | CHD-C1D-ND  | -2.33 | 122.31      | 124.45   |
| 14  | 1     | 1612 | CLA  | C1B-CHB-C4A | -2.33 | 125.50      | 130.12   |
| 14  | 2     | 833  | CLA  | C1B-CHB-C4A | -2.33 | 125.50      | 130.12   |
| 17  | 1     | 1648 | BCR  | C37-C22-C21 | -2.33 | 119.66      | 122.92   |
| 14  | A     | 824  | CLA  | O2D-CGD-CBD | 2.33  | 115.41      | 111.27   |
| 14  | b     | 814  | CLA  | CHB-C4A-NA  | 2.33  | 127.73      | 124.51   |
| 14  | f     | 203  | CLA  | CHB-C4A-NA  | 2.33  | 127.73      | 124.51   |
| 14  | 2     | 821  | CLA  | CHB-C4A-NA  | 2.33  | 127.73      | 124.51   |
| 14  | 1     | 1640 | CLA  | C1B-CHB-C4A | -2.33 | 125.50      | 130.12   |
| 17  | A     | 850  | BCR  | C38-C26-C25 | -2.33 | 121.91      | 124.53   |
| 17  | a     | 850  | BCR  | C8-C7-C6    | -2.33 | 120.67      | 127.20   |
| 14  | b     | 806  | CLA  | C1B-CHB-C4A | -2.33 | 125.51      | 130.12   |
| 14  | 2     | 812  | CLA  | C1B-CHB-C4A | -2.33 | 125.51      | 130.12   |
| 17  | a     | 848  | BCR  | C8-C7-C6    | -2.33 | 120.67      | 127.20   |
| 14  | A     | 839  | CLA  | C1B-CHB-C4A | -2.33 | 125.51      | 130.12   |
| 14  | 1     | 1621 | CLA  | O2A-CGA-O1A | -2.33 | 117.72      | 123.59   |
| 14  | B     | 824  | CLA  | C1B-CHB-C4A | -2.33 | 125.51      | 130.12   |
| 14  | a     | 820  | CLA  | O2A-CGA-O1A | -2.33 | 117.72      | 123.59   |
| 14  | f     | 203  | CLA  | C1-C2-C3    | -2.33 | 122.99      | 126.75   |
| 14  | B     | 832  | CLA  | C1B-CHB-C4A | -2.32 | 125.51      | 130.12   |
| 14  | 1     | 1606 | CLA  | C1B-CHB-C4A | -2.32 | 125.51      | 130.12   |
| 14  | b     | 825  | CLA  | C1B-CHB-C4A | -2.32 | 125.51      | 130.12   |
| 14  | 9     | 103  | CLA  | C1B-CHB-C4A | -2.32 | 125.51      | 130.12   |
| 14  | A     | 804  | CLA  | C1B-CHB-C4A | -2.32 | 125.51      | 130.12   |
| 14  | b     | 842  | CLA  | C1B-CHB-C4A | -2.32 | 125.51      | 130.12   |
| 14  | b     | 842  | CLA  | CHD-C1D-ND  | -2.32 | 122.32      | 124.45   |
| 17  | a     | 847  | BCR  | C37-C22-C21 | -2.32 | 119.67      | 122.92   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 841  | CLA  | C1B-CHB-C4A | -2.32 | 125.52      | 130.12   |
| 14  | A     | 828  | CLA  | CHB-C4A-NA  | 2.32  | 127.72      | 124.51   |
| 14  | 2     | 813  | CLA  | CHB-C4A-NA  | 2.32  | 127.72      | 124.51   |
| 14  | a     | 811  | CLA  | CMB-C2B-C3B | 2.32  | 129.02      | 124.68   |
| 14  | A     | 827  | CLA  | CHD-C1D-ND  | -2.32 | 122.32      | 124.45   |
| 14  | B     | 826  | CLA  | C1B-CHB-C4A | -2.32 | 125.52      | 130.12   |
| 14  | a     | 824  | CLA  | O2D-CGD-CBD | 2.32  | 115.39      | 111.27   |
| 17  | A     | 850  | BCR  | C8-C7-C6    | -2.32 | 120.69      | 127.20   |
| 14  | z     | 102  | CLA  | CHB-C4A-NA  | 2.32  | 127.72      | 124.51   |
| 14  | 2     | 827  | CLA  | C1B-CHB-C4A | -2.32 | 125.52      | 130.12   |
| 14  | a     | 802  | CLA  | O2A-CGA-O1A | -2.32 | 117.74      | 123.59   |
| 14  | k     | 103  | CLA  | C1B-CHB-C4A | -2.32 | 125.53      | 130.12   |
| 14  | 1     | 1603 | CLA  | O2A-CGA-O1A | -2.32 | 117.74      | 123.59   |
| 17  | 6     | 202  | BCR  | C8-C7-C6    | -2.32 | 120.69      | 127.20   |
| 18  | 1     | 1655 | LHG  | O8-C23-C24  | 2.32  | 119.18      | 111.91   |
| 14  | a     | 839  | CLA  | C1B-CHB-C4A | -2.32 | 125.53      | 130.12   |
| 14  | a     | 811  | CLA  | C1B-CHB-C4A | -2.32 | 125.53      | 130.12   |
| 14  | 1     | 1619 | CLA  | C1B-CHB-C4A | -2.32 | 125.53      | 130.12   |
| 14  | 1     | 1625 | CLA  | O2D-CGD-CBD | 2.32  | 115.39      | 111.27   |
| 14  | a     | 818  | CLA  | C1B-CHB-C4A | -2.32 | 125.53      | 130.12   |
| 17  | b     | 847  | BCR  | C35-C13-C14 | -2.32 | 119.68      | 122.92   |
| 17  | k     | 102  | BCR  | C24-C23-C22 | -2.32 | 122.74      | 126.23   |
| 14  | 2     | 832  | CLA  | C1B-CHB-C4A | -2.31 | 125.53      | 130.12   |
| 17  | 1     | 1651 | BCR  | C8-C7-C6    | -2.31 | 120.70      | 127.20   |
| 14  | B     | 829  | CLA  | C1B-CHB-C4A | -2.31 | 125.53      | 130.12   |
| 14  | b     | 812  | CLA  | C1B-CHB-C4A | -2.31 | 125.53      | 130.12   |
| 14  | b     | 826  | CLA  | CHB-C4A-NA  | 2.31  | 127.71      | 124.51   |
| 17  | f     | 204  | BCR  | C24-C23-C22 | -2.31 | 122.74      | 126.23   |
| 14  | a     | 813  | CLA  | C1B-CHB-C4A | -2.31 | 125.54      | 130.12   |
| 18  | B     | 850  | LHG  | C11-C10-C9  | -2.31 | 102.69      | 114.42   |
| 14  | B     | 813  | CLA  | CHB-C4A-NA  | 2.31  | 127.71      | 124.51   |
| 14  | b     | 833  | CLA  | C1B-CHB-C4A | -2.31 | 125.54      | 130.12   |
| 14  | 2     | 825  | CLA  | C1B-CHB-C4A | -2.31 | 125.54      | 130.12   |
| 17  | a     | 850  | BCR  | C38-C26-C25 | -2.31 | 121.93      | 124.53   |
| 14  | 1     | 1627 | CLA  | C6-C5-C3    | 2.31  | 119.51      | 113.45   |
| 14  | k     | 103  | CLA  | CHD-C1D-ND  | -2.31 | 122.33      | 124.45   |
| 17  | A     | 850  | BCR  | C2-C1-C6    | 2.31  | 114.04      | 110.48   |
| 14  | X     | 1701 | CLA  | CHB-C4A-NA  | 2.31  | 127.71      | 124.51   |
| 14  | 2     | 814  | CLA  | C5-C3-C2    | 2.31  | 125.79      | 121.12   |
| 14  | B     | 808  | CLA  | C1B-CHB-C4A | -2.31 | 125.54      | 130.12   |
| 14  | 2     | 834  | CLA  | CHB-C4A-NA  | 2.31  | 127.70      | 124.51   |
| 14  | b     | 835  | CLA  | C1B-CHB-C4A | -2.31 | 125.55      | 130.12   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 20  | 2     | 850  | LMG  | O3-C3-C2    | -2.31 | 105.01      | 110.35   |
| 14  | b     | 834  | CLA  | CHB-C4A-NA  | 2.31  | 127.70      | 124.51   |
| 18  | b     | 851  | LHG  | C11-C10-C9  | -2.31 | 102.71      | 114.42   |
| 14  | B     | 834  | CLA  | C1B-CHB-C4A | -2.31 | 125.55      | 130.12   |
| 14  | F     | 204  | CLA  | CHB-C4A-NA  | 2.31  | 127.70      | 124.51   |
| 14  | A     | 802  | CLA  | O2A-CGA-O1A | -2.31 | 117.77      | 123.59   |
| 18  | z     | 101  | LHG  | C11-C10-C9  | -2.31 | 102.72      | 114.42   |
| 14  | A     | 829  | CLA  | O1D-CGD-CBD | 2.31  | 129.20      | 124.48   |
| 17  | I     | 101  | BCR  | C8-C7-C6    | -2.30 | 120.73      | 127.20   |
| 14  | A     | 833  | CLA  | CHB-C4A-NA  | 2.30  | 127.70      | 124.51   |
| 14  | b     | 832  | CLA  | C1B-CHB-C4A | -2.30 | 125.55      | 130.12   |
| 14  | 6     | 203  | CLA  | C1-C2-C3    | -2.30 | 123.03      | 126.75   |
| 14  | 2     | 807  | CLA  | C1B-CHB-C4A | -2.30 | 125.56      | 130.12   |
| 14  | 2     | 835  | CLA  | C1B-CHB-C4A | -2.30 | 125.56      | 130.12   |
| 17  | F     | 202  | BCR  | C8-C7-C6    | -2.30 | 120.73      | 127.20   |
| 17  | 1     | 1651 | BCR  | C38-C26-C25 | -2.30 | 121.94      | 124.53   |
| 14  | l     | 206  | CLA  | O2D-CGD-CBD | 2.30  | 115.36      | 111.27   |
| 14  | b     | 824  | CLA  | CHD-C1D-ND  | -2.30 | 122.34      | 124.45   |
| 14  | 1     | 1628 | CLA  | CHD-C1D-ND  | -2.30 | 122.34      | 124.45   |
| 14  | 6     | 203  | CLA  | CHB-C4A-NA  | 2.30  | 127.70      | 124.51   |
| 14  | A     | 826  | CLA  | C6-C5-C3    | 2.30  | 119.49      | 113.45   |
| 14  | b     | 822  | CLA  | C1B-CHB-C4A | -2.30 | 125.56      | 130.12   |
| 20  | 2     | 850  | LMG  | C40-C39-C38 | -2.30 | 102.74      | 114.42   |
| 14  | B     | 806  | CLA  | O2D-CGD-O1D | -2.30 | 119.34      | 123.84   |
| 17  | 1     | 1651 | BCR  | C2-C1-C6    | 2.30  | 114.02      | 110.48   |
| 14  | b     | 803  | CLA  | C11-C10-C8  | -2.30 | 108.48      | 115.92   |
| 14  | 2     | 803  | CLA  | C11-C10-C8  | -2.30 | 108.48      | 115.92   |
| 20  | b     | 850  | LMG  | C40-C39-C38 | -2.30 | 102.75      | 114.42   |
| 14  | B     | 831  | CLA  | C1B-CHB-C4A | -2.30 | 125.56      | 130.12   |
| 14  | 2     | 826  | CLA  | CHB-C4A-NA  | 2.30  | 127.69      | 124.51   |
| 14  | B     | 813  | CLA  | C5-C3-C2    | 2.30  | 125.77      | 121.12   |
| 17  | A     | 856  | BCR  | C38-C26-C25 | -2.30 | 121.95      | 124.53   |
| 17  | i     | 101  | BCR  | C8-C7-C6    | -2.30 | 120.75      | 127.20   |
| 14  | b     | 807  | CLA  | O2D-CGD-O1D | -2.30 | 119.34      | 123.84   |
| 14  | j     | 1301 | CLA  | O1D-CGD-CBD | 2.30  | 129.19      | 124.48   |
| 14  | K     | 103  | CLA  | C1B-CHB-C4A | -2.30 | 125.57      | 130.12   |
| 14  | B     | 807  | CLA  | C1-C2-C3    | -2.30 | 122.07      | 126.04   |
| 20  | B     | 849  | LMG  | C40-C39-C38 | -2.30 | 102.77      | 114.42   |
| 14  | b     | 830  | CLA  | C3C-C4C-NC  | -2.30 | 108.00      | 110.57   |
| 17  | 7     | 101  | BCR  | C8-C7-C6    | -2.30 | 120.75      | 127.20   |
| 20  | B     | 849  | LMG  | O3-C3-C2    | -2.30 | 105.04      | 110.35   |
| 17  | f     | 202  | BCR  | C8-C7-C6    | -2.30 | 120.75      | 127.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | A     | 847  | BCR  | C37-C22-C21 | -2.30 | 119.71      | 122.92   |
| 14  | a     | 829  | CLA  | O1D-CGD-CBD | 2.30  | 129.18      | 124.48   |
| 17  | 1     | 1648 | BCR  | C38-C26-C25 | -2.29 | 121.95      | 124.53   |
| 20  | b     | 850  | LMG  | O3-C3-C2    | -2.29 | 105.04      | 110.35   |
| 14  | 1     | 1634 | CLA  | C1B-CHB-C4A | -2.29 | 125.57      | 130.12   |
| 14  | B     | 802  | CLA  | C11-C10-C8  | -2.29 | 108.50      | 115.92   |
| 14  | B     | 825  | CLA  | CHB-C4A-NA  | 2.29  | 127.68      | 124.51   |
| 17  | a     | 850  | BCR  | C2-C1-C6    | 2.29  | 114.01      | 110.48   |
| 14  | F     | 203  | CLA  | O1D-CGD-CBD | 2.29  | 129.17      | 124.48   |
| 14  | B     | 833  | CLA  | CHB-C4A-NA  | 2.29  | 127.68      | 124.51   |
| 14  | B     | 811  | CLA  | CHD-C1D-ND  | -2.29 | 122.35      | 124.45   |
| 14  | 1     | 1605 | CLA  | C1B-CHB-C4A | -2.29 | 125.58      | 130.12   |
| 14  | 0     | 207  | CLA  | O2D-CGD-CBD | 2.29  | 115.34      | 111.27   |
| 14  | 2     | 809  | CLA  | C1B-CHB-C4A | -2.29 | 125.58      | 130.12   |
| 17  | B     | 846  | BCR  | C35-C13-C14 | -2.29 | 119.72      | 122.92   |
| 14  | 8     | 1301 | CLA  | O1D-CGD-CBD | 2.29  | 129.17      | 124.48   |
| 14  | a     | 826  | CLA  | C6-C5-C3    | 2.29  | 119.46      | 113.45   |
| 14  | b     | 814  | CLA  | C5-C3-C2    | 2.29  | 125.75      | 121.12   |
| 14  | A     | 811  | CLA  | CMB-C2B-C3B | 2.29  | 128.96      | 124.68   |
| 14  | A     | 833  | CLA  | C1B-CHB-C4A | -2.29 | 125.59      | 130.12   |
| 17  | a     | 851  | BCR  | C38-C26-C25 | -2.29 | 121.96      | 124.53   |
| 17  | K     | 102  | BCR  | C24-C23-C22 | -2.29 | 122.78      | 126.23   |
| 14  | B     | 821  | CLA  | C1B-CHB-C4A | -2.29 | 125.59      | 130.12   |
| 14  | a     | 844  | CLA  | CHD-C1D-ND  | -2.29 | 122.35      | 124.45   |
| 14  | 9     | 101  | CLA  | C1B-CHB-C4A | -2.29 | 125.59      | 130.12   |
| 17  | a     | 847  | BCR  | C38-C26-C25 | -2.28 | 121.96      | 124.53   |
| 14  | a     | 804  | CLA  | C1B-CHB-C4A | -2.28 | 125.59      | 130.12   |
| 14  | a     | 827  | CLA  | CHD-C1D-ND  | -2.28 | 122.36      | 124.45   |
| 14  | 9     | 103  | CLA  | CHD-C1D-ND  | -2.28 | 122.36      | 124.45   |
| 14  | A     | 818  | CLA  | C1B-CHB-C4A | -2.28 | 125.59      | 130.12   |
| 17  | k     | 102  | BCR  | C27-C26-C25 | 2.28  | 126.04      | 122.73   |
| 17  | 2     | 847  | BCR  | C35-C13-C14 | -2.28 | 119.73      | 122.92   |
| 14  | B     | 806  | CLA  | C1B-CHB-C4A | -2.28 | 125.60      | 130.12   |
| 14  | B     | 829  | CLA  | C3C-C4C-NC  | -2.28 | 108.01      | 110.57   |
| 17  | j     | 1304 | BCR  | C24-C23-C22 | -2.28 | 122.79      | 126.23   |
| 14  | a     | 805  | CLA  | O2D-CGD-CBD | 2.28  | 115.32      | 111.27   |
| 14  | 1     | 1630 | CLA  | O1D-CGD-CBD | 2.28  | 129.15      | 124.48   |
| 20  | 2     | 850  | LMG  | O2-C2-C1    | -2.28 | 104.51      | 110.05   |
| 14  | b     | 809  | CLA  | C1B-CHB-C4A | -2.28 | 125.61      | 130.12   |
| 14  | b     | 811  | CLA  | C1B-CHB-C4A | -2.28 | 125.61      | 130.12   |
| 14  | K     | 103  | CLA  | CHD-C1D-ND  | -2.28 | 122.36      | 124.45   |
| 14  | a     | 803  | CLA  | CHD-C1D-ND  | -2.28 | 122.36      | 124.45   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | 2     | 822  | CLA  | C1B-CHB-C4A | -2.28 | 125.61      | 130.12   |
| 13  | A     | 801  | CL0  | CMB-C2B-C3B | 2.28  | 128.94      | 124.68   |
| 14  | 1     | 1612 | CLA  | CMB-C2B-C3B | 2.28  | 128.94      | 124.68   |
| 14  | L     | 205  | CLA  | O2D-CGD-CBD | 2.28  | 115.31      | 111.27   |
| 17  | a     | 852  | BCR  | C8-C7-C6    | -2.28 | 120.81      | 127.20   |
| 17  | 8     | 1305 | BCR  | C38-C26-C25 | -2.28 | 121.97      | 124.53   |
| 14  | 2     | 824  | CLA  | CHD-C1D-ND  | -2.27 | 122.36      | 124.45   |
| 13  | a     | 801  | CL0  | CMB-C2B-C3B | 2.27  | 128.93      | 124.68   |
| 14  | b     | 808  | CLA  | C1-C2-C3    | -2.27 | 122.11      | 126.04   |
| 14  | 6     | 201  | CLA  | C1-C2-C3    | -2.27 | 122.11      | 126.04   |
| 14  | a     | 833  | CLA  | C1B-CHB-C4A | -2.27 | 125.61      | 130.12   |
| 14  | b     | 811  | CLA  | C2A-C1A-CHA | 2.27  | 127.83      | 123.86   |
| 14  | B     | 810  | CLA  | C1B-CHB-C4A | -2.27 | 125.61      | 130.12   |
| 14  | b     | 812  | CLA  | CHD-C1D-ND  | -2.27 | 122.36      | 124.45   |
| 14  | a     | 843  | CLA  | CMB-C2B-C3B | 2.27  | 128.93      | 124.68   |
| 14  | 1     | 1606 | CLA  | O2D-CGD-CBD | 2.27  | 115.31      | 111.27   |
| 14  | B     | 814  | CLA  | C1B-CHB-C4A | -2.27 | 125.62      | 130.12   |
| 17  | B     | 848  | BCR  | C24-C23-C22 | -2.27 | 122.80      | 126.23   |
| 14  | b     | 807  | CLA  | C1B-CHB-C4A | -2.27 | 125.62      | 130.12   |
| 17  | A     | 851  | BCR  | C38-C26-C25 | -2.27 | 121.98      | 124.53   |
| 17  | b     | 848  | BCR  | C15-C14-C13 | -2.27 | 124.07      | 127.31   |
| 14  | B     | 810  | CLA  | C2A-C1A-CHA | 2.27  | 127.83      | 123.86   |
| 17  | 8     | 1304 | BCR  | C24-C23-C22 | -2.27 | 122.80      | 126.23   |
| 14  | 1     | 1642 | CLA  | C1-C2-C3    | -2.27 | 122.12      | 126.04   |
| 14  | b     | 836  | CLA  | C1B-CHB-C4A | -2.27 | 125.62      | 130.12   |
| 14  | 2     | 811  | CLA  | C2A-C1A-CHA | 2.27  | 127.83      | 123.86   |
| 14  | 2     | 836  | CLA  | C1B-CHB-C4A | -2.27 | 125.62      | 130.12   |
| 14  | 2     | 808  | CLA  | C1-C2-C3    | -2.27 | 122.12      | 126.04   |
| 14  | A     | 803  | CLA  | CHD-C1D-ND  | -2.27 | 122.37      | 124.45   |
| 14  | 2     | 812  | CLA  | CHD-C1D-ND  | -2.27 | 122.37      | 124.45   |
| 17  | M     | 103  | BCR  | C8-C7-C6    | -2.27 | 120.83      | 127.20   |
| 14  | B     | 835  | CLA  | C1B-CHB-C4A | -2.27 | 125.62      | 130.12   |
| 14  | b     | 815  | CLA  | C1B-CHB-C4A | -2.27 | 125.63      | 130.12   |
| 14  | F     | 201  | CLA  | C1-C2-C3    | -2.27 | 122.12      | 126.04   |
| 14  | B     | 815  | CLA  | CHB-C4A-NA  | 2.27  | 127.64      | 124.51   |
| 14  | b     | 816  | CLA  | CHB-C4A-NA  | 2.27  | 127.64      | 124.51   |
| 14  | b     | 823  | CLA  | CHB-C4A-NA  | 2.27  | 127.64      | 124.51   |
| 14  | f     | 201  | CLA  | C1-C2-C3    | -2.27 | 122.12      | 126.04   |
| 14  | k     | 101  | CLA  | C1B-CHB-C4A | -2.27 | 125.63      | 130.12   |
| 17  | j     | 1305 | BCR  | C36-C18-C17 | -2.27 | 119.75      | 122.92   |
| 17  | K     | 102  | BCR  | C27-C26-C25 | 2.26  | 126.02      | 122.73   |
| 14  | b     | 820  | CLA  | CHD-C1D-ND  | -2.26 | 122.37      | 124.45   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | j     | 1305 | BCR  | C38-C26-C25 | -2.26 | 121.99      | 124.53   |
| 17  | 1     | 1653 | BCR  | C8-C7-C6    | -2.26 | 120.85      | 127.20   |
| 20  | B     | 849  | LMG  | O2-C2-C1    | -2.26 | 104.55      | 110.05   |
| 17  | A     | 852  | BCR  | C8-C7-C6    | -2.26 | 120.85      | 127.20   |
| 14  | a     | 841  | CLA  | C1-C2-C3    | -2.26 | 122.13      | 126.04   |
| 14  | a     | 826  | CLA  | C1B-CHB-C4A | -2.26 | 125.64      | 130.12   |
| 14  | B     | 819  | CLA  | CHD-C1D-ND  | -2.26 | 122.38      | 124.45   |
| 14  | 2     | 807  | CLA  | O2D-CGD-O1D | -2.26 | 119.42      | 123.84   |
| 14  | 1     | 1601 | CLA  | CHB-C4A-NA  | 2.26  | 127.64      | 124.51   |
| 17  | 9     | 102  | BCR  | C27-C26-C25 | 2.26  | 126.01      | 122.73   |
| 14  | K     | 101  | CLA  | C1B-CHB-C4A | -2.26 | 125.64      | 130.12   |
| 14  | L     | 203  | CLA  | C1-C2-C3    | -2.26 | 122.14      | 126.04   |
| 17  | m     | 102  | BCR  | C8-C7-C6    | -2.26 | 120.86      | 127.20   |
| 14  | M     | 102  | CLA  | CHB-C4A-NA  | 2.26  | 127.63      | 124.51   |
| 14  | A     | 843  | CLA  | CMB-C2B-C3B | 2.26  | 128.90      | 124.68   |
| 17  | y     | 102  | BCR  | C8-C7-C6    | -2.26 | 120.86      | 127.20   |
| 20  | b     | 850  | LMG  | O2-C2-C1    | -2.26 | 104.56      | 110.05   |
| 14  | 2     | 820  | CLA  | CHB-C4A-NA  | 2.26  | 127.63      | 124.51   |
| 14  | B     | 804  | CLA  | C1-C2-C3    | -2.26 | 122.14      | 126.04   |
| 14  | 1     | 1609 | CLA  | C1B-CHB-C4A | -2.26 | 125.65      | 130.12   |
| 14  | A     | 808  | CLA  | C1B-CHB-C4A | -2.26 | 125.65      | 130.12   |
| 20  | B     | 849  | LMG  | O1-C1-C2    | -2.26 | 104.78      | 108.30   |
| 14  | 2     | 816  | CLA  | CHB-C4A-NA  | 2.25  | 127.63      | 124.51   |
| 17  | b     | 847  | BCR  | C7-C8-C9    | -2.25 | 122.83      | 126.23   |
| 14  | B     | 819  | CLA  | CHB-C4A-NA  | 2.25  | 127.63      | 124.51   |
| 14  | l     | 204  | CLA  | C1-C2-C3    | -2.25 | 122.14      | 126.04   |
| 14  | A     | 844  | CLA  | CHD-C1D-ND  | -2.25 | 122.38      | 124.45   |
| 14  | a     | 828  | CLA  | CHB-C4A-NA  | 2.25  | 127.63      | 124.51   |
| 14  | A     | 805  | CLA  | O2D-CGD-CBD | 2.25  | 115.27      | 111.27   |
| 17  | J     | 103  | BCR  | C24-C23-C22 | -2.25 | 122.83      | 126.23   |
| 14  | j     | 1302 | CLA  | O2A-CGA-O1A | -2.25 | 117.69      | 123.30   |
| 18  | z     | 101  | LHG  | C27-C26-C25 | -2.25 | 102.99      | 114.42   |
| 17  | b     | 849  | BCR  | C36-C18-C17 | -2.25 | 119.77      | 122.92   |
| 14  | 1     | 1604 | CLA  | CHD-C1D-ND  | -2.25 | 122.39      | 124.45   |
| 17  | A     | 856  | BCR  | C8-C7-C6    | -2.25 | 120.88      | 127.20   |
| 14  | a     | 817  | CLA  | C1B-CHB-C4A | -2.25 | 125.66      | 130.12   |
| 20  | b     | 850  | LMG  | O1-C1-C2    | -2.25 | 104.79      | 108.30   |
| 18  | B     | 850  | LHG  | C27-C26-C25 | -2.25 | 103.01      | 114.42   |
| 14  | 8     | 1302 | CLA  | O2A-CGA-O1A | -2.25 | 117.69      | 123.30   |
| 14  | 1     | 1629 | CLA  | CHB-C4A-NA  | 2.25  | 127.62      | 124.51   |
| 13  | 1     | 1602 | CL0  | C1B-CHB-C4A | -2.25 | 125.66      | 130.12   |
| 14  | a     | 823  | CLA  | CHD-C1D-ND  | -2.25 | 122.39      | 124.45   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | 2     | 830  | CLA  | C3C-C4C-NC  | -2.25 | 108.05      | 110.57   |
| 17  | 0     | 203  | BCR  | C15-C14-C13 | -2.25 | 124.10      | 127.31   |
| 14  | b     | 805  | CLA  | C1-C2-C3    | -2.25 | 122.16      | 126.04   |
| 18  | b     | 851  | LHG  | C20-C19-C18 | -2.25 | 103.02      | 114.42   |
| 17  | l     | 202  | BCR  | C15-C14-C13 | -2.25 | 124.11      | 127.31   |
| 14  | 2     | 811  | CLA  | C1B-CHB-C4A | -2.25 | 125.67      | 130.12   |
| 14  | 2     | 815  | CLA  | C1B-CHB-C4A | -2.25 | 125.67      | 130.12   |
| 18  | b     | 851  | LHG  | C27-C26-C25 | -2.24 | 103.03      | 114.42   |
| 14  | 1     | 1622 | CLA  | C1B-CHB-C4A | -2.24 | 125.67      | 130.12   |
| 17  | 2     | 847  | BCR  | C7-C8-C9    | -2.24 | 122.85      | 126.23   |
| 14  | A     | 808  | CLA  | CHD-C1D-ND  | -2.24 | 122.39      | 124.45   |
| 14  | a     | 810  | CLA  | C1B-CHB-C4A | -2.24 | 125.67      | 130.12   |
| 14  | a     | 812  | CLA  | CHB-C4A-NA  | 2.24  | 127.61      | 124.51   |
| 14  | A     | 841  | CLA  | C1-C2-C3    | -2.24 | 122.17      | 126.04   |
| 17  | b     | 849  | BCR  | C24-C23-C22 | -2.24 | 122.85      | 126.23   |
| 14  | 1     | 1607 | CLA  | C2D-C1D-ND  | -2.24 | 108.45      | 110.10   |
| 18  | B     | 850  | LHG  | C20-C19-C18 | -2.24 | 103.05      | 114.42   |
| 14  | a     | 808  | CLA  | C1B-CHB-C4A | -2.24 | 125.68      | 130.12   |
| 14  | 1     | 1627 | CLA  | C1B-CHB-C4A | -2.24 | 125.68      | 130.12   |
| 14  | 2     | 805  | CLA  | CHD-C1D-ND  | -2.24 | 122.39      | 124.45   |
| 14  | 2     | 820  | CLA  | CHD-C1D-ND  | -2.24 | 122.39      | 124.45   |
| 14  | A     | 806  | CLA  | C2D-C1D-ND  | -2.24 | 108.45      | 110.10   |
| 14  | 1     | 1632 | CLA  | C2D-C1D-ND  | -2.24 | 108.45      | 110.10   |
| 14  | A     | 812  | CLA  | CHB-C4A-NA  | 2.24  | 127.61      | 124.51   |
| 13  | a     | 801  | CL0  | C1B-CHB-C4A | -2.24 | 125.68      | 130.12   |
| 18  | z     | 101  | LHG  | C20-C19-C18 | -2.24 | 103.05      | 114.42   |
| 14  | B     | 823  | CLA  | CHD-C1D-ND  | -2.24 | 122.40      | 124.45   |
| 14  | b     | 839  | CLA  | C1B-CHB-C4A | -2.24 | 125.68      | 130.12   |
| 17  | 8     | 1304 | BCR  | C15-C16-C17 | -2.24 | 118.89      | 123.47   |
| 14  | 2     | 839  | CLA  | C1B-CHB-C4A | -2.24 | 125.69      | 130.12   |
| 17  | B     | 847  | BCR  | C15-C14-C13 | -2.24 | 124.12      | 127.31   |
| 13  | 1     | 1602 | CL0  | CMB-C2B-C3B | 2.24  | 128.86      | 124.68   |
| 17  | f     | 204  | BCR  | C15-C16-C17 | -2.24 | 118.89      | 123.47   |
| 14  | 2     | 805  | CLA  | C1-C2-C3    | -2.24 | 122.17      | 126.04   |
| 14  | 1     | 1632 | CLA  | O2D-CGD-CBD | 2.24  | 115.24      | 111.27   |
| 14  | 1     | 1644 | CLA  | CMB-C2B-C3B | 2.24  | 128.86      | 124.68   |
| 14  | A     | 857  | CLA  | CHB-C4A-NA  | 2.24  | 127.60      | 124.51   |
| 14  | 1     | 1624 | CLA  | CHD-C1D-ND  | -2.24 | 122.40      | 124.45   |
| 14  | A     | 817  | CLA  | C1B-CHB-C4A | -2.24 | 125.69      | 130.12   |
| 14  | A     | 826  | CLA  | C1B-CHB-C4A | -2.24 | 125.69      | 130.12   |
| 14  | b     | 837  | CLA  | C1B-CHB-C4A | -2.24 | 125.69      | 130.12   |
| 14  | J     | 101  | CLA  | O2A-CGA-O1A | -2.23 | 117.73      | 123.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 805  | CLA  | O2A-CGA-O1A | -2.23 | 117.95      | 123.59   |
| 17  | J     | 103  | BCR  | C38-C26-C25 | -2.23 | 122.02      | 124.53   |
| 14  | b     | 806  | CLA  | O2A-CGA-O1A | -2.23 | 117.95      | 123.59   |
| 14  | 2     | 837  | CLA  | C1B-CHB-C4A | -2.23 | 125.69      | 130.12   |
| 17  | b     | 849  | BCR  | C8-C7-C6    | -2.23 | 120.93      | 127.20   |
| 17  | b     | 847  | BCR  | C15-C14-C13 | -2.23 | 124.12      | 127.31   |
| 14  | 1     | 1609 | CLA  | CHD-C1D-ND  | -2.23 | 122.40      | 124.45   |
| 17  | 1     | 1652 | BCR  | C38-C26-C25 | -2.23 | 122.02      | 124.53   |
| 17  | 8     | 1305 | BCR  | C8-C7-C6    | -2.23 | 120.93      | 127.20   |
| 14  | B     | 836  | CLA  | C1B-CHB-C4A | -2.23 | 125.70      | 130.12   |
| 14  | B     | 840  | CLA  | C3A-C2A-C1A | 2.23  | 104.68      | 101.34   |
| 17  | j     | 1305 | BCR  | C8-C7-C6    | -2.23 | 120.94      | 127.20   |
| 17  | 2     | 849  | BCR  | C36-C18-C17 | -2.23 | 119.80      | 122.92   |
| 13  | A     | 801  | CL0  | C2A-C1A-CHA | 2.23  | 127.76      | 123.86   |
| 17  | B     | 846  | BCR  | C15-C14-C13 | -2.23 | 124.13      | 127.31   |
| 17  | 9     | 102  | BCR  | C15-C14-C13 | -2.23 | 124.13      | 127.31   |
| 14  | b     | 833  | CLA  | CHD-C1D-ND  | -2.23 | 122.41      | 124.45   |
| 17  | B     | 848  | BCR  | C8-C7-C6    | -2.23 | 120.94      | 127.20   |
| 17  | 2     | 848  | BCR  | C15-C14-C13 | -2.23 | 124.13      | 127.31   |
| 17  | A     | 856  | BCR  | C36-C18-C17 | -2.23 | 119.80      | 122.92   |
| 14  | b     | 814  | CLA  | C6-C5-C3    | 2.23  | 119.30      | 113.45   |
| 17  | 2     | 849  | BCR  | C8-C7-C6    | -2.23 | 120.94      | 127.20   |
| 14  | a     | 831  | CLA  | C2D-C1D-ND  | -2.23 | 108.46      | 110.10   |
| 17  | B     | 846  | BCR  | C7-C8-C9    | -2.23 | 122.87      | 126.23   |
| 14  | 1     | 1618 | CLA  | C1B-CHB-C4A | -2.23 | 125.70      | 130.12   |
| 14  | B     | 804  | CLA  | CHD-C1D-ND  | -2.23 | 122.41      | 124.45   |
| 14  | 1     | 1626 | CLA  | CHD-C1D-ND  | -2.23 | 122.41      | 124.45   |
| 14  | 2     | 813  | CLA  | O2D-CGD-CBD | 2.23  | 115.22      | 111.27   |
| 14  | B     | 813  | CLA  | C6-C5-C3    | 2.23  | 119.29      | 113.45   |
| 20  | 2     | 850  | LMG  | O1-C1-C2    | -2.23 | 104.83      | 108.30   |
| 17  | F     | 205  | BCR  | C15-C16-C17 | -2.23 | 118.92      | 123.47   |
| 14  | A     | 810  | CLA  | C1B-CHB-C4A | -2.22 | 125.71      | 130.12   |
| 14  | a     | 837  | CLA  | CHB-C4A-NA  | 2.22  | 127.59      | 124.51   |
| 17  | 2     | 849  | BCR  | C24-C23-C22 | -2.22 | 122.87      | 126.23   |
| 14  | b     | 841  | CLA  | C3A-C2A-C1A | 2.22  | 104.67      | 101.34   |
| 14  | 2     | 806  | CLA  | O2A-CGA-O1A | -2.22 | 117.98      | 123.59   |
| 17  | B     | 848  | BCR  | C36-C18-C17 | -2.22 | 119.81      | 122.92   |
| 17  | 8     | 1305 | BCR  | C36-C18-C17 | -2.22 | 119.81      | 122.92   |
| 14  | B     | 839  | CLA  | CHB-C4A-NA  | 2.22  | 127.58      | 124.51   |
| 14  | 1     | 1613 | CLA  | CHB-C4A-NA  | 2.22  | 127.58      | 124.51   |
| 14  | a     | 834  | CLA  | C6-C5-C3    | 2.22  | 119.28      | 113.45   |
| 14  | 1     | 1635 | CLA  | C6-C5-C3    | 2.22  | 119.28      | 113.45   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 13  | A     | 801  | CL0  | C1B-CHB-C4A | -2.22 | 125.72      | 130.12   |
| 14  | B     | 838  | CLA  | C1B-CHB-C4A | -2.22 | 125.72      | 130.12   |
| 14  | A     | 834  | CLA  | C6-C5-C3    | 2.22  | 119.27      | 113.45   |
| 14  | b     | 820  | CLA  | CHB-C4A-NA  | 2.22  | 127.58      | 124.51   |
| 14  | 0     | 205  | CLA  | C1-C2-C3    | -2.22 | 122.21      | 126.04   |
| 14  | B     | 822  | CLA  | CHB-C4A-NA  | 2.22  | 127.58      | 124.51   |
| 14  | A     | 828  | CLA  | C1B-CHB-C4A | -2.22 | 125.73      | 130.12   |
| 14  | A     | 823  | CLA  | CHD-C1D-ND  | -2.22 | 122.42      | 124.45   |
| 14  | 1     | 1625 | CLA  | CMB-C2B-C3B | 2.22  | 128.82      | 124.68   |
| 14  | B     | 812  | CLA  | O2D-CGD-CBD | 2.22  | 115.21      | 111.27   |
| 14  | a     | 806  | CLA  | C2D-C1D-ND  | -2.22 | 108.47      | 110.10   |
| 14  | A     | 821  | CLA  | C1B-CHB-C4A | -2.22 | 125.73      | 130.12   |
| 17  | 8     | 1306 | BCR  | C33-C5-C6   | -2.22 | 122.04      | 124.53   |
| 14  | 6     | 201  | CLA  | CHD-C1D-ND  | -2.22 | 122.42      | 124.45   |
| 14  | A     | 835  | CLA  | C1B-CHB-C4A | -2.22 | 125.73      | 130.12   |
| 17  | j     | 1304 | BCR  | C15-C16-C17 | -2.22 | 118.94      | 123.47   |
| 14  | B     | 807  | CLA  | O2A-CGA-O1A | -2.22 | 118.00      | 123.59   |
| 14  | a     | 831  | CLA  | O2A-CGA-O1A | -2.22 | 118.00      | 123.59   |
| 14  | 2     | 814  | CLA  | C6-C5-C3    | 2.21  | 119.26      | 113.45   |
| 14  | 1     | 1621 | CLA  | C1B-CHB-C4A | -2.21 | 125.73      | 130.12   |
| 17  | L     | 201  | BCR  | C15-C14-C13 | -2.21 | 124.15      | 127.31   |
| 17  | 1     | 1650 | BCR  | C38-C26-C25 | -2.21 | 122.04      | 124.53   |
| 14  | L     | 205  | CLA  | O2A-CGA-O1A | -2.21 | 118.01      | 123.59   |
| 17  | 8     | 1304 | BCR  | C38-C26-C25 | -2.21 | 122.04      | 124.53   |
| 17  | L     | 207  | BCR  | C24-C23-C22 | -2.21 | 122.89      | 126.23   |
| 14  | 0     | 207  | CLA  | C1-C2-C3    | -2.21 | 122.22      | 126.04   |
| 14  | b     | 828  | CLA  | CHB-C4A-NA  | 2.21  | 127.57      | 124.51   |
| 14  | a     | 810  | CLA  | CHD-C1D-ND  | -2.21 | 122.42      | 124.45   |
| 14  | f     | 201  | CLA  | CHD-C1D-ND  | -2.21 | 122.42      | 124.45   |
| 14  | A     | 837  | CLA  | CHB-C4A-NA  | 2.21  | 127.57      | 124.51   |
| 14  | b     | 813  | CLA  | O2D-CGD-CBD | 2.21  | 115.19      | 111.27   |
| 14  | A     | 828  | CLA  | C1-C2-C3    | -2.21 | 122.22      | 126.04   |
| 14  | B     | 835  | CLA  | O2A-CGA-O1A | -2.21 | 118.02      | 123.59   |
| 14  | a     | 821  | CLA  | C1B-CHB-C4A | -2.21 | 125.74      | 130.12   |
| 14  | B     | 816  | CLA  | O2A-CGA-O1A | -2.21 | 118.02      | 123.59   |
| 14  | 1     | 1611 | CLA  | C1B-CHB-C4A | -2.21 | 125.74      | 130.12   |
| 17  | A     | 851  | BCR  | C8-C7-C6    | -2.21 | 121.00      | 127.20   |
| 14  | A     | 809  | CLA  | CHD-C1D-ND  | -2.21 | 122.42      | 124.45   |
| 14  | l     | 206  | CLA  | O2A-CGA-O1A | -2.21 | 118.02      | 123.59   |
| 14  | 1     | 1629 | CLA  | C1-C2-C3    | -2.21 | 122.22      | 126.04   |
| 14  | 1     | 1636 | CLA  | C1B-CHB-C4A | -2.21 | 125.75      | 130.12   |
| 17  | 2     | 847  | BCR  | C15-C14-C13 | -2.21 | 124.16      | 127.31   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 840  | CLA  | C5-C3-C2    | 2.21  | 125.58      | 121.12   |
| 14  | b     | 833  | CLA  | C1-C2-C3    | -2.21 | 122.23      | 126.04   |
| 14  | B     | 832  | CLA  | C1-C2-C3    | -2.21 | 122.23      | 126.04   |
| 14  | A     | 820  | CLA  | C1B-CHB-C4A | -2.21 | 125.75      | 130.12   |
| 14  | 2     | 808  | CLA  | O2A-CGA-O1A | -2.21 | 118.03      | 123.59   |
| 14  | 2     | 836  | CLA  | O2A-CGA-O1A | -2.21 | 118.03      | 123.59   |
| 17  | j     | 1305 | BCR  | C28-C27-C26 | -2.20 | 110.14      | 114.08   |
| 14  | b     | 805  | CLA  | O2A-CGA-O1A | -2.20 | 118.03      | 123.59   |
| 14  | b     | 808  | CLA  | O2A-CGA-O1A | -2.20 | 118.03      | 123.59   |
| 14  | a     | 835  | CLA  | C1B-CHB-C4A | -2.20 | 125.75      | 130.12   |
| 14  | A     | 840  | CLA  | C5-C3-C2    | 2.20  | 125.58      | 121.12   |
| 17  | B     | 844  | BCR  | C28-C27-C26 | -2.20 | 110.14      | 114.08   |
| 14  | b     | 836  | CLA  | O2A-CGA-O1A | -2.20 | 118.03      | 123.59   |
| 14  | 1     | 1632 | CLA  | O2A-CGA-O1A | -2.20 | 118.03      | 123.59   |
| 14  | b     | 805  | CLA  | CHD-C1D-ND  | -2.20 | 122.43      | 124.45   |
| 14  | 1     | 1645 | CLA  | CHD-C1D-ND  | -2.20 | 122.43      | 124.45   |
| 17  | K     | 102  | BCR  | C15-C14-C13 | -2.20 | 124.17      | 127.31   |
| 14  | a     | 814  | CLA  | CHB-C4A-NA  | 2.20  | 127.56      | 124.51   |
| 14  | B     | 804  | CLA  | O2A-CGA-O1A | -2.20 | 118.04      | 123.59   |
| 14  | 2     | 805  | CLA  | O2A-CGA-O1A | -2.20 | 118.04      | 123.59   |
| 13  | a     | 801  | CL0  | C2A-C1A-CHA | 2.20  | 127.71      | 123.86   |
| 18  | 1     | 1654 | LHG  | C18-C17-C16 | -2.20 | 103.26      | 114.42   |
| 14  | 1     | 206  | CLA  | C1-C2-C3    | -2.20 | 122.24      | 126.04   |
| 14  | 2     | 833  | CLA  | C1-C2-C3    | -2.20 | 122.24      | 126.04   |
| 14  | A     | 831  | CLA  | O2D-CGD-CBD | 2.20  | 115.18      | 111.27   |
| 13  | 1     | 1602 | CL0  | C2A-C1A-CHA | 2.20  | 127.70      | 123.86   |
| 14  | F     | 201  | CLA  | CHD-C1D-ND  | -2.20 | 122.43      | 124.45   |
| 14  | A     | 831  | CLA  | O2A-CGA-O1A | -2.20 | 118.04      | 123.59   |
| 14  | a     | 831  | CLA  | O2D-CGD-CBD | 2.20  | 115.17      | 111.27   |
| 18  | a     | 853  | LHG  | C18-C17-C16 | -2.20 | 103.27      | 114.42   |
| 14  | A     | 810  | CLA  | CHD-C1D-ND  | -2.20 | 122.44      | 124.45   |
| 14  | A     | 814  | CLA  | CHB-C4A-NA  | 2.20  | 127.55      | 124.51   |
| 17  | b     | 845  | BCR  | C28-C27-C26 | -2.20 | 110.16      | 114.08   |
| 14  | 2     | 817  | CLA  | O2A-CGA-O1A | -2.20 | 118.05      | 123.59   |
| 14  | a     | 808  | CLA  | CHD-C1D-ND  | -2.20 | 122.44      | 124.45   |
| 14  | b     | 807  | CLA  | CHD-C1D-ND  | -2.20 | 122.44      | 124.45   |
| 14  | 1     | 1615 | CLA  | CHB-C4A-NA  | 2.20  | 127.55      | 124.51   |
| 17  | a     | 851  | BCR  | C8-C7-C6    | -2.20 | 121.04      | 127.20   |
| 14  | 2     | 833  | CLA  | CHD-C1D-ND  | -2.19 | 122.44      | 124.45   |
| 14  | 8     | 1301 | CLA  | CHB-C4A-NA  | 2.19  | 127.55      | 124.51   |
| 17  | 1     | 1652 | BCR  | C8-C7-C6    | -2.19 | 121.04      | 127.20   |
| 14  | 1     | 1641 | CLA  | C5-C3-C2    | 2.19  | 125.56      | 121.12   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 842  | CLA  | O2A-CGA-O1A | -2.19 | 118.06      | 123.59   |
| 14  | 2     | 841  | CLA  | C3A-C2A-C1A | 2.19  | 104.62      | 101.34   |
| 14  | 2     | 823  | CLA  | CHB-C4A-NA  | 2.19  | 127.54      | 124.51   |
| 14  | a     | 828  | CLA  | C1-C2-C3    | -2.19 | 122.25      | 126.04   |
| 17  | B     | 851  | BCR  | C33-C5-C6   | -2.19 | 122.07      | 124.53   |
| 14  | a     | 820  | CLA  | C1B-CHB-C4A | -2.19 | 125.78      | 130.12   |
| 14  | 0     | 207  | CLA  | O2A-CGA-O1A | -2.19 | 118.06      | 123.59   |
| 18  | A     | 853  | LHG  | C18-C17-C16 | -2.19 | 103.31      | 114.42   |
| 17  | J     | 103  | BCR  | C15-C16-C17 | -2.19 | 118.99      | 123.47   |
| 14  | B     | 803  | CLA  | O1D-CGD-CBD | 2.19  | 128.96      | 124.48   |
| 17  | 2     | 845  | BCR  | C28-C27-C26 | -2.19 | 110.17      | 114.08   |
| 14  | B     | 827  | CLA  | CHB-C4A-NA  | 2.19  | 127.54      | 124.51   |
| 14  | j     | 1301 | CLA  | CHB-C4A-NA  | 2.19  | 127.54      | 124.51   |
| 17  | a     | 849  | BCR  | C38-C26-C25 | -2.19 | 122.07      | 124.53   |
| 14  | 1     | 1628 | CLA  | O2D-CGD-CBD | 2.19  | 115.16      | 111.27   |
| 14  | A     | 825  | CLA  | CHD-C1D-ND  | -2.19 | 122.44      | 124.45   |
| 14  | a     | 834  | CLA  | C5-C3-C2    | 2.19  | 125.54      | 121.12   |
| 17  | b     | 852  | BCR  | C33-C5-C6   | -2.19 | 122.07      | 124.53   |
| 14  | 1     | 1611 | CLA  | CHD-C1D-ND  | -2.19 | 122.44      | 124.45   |
| 14  | 1     | 1638 | CLA  | CHB-C4A-NA  | 2.19  | 127.53      | 124.51   |
| 14  | a     | 843  | CLA  | C1B-CHB-C4A | -2.19 | 125.79      | 130.12   |
| 14  | 1     | 1629 | CLA  | C1B-CHB-C4A | -2.19 | 125.79      | 130.12   |
| 17  | B     | 851  | BCR  | C20-C21-C22 | -2.18 | 124.19      | 127.31   |
| 17  | 8     | 1305 | BCR  | C28-C27-C26 | -2.18 | 110.18      | 114.08   |
| 17  | 6     | 204  | BCR  | C15-C16-C17 | -2.18 | 119.00      | 123.47   |
| 14  | 2     | 828  | CLA  | CHB-C4A-NA  | 2.18  | 127.53      | 124.51   |
| 14  | b     | 817  | CLA  | O2A-CGA-O1A | -2.18 | 118.08      | 123.59   |
| 17  | A     | 856  | BCR  | C28-C27-C26 | -2.18 | 110.18      | 114.08   |
| 17  | B     | 847  | BCR  | C8-C7-C6    | -2.18 | 121.07      | 127.20   |
| 17  | B     | 851  | BCR  | C27-C26-C25 | 2.18  | 125.90      | 122.73   |
| 17  | b     | 848  | BCR  | C8-C7-C6    | -2.18 | 121.07      | 127.20   |
| 14  | A     | 831  | CLA  | C2D-C1D-ND  | -2.18 | 108.50      | 110.10   |
| 17  | b     | 848  | BCR  | C2-C1-C6    | 2.18  | 113.84      | 110.48   |
| 14  | b     | 840  | CLA  | CHB-C4A-NA  | 2.18  | 127.53      | 124.51   |
| 14  | a     | 828  | CLA  | C1B-CHB-C4A | -2.18 | 125.80      | 130.12   |
| 14  | L     | 205  | CLA  | C1-C2-C3    | -2.18 | 122.27      | 126.04   |
| 14  | a     | 809  | CLA  | CHD-C1D-ND  | -2.18 | 122.45      | 124.45   |
| 18  | y     | 101  | LHG  | C20-C19-C18 | -2.18 | 103.36      | 114.42   |
| 17  | 2     | 848  | BCR  | C8-C7-C6    | -2.18 | 121.08      | 127.20   |
| 18  | m     | 101  | LHG  | C20-C19-C18 | -2.18 | 103.36      | 114.42   |
| 14  | 1     | 1638 | CLA  | O2A-CGA-O1A | -2.18 | 117.87      | 123.30   |
| 17  | A     | 849  | BCR  | C38-C26-C25 | -2.18 | 122.08      | 124.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | 1     | 1648 | BCR  | C24-C23-C22 | -2.18 | 122.94      | 126.23   |
| 14  | 2     | 803  | CLA  | CHB-C4A-NA  | 2.18  | 127.52      | 124.51   |
| 17  | B     | 845  | BCR  | C8-C7-C6    | -2.18 | 121.09      | 127.20   |
| 14  | a     | 824  | CLA  | CMB-C2B-C3B | 2.18  | 128.75      | 124.68   |
| 17  | 1     | 1650 | BCR  | C27-C26-C25 | 2.18  | 125.89      | 122.73   |
| 14  | b     | 804  | CLA  | O1D-CGD-CBD | 2.18  | 128.94      | 124.48   |
| 14  | a     | 827  | CLA  | O2D-CGD-CBD | 2.17  | 115.13      | 111.27   |
| 14  | 2     | 825  | CLA  | CHA-C1A-NA  | -2.17 | 121.42      | 126.40   |
| 14  | 1     | 1627 | CLA  | CAA-CBA-CGA | -2.17 | 106.91      | 113.25   |
| 14  | b     | 809  | CLA  | O2D-CGD-CBD | 2.17  | 115.13      | 111.27   |
| 17  | 0     | 201  | BCR  | C24-C23-C22 | -2.17 | 122.95      | 126.23   |
| 14  | A     | 834  | CLA  | C5-C3-C2    | 2.17  | 125.51      | 121.12   |
| 14  | 1     | 1635 | CLA  | C5-C3-C2    | 2.17  | 125.51      | 121.12   |
| 18  | M     | 101  | LHG  | C20-C19-C18 | -2.17 | 103.40      | 114.42   |
| 14  | 0     | 206  | CLA  | C1-C2-C3    | -2.17 | 122.29      | 126.04   |
| 14  | j     | 1303 | CLA  | C2D-C1D-ND  | -2.17 | 108.50      | 110.10   |
| 14  | A     | 842  | CLA  | O2A-CGA-O1A | -2.17 | 118.12      | 123.59   |
| 17  | B     | 847  | BCR  | C2-C1-C6    | 2.17  | 113.82      | 110.48   |
| 14  | 2     | 840  | CLA  | CHB-C4A-NA  | 2.17  | 127.51      | 124.51   |
| 14  | A     | 843  | CLA  | C1B-CHB-C4A | -2.17 | 125.82      | 130.12   |
| 14  | l     | 205  | CLA  | C1-C2-C3    | -2.17 | 122.29      | 126.04   |
| 14  | B     | 808  | CLA  | O2D-CGD-CBD | 2.17  | 115.12      | 111.27   |
| 14  | a     | 822  | CLA  | CHD-C1D-ND  | -2.17 | 122.46      | 124.45   |
| 14  | 1     | 1643 | CLA  | O2A-CGA-O1A | -2.17 | 118.12      | 123.59   |
| 14  | A     | 824  | CLA  | CMB-C2B-C3B | 2.17  | 128.74      | 124.68   |
| 17  | 0     | 209  | BCR  | C24-C23-C22 | -2.17 | 122.96      | 126.23   |
| 17  | b     | 846  | BCR  | C8-C7-C6    | -2.17 | 121.11      | 127.20   |
| 14  | B     | 832  | CLA  | CHD-C1D-ND  | -2.17 | 122.46      | 124.45   |
| 14  | 2     | 806  | CLA  | CHD-C1D-ND  | -2.17 | 122.46      | 124.45   |
| 14  | a     | 826  | CLA  | CAA-CBA-CGA | -2.17 | 106.92      | 113.25   |
| 14  | A     | 837  | CLA  | O2A-CGA-O1A | -2.17 | 117.90      | 123.30   |
| 14  | F     | 203  | CLA  | CHB-C4A-NA  | 2.17  | 127.51      | 124.51   |
| 14  | L     | 204  | CLA  | C1-C2-C3    | -2.17 | 122.30      | 126.04   |
| 14  | 2     | 804  | CLA  | O1D-CGD-CBD | 2.17  | 128.92      | 124.48   |
| 17  | A     | 849  | BCR  | C24-C23-C22 | -2.17 | 122.96      | 126.23   |
| 14  | A     | 826  | CLA  | CAA-CBA-CGA | -2.17 | 106.92      | 113.25   |
| 14  | B     | 824  | CLA  | CHA-C1A-NA  | -2.17 | 121.44      | 126.40   |
| 17  | 0     | 208  | BCR  | C28-C27-C26 | -2.16 | 110.21      | 114.08   |
| 17  | j     | 1304 | BCR  | C38-C26-C25 | -2.16 | 122.10      | 124.53   |
| 17  | 2     | 848  | BCR  | C2-C1-C6    | 2.16  | 113.81      | 110.48   |
| 17  | 1     | 1650 | BCR  | C24-C23-C22 | -2.16 | 122.97      | 126.23   |
| 17  | 2     | 846  | BCR  | C8-C7-C6    | -2.16 | 121.13      | 127.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | 1     | 1644 | CLA  | C1B-CHB-C4A | -2.16 | 125.83      | 130.12   |
| 14  | 2     | 809  | CLA  | O2D-CGD-CBD | 2.16  | 115.11      | 111.27   |
| 14  | 2     | 816  | CLA  | O2A-CGA-O1A | -2.16 | 118.14      | 123.59   |
| 14  | B     | 802  | CLA  | CHB-C4A-NA  | 2.16  | 127.50      | 124.51   |
| 14  | l     | 205  | CLA  | CHD-C1D-ND  | -2.16 | 122.47      | 124.45   |
| 17  | k     | 102  | BCR  | C15-C14-C13 | -2.16 | 124.23      | 127.31   |
| 14  | b     | 803  | CLA  | CHB-C4A-NA  | 2.16  | 127.50      | 124.51   |
| 14  | A     | 827  | CLA  | O2D-CGD-CBD | 2.16  | 115.10      | 111.27   |
| 14  | 2     | 829  | CLA  | C2D-C1D-ND  | -2.16 | 108.52      | 110.10   |
| 17  | B     | 851  | BCR  | C38-C26-C25 | -2.16 | 122.11      | 124.53   |
| 14  | 8     | 1303 | CLA  | C2D-C1D-ND  | -2.15 | 108.52      | 110.10   |
| 14  | 1     | 1610 | CLA  | CHD-C1D-ND  | -2.15 | 122.47      | 124.45   |
| 17  | k     | 104  | BCR  | C8-C7-C6    | -2.15 | 121.16      | 127.20   |
| 17  | 6     | 202  | BCR  | C37-C22-C21 | -2.15 | 119.91      | 122.92   |
| 17  | b     | 847  | BCR  | C36-C18-C19 | 2.15  | 121.47      | 118.08   |
| 14  | j     | 1301 | CLA  | O2D-CGD-O1D | -2.15 | 119.63      | 123.84   |
| 17  | 1     | 1648 | BCR  | C8-C7-C6    | -2.15 | 121.16      | 127.20   |
| 14  | K     | 101  | CLA  | CHD-C1D-ND  | -2.15 | 122.48      | 124.45   |
| 17  | a     | 849  | BCR  | C27-C26-C25 | 2.15  | 125.85      | 122.73   |
| 14  | J     | 102  | CLA  | C2D-C1D-ND  | -2.15 | 108.52      | 110.10   |
| 14  | B     | 816  | CLA  | C1B-CHB-C4A | -2.15 | 125.86      | 130.12   |
| 14  | a     | 837  | CLA  | O2A-CGA-O1A | -2.15 | 117.94      | 123.30   |
| 14  | b     | 817  | CLA  | C1B-CHB-C4A | -2.15 | 125.86      | 130.12   |
| 14  | 1     | 1617 | CLA  | CHD-C1D-ND  | -2.15 | 122.48      | 124.45   |
| 14  | a     | 824  | CLA  | C1-C2-C3    | -2.15 | 122.33      | 126.04   |
| 17  | A     | 847  | BCR  | C8-C7-C6    | -2.15 | 121.17      | 127.20   |
| 17  | 2     | 847  | BCR  | C36-C18-C19 | 2.15  | 121.46      | 118.08   |
| 14  | B     | 840  | CLA  | C2D-C1D-ND  | -2.15 | 108.52      | 110.10   |
| 17  | a     | 847  | BCR  | C8-C7-C6    | -2.15 | 121.17      | 127.20   |
| 14  | b     | 807  | CLA  | O1D-CGD-CBD | 2.15  | 128.88      | 124.48   |
| 14  | b     | 841  | CLA  | C2D-C1D-ND  | -2.15 | 108.52      | 110.10   |
| 17  | 8     | 1306 | BCR  | C37-C22-C21 | -2.15 | 119.92      | 122.92   |
| 14  | a     | 825  | CLA  | CHD-C1D-ND  | -2.15 | 122.48      | 124.45   |
| 14  | A     | 824  | CLA  | C1-C2-C3    | -2.15 | 122.33      | 126.04   |
| 14  | 1     | 1638 | CLA  | O1A-CGA-CBA | 2.15  | 129.97      | 123.08   |
| 17  | K     | 104  | BCR  | C8-C7-C6    | -2.15 | 121.18      | 127.20   |
| 14  | 8     | 1301 | CLA  | O2D-CGD-O1D | -2.15 | 119.64      | 123.84   |
| 14  | A     | 837  | CLA  | O1A-CGA-CBA | 2.14  | 129.97      | 123.08   |
| 14  | b     | 816  | CLA  | O2A-CGA-O1A | -2.14 | 118.18      | 123.59   |
| 17  | B     | 844  | BCR  | C38-C26-C25 | -2.14 | 122.12      | 124.53   |
| 17  | 8     | 1306 | BCR  | C38-C26-C25 | -2.14 | 122.12      | 124.53   |
| 17  | 8     | 1306 | BCR  | C37-C22-C23 | 2.14  | 121.45      | 118.08   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | 9     | 104  | BCR  | C8-C7-C6    | -2.14 | 121.18      | 127.20   |
| 18  | A     | 854  | LHG  | C11-C10-C9  | -2.14 | 103.55      | 114.42   |
| 17  | 0     | 201  | BCR  | C8-C7-C6    | -2.14 | 121.19      | 127.20   |
| 14  | B     | 815  | CLA  | O2A-CGA-O1A | -2.14 | 118.19      | 123.59   |
| 18  | 1     | 1655 | LHG  | C11-C10-C9  | -2.14 | 103.56      | 114.42   |
| 17  | F     | 202  | BCR  | C37-C22-C21 | -2.14 | 119.93      | 122.92   |
| 14  | J     | 102  | CLA  | CHD-C1D-ND  | -2.14 | 122.49      | 124.45   |
| 17  | 8     | 1306 | BCR  | C27-C26-C25 | 2.14  | 125.84      | 122.73   |
| 14  | 2     | 841  | CLA  | O2A-CGA-O1A | -2.14 | 118.19      | 123.59   |
| 14  | B     | 806  | CLA  | CHD-C1D-ND  | -2.14 | 122.49      | 124.45   |
| 17  | L     | 206  | BCR  | C28-C27-C26 | -2.14 | 110.26      | 114.08   |
| 14  | b     | 825  | CLA  | CHA-C1A-NA  | -2.14 | 121.50      | 126.40   |
| 17  | b     | 844  | BCR  | C8-C7-C6    | -2.14 | 121.20      | 127.20   |
| 17  | f     | 202  | BCR  | C37-C22-C21 | -2.14 | 119.93      | 122.92   |
| 17  | b     | 845  | BCR  | C38-C26-C25 | -2.14 | 122.13      | 124.53   |
| 20  | b     | 850  | LMG  | C38-C37-C36 | -2.14 | 103.58      | 114.42   |
| 17  | b     | 852  | BCR  | C20-C21-C22 | -2.14 | 124.26      | 127.31   |
| 14  | a     | 806  | CLA  | C1-O2A-CGA  | 2.14  | 122.05      | 116.44   |
| 14  | B     | 828  | CLA  | C2D-C1D-ND  | -2.14 | 108.53      | 110.10   |
| 14  | 2     | 817  | CLA  | C1B-CHB-C4A | -2.14 | 125.89      | 130.12   |
| 14  | F     | 203  | CLA  | O2D-CGD-O1D | -2.13 | 119.66      | 123.84   |
| 17  | L     | 207  | BCR  | C8-C7-C6    | -2.13 | 121.21      | 127.20   |
| 18  | A     | 854  | LHG  | O8-C23-O10  | -2.13 | 118.21      | 123.59   |
| 18  | a     | 854  | LHG  | C11-C10-C9  | -2.13 | 103.59      | 114.42   |
| 20  | B     | 849  | LMG  | C38-C37-C36 | -2.13 | 103.60      | 114.42   |
| 18  | a     | 854  | LHG  | O8-C23-O10  | -2.13 | 118.21      | 123.59   |
| 18  | l     | 201  | LHG  | C20-C19-C18 | -2.13 | 103.60      | 114.42   |
| 17  | b     | 852  | BCR  | C37-C22-C23 | 2.13  | 121.44      | 118.08   |
| 17  | A     | 849  | BCR  | C27-C26-C25 | 2.13  | 125.83      | 122.73   |
| 17  | A     | 847  | BCR  | C24-C23-C22 | -2.13 | 123.01      | 126.23   |
| 14  | A     | 806  | CLA  | C1-O2A-CGA  | 2.13  | 122.04      | 116.44   |
| 14  | k     | 101  | CLA  | CHD-C1D-ND  | -2.13 | 122.50      | 124.45   |
| 17  | l     | 207  | BCR  | C28-C27-C26 | -2.13 | 110.27      | 114.08   |
| 17  | 0     | 209  | BCR  | C8-C7-C6    | -2.13 | 121.22      | 127.20   |
| 18  | L     | 208  | LHG  | C20-C19-C18 | -2.13 | 103.61      | 114.42   |
| 20  | 2     | 850  | LMG  | C38-C37-C36 | -2.13 | 103.62      | 114.42   |
| 18  | 0     | 202  | LHG  | C20-C19-C18 | -2.13 | 103.63      | 114.42   |
| 17  | a     | 849  | BCR  | C24-C23-C22 | -2.13 | 123.02      | 126.23   |
| 17  | 8     | 1306 | BCR  | C20-C21-C22 | -2.13 | 124.28      | 127.31   |
| 14  | b     | 835  | CLA  | O2A-CGA-O1A | -2.12 | 118.23      | 123.59   |
| 14  | a     | 837  | CLA  | O1A-CGA-CBA | 2.12  | 129.91      | 123.08   |
| 14  | 1     | 1607 | CLA  | C1-O2A-CGA  | 2.12  | 122.02      | 116.44   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | L     | 204  | CLA  | CHD-C1D-ND  | -2.12 | 122.50      | 124.45   |
| 14  | 2     | 822  | CLA  | CHD-C1D-ND  | -2.12 | 122.50      | 124.45   |
| 18  | 1     | 1655 | LHG  | O8-C23-O10  | -2.12 | 118.23      | 123.59   |
| 17  | b     | 852  | BCR  | C27-C26-C25 | 2.12  | 125.81      | 122.73   |
| 14  | b     | 831  | CLA  | O2D-CGD-CBD | 2.12  | 115.04      | 111.27   |
| 14  | B     | 806  | CLA  | O1D-CGD-CBD | 2.12  | 128.82      | 124.48   |
| 17  | 2     | 844  | BCR  | C8-C7-C6    | -2.12 | 121.25      | 127.20   |
| 17  | B     | 846  | BCR  | C36-C18-C19 | 2.12  | 121.42      | 118.08   |
| 14  | A     | 809  | CLA  | O2A-CGA-O1A | -2.12 | 118.25      | 123.59   |
| 17  | a     | 849  | BCR  | C8-C7-C6    | -2.12 | 121.25      | 127.20   |
| 14  | B     | 834  | CLA  | O2A-CGA-O1A | -2.12 | 118.25      | 123.59   |
| 14  | B     | 826  | CLA  | C2D-C1D-ND  | -2.12 | 108.54      | 110.10   |
| 17  | 0     | 203  | BCR  | C27-C26-C25 | 2.12  | 125.81      | 122.73   |
| 17  | a     | 847  | BCR  | C24-C23-C22 | -2.12 | 123.03      | 126.23   |
| 14  | b     | 806  | CLA  | CHD-C1D-ND  | -2.12 | 122.51      | 124.45   |
| 17  | 8     | 1305 | BCR  | C29-C30-C25 | 2.12  | 113.74      | 110.48   |
| 17  | B     | 851  | BCR  | C37-C22-C23 | 2.12  | 121.41      | 118.08   |
| 14  | 1     | 1640 | CLA  | CHB-C4A-NA  | 2.12  | 127.44      | 124.51   |
| 14  | 1     | 1625 | CLA  | C1-C2-C3    | -2.12 | 122.39      | 126.04   |
| 17  | A     | 849  | BCR  | C8-C7-C6    | -2.11 | 121.26      | 127.20   |
| 14  | a     | 809  | CLA  | O2A-CGA-O1A | -2.11 | 118.26      | 123.59   |
| 14  | 1     | 1639 | CLA  | C1B-CHB-C4A | -2.11 | 125.93      | 130.12   |
| 14  | b     | 829  | CLA  | C2D-C1D-ND  | -2.11 | 108.55      | 110.10   |
| 17  | B     | 843  | BCR  | C8-C7-C6    | -2.11 | 121.27      | 127.20   |
| 14  | A     | 819  | CLA  | CHB-C4A-NA  | 2.11  | 127.43      | 124.51   |
| 14  | a     | 803  | CLA  | CHB-C4A-NA  | 2.11  | 127.43      | 124.51   |
| 17  | b     | 852  | BCR  | C38-C26-C25 | -2.11 | 122.16      | 124.53   |
| 17  | 1     | 1652 | BCR  | C7-C8-C9    | -2.11 | 123.05      | 126.23   |
| 14  | 2     | 831  | CLA  | O2D-CGD-CBD | 2.11  | 115.02      | 111.27   |
| 14  | 1     | 1620 | CLA  | CHB-C4A-NA  | 2.11  | 127.43      | 124.51   |
| 14  | 2     | 807  | CLA  | CHD-C1D-ND  | -2.11 | 122.52      | 124.45   |
| 14  | 9     | 101  | CLA  | CHD-C1D-ND  | -2.11 | 122.52      | 124.45   |
| 14  | a     | 839  | CLA  | O2A-CGA-O1A | -2.11 | 118.27      | 123.59   |
| 14  | 1     | 1640 | CLA  | O2A-CGA-O1A | -2.11 | 118.27      | 123.59   |
| 14  | a     | 816  | CLA  | CHD-C1D-ND  | -2.11 | 122.52      | 124.45   |
| 14  | A     | 803  | CLA  | CHB-C4A-NA  | 2.11  | 127.43      | 124.51   |
| 17  | 0     | 201  | BCR  | C7-C8-C9    | -2.11 | 123.05      | 126.23   |
| 17  | A     | 850  | BCR  | C27-C26-C25 | 2.11  | 125.79      | 122.73   |
| 14  | 1     | 1629 | CLA  | CHD-C1D-ND  | -2.11 | 122.52      | 124.45   |
| 14  | B     | 840  | CLA  | O2A-CGA-O1A | -2.11 | 118.27      | 123.59   |
| 17  | 1     | 1650 | BCR  | C8-C7-C6    | -2.11 | 121.28      | 127.20   |
| 17  | 0     | 209  | BCR  | C20-C21-C22 | -2.11 | 124.30      | 127.31   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | b     | 841  | CLA  | O2A-CGA-O1A | -2.11 | 118.28      | 123.59   |
| 14  | 0     | 206  | CLA  | CHD-C1D-ND  | -2.11 | 122.52      | 124.45   |
| 17  | 0     | 201  | BCR  | C20-C21-C22 | -2.11 | 124.30      | 127.31   |
| 17  | l     | 202  | BCR  | C27-C26-C25 | 2.11  | 125.79      | 122.73   |
| 20  | B     | 849  | LMG  | C42-C41-C40 | -2.10 | 103.74      | 114.42   |
| 14  | A     | 816  | CLA  | CHD-C1D-ND  | -2.10 | 122.52      | 124.45   |
| 14  | A     | 838  | CLA  | C1B-CHB-C4A | -2.10 | 125.95      | 130.12   |
| 17  | L     | 201  | BCR  | C27-C26-C25 | 2.10  | 125.78      | 122.73   |
| 14  | j     | 1303 | CLA  | CHD-C1D-ND  | -2.10 | 122.52      | 124.45   |
| 14  | 2     | 835  | CLA  | O2A-CGA-O1A | -2.10 | 118.28      | 123.59   |
| 20  | b     | 850  | LMG  | C42-C41-C40 | -2.10 | 103.75      | 114.42   |
| 14  | a     | 838  | CLA  | C1B-CHB-C4A | -2.10 | 125.95      | 130.12   |
| 14  | B     | 805  | CLA  | CHD-C1D-ND  | -2.10 | 122.52      | 124.45   |
| 17  | A     | 851  | BCR  | C7-C8-C9    | -2.10 | 123.06      | 126.23   |
| 17  | 6     | 204  | BCR  | C37-C22-C21 | -2.10 | 119.98      | 122.92   |
| 14  | a     | 817  | CLA  | O2A-CGA-O1A | -2.10 | 118.29      | 123.59   |
| 14  | A     | 811  | CLA  | CHD-C1D-ND  | -2.10 | 122.52      | 124.45   |
| 14  | 1     | 1610 | CLA  | O2A-CGA-O1A | -2.10 | 118.29      | 123.59   |
| 20  | 2     | 850  | LMG  | C42-C41-C40 | -2.10 | 103.77      | 114.42   |
| 14  | b     | 802  | CLA  | CHB-C4A-NA  | 2.10  | 127.41      | 124.51   |
| 17  | 2     | 845  | BCR  | C38-C26-C25 | -2.10 | 122.17      | 124.53   |
| 14  | b     | 822  | CLA  | CHD-C1D-ND  | -2.10 | 122.53      | 124.45   |
| 14  | A     | 855  | CLA  | CHB-C4A-NA  | 2.10  | 127.41      | 124.51   |
| 14  | 2     | 808  | CLA  | C2D-C1D-ND  | -2.10 | 108.56      | 110.10   |
| 17  | a     | 849  | BCR  | C7-C8-C9    | -2.10 | 123.07      | 126.23   |
| 14  | 0     | 205  | CLA  | O2A-CGA-O1A | -2.10 | 118.30      | 123.59   |
| 14  | B     | 820  | CLA  | O2A-CGA-O1A | -2.10 | 118.30      | 123.59   |
| 14  | 1     | 1635 | CLA  | C16-C15-C13 | -2.10 | 109.14      | 115.92   |
| 14  | a     | 819  | CLA  | CHB-C4A-NA  | 2.10  | 127.41      | 124.51   |
| 17  | j     | 1305 | BCR  | C16-C15-C14 | -2.10 | 119.18      | 123.47   |
| 14  | 1     | 1614 | CLA  | O2D-CGD-CBD | 2.09  | 114.99      | 111.27   |
| 14  | A     | 828  | CLA  | CHD-C1D-ND  | -2.09 | 122.53      | 124.45   |
| 14  | a     | 828  | CLA  | CHD-C1D-ND  | -2.09 | 122.53      | 124.45   |
| 14  | b     | 841  | CLA  | CHD-C1D-ND  | -2.09 | 122.53      | 124.45   |
| 14  | 8     | 1303 | CLA  | CHD-C1D-ND  | -2.09 | 122.53      | 124.45   |
| 14  | A     | 817  | CLA  | O2A-CGA-O1A | -2.09 | 118.31      | 123.59   |
| 17  | 1     | 1651 | BCR  | C27-C26-C25 | 2.09  | 125.77      | 122.73   |
| 17  | 1     | 1650 | BCR  | C7-C8-C9    | -2.09 | 123.07      | 126.23   |
| 14  | 2     | 822  | CLA  | O2D-CGD-CBD | 2.09  | 114.98      | 111.27   |
| 14  | a     | 819  | CLA  | C1-C2-C3    | -2.09 | 122.43      | 126.04   |
| 17  | A     | 856  | BCR  | C29-C30-C25 | 2.09  | 113.70      | 110.48   |
| 14  | A     | 813  | CLA  | O2D-CGD-CBD | 2.09  | 114.98      | 111.27   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | a     | 851  | BCR  | C7-C8-C9    | -2.09 | 123.08      | 126.23   |
| 14  | A     | 839  | CLA  | O2A-CGA-O1A | -2.09 | 118.32      | 123.59   |
| 14  | l     | 204  | CLA  | O2A-CGA-O1A | -2.09 | 118.32      | 123.59   |
| 14  | B     | 821  | CLA  | CHD-C1D-ND  | -2.09 | 122.53      | 124.45   |
| 14  | 2     | 841  | CLA  | CHD-C1D-ND  | -2.09 | 122.53      | 124.45   |
| 14  | 1     | 1604 | CLA  | CHB-C4A-NA  | 2.09  | 127.40      | 124.51   |
| 14  | 2     | 802  | CLA  | CHB-C4A-NA  | 2.09  | 127.40      | 124.51   |
| 17  | 8     | 1305 | BCR  | C16-C15-C14 | -2.09 | 119.19      | 123.47   |
| 17  | A     | 856  | BCR  | C24-C23-C22 | -2.09 | 123.08      | 126.23   |
| 14  | 2     | 827  | CLA  | C2D-C1D-ND  | -2.09 | 108.56      | 110.10   |
| 17  | b     | 852  | BCR  | C37-C22-C21 | -2.09 | 120.00      | 122.92   |
| 17  | A     | 849  | BCR  | C7-C8-C9    | -2.09 | 123.08      | 126.23   |
| 14  | A     | 822  | CLA  | CHD-C1D-ND  | -2.09 | 122.54      | 124.45   |
| 14  | B     | 830  | CLA  | O2D-CGD-CBD | 2.09  | 114.98      | 111.27   |
| 14  | 2     | 838  | CLA  | O2D-CGD-CBD | 2.09  | 114.98      | 111.27   |
| 17  | a     | 850  | BCR  | C27-C26-C25 | 2.09  | 125.76      | 122.73   |
| 14  | b     | 822  | CLA  | O2D-CGD-CBD | 2.09  | 114.97      | 111.27   |
| 14  | 1     | 1620 | CLA  | C1-C2-C3    | -2.09 | 122.44      | 126.04   |
| 14  | 2     | 841  | CLA  | C2D-C1D-ND  | -2.08 | 108.57      | 110.10   |
| 14  | A     | 806  | CLA  | C3C-C4C-NC  | -2.08 | 108.23      | 110.57   |
| 17  | 2     | 844  | BCR  | C27-C26-C25 | 2.08  | 125.76      | 122.73   |
| 14  | b     | 837  | CLA  | CHB-C4A-NA  | 2.08  | 127.39      | 124.51   |
| 14  | A     | 841  | CLA  | O2A-CGA-O1A | -2.08 | 118.33      | 123.59   |
| 14  | 1     | 1618 | CLA  | O2A-CGA-O1A | -2.08 | 118.33      | 123.59   |
| 17  | L     | 207  | BCR  | C7-C8-C9    | -2.08 | 123.09      | 126.23   |
| 17  | 8     | 1305 | BCR  | C24-C23-C22 | -2.08 | 123.09      | 126.23   |
| 14  | 2     | 807  | CLA  | O1D-CGD-CBD | 2.08  | 128.74      | 124.48   |
| 17  | b     | 848  | BCR  | C36-C18-C19 | 2.08  | 121.36      | 118.08   |
| 17  | L     | 207  | BCR  | C20-C21-C22 | -2.08 | 124.34      | 127.31   |
| 17  | f     | 204  | BCR  | C37-C22-C21 | -2.08 | 120.01      | 122.92   |
| 14  | B     | 817  | CLA  | C2D-C1D-ND  | -2.08 | 108.57      | 110.10   |
| 17  | b     | 847  | BCR  | C8-C7-C6    | -2.08 | 121.36      | 127.20   |
| 17  | 0     | 209  | BCR  | C7-C8-C9    | -2.08 | 123.09      | 126.23   |
| 14  | a     | 839  | CLA  | CHB-C4A-NA  | 2.08  | 127.39      | 124.51   |
| 17  | A     | 850  | BCR  | C33-C5-C6   | -2.08 | 122.19      | 124.53   |
| 17  | L     | 206  | BCR  | C8-C7-C6    | -2.08 | 121.36      | 127.20   |
| 14  | 1     | 1642 | CLA  | O2A-CGA-O1A | -2.08 | 118.35      | 123.59   |
| 17  | a     | 850  | BCR  | C33-C5-C6   | -2.08 | 122.19      | 124.53   |
| 14  | j     | 1302 | CLA  | CHD-C1D-ND  | -2.08 | 122.54      | 124.45   |
| 14  | B     | 821  | CLA  | O2D-CGD-CBD | 2.08  | 114.96      | 111.27   |
| 17  | B     | 851  | BCR  | C37-C22-C21 | -2.08 | 120.01      | 122.92   |
| 17  | 2     | 848  | BCR  | C36-C18-C19 | 2.08  | 121.35      | 118.08   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | l     | 207  | BCR  | C8-C7-C6    | -2.08 | 121.37      | 127.20   |
| 14  | b     | 821  | CLA  | O2A-CGA-O1A | -2.08 | 118.35      | 123.59   |
| 14  | F     | 204  | CLA  | CHD-C1D-ND  | -2.08 | 122.55      | 124.45   |
| 14  | 1     | 1623 | CLA  | CHD-C1D-ND  | -2.08 | 122.55      | 124.45   |
| 14  | B     | 836  | CLA  | CHB-C4A-NA  | 2.08  | 127.38      | 124.51   |
| 14  | a     | 841  | CLA  | O2A-CGA-O1A | -2.08 | 118.35      | 123.59   |
| 14  | L     | 203  | CLA  | O2A-CGA-O1A | -2.08 | 118.35      | 123.59   |
| 14  | b     | 812  | CLA  | C1-C2-C3    | -2.08 | 122.45      | 126.04   |
| 14  | 2     | 819  | CLA  | CHD-C1D-ND  | -2.08 | 122.55      | 124.45   |
| 14  | a     | 806  | CLA  | C3C-C4C-NC  | -2.07 | 108.24      | 110.57   |
| 14  | B     | 814  | CLA  | C2D-C1D-ND  | -2.07 | 108.58      | 110.10   |
| 14  | 2     | 818  | CLA  | C2D-C1D-ND  | -2.07 | 108.58      | 110.10   |
| 14  | A     | 834  | CLA  | C16-C15-C13 | -2.07 | 109.21      | 115.92   |
| 14  | f     | 203  | CLA  | CHD-C1D-ND  | -2.07 | 122.55      | 124.45   |
| 14  | A     | 813  | CLA  | C2D-C1D-ND  | -2.07 | 108.58      | 110.10   |
| 14  | l     | 206  | CLA  | C2D-C1D-ND  | -2.07 | 108.58      | 110.10   |
| 14  | b     | 805  | CLA  | O1D-CGD-CBD | 2.07  | 128.72      | 124.48   |
| 17  | l     | 202  | BCR  | C37-C22-C23 | 2.07  | 121.34      | 118.08   |
| 14  | a     | 813  | CLA  | O2D-CGD-CBD | 2.07  | 114.95      | 111.27   |
| 17  | 1     | 1651 | BCR  | C33-C5-C6   | -2.07 | 122.20      | 124.53   |
| 14  | b     | 818  | CLA  | C2D-C1D-ND  | -2.07 | 108.58      | 110.10   |
| 14  | b     | 835  | CLA  | C2D-C1D-ND  | -2.07 | 108.58      | 110.10   |
| 17  | 0     | 203  | BCR  | C37-C22-C23 | 2.07  | 121.34      | 118.08   |
| 14  | a     | 815  | CLA  | CHD-C1D-ND  | -2.07 | 122.55      | 124.45   |
| 14  | A     | 819  | CLA  | C1-C2-C3    | -2.07 | 122.47      | 126.04   |
| 14  | a     | 834  | CLA  | C16-C15-C13 | -2.07 | 109.24      | 115.92   |
| 17  | B     | 847  | BCR  | C36-C18-C19 | 2.07  | 121.33      | 118.08   |
| 14  | 2     | 821  | CLA  | O2A-CGA-O1A | -2.07 | 118.38      | 123.59   |
| 17  | F     | 205  | BCR  | C37-C22-C21 | -2.07 | 120.03      | 122.92   |
| 17  | b     | 844  | BCR  | C27-C26-C25 | 2.07  | 125.73      | 122.73   |
| 17  | 2     | 847  | BCR  | C8-C7-C6    | -2.07 | 121.40      | 127.20   |
| 14  | 2     | 837  | CLA  | CHB-C4A-NA  | 2.07  | 127.37      | 124.51   |
| 14  | a     | 811  | CLA  | CHD-C1D-ND  | -2.07 | 122.56      | 124.45   |
| 14  | b     | 827  | CLA  | C2D-C1D-ND  | -2.07 | 108.58      | 110.10   |
| 14  | A     | 839  | CLA  | CHB-C4A-NA  | 2.06  | 127.37      | 124.51   |
| 17  | j     | 1305 | BCR  | C24-C23-C22 | -2.06 | 123.12      | 126.23   |
| 14  | B     | 817  | CLA  | O2A-CGA-O1A | -2.06 | 118.38      | 123.59   |
| 17  | L     | 201  | BCR  | C37-C22-C23 | 2.06  | 121.33      | 118.08   |
| 14  | b     | 835  | CLA  | CAA-CBA-CGA | -2.06 | 107.22      | 113.25   |
| 14  | 1     | 1616 | CLA  | CHD-C1D-ND  | -2.06 | 122.56      | 124.45   |
| 14  | 2     | 805  | CLA  | O1D-CGD-CBD | 2.06  | 128.71      | 124.48   |
| 17  | A     | 856  | BCR  | C16-C15-C14 | -2.06 | 119.25      | 123.47   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | 2     | 830  | CLA  | CAC-C3C-C4C | 2.06  | 127.49      | 124.81   |
| 14  | B     | 811  | CLA  | C1-C2-C3    | -2.06 | 122.48      | 126.04   |
| 14  | B     | 837  | CLA  | O2D-CGD-CBD | 2.06  | 114.93      | 111.27   |
| 14  | 1     | 1612 | CLA  | CHD-C1D-ND  | -2.06 | 122.56      | 124.45   |
| 17  | 0     | 208  | BCR  | C8-C7-C6    | -2.06 | 121.41      | 127.20   |
| 14  | 2     | 812  | CLA  | C1-C2-C3    | -2.06 | 122.48      | 126.04   |
| 17  | a     | 852  | BCR  | C36-C18-C19 | 2.06  | 119.15      | 114.60   |
| 14  | A     | 826  | CLA  | O2A-CGA-O1A | -2.06 | 118.39      | 123.59   |
| 14  | 2     | 815  | CLA  | C2D-C1D-ND  | -2.06 | 108.59      | 110.10   |
| 14  | b     | 818  | CLA  | O2A-CGA-O1A | -2.06 | 118.39      | 123.59   |
| 14  | A     | 804  | CLA  | O2D-CGD-CBD | 2.06  | 114.93      | 111.27   |
| 14  | b     | 822  | CLA  | O2A-CGA-O1A | -2.06 | 118.17      | 123.30   |
| 17  | B     | 843  | BCR  | C27-C26-C25 | 2.06  | 125.72      | 122.73   |
| 14  | A     | 815  | CLA  | CHD-C1D-ND  | -2.06 | 122.56      | 124.45   |
| 14  | 2     | 818  | CLA  | O2A-CGA-O1A | -2.06 | 118.41      | 123.59   |
| 17  | B     | 846  | BCR  | C8-C7-C6    | -2.05 | 121.43      | 127.20   |
| 14  | B     | 818  | CLA  | CHD-C1D-ND  | -2.05 | 122.57      | 124.45   |
| 17  | 1     | 1653 | BCR  | C36-C18-C19 | 2.05  | 119.14      | 114.60   |
| 14  | B     | 818  | CLA  | O2A-CGA-O1A | -2.05 | 118.41      | 123.59   |
| 17  | j     | 1305 | BCR  | C29-C30-C25 | 2.05  | 113.64      | 110.48   |
| 14  | b     | 819  | CLA  | CHD-C1D-ND  | -2.05 | 122.57      | 124.45   |
| 14  | a     | 835  | CLA  | CMB-C2B-C3B | 2.05  | 128.52      | 124.68   |
| 14  | a     | 804  | CLA  | O2D-CGD-CBD | 2.05  | 114.91      | 111.27   |
| 14  | 2     | 835  | CLA  | CAA-CBA-CGA | -2.05 | 107.26      | 113.25   |
| 14  | B     | 807  | CLA  | C2D-C1D-ND  | -2.05 | 108.59      | 110.10   |
| 14  | B     | 834  | CLA  | CAA-CBA-CGA | -2.05 | 107.26      | 113.25   |
| 14  | a     | 826  | CLA  | O2A-CGA-O1A | -2.05 | 118.42      | 123.59   |
| 14  | A     | 812  | CLA  | CHD-C1D-ND  | -2.05 | 122.57      | 124.45   |
| 14  | 1     | 1625 | CLA  | CHD-C1D-ND  | -2.05 | 122.57      | 124.45   |
| 14  | 6     | 203  | CLA  | CHD-C1D-ND  | -2.05 | 122.57      | 124.45   |
| 14  | 1     | 1627 | CLA  | O2A-CGA-O1A | -2.05 | 118.42      | 123.59   |
| 14  | J     | 101  | CLA  | CHD-C1D-ND  | -2.05 | 122.57      | 124.45   |
| 14  | b     | 808  | CLA  | C2D-C1D-ND  | -2.05 | 108.59      | 110.10   |
| 14  | 2     | 835  | CLA  | C2D-C1D-ND  | -2.05 | 108.59      | 110.10   |
| 14  | L     | 205  | CLA  | C2D-C1D-ND  | -2.05 | 108.60      | 110.10   |
| 14  | A     | 834  | CLA  | O1D-CGD-CBD | 2.05  | 128.67      | 124.48   |
| 14  | 1     | 1607 | CLA  | C3C-C4C-NC  | -2.05 | 108.28      | 110.57   |
| 14  | b     | 830  | CLA  | CAC-C3C-C4C | 2.05  | 127.46      | 124.81   |
| 14  | a     | 829  | CLA  | O2A-CGA-O1A | -2.05 | 118.43      | 123.59   |
| 14  | 1     | 1635 | CLA  | O1D-CGD-CBD | 2.04  | 128.67      | 124.48   |
| 14  | 2     | 839  | CLA  | CHB-C4A-NA  | 2.04  | 127.34      | 124.51   |
| 17  | 8     | 1304 | BCR  | C16-C15-C14 | -2.04 | 119.29      | 123.47   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | 1     | 1636 | CLA  | CMB-C2B-C3B | 2.04  | 128.50      | 124.68   |
| 20  | B     | 849  | LMG  | O1-C7-C8    | -2.04 | 105.97      | 110.90   |
| 14  | 2     | 822  | CLA  | O2A-CGA-O1A | -2.04 | 118.21      | 123.30   |
| 20  | b     | 850  | LMG  | O1-C7-C8    | -2.04 | 105.97      | 110.90   |
| 14  | 2     | 814  | CLA  | O2A-CGA-O1A | -2.04 | 118.44      | 123.59   |
| 17  | A     | 852  | BCR  | C36-C18-C19 | 2.04  | 119.11      | 114.60   |
| 14  | a     | 823  | CLA  | O2A-CGA-O1A | -2.04 | 118.21      | 123.30   |
| 14  | b     | 815  | CLA  | C2D-C1D-ND  | -2.04 | 108.60      | 110.10   |
| 14  | 2     | 819  | CLA  | O2A-CGA-O1A | -2.04 | 118.44      | 123.59   |
| 14  | A     | 835  | CLA  | CMB-C2B-C3B | 2.04  | 128.50      | 124.68   |
| 14  | B     | 804  | CLA  | O1D-CGD-CBD | 2.04  | 128.66      | 124.48   |
| 14  | a     | 805  | CLA  | O2A-CGA-O1A | -2.04 | 118.44      | 123.59   |
| 14  | B     | 821  | CLA  | O2A-CGA-O1A | -2.04 | 118.22      | 123.30   |
| 14  | a     | 824  | CLA  | CHD-C1D-ND  | -2.04 | 122.58      | 124.45   |
| 14  | a     | 834  | CLA  | O1D-CGD-CBD | 2.04  | 128.65      | 124.48   |
| 14  | b     | 819  | CLA  | O2A-CGA-O1A | -2.04 | 118.45      | 123.59   |
| 20  | 2     | 850  | LMG  | O1-C7-C8    | -2.04 | 105.99      | 110.90   |
| 17  | j     | 1304 | BCR  | C16-C15-C14 | -2.04 | 119.30      | 123.47   |
| 14  | B     | 813  | CLA  | O2A-CGA-O1A | -2.04 | 118.46      | 123.59   |
| 14  | b     | 814  | CLA  | O2A-CGA-O1A | -2.03 | 118.46      | 123.59   |
| 17  | b     | 848  | BCR  | C36-C18-C17 | -2.03 | 120.07      | 122.92   |
| 14  | 1     | 1605 | CLA  | O2D-CGD-CBD | 2.03  | 114.88      | 111.27   |
| 14  | A     | 823  | CLA  | O2A-CGA-O1A | -2.03 | 118.23      | 123.30   |
| 14  | b     | 805  | CLA  | C2D-C1D-ND  | -2.03 | 108.61      | 110.10   |
| 14  | a     | 814  | CLA  | CHD-C1D-ND  | -2.03 | 122.59      | 124.45   |
| 14  | 2     | 811  | CLA  | CAC-C3C-C4C | 2.03  | 127.45      | 124.81   |
| 14  | B     | 831  | CLA  | CHD-C1D-ND  | -2.03 | 122.59      | 124.45   |
| 14  | 1     | 1610 | CLA  | O2D-CGD-CBD | 2.03  | 114.88      | 111.27   |
| 17  | K     | 104  | BCR  | C16-C15-C14 | -2.03 | 119.31      | 123.47   |
| 14  | A     | 805  | CLA  | O2A-CGA-O1A | -2.03 | 118.47      | 123.59   |
| 14  | B     | 834  | CLA  | C2D-C1D-ND  | -2.03 | 108.61      | 110.10   |
| 14  | 1     | 1613 | CLA  | CHD-C1D-ND  | -2.03 | 122.59      | 124.45   |
| 14  | a     | 835  | CLA  | O2D-CGD-CBD | 2.03  | 114.87      | 111.27   |
| 14  | B     | 829  | CLA  | CAC-C3C-C4C | 2.03  | 127.44      | 124.81   |
| 14  | B     | 810  | CLA  | CAC-C3C-C4C | 2.03  | 127.44      | 124.81   |
| 14  | A     | 814  | CLA  | CHD-C1D-ND  | -2.03 | 122.59      | 124.45   |
| 14  | 9     | 103  | CLA  | C1-C2-C3    | -2.02 | 122.54      | 126.04   |
| 14  | b     | 805  | CLA  | C4-C3-C5    | 2.02  | 118.68      | 115.27   |
| 14  | 8     | 1302 | CLA  | CHD-C1D-ND  | -2.02 | 122.59      | 124.45   |
| 14  | a     | 820  | CLA  | C1-C2-C3    | -2.02 | 122.54      | 126.04   |
| 14  | A     | 803  | CLA  | CMB-C2B-C3B | 2.02  | 128.46      | 124.68   |
| 14  | B     | 830  | CLA  | O2A-CGA-O1A | -2.02 | 118.49      | 123.59   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | b     | 838  | CLA  | O2D-CGD-CBD | 2.02  | 114.86      | 111.27   |
| 13  | a     | 801  | CL0  | O2A-CGA-O1A | -2.02 | 118.49      | 123.59   |
| 17  | J     | 103  | BCR  | C16-C15-C14 | -2.02 | 119.33      | 123.47   |
| 14  | B     | 809  | CLA  | C3C-C4C-NC  | -2.02 | 108.30      | 110.57   |
| 14  | a     | 809  | CLA  | O2D-CGD-CBD | 2.02  | 114.86      | 111.27   |
| 17  | b     | 847  | BCR  | C37-C22-C21 | -2.02 | 120.09      | 122.92   |
| 14  | K     | 103  | CLA  | C1-C2-C3    | -2.02 | 122.55      | 126.04   |
| 13  | 1     | 1602 | CL0  | O2A-CGA-O1A | -2.02 | 118.49      | 123.59   |
| 14  | b     | 812  | CLA  | C4-C3-C5    | 2.02  | 118.67      | 115.27   |
| 14  | A     | 834  | CLA  | C2D-C1D-ND  | -2.02 | 108.61      | 110.10   |
| 14  | A     | 803  | CLA  | O2A-CGA-O1A | -2.02 | 118.49      | 123.59   |
| 14  | 2     | 840  | CLA  | O2A-CGA-O1A | -2.02 | 118.49      | 123.59   |
| 14  | 1     | 1621 | CLA  | C1-C2-C3    | -2.02 | 122.55      | 126.04   |
| 13  | A     | 801  | CL0  | O2A-CGA-O1A | -2.02 | 118.50      | 123.59   |
| 14  | 1     | 1606 | CLA  | O2A-CGA-O1A | -2.02 | 118.50      | 123.59   |
| 14  | b     | 821  | CLA  | CHD-C1D-ND  | -2.02 | 122.60      | 124.45   |
| 14  | 1     | 1626 | CLA  | O2A-CGA-O1A | -2.02 | 118.50      | 123.59   |
| 14  | 2     | 831  | CLA  | O2A-CGA-O1A | -2.02 | 118.50      | 123.59   |
| 17  | a     | 848  | BCR  | C36-C18-C17 | -2.02 | 120.10      | 122.92   |
| 14  | A     | 820  | CLA  | C1-C2-C3    | -2.02 | 122.55      | 126.04   |
| 17  | 1     | 1649 | BCR  | C36-C18-C17 | -2.02 | 120.10      | 122.92   |
| 14  | B     | 803  | CLA  | CAC-C3C-C4C | 2.02  | 127.43      | 124.81   |
| 14  | B     | 802  | CLA  | O2A-CGA-O1A | -2.02 | 118.50      | 123.59   |
| 14  | k     | 103  | CLA  | O2A-CGA-O1A | -2.02 | 118.50      | 123.59   |
| 14  | B     | 807  | CLA  | O2D-CGD-CBD | 2.02  | 114.85      | 111.27   |
| 14  | 1     | 1630 | CLA  | O2A-CGA-O1A | -2.02 | 118.51      | 123.59   |
| 14  | b     | 804  | CLA  | CAC-C3C-C4C | 2.01  | 127.42      | 124.81   |
| 14  | 2     | 804  | CLA  | CAC-C3C-C4C | 2.01  | 127.42      | 124.81   |
| 14  | B     | 839  | CLA  | O2A-CGA-O1A | -2.01 | 118.51      | 123.59   |
| 14  | B     | 804  | CLA  | C4-C3-C5    | 2.01  | 118.66      | 115.27   |
| 14  | B     | 811  | CLA  | C4-C3-C5    | 2.01  | 118.66      | 115.27   |
| 17  | A     | 848  | BCR  | C36-C18-C17 | -2.01 | 120.10      | 122.92   |
| 14  | 1     | 1604 | CLA  | O2A-CGA-O1A | -2.01 | 118.51      | 123.59   |
| 14  | A     | 819  | CLA  | C6-C5-C3    | 2.01  | 118.73      | 113.45   |
| 14  | 1     | 1615 | CLA  | O2A-CGA-O1A | -2.01 | 118.51      | 123.59   |
| 14  | 1     | 1624 | CLA  | O2A-CGA-O1A | -2.01 | 118.28      | 123.30   |
| 17  | B     | 847  | BCR  | C36-C18-C17 | -2.01 | 120.10      | 122.92   |
| 17  | 8     | 1304 | BCR  | C29-C30-C25 | 2.01  | 113.58      | 110.48   |
| 14  | A     | 830  | CLA  | O1D-CGD-CBD | 2.01  | 128.60      | 124.48   |
| 14  | b     | 803  | CLA  | O2A-CGA-O1A | -2.01 | 118.52      | 123.59   |
| 14  | 1     | 1620 | CLA  | C6-C5-C3    | 2.01  | 118.73      | 113.45   |
| 14  | B     | 840  | CLA  | CHD-C1D-ND  | -2.01 | 122.61      | 124.45   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 825  | CLA  | O2A-CGA-O1A | -2.01 | 118.52      | 123.59   |
| 14  | k     | 103  | CLA  | C1-C2-C3    | -2.01 | 122.57      | 126.04   |
| 14  | 2     | 829  | CLA  | CHB-C4A-NA  | 2.01  | 127.29      | 124.51   |
| 17  | j     | 1304 | BCR  | C8-C7-C6    | -2.01 | 121.56      | 127.20   |
| 17  | k     | 104  | BCR  | C16-C15-C14 | -2.01 | 119.36      | 123.47   |
| 14  | a     | 819  | CLA  | C6-C5-C3    | 2.01  | 118.72      | 113.45   |
| 14  | 2     | 803  | CLA  | O2A-CGA-O1A | -2.01 | 118.52      | 123.59   |
| 14  | 2     | 805  | CLA  | C4-C3-C5    | 2.01  | 118.65      | 115.27   |
| 14  | 1     | 1604 | CLA  | CMB-C2B-C3B | 2.01  | 128.44      | 124.68   |
| 14  | b     | 810  | CLA  | C3C-C4C-NC  | -2.01 | 108.32      | 110.57   |
| 17  | j     | 1304 | BCR  | C29-C30-C25 | 2.01  | 113.57      | 110.48   |
| 20  | B     | 849  | LMG  | O7-C10-O9   | -2.01 | 118.85      | 123.70   |
| 14  | A     | 807  | CLA  | O2D-CGD-O1D | -2.01 | 119.91      | 123.84   |
| 14  | K     | 103  | CLA  | O2A-CGA-O1A | -2.01 | 118.53      | 123.59   |
| 14  | 1     | 1614 | CLA  | C2D-C1D-ND  | -2.01 | 108.62      | 110.10   |
| 14  | A     | 829  | CLA  | O2A-CGA-O1A | -2.01 | 118.53      | 123.59   |
| 14  | 9     | 103  | CLA  | O2A-CGA-O1A | -2.01 | 118.53      | 123.59   |
| 14  | b     | 812  | CLA  | O2A-CGA-O1A | -2.01 | 118.53      | 123.59   |
| 14  | 2     | 812  | CLA  | O2A-CGA-O1A | -2.01 | 118.53      | 123.59   |
| 17  | J     | 103  | BCR  | C8-C7-C6    | -2.01 | 121.57      | 127.20   |
| 14  | A     | 814  | CLA  | O2A-CGA-O1A | -2.01 | 118.53      | 123.59   |
| 14  | a     | 819  | CLA  | O2D-CGD-CBD | 2.01  | 114.83      | 111.27   |
| 17  | 9     | 104  | BCR  | C16-C15-C14 | -2.00 | 119.37      | 123.47   |
| 17  | 8     | 1304 | BCR  | C8-C7-C6    | -2.00 | 121.57      | 127.20   |
| 14  | B     | 838  | CLA  | CHB-C4A-NA  | 2.00  | 127.28      | 124.51   |
| 14  | B     | 828  | CLA  | CHD-C1D-ND  | -2.00 | 122.61      | 124.45   |
| 14  | a     | 830  | CLA  | O1D-CGD-CBD | 2.00  | 128.58      | 124.48   |
| 20  | b     | 850  | LMG  | O7-C10-O9   | -2.00 | 118.86      | 123.70   |
| 14  | a     | 814  | CLA  | O2A-CGA-O1A | -2.00 | 118.54      | 123.59   |
| 14  | 2     | 819  | CLA  | O1D-CGD-CBD | 2.00  | 128.58      | 124.48   |
| 14  | b     | 831  | CLA  | O2A-CGA-O1A | -2.00 | 118.54      | 123.59   |
| 14  | A     | 824  | CLA  | CHD-C1D-ND  | -2.00 | 122.62      | 124.45   |

All (294) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 13  | A     | 801 | CL0  | NC   |
| 13  | A     | 801 | CL0  | ND   |
| 13  | A     | 801 | CL0  | NA   |
| 13  | a     | 801 | CL0  | NC   |
| 13  | a     | 801 | CL0  | ND   |
| 13  | a     | 801 | CL0  | NA   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 13  | 1     | 1602 | CL0  | NC   |
| 13  | 1     | 1602 | CL0  | ND   |
| 13  | 1     | 1602 | CL0  | NA   |
| 14  | A     | 802  | CLA  | ND   |
| 14  | A     | 803  | CLA  | ND   |
| 14  | A     | 804  | CLA  | ND   |
| 14  | A     | 805  | CLA  | ND   |
| 14  | A     | 806  | CLA  | ND   |
| 14  | A     | 807  | CLA  | ND   |
| 14  | A     | 808  | CLA  | ND   |
| 14  | A     | 809  | CLA  | ND   |
| 14  | A     | 810  | CLA  | ND   |
| 14  | A     | 811  | CLA  | ND   |
| 14  | A     | 812  | CLA  | ND   |
| 14  | A     | 813  | CLA  | ND   |
| 14  | A     | 814  | CLA  | ND   |
| 14  | A     | 815  | CLA  | ND   |
| 14  | A     | 816  | CLA  | ND   |
| 14  | A     | 817  | CLA  | ND   |
| 14  | A     | 818  | CLA  | ND   |
| 14  | A     | 819  | CLA  | ND   |
| 14  | A     | 820  | CLA  | ND   |
| 14  | A     | 821  | CLA  | ND   |
| 14  | A     | 822  | CLA  | ND   |
| 14  | A     | 823  | CLA  | ND   |
| 14  | A     | 824  | CLA  | ND   |
| 14  | A     | 825  | CLA  | ND   |
| 14  | A     | 826  | CLA  | ND   |
| 14  | A     | 827  | CLA  | ND   |
| 14  | A     | 828  | CLA  | ND   |
| 14  | A     | 829  | CLA  | ND   |
| 14  | A     | 830  | CLA  | ND   |
| 14  | A     | 831  | CLA  | ND   |
| 14  | A     | 832  | CLA  | ND   |
| 14  | A     | 833  | CLA  | ND   |
| 14  | A     | 834  | CLA  | ND   |
| 14  | A     | 835  | CLA  | ND   |
| 14  | A     | 836  | CLA  | ND   |
| 14  | A     | 837  | CLA  | ND   |
| 14  | A     | 838  | CLA  | ND   |
| 14  | A     | 839  | CLA  | ND   |
| 14  | A     | 840  | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14  | A     | 841 | CLA  | ND   |
| 14  | A     | 842 | CLA  | ND   |
| 14  | A     | 843 | CLA  | ND   |
| 14  | A     | 844 | CLA  | ND   |
| 14  | A     | 855 | CLA  | ND   |
| 14  | A     | 857 | CLA  | ND   |
| 14  | B     | 802 | CLA  | ND   |
| 14  | B     | 803 | CLA  | ND   |
| 14  | B     | 804 | CLA  | ND   |
| 14  | B     | 805 | CLA  | ND   |
| 14  | B     | 806 | CLA  | ND   |
| 14  | B     | 807 | CLA  | ND   |
| 14  | B     | 808 | CLA  | ND   |
| 14  | B     | 809 | CLA  | ND   |
| 14  | B     | 810 | CLA  | ND   |
| 14  | B     | 811 | CLA  | ND   |
| 14  | B     | 812 | CLA  | ND   |
| 14  | B     | 813 | CLA  | ND   |
| 14  | B     | 814 | CLA  | ND   |
| 14  | B     | 815 | CLA  | ND   |
| 14  | B     | 816 | CLA  | ND   |
| 14  | B     | 817 | CLA  | ND   |
| 14  | B     | 818 | CLA  | ND   |
| 14  | B     | 819 | CLA  | ND   |
| 14  | B     | 820 | CLA  | ND   |
| 14  | B     | 821 | CLA  | ND   |
| 14  | B     | 822 | CLA  | ND   |
| 14  | B     | 823 | CLA  | ND   |
| 14  | B     | 824 | CLA  | ND   |
| 14  | B     | 825 | CLA  | ND   |
| 14  | B     | 826 | CLA  | ND   |
| 14  | B     | 827 | CLA  | ND   |
| 14  | B     | 828 | CLA  | ND   |
| 14  | B     | 829 | CLA  | ND   |
| 14  | B     | 830 | CLA  | ND   |
| 14  | B     | 831 | CLA  | ND   |
| 14  | B     | 832 | CLA  | ND   |
| 14  | B     | 833 | CLA  | ND   |
| 14  | B     | 834 | CLA  | ND   |
| 14  | B     | 835 | CLA  | ND   |
| 14  | B     | 836 | CLA  | ND   |
| 14  | B     | 837 | CLA  | ND   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 14  | B     | 838  | CLA  | ND   |
| 14  | B     | 840  | CLA  | ND   |
| 14  | B     | 841  | CLA  | ND   |
| 14  | F     | 201  | CLA  | ND   |
| 14  | F     | 203  | CLA  | ND   |
| 14  | F     | 204  | CLA  | ND   |
| 14  | J     | 101  | CLA  | ND   |
| 14  | J     | 102  | CLA  | ND   |
| 14  | K     | 101  | CLA  | ND   |
| 14  | K     | 103  | CLA  | ND   |
| 14  | L     | 203  | CLA  | ND   |
| 14  | L     | 204  | CLA  | ND   |
| 14  | L     | 205  | CLA  | ND   |
| 14  | M     | 102  | CLA  | ND   |
| 14  | X     | 1701 | CLA  | ND   |
| 14  | a     | 802  | CLA  | ND   |
| 14  | a     | 803  | CLA  | ND   |
| 14  | a     | 804  | CLA  | ND   |
| 14  | a     | 805  | CLA  | ND   |
| 14  | a     | 806  | CLA  | ND   |
| 14  | a     | 807  | CLA  | ND   |
| 14  | a     | 808  | CLA  | ND   |
| 14  | a     | 809  | CLA  | ND   |
| 14  | a     | 810  | CLA  | ND   |
| 14  | a     | 811  | CLA  | ND   |
| 14  | a     | 812  | CLA  | ND   |
| 14  | a     | 813  | CLA  | ND   |
| 14  | a     | 814  | CLA  | ND   |
| 14  | a     | 815  | CLA  | ND   |
| 14  | a     | 816  | CLA  | ND   |
| 14  | a     | 817  | CLA  | ND   |
| 14  | a     | 818  | CLA  | ND   |
| 14  | a     | 819  | CLA  | ND   |
| 14  | a     | 820  | CLA  | ND   |
| 14  | a     | 821  | CLA  | ND   |
| 14  | a     | 822  | CLA  | ND   |
| 14  | a     | 823  | CLA  | ND   |
| 14  | a     | 824  | CLA  | ND   |
| 14  | a     | 825  | CLA  | ND   |
| 14  | a     | 826  | CLA  | ND   |
| 14  | a     | 827  | CLA  | ND   |
| 14  | a     | 828  | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14  | a     | 829 | CLA  | ND   |
| 14  | a     | 830 | CLA  | ND   |
| 14  | a     | 831 | CLA  | ND   |
| 14  | a     | 832 | CLA  | ND   |
| 14  | a     | 833 | CLA  | ND   |
| 14  | a     | 834 | CLA  | ND   |
| 14  | a     | 835 | CLA  | ND   |
| 14  | a     | 836 | CLA  | ND   |
| 14  | a     | 837 | CLA  | ND   |
| 14  | a     | 838 | CLA  | ND   |
| 14  | a     | 839 | CLA  | ND   |
| 14  | a     | 840 | CLA  | ND   |
| 14  | a     | 841 | CLA  | ND   |
| 14  | a     | 842 | CLA  | ND   |
| 14  | a     | 843 | CLA  | ND   |
| 14  | a     | 844 | CLA  | ND   |
| 14  | b     | 802 | CLA  | ND   |
| 14  | b     | 803 | CLA  | ND   |
| 14  | b     | 804 | CLA  | ND   |
| 14  | b     | 805 | CLA  | ND   |
| 14  | b     | 806 | CLA  | ND   |
| 14  | b     | 807 | CLA  | ND   |
| 14  | b     | 808 | CLA  | ND   |
| 14  | b     | 809 | CLA  | ND   |
| 14  | b     | 810 | CLA  | ND   |
| 14  | b     | 811 | CLA  | ND   |
| 14  | b     | 812 | CLA  | ND   |
| 14  | b     | 813 | CLA  | ND   |
| 14  | b     | 814 | CLA  | ND   |
| 14  | b     | 815 | CLA  | ND   |
| 14  | b     | 816 | CLA  | ND   |
| 14  | b     | 817 | CLA  | ND   |
| 14  | b     | 818 | CLA  | ND   |
| 14  | b     | 819 | CLA  | ND   |
| 14  | b     | 820 | CLA  | ND   |
| 14  | b     | 821 | CLA  | ND   |
| 14  | b     | 822 | CLA  | ND   |
| 14  | b     | 823 | CLA  | ND   |
| 14  | b     | 824 | CLA  | ND   |
| 14  | b     | 825 | CLA  | ND   |
| 14  | b     | 826 | CLA  | ND   |
| 14  | b     | 827 | CLA  | ND   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 14  | b     | 828  | CLA  | ND   |
| 14  | b     | 829  | CLA  | ND   |
| 14  | b     | 830  | CLA  | ND   |
| 14  | b     | 831  | CLA  | ND   |
| 14  | b     | 832  | CLA  | ND   |
| 14  | b     | 833  | CLA  | ND   |
| 14  | b     | 834  | CLA  | ND   |
| 14  | b     | 835  | CLA  | ND   |
| 14  | b     | 836  | CLA  | ND   |
| 14  | b     | 837  | CLA  | ND   |
| 14  | b     | 838  | CLA  | ND   |
| 14  | b     | 839  | CLA  | ND   |
| 14  | b     | 841  | CLA  | ND   |
| 14  | b     | 842  | CLA  | ND   |
| 14  | f     | 201  | CLA  | ND   |
| 14  | f     | 203  | CLA  | ND   |
| 14  | j     | 1301 | CLA  | ND   |
| 14  | j     | 1302 | CLA  | ND   |
| 14  | j     | 1303 | CLA  | ND   |
| 14  | k     | 101  | CLA  | ND   |
| 14  | k     | 103  | CLA  | ND   |
| 14  | l     | 204  | CLA  | ND   |
| 14  | l     | 205  | CLA  | ND   |
| 14  | l     | 206  | CLA  | ND   |
| 14  | x     | 1701 | CLA  | ND   |
| 14  | 1     | 1601 | CLA  | ND   |
| 14  | 1     | 1603 | CLA  | ND   |
| 14  | 1     | 1604 | CLA  | ND   |
| 14  | 1     | 1605 | CLA  | ND   |
| 14  | 1     | 1606 | CLA  | ND   |
| 14  | 1     | 1607 | CLA  | ND   |
| 14  | 1     | 1608 | CLA  | ND   |
| 14  | 1     | 1609 | CLA  | ND   |
| 14  | 1     | 1610 | CLA  | ND   |
| 14  | 1     | 1611 | CLA  | ND   |
| 14  | 1     | 1612 | CLA  | ND   |
| 14  | 1     | 1613 | CLA  | ND   |
| 14  | 1     | 1614 | CLA  | ND   |
| 14  | 1     | 1615 | CLA  | ND   |
| 14  | 1     | 1616 | CLA  | ND   |
| 14  | 1     | 1617 | CLA  | ND   |
| 14  | 1     | 1618 | CLA  | ND   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 14  | 1     | 1619 | CLA  | ND   |
| 14  | 1     | 1620 | CLA  | ND   |
| 14  | 1     | 1621 | CLA  | ND   |
| 14  | 1     | 1622 | CLA  | ND   |
| 14  | 1     | 1623 | CLA  | ND   |
| 14  | 1     | 1624 | CLA  | ND   |
| 14  | 1     | 1625 | CLA  | ND   |
| 14  | 1     | 1626 | CLA  | ND   |
| 14  | 1     | 1627 | CLA  | ND   |
| 14  | 1     | 1628 | CLA  | ND   |
| 14  | 1     | 1629 | CLA  | ND   |
| 14  | 1     | 1630 | CLA  | ND   |
| 14  | 1     | 1631 | CLA  | ND   |
| 14  | 1     | 1632 | CLA  | ND   |
| 14  | 1     | 1633 | CLA  | ND   |
| 14  | 1     | 1634 | CLA  | ND   |
| 14  | 1     | 1635 | CLA  | ND   |
| 14  | 1     | 1636 | CLA  | ND   |
| 14  | 1     | 1637 | CLA  | ND   |
| 14  | 1     | 1638 | CLA  | ND   |
| 14  | 1     | 1639 | CLA  | ND   |
| 14  | 1     | 1640 | CLA  | ND   |
| 14  | 1     | 1641 | CLA  | ND   |
| 14  | 1     | 1642 | CLA  | ND   |
| 14  | 1     | 1643 | CLA  | ND   |
| 14  | 1     | 1644 | CLA  | ND   |
| 14  | 1     | 1645 | CLA  | ND   |
| 14  | 2     | 802  | CLA  | ND   |
| 14  | 2     | 803  | CLA  | ND   |
| 14  | 2     | 804  | CLA  | ND   |
| 14  | 2     | 805  | CLA  | ND   |
| 14  | 2     | 806  | CLA  | ND   |
| 14  | 2     | 807  | CLA  | ND   |
| 14  | 2     | 808  | CLA  | ND   |
| 14  | 2     | 809  | CLA  | ND   |
| 14  | 2     | 810  | CLA  | ND   |
| 14  | 2     | 811  | CLA  | ND   |
| 14  | 2     | 812  | CLA  | ND   |
| 14  | 2     | 813  | CLA  | ND   |
| 14  | 2     | 814  | CLA  | ND   |
| 14  | 2     | 815  | CLA  | ND   |
| 14  | 2     | 816  | CLA  | ND   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 14  | 2     | 817  | CLA  | ND   |
| 14  | 2     | 818  | CLA  | ND   |
| 14  | 2     | 819  | CLA  | ND   |
| 14  | 2     | 820  | CLA  | ND   |
| 14  | 2     | 821  | CLA  | ND   |
| 14  | 2     | 822  | CLA  | ND   |
| 14  | 2     | 823  | CLA  | ND   |
| 14  | 2     | 824  | CLA  | ND   |
| 14  | 2     | 825  | CLA  | ND   |
| 14  | 2     | 826  | CLA  | ND   |
| 14  | 2     | 827  | CLA  | ND   |
| 14  | 2     | 828  | CLA  | ND   |
| 14  | 2     | 829  | CLA  | ND   |
| 14  | 2     | 830  | CLA  | ND   |
| 14  | 2     | 831  | CLA  | ND   |
| 14  | 2     | 832  | CLA  | ND   |
| 14  | 2     | 833  | CLA  | ND   |
| 14  | 2     | 834  | CLA  | ND   |
| 14  | 2     | 835  | CLA  | ND   |
| 14  | 2     | 836  | CLA  | ND   |
| 14  | 2     | 837  | CLA  | ND   |
| 14  | 2     | 838  | CLA  | ND   |
| 14  | 2     | 839  | CLA  | ND   |
| 14  | 2     | 841  | CLA  | ND   |
| 14  | 2     | 842  | CLA  | ND   |
| 14  | 6     | 201  | CLA  | ND   |
| 14  | 6     | 203  | CLA  | ND   |
| 14  | 8     | 1301 | CLA  | ND   |
| 14  | 8     | 1302 | CLA  | ND   |
| 14  | 8     | 1303 | CLA  | ND   |
| 14  | 9     | 101  | CLA  | ND   |
| 14  | 9     | 103  | CLA  | ND   |
| 14  | 0     | 205  | CLA  | ND   |
| 14  | 0     | 206  | CLA  | ND   |
| 14  | 0     | 207  | CLA  | ND   |
| 14  | z     | 102  | CLA  | ND   |

All (4211) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | A     | 802 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 803 | CLA  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | A     | 804 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 804 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 805 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 805 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 805 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 805 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 806 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 806 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 806 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 806 | CLA  | CAD-CBD-CGD-O1D |
| 14  | A     | 806 | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 806 | CLA  | O2A-C1-C2-C3    |
| 14  | A     | 807 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 807 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 809 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 809 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 809 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 812 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 812 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 812 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 814 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 814 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 814 | CLA  | CAD-CBD-CGD-O1D |
| 14  | A     | 814 | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 815 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 816 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 816 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 816 | CLA  | CAD-CBD-CGD-O1D |
| 14  | A     | 816 | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 816 | CLA  | O2A-C1-C2-C3    |
| 14  | A     | 817 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 819 | CLA  | C2-C3-C5-C6     |
| 14  | A     | 819 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 820 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 820 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 821 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 823 | CLA  | CAD-CBD-CGD-O1D |
| 14  | A     | 823 | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 823 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 824 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 824 | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 825 | CLA  | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | A     | 825 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 829 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 829 | CLA  | O2A-C1-C2-C3    |
| 14  | A     | 830 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 831 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 835 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 835 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 836 | CLA  | C2-C3-C5-C6     |
| 14  | A     | 836 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 837 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 837 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 839 | CLA  | CAD-CBD-CGD-O1D |
| 14  | A     | 839 | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 842 | CLA  | C2-C3-C5-C6     |
| 14  | A     | 842 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 844 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 844 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 855 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 855 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 855 | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 803 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 804 | CLA  | C11-C12-C13-C14 |
| 14  | B     | 805 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 805 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 805 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 805 | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 805 | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 809 | CLA  | C2-C3-C5-C6     |
| 14  | B     | 809 | CLA  | C4-C3-C5-C6     |
| 14  | B     | 817 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 817 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 818 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 818 | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 818 | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 819 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 820 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 820 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 822 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 824 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 824 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 824 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 825 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 825  | CLA  | C11-C10-C8-C7   |
| 14  | B     | 826  | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 826  | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 827  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 827  | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 829  | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 829  | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 830  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 830  | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 831  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 832  | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 832  | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 834  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 834  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 841  | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 841  | CLA  | CAD-CBD-CGD-O2D |
| 14  | F     | 201  | CLA  | CHA-CBD-CGD-O1D |
| 14  | F     | 201  | CLA  | CBD-CGD-O2D-CED |
| 14  | F     | 204  | CLA  | C1A-C2A-CAA-CBA |
| 14  | F     | 204  | CLA  | C3A-C2A-CAA-CBA |
| 14  | K     | 101  | CLA  | C3A-C2A-CAA-CBA |
| 14  | K     | 101  | CLA  | CHA-CBD-CGD-O1D |
| 14  | K     | 101  | CLA  | CHA-CBD-CGD-O2D |
| 14  | K     | 101  | CLA  | CAD-CBD-CGD-O1D |
| 14  | K     | 103  | CLA  | CAD-CBD-CGD-O1D |
| 14  | K     | 103  | CLA  | CAD-CBD-CGD-O2D |
| 14  | L     | 203  | CLA  | C1A-C2A-CAA-CBA |
| 14  | L     | 203  | CLA  | C3A-C2A-CAA-CBA |
| 14  | X     | 1701 | CLA  | CAD-CBD-CGD-O1D |
| 14  | X     | 1701 | CLA  | CAD-CBD-CGD-O2D |
| 14  | a     | 802  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 803  | CLA  | C6-C7-C8-C9     |
| 14  | a     | 804  | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 804  | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 805  | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 805  | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 805  | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 805  | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 806  | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 806  | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 806  | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 806  | CLA  | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | a     | 806 | CLA  | CAD-CBD-CGD-O2D |
| 14  | a     | 806 | CLA  | O2A-C1-C2-C3    |
| 14  | a     | 807 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 807 | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 809 | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 809 | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 809 | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 812 | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 812 | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 812 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 814 | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 814 | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 814 | CLA  | CAD-CBD-CGD-O1D |
| 14  | a     | 814 | CLA  | CAD-CBD-CGD-O2D |
| 14  | a     | 815 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 816 | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 816 | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 816 | CLA  | CAD-CBD-CGD-O1D |
| 14  | a     | 816 | CLA  | CAD-CBD-CGD-O2D |
| 14  | a     | 816 | CLA  | O2A-C1-C2-C3    |
| 14  | a     | 817 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 819 | CLA  | C2-C3-C5-C6     |
| 14  | a     | 819 | CLA  | C4-C3-C5-C6     |
| 14  | a     | 820 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 820 | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 821 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 823 | CLA  | CAD-CBD-CGD-O1D |
| 14  | a     | 823 | CLA  | CAD-CBD-CGD-O2D |
| 14  | a     | 823 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 824 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 824 | CLA  | CAD-CBD-CGD-O2D |
| 14  | a     | 825 | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 825 | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 829 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 829 | CLA  | O2A-C1-C2-C3    |
| 14  | a     | 830 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 831 | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 835 | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 835 | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 836 | CLA  | C2-C3-C5-C6     |
| 14  | a     | 836 | CLA  | C4-C3-C5-C6     |
| 14  | a     | 837 | CLA  | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | a     | 837 | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 839 | CLA  | CAD-CBD-CGD-O1D |
| 14  | a     | 839 | CLA  | CAD-CBD-CGD-O2D |
| 14  | a     | 842 | CLA  | C2-C3-C5-C6     |
| 14  | a     | 842 | CLA  | C4-C3-C5-C6     |
| 14  | a     | 844 | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 844 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 802 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 802 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 802 | CLA  | CAD-CBD-CGD-O1D |
| 14  | b     | 804 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 805 | CLA  | C11-C12-C13-C14 |
| 14  | b     | 806 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 806 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 806 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 806 | CLA  | CAD-CBD-CGD-O1D |
| 14  | b     | 806 | CLA  | CAD-CBD-CGD-O2D |
| 14  | b     | 810 | CLA  | C2-C3-C5-C6     |
| 14  | b     | 810 | CLA  | C4-C3-C5-C6     |
| 14  | b     | 818 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 818 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 819 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 819 | CLA  | CAD-CBD-CGD-O1D |
| 14  | b     | 819 | CLA  | CAD-CBD-CGD-O2D |
| 14  | b     | 820 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 821 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 821 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 823 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 825 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 825 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 825 | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 826 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 826 | CLA  | C11-C10-C8-C7   |
| 14  | b     | 827 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 827 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 828 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 828 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 830 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 830 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 831 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 831 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 832 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 833  | CLA  | CAD-CBD-CGD-O1D |
| 14  | b     | 833  | CLA  | CAD-CBD-CGD-O2D |
| 14  | b     | 835  | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 835  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 842  | CLA  | CAD-CBD-CGD-O1D |
| 14  | b     | 842  | CLA  | CAD-CBD-CGD-O2D |
| 14  | f     | 201  | CLA  | CHA-CBD-CGD-O1D |
| 14  | f     | 201  | CLA  | CBD-CGD-O2D-CED |
| 14  | f     | 203  | CLA  | C1A-C2A-CAA-CBA |
| 14  | f     | 203  | CLA  | C3A-C2A-CAA-CBA |
| 14  | k     | 101  | CLA  | C3A-C2A-CAA-CBA |
| 14  | k     | 101  | CLA  | CHA-CBD-CGD-O1D |
| 14  | k     | 101  | CLA  | CHA-CBD-CGD-O2D |
| 14  | k     | 101  | CLA  | CAD-CBD-CGD-O1D |
| 14  | k     | 103  | CLA  | CAD-CBD-CGD-O1D |
| 14  | k     | 103  | CLA  | CAD-CBD-CGD-O2D |
| 14  | l     | 204  | CLA  | C1A-C2A-CAA-CBA |
| 14  | l     | 204  | CLA  | C3A-C2A-CAA-CBA |
| 14  | x     | 1701 | CLA  | CAD-CBD-CGD-O1D |
| 14  | x     | 1701 | CLA  | CAD-CBD-CGD-O2D |
| 14  | 1     | 1603 | CLA  | CBD-CGD-O2D-CED |
| 14  | 1     | 1605 | CLA  | CHA-CBD-CGD-O1D |
| 14  | 1     | 1605 | CLA  | CHA-CBD-CGD-O2D |
| 14  | 1     | 1606 | CLA  | C1A-C2A-CAA-CBA |
| 14  | 1     | 1606 | CLA  | C3A-C2A-CAA-CBA |
| 14  | 1     | 1606 | CLA  | CHA-CBD-CGD-O1D |
| 14  | 1     | 1606 | CLA  | CHA-CBD-CGD-O2D |
| 14  | 1     | 1607 | CLA  | C1A-C2A-CAA-CBA |
| 14  | 1     | 1607 | CLA  | CHA-CBD-CGD-O1D |
| 14  | 1     | 1607 | CLA  | CHA-CBD-CGD-O2D |
| 14  | 1     | 1607 | CLA  | CAD-CBD-CGD-O1D |
| 14  | 1     | 1607 | CLA  | CAD-CBD-CGD-O2D |
| 14  | 1     | 1607 | CLA  | O2A-C1-C2-C3    |
| 14  | 1     | 1608 | CLA  | C1A-C2A-CAA-CBA |
| 14  | 1     | 1608 | CLA  | C3A-C2A-CAA-CBA |
| 14  | 1     | 1610 | CLA  | C3A-C2A-CAA-CBA |
| 14  | 1     | 1610 | CLA  | CHA-CBD-CGD-O1D |
| 14  | 1     | 1610 | CLA  | CHA-CBD-CGD-O2D |
| 14  | 1     | 1613 | CLA  | CHA-CBD-CGD-O1D |
| 14  | 1     | 1613 | CLA  | CHA-CBD-CGD-O2D |
| 14  | 1     | 1613 | CLA  | CBD-CGD-O2D-CED |
| 14  | 1     | 1615 | CLA  | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | 1     | 1615 | CLA  | CHA-CBD-CGD-O2D |
| 14  | 1     | 1615 | CLA  | CAD-CBD-CGD-O1D |
| 14  | 1     | 1615 | CLA  | CAD-CBD-CGD-O2D |
| 14  | 1     | 1616 | CLA  | C1A-C2A-CAA-CBA |
| 14  | 1     | 1617 | CLA  | CHA-CBD-CGD-O1D |
| 14  | 1     | 1617 | CLA  | CHA-CBD-CGD-O2D |
| 14  | 1     | 1617 | CLA  | CAD-CBD-CGD-O1D |
| 14  | 1     | 1617 | CLA  | CAD-CBD-CGD-O2D |
| 14  | 1     | 1617 | CLA  | O2A-C1-C2-C3    |
| 14  | 1     | 1618 | CLA  | CBD-CGD-O2D-CED |
| 14  | 1     | 1620 | CLA  | C2-C3-C5-C6     |
| 14  | 1     | 1620 | CLA  | C4-C3-C5-C6     |
| 14  | 1     | 1621 | CLA  | C1A-C2A-CAA-CBA |
| 14  | 1     | 1621 | CLA  | C3A-C2A-CAA-CBA |
| 14  | 1     | 1622 | CLA  | CBD-CGD-O2D-CED |
| 14  | 1     | 1624 | CLA  | CAD-CBD-CGD-O1D |
| 14  | 1     | 1624 | CLA  | CAD-CBD-CGD-O2D |
| 14  | 1     | 1624 | CLA  | CBD-CGD-O2D-CED |
| 14  | 1     | 1625 | CLA  | C1A-C2A-CAA-CBA |
| 14  | 1     | 1625 | CLA  | CAD-CBD-CGD-O2D |
| 14  | 1     | 1626 | CLA  | CHA-CBD-CGD-O1D |
| 14  | 1     | 1626 | CLA  | CHA-CBD-CGD-O2D |
| 14  | 1     | 1630 | CLA  | CBD-CGD-O2D-CED |
| 14  | 1     | 1630 | CLA  | O2A-C1-C2-C3    |
| 14  | 1     | 1631 | CLA  | C1A-C2A-CAA-CBA |
| 14  | 1     | 1632 | CLA  | CHA-CBD-CGD-O2D |
| 14  | 1     | 1636 | CLA  | CHA-CBD-CGD-O1D |
| 14  | 1     | 1636 | CLA  | CHA-CBD-CGD-O2D |
| 14  | 1     | 1637 | CLA  | C2-C3-C5-C6     |
| 14  | 1     | 1637 | CLA  | C4-C3-C5-C6     |
| 14  | 1     | 1638 | CLA  | CHA-CBD-CGD-O1D |
| 14  | 1     | 1638 | CLA  | CHA-CBD-CGD-O2D |
| 14  | 1     | 1640 | CLA  | CAD-CBD-CGD-O1D |
| 14  | 1     | 1640 | CLA  | CAD-CBD-CGD-O2D |
| 14  | 1     | 1643 | CLA  | C2-C3-C5-C6     |
| 14  | 1     | 1643 | CLA  | C4-C3-C5-C6     |
| 14  | 1     | 1645 | CLA  | CHA-CBD-CGD-O1D |
| 14  | 1     | 1645 | CLA  | CHA-CBD-CGD-O2D |
| 14  | 2     | 802  | CLA  | CHA-CBD-CGD-O1D |
| 14  | 2     | 802  | CLA  | CHA-CBD-CGD-O2D |
| 14  | 2     | 802  | CLA  | CAD-CBD-CGD-O1D |
| 14  | 2     | 804  | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | 2     | 805 | CLA  | C11-C12-C13-C14 |
| 14  | 2     | 806 | CLA  | C3A-C2A-CAA-CBA |
| 14  | 2     | 806 | CLA  | CHA-CBD-CGD-O1D |
| 14  | 2     | 806 | CLA  | CHA-CBD-CGD-O2D |
| 14  | 2     | 806 | CLA  | CAD-CBD-CGD-O1D |
| 14  | 2     | 806 | CLA  | CAD-CBD-CGD-O2D |
| 14  | 2     | 810 | CLA  | C2-C3-C5-C6     |
| 14  | 2     | 810 | CLA  | C4-C3-C5-C6     |
| 14  | 2     | 818 | CLA  | C1A-C2A-CAA-CBA |
| 14  | 2     | 818 | CLA  | C3A-C2A-CAA-CBA |
| 14  | 2     | 819 | CLA  | C3A-C2A-CAA-CBA |
| 14  | 2     | 819 | CLA  | CAD-CBD-CGD-O1D |
| 14  | 2     | 819 | CLA  | CAD-CBD-CGD-O2D |
| 14  | 2     | 820 | CLA  | CBD-CGD-O2D-CED |
| 14  | 2     | 821 | CLA  | C1A-C2A-CAA-CBA |
| 14  | 2     | 821 | CLA  | C3A-C2A-CAA-CBA |
| 14  | 2     | 823 | CLA  | CBD-CGD-O2D-CED |
| 14  | 2     | 825 | CLA  | C1A-C2A-CAA-CBA |
| 14  | 2     | 825 | CLA  | C3A-C2A-CAA-CBA |
| 14  | 2     | 825 | CLA  | C2A-CAA-CBA-CGA |
| 14  | 2     | 826 | CLA  | C1A-C2A-CAA-CBA |
| 14  | 2     | 826 | CLA  | C11-C10-C8-C7   |
| 14  | 2     | 827 | CLA  | CHA-CBD-CGD-O1D |
| 14  | 2     | 827 | CLA  | CHA-CBD-CGD-O2D |
| 14  | 2     | 828 | CLA  | C1A-C2A-CAA-CBA |
| 14  | 2     | 828 | CLA  | C3A-C2A-CAA-CBA |
| 14  | 2     | 830 | CLA  | CHA-CBD-CGD-O1D |
| 14  | 2     | 830 | CLA  | CHA-CBD-CGD-O2D |
| 14  | 2     | 831 | CLA  | C1A-C2A-CAA-CBA |
| 14  | 2     | 831 | CLA  | C3A-C2A-CAA-CBA |
| 14  | 2     | 832 | CLA  | C1A-C2A-CAA-CBA |
| 14  | 2     | 833 | CLA  | CAD-CBD-CGD-O1D |
| 14  | 2     | 833 | CLA  | CAD-CBD-CGD-O2D |
| 14  | 2     | 835 | CLA  | C1A-C2A-CAA-CBA |
| 14  | 2     | 835 | CLA  | CBD-CGD-O2D-CED |
| 14  | 2     | 842 | CLA  | CAD-CBD-CGD-O1D |
| 14  | 2     | 842 | CLA  | CAD-CBD-CGD-O2D |
| 14  | 6     | 201 | CLA  | CHA-CBD-CGD-O1D |
| 14  | 6     | 201 | CLA  | CBD-CGD-O2D-CED |
| 14  | 6     | 203 | CLA  | C1A-C2A-CAA-CBA |
| 14  | 6     | 203 | CLA  | C3A-C2A-CAA-CBA |
| 14  | 9     | 101 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | 9     | 101 | CLA  | CHA-CBD-CGD-O1D |
| 14  | 9     | 101 | CLA  | CHA-CBD-CGD-O2D |
| 14  | 9     | 101 | CLA  | CAD-CBD-CGD-O1D |
| 14  | 9     | 103 | CLA  | CAD-CBD-CGD-O1D |
| 14  | 9     | 103 | CLA  | CAD-CBD-CGD-O2D |
| 14  | 0     | 205 | CLA  | C1A-C2A-CAA-CBA |
| 14  | 0     | 205 | CLA  | C3A-C2A-CAA-CBA |
| 14  | z     | 102 | CLA  | CAD-CBD-CGD-O1D |
| 14  | z     | 102 | CLA  | CAD-CBD-CGD-O2D |
| 17  | A     | 847 | BCR  | C7-C8-C9-C34    |
| 17  | A     | 847 | BCR  | C11-C12-C13-C35 |
| 17  | A     | 847 | BCR  | C36-C18-C19-C20 |
| 17  | A     | 847 | BCR  | C22-C23-C24-C25 |
| 17  | A     | 847 | BCR  | C23-C24-C25-C30 |
| 17  | A     | 848 | BCR  | C7-C8-C9-C34    |
| 17  | A     | 848 | BCR  | C12-C13-C14-C15 |
| 17  | A     | 848 | BCR  | C35-C13-C14-C15 |
| 17  | A     | 848 | BCR  | C13-C14-C15-C16 |
| 17  | A     | 848 | BCR  | C14-C15-C16-C17 |
| 17  | A     | 848 | BCR  | C16-C17-C18-C19 |
| 17  | A     | 848 | BCR  | C16-C17-C18-C36 |
| 17  | A     | 848 | BCR  | C20-C21-C22-C37 |
| 17  | A     | 849 | BCR  | C20-C21-C22-C37 |
| 17  | A     | 850 | BCR  | C36-C18-C19-C20 |
| 17  | A     | 850 | BCR  | C20-C21-C22-C37 |
| 17  | A     | 850 | BCR  | C21-C22-C23-C24 |
| 17  | A     | 851 | BCR  | C1-C6-C7-C8     |
| 17  | A     | 851 | BCR  | C7-C8-C9-C34    |
| 17  | A     | 851 | BCR  | C16-C17-C18-C36 |
| 17  | A     | 851 | BCR  | C18-C19-C20-C21 |
| 17  | A     | 851 | BCR  | C20-C21-C22-C23 |
| 17  | A     | 851 | BCR  | C20-C21-C22-C37 |
| 17  | A     | 851 | BCR  | C21-C22-C23-C24 |
| 17  | A     | 851 | BCR  | C37-C22-C23-C24 |
| 17  | A     | 851 | BCR  | C23-C24-C25-C26 |
| 17  | A     | 851 | BCR  | C23-C24-C25-C30 |
| 17  | A     | 852 | BCR  | C7-C8-C9-C10    |
| 17  | A     | 852 | BCR  | C7-C8-C9-C34    |
| 17  | A     | 852 | BCR  | C16-C17-C18-C36 |
| 17  | A     | 856 | BCR  | C7-C8-C9-C34    |
| 17  | A     | 856 | BCR  | C14-C15-C16-C17 |
| 17  | A     | 856 | BCR  | C21-C22-C23-C24 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 17  | B     | 843 | BCR  | C7-C8-C9-C10    |
| 17  | B     | 843 | BCR  | C16-C17-C18-C36 |
| 17  | B     | 843 | BCR  | C17-C18-C19-C20 |
| 17  | B     | 843 | BCR  | C21-C22-C23-C24 |
| 17  | B     | 843 | BCR  | C22-C23-C24-C25 |
| 17  | B     | 844 | BCR  | C1-C6-C7-C8     |
| 17  | B     | 844 | BCR  | C6-C7-C8-C9     |
| 17  | B     | 844 | BCR  | C7-C8-C9-C10    |
| 17  | B     | 844 | BCR  | C7-C8-C9-C34    |
| 17  | B     | 844 | BCR  | C21-C22-C23-C24 |
| 17  | B     | 845 | BCR  | C7-C8-C9-C34    |
| 17  | B     | 845 | BCR  | C20-C21-C22-C23 |
| 17  | B     | 845 | BCR  | C20-C21-C22-C37 |
| 17  | B     | 845 | BCR  | C37-C22-C23-C24 |
| 17  | B     | 846 | BCR  | C6-C7-C8-C9     |
| 17  | B     | 846 | BCR  | C7-C8-C9-C34    |
| 17  | B     | 846 | BCR  | C14-C15-C16-C17 |
| 17  | B     | 846 | BCR  | C20-C21-C22-C37 |
| 17  | B     | 846 | BCR  | C23-C24-C25-C30 |
| 17  | B     | 847 | BCR  | C6-C7-C8-C9     |
| 17  | B     | 847 | BCR  | C11-C12-C13-C14 |
| 17  | B     | 847 | BCR  | C11-C12-C13-C35 |
| 17  | B     | 847 | BCR  | C37-C22-C23-C24 |
| 17  | B     | 851 | BCR  | C36-C18-C19-C20 |
| 17  | B     | 851 | BCR  | C18-C19-C20-C21 |
| 17  | B     | 851 | BCR  | C20-C21-C22-C37 |
| 17  | B     | 851 | BCR  | C22-C23-C24-C25 |
| 17  | F     | 202 | BCR  | C7-C8-C9-C34    |
| 17  | F     | 202 | BCR  | C37-C22-C23-C24 |
| 17  | F     | 205 | BCR  | C12-C13-C14-C15 |
| 17  | F     | 205 | BCR  | C37-C22-C23-C24 |
| 17  | F     | 205 | BCR  | C23-C24-C25-C30 |
| 17  | I     | 101 | BCR  | C7-C8-C9-C34    |
| 17  | J     | 103 | BCR  | C1-C6-C7-C8     |
| 17  | J     | 103 | BCR  | C6-C7-C8-C9     |
| 17  | J     | 103 | BCR  | C7-C8-C9-C10    |
| 17  | J     | 103 | BCR  | C7-C8-C9-C34    |
| 17  | J     | 103 | BCR  | C36-C18-C19-C20 |
| 17  | J     | 103 | BCR  | C37-C22-C23-C24 |
| 17  | K     | 102 | BCR  | C6-C7-C8-C9     |
| 17  | K     | 102 | BCR  | C7-C8-C9-C34    |
| 17  | L     | 201 | BCR  | C7-C8-C9-C34    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 17  | L     | 201 | BCR  | C20-C21-C22-C23 |
| 17  | L     | 201 | BCR  | C20-C21-C22-C37 |
| 17  | L     | 206 | BCR  | C7-C8-C9-C10    |
| 17  | L     | 206 | BCR  | C7-C8-C9-C34    |
| 17  | L     | 206 | BCR  | C21-C22-C23-C24 |
| 17  | L     | 207 | BCR  | C11-C12-C13-C35 |
| 17  | M     | 103 | BCR  | C7-C8-C9-C34    |
| 17  | M     | 103 | BCR  | C21-C22-C23-C24 |
| 17  | a     | 847 | BCR  | C7-C8-C9-C34    |
| 17  | a     | 847 | BCR  | C11-C12-C13-C35 |
| 17  | a     | 847 | BCR  | C36-C18-C19-C20 |
| 17  | a     | 847 | BCR  | C22-C23-C24-C25 |
| 17  | a     | 847 | BCR  | C23-C24-C25-C30 |
| 17  | a     | 848 | BCR  | C7-C8-C9-C34    |
| 17  | a     | 848 | BCR  | C12-C13-C14-C15 |
| 17  | a     | 848 | BCR  | C35-C13-C14-C15 |
| 17  | a     | 848 | BCR  | C13-C14-C15-C16 |
| 17  | a     | 848 | BCR  | C14-C15-C16-C17 |
| 17  | a     | 848 | BCR  | C16-C17-C18-C19 |
| 17  | a     | 848 | BCR  | C16-C17-C18-C36 |
| 17  | a     | 848 | BCR  | C20-C21-C22-C37 |
| 17  | a     | 849 | BCR  | C20-C21-C22-C37 |
| 17  | a     | 850 | BCR  | C36-C18-C19-C20 |
| 17  | a     | 850 | BCR  | C20-C21-C22-C37 |
| 17  | a     | 850 | BCR  | C21-C22-C23-C24 |
| 17  | a     | 851 | BCR  | C1-C6-C7-C8     |
| 17  | a     | 851 | BCR  | C7-C8-C9-C34    |
| 17  | a     | 851 | BCR  | C16-C17-C18-C36 |
| 17  | a     | 851 | BCR  | C18-C19-C20-C21 |
| 17  | a     | 851 | BCR  | C20-C21-C22-C23 |
| 17  | a     | 851 | BCR  | C20-C21-C22-C37 |
| 17  | a     | 851 | BCR  | C21-C22-C23-C24 |
| 17  | a     | 851 | BCR  | C37-C22-C23-C24 |
| 17  | a     | 851 | BCR  | C23-C24-C25-C26 |
| 17  | a     | 851 | BCR  | C23-C24-C25-C30 |
| 17  | a     | 852 | BCR  | C7-C8-C9-C10    |
| 17  | a     | 852 | BCR  | C7-C8-C9-C34    |
| 17  | a     | 852 | BCR  | C16-C17-C18-C36 |
| 17  | b     | 844 | BCR  | C7-C8-C9-C10    |
| 17  | b     | 844 | BCR  | C16-C17-C18-C36 |
| 17  | b     | 844 | BCR  | C17-C18-C19-C20 |
| 17  | b     | 844 | BCR  | C21-C22-C23-C24 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | b     | 844  | BCR  | C22-C23-C24-C25 |
| 17  | b     | 845  | BCR  | C1-C6-C7-C8     |
| 17  | b     | 845  | BCR  | C6-C7-C8-C9     |
| 17  | b     | 845  | BCR  | C7-C8-C9-C10    |
| 17  | b     | 845  | BCR  | C7-C8-C9-C34    |
| 17  | b     | 845  | BCR  | C21-C22-C23-C24 |
| 17  | b     | 846  | BCR  | C7-C8-C9-C34    |
| 17  | b     | 846  | BCR  | C20-C21-C22-C23 |
| 17  | b     | 846  | BCR  | C20-C21-C22-C37 |
| 17  | b     | 846  | BCR  | C37-C22-C23-C24 |
| 17  | b     | 847  | BCR  | C6-C7-C8-C9     |
| 17  | b     | 847  | BCR  | C7-C8-C9-C34    |
| 17  | b     | 847  | BCR  | C14-C15-C16-C17 |
| 17  | b     | 847  | BCR  | C20-C21-C22-C37 |
| 17  | b     | 847  | BCR  | C23-C24-C25-C30 |
| 17  | b     | 848  | BCR  | C6-C7-C8-C9     |
| 17  | b     | 848  | BCR  | C11-C12-C13-C14 |
| 17  | b     | 848  | BCR  | C11-C12-C13-C35 |
| 17  | b     | 848  | BCR  | C37-C22-C23-C24 |
| 17  | b     | 852  | BCR  | C36-C18-C19-C20 |
| 17  | b     | 852  | BCR  | C18-C19-C20-C21 |
| 17  | b     | 852  | BCR  | C20-C21-C22-C37 |
| 17  | b     | 852  | BCR  | C22-C23-C24-C25 |
| 17  | f     | 202  | BCR  | C7-C8-C9-C34    |
| 17  | f     | 202  | BCR  | C37-C22-C23-C24 |
| 17  | f     | 204  | BCR  | C12-C13-C14-C15 |
| 17  | f     | 204  | BCR  | C37-C22-C23-C24 |
| 17  | f     | 204  | BCR  | C23-C24-C25-C30 |
| 17  | i     | 101  | BCR  | C7-C8-C9-C34    |
| 17  | j     | 1304 | BCR  | C1-C6-C7-C8     |
| 17  | j     | 1304 | BCR  | C6-C7-C8-C9     |
| 17  | j     | 1304 | BCR  | C7-C8-C9-C10    |
| 17  | j     | 1304 | BCR  | C7-C8-C9-C34    |
| 17  | j     | 1304 | BCR  | C36-C18-C19-C20 |
| 17  | j     | 1304 | BCR  | C37-C22-C23-C24 |
| 17  | j     | 1305 | BCR  | C7-C8-C9-C34    |
| 17  | j     | 1305 | BCR  | C14-C15-C16-C17 |
| 17  | j     | 1305 | BCR  | C21-C22-C23-C24 |
| 17  | k     | 102  | BCR  | C6-C7-C8-C9     |
| 17  | k     | 102  | BCR  | C7-C8-C9-C34    |
| 17  | l     | 202  | BCR  | C7-C8-C9-C34    |
| 17  | l     | 202  | BCR  | C20-C21-C22-C23 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | l     | 202  | BCR  | C20-C21-C22-C37 |
| 17  | l     | 207  | BCR  | C7-C8-C9-C10    |
| 17  | l     | 207  | BCR  | C7-C8-C9-C34    |
| 17  | l     | 207  | BCR  | C21-C22-C23-C24 |
| 17  | m     | 102  | BCR  | C7-C8-C9-C34    |
| 17  | m     | 102  | BCR  | C21-C22-C23-C24 |
| 17  | 1     | 1648 | BCR  | C7-C8-C9-C34    |
| 17  | 1     | 1648 | BCR  | C36-C18-C19-C20 |
| 17  | 1     | 1648 | BCR  | C22-C23-C24-C25 |
| 17  | 1     | 1648 | BCR  | C23-C24-C25-C30 |
| 17  | 1     | 1649 | BCR  | C7-C8-C9-C34    |
| 17  | 1     | 1649 | BCR  | C12-C13-C14-C15 |
| 17  | 1     | 1649 | BCR  | C35-C13-C14-C15 |
| 17  | 1     | 1649 | BCR  | C13-C14-C15-C16 |
| 17  | 1     | 1649 | BCR  | C14-C15-C16-C17 |
| 17  | 1     | 1649 | BCR  | C16-C17-C18-C19 |
| 17  | 1     | 1649 | BCR  | C16-C17-C18-C36 |
| 17  | 1     | 1649 | BCR  | C20-C21-C22-C37 |
| 17  | 1     | 1650 | BCR  | C20-C21-C22-C37 |
| 17  | 1     | 1651 | BCR  | C36-C18-C19-C20 |
| 17  | 1     | 1651 | BCR  | C20-C21-C22-C37 |
| 17  | 1     | 1651 | BCR  | C21-C22-C23-C24 |
| 17  | 1     | 1652 | BCR  | C7-C8-C9-C34    |
| 17  | 1     | 1652 | BCR  | C16-C17-C18-C36 |
| 17  | 1     | 1652 | BCR  | C18-C19-C20-C21 |
| 17  | 1     | 1652 | BCR  | C20-C21-C22-C23 |
| 17  | 1     | 1652 | BCR  | C20-C21-C22-C37 |
| 17  | 1     | 1652 | BCR  | C21-C22-C23-C24 |
| 17  | 1     | 1652 | BCR  | C37-C22-C23-C24 |
| 17  | 1     | 1652 | BCR  | C23-C24-C25-C26 |
| 17  | 1     | 1652 | BCR  | C23-C24-C25-C30 |
| 17  | 1     | 1653 | BCR  | C7-C8-C9-C10    |
| 17  | 1     | 1653 | BCR  | C7-C8-C9-C34    |
| 17  | 1     | 1653 | BCR  | C16-C17-C18-C36 |
| 17  | 2     | 844  | BCR  | C7-C8-C9-C10    |
| 17  | 2     | 844  | BCR  | C16-C17-C18-C36 |
| 17  | 2     | 844  | BCR  | C17-C18-C19-C20 |
| 17  | 2     | 844  | BCR  | C21-C22-C23-C24 |
| 17  | 2     | 844  | BCR  | C22-C23-C24-C25 |
| 17  | 2     | 845  | BCR  | C1-C6-C7-C8     |
| 17  | 2     | 845  | BCR  | C6-C7-C8-C9     |
| 17  | 2     | 845  | BCR  | C7-C8-C9-C10    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | 2     | 845  | BCR  | C7-C8-C9-C34    |
| 17  | 2     | 845  | BCR  | C21-C22-C23-C24 |
| 17  | 2     | 846  | BCR  | C7-C8-C9-C34    |
| 17  | 2     | 846  | BCR  | C20-C21-C22-C23 |
| 17  | 2     | 846  | BCR  | C20-C21-C22-C37 |
| 17  | 2     | 846  | BCR  | C37-C22-C23-C24 |
| 17  | 2     | 847  | BCR  | C6-C7-C8-C9     |
| 17  | 2     | 847  | BCR  | C7-C8-C9-C34    |
| 17  | 2     | 847  | BCR  | C14-C15-C16-C17 |
| 17  | 2     | 847  | BCR  | C20-C21-C22-C37 |
| 17  | 2     | 847  | BCR  | C23-C24-C25-C30 |
| 17  | 2     | 848  | BCR  | C6-C7-C8-C9     |
| 17  | 2     | 848  | BCR  | C11-C12-C13-C14 |
| 17  | 2     | 848  | BCR  | C11-C12-C13-C35 |
| 17  | 2     | 848  | BCR  | C37-C22-C23-C24 |
| 17  | 6     | 202  | BCR  | C7-C8-C9-C34    |
| 17  | 6     | 202  | BCR  | C37-C22-C23-C24 |
| 17  | 6     | 204  | BCR  | C12-C13-C14-C15 |
| 17  | 6     | 204  | BCR  | C37-C22-C23-C24 |
| 17  | 6     | 204  | BCR  | C23-C24-C25-C30 |
| 17  | 7     | 101  | BCR  | C7-C8-C9-C34    |
| 17  | 8     | 1304 | BCR  | C1-C6-C7-C8     |
| 17  | 8     | 1304 | BCR  | C6-C7-C8-C9     |
| 17  | 8     | 1304 | BCR  | C7-C8-C9-C10    |
| 17  | 8     | 1304 | BCR  | C7-C8-C9-C34    |
| 17  | 8     | 1304 | BCR  | C36-C18-C19-C20 |
| 17  | 8     | 1304 | BCR  | C37-C22-C23-C24 |
| 17  | 8     | 1305 | BCR  | C7-C8-C9-C34    |
| 17  | 8     | 1305 | BCR  | C14-C15-C16-C17 |
| 17  | 8     | 1305 | BCR  | C21-C22-C23-C24 |
| 17  | 8     | 1306 | BCR  | C36-C18-C19-C20 |
| 17  | 8     | 1306 | BCR  | C18-C19-C20-C21 |
| 17  | 8     | 1306 | BCR  | C20-C21-C22-C37 |
| 17  | 8     | 1306 | BCR  | C22-C23-C24-C25 |
| 17  | 9     | 102  | BCR  | C6-C7-C8-C9     |
| 17  | 9     | 102  | BCR  | C7-C8-C9-C34    |
| 17  | 0     | 201  | BCR  | C11-C12-C13-C35 |
| 17  | 0     | 203  | BCR  | C7-C8-C9-C34    |
| 17  | 0     | 203  | BCR  | C20-C21-C22-C23 |
| 17  | 0     | 203  | BCR  | C20-C21-C22-C37 |
| 17  | 0     | 208  | BCR  | C7-C8-C9-C10    |
| 17  | 0     | 208  | BCR  | C7-C8-C9-C34    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | 0     | 208  | BCR  | C21-C22-C23-C24 |
| 17  | 0     | 209  | BCR  | C11-C12-C13-C35 |
| 17  | y     | 102  | BCR  | C7-C8-C9-C34    |
| 17  | y     | 102  | BCR  | C21-C22-C23-C24 |
| 18  | A     | 854  | LHG  | C4-O6-P-O5      |
| 18  | B     | 850  | LHG  | C3-O3-P-O5      |
| 18  | B     | 850  | LHG  | C4-O6-P-O5      |
| 18  | B     | 850  | LHG  | C8-C7-O7-C5     |
| 18  | L     | 208  | LHG  | O1-C1-C2-C3     |
| 18  | L     | 208  | LHG  | C1-C2-C3-O3     |
| 18  | L     | 208  | LHG  | C2-C3-O3-P      |
| 18  | L     | 208  | LHG  | C4-O6-P-O4      |
| 18  | M     | 101  | LHG  | C3-O3-P-O4      |
| 18  | M     | 101  | LHG  | C3-O3-P-O5      |
| 18  | M     | 101  | LHG  | C3-O3-P-O6      |
| 18  | M     | 101  | LHG  | C4-O6-P-O5      |
| 18  | M     | 101  | LHG  | O10-C23-O8-C6   |
| 18  | M     | 101  | LHG  | C24-C23-O8-C6   |
| 18  | a     | 854  | LHG  | C4-O6-P-O5      |
| 18  | b     | 851  | LHG  | C3-O3-P-O5      |
| 18  | b     | 851  | LHG  | C4-O6-P-O5      |
| 18  | b     | 851  | LHG  | C8-C7-O7-C5     |
| 18  | l     | 201  | LHG  | O1-C1-C2-C3     |
| 18  | l     | 201  | LHG  | C1-C2-C3-O3     |
| 18  | l     | 201  | LHG  | C2-C3-O3-P      |
| 18  | l     | 201  | LHG  | C4-O6-P-O4      |
| 18  | m     | 101  | LHG  | C3-O3-P-O4      |
| 18  | m     | 101  | LHG  | C3-O3-P-O5      |
| 18  | m     | 101  | LHG  | C3-O3-P-O6      |
| 18  | m     | 101  | LHG  | C4-O6-P-O5      |
| 18  | m     | 101  | LHG  | O10-C23-O8-C6   |
| 18  | m     | 101  | LHG  | C24-C23-O8-C6   |
| 18  | 1     | 1655 | LHG  | C4-O6-P-O5      |
| 18  | 0     | 202  | LHG  | O1-C1-C2-C3     |
| 18  | 0     | 202  | LHG  | C1-C2-C3-O3     |
| 18  | 0     | 202  | LHG  | C2-C3-O3-P      |
| 18  | 0     | 202  | LHG  | C4-O6-P-O4      |
| 18  | y     | 101  | LHG  | C3-O3-P-O4      |
| 18  | y     | 101  | LHG  | C3-O3-P-O5      |
| 18  | y     | 101  | LHG  | C3-O3-P-O6      |
| 18  | y     | 101  | LHG  | C4-O6-P-O5      |
| 18  | y     | 101  | LHG  | O10-C23-O8-C6   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | y     | 101  | LHG  | C24-C23-O8-C6   |
| 18  | z     | 101  | LHG  | C3-O3-P-O5      |
| 18  | z     | 101  | LHG  | C4-O6-P-O5      |
| 18  | z     | 101  | LHG  | C8-C7-O7-C5     |
| 14  | A     | 817  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 824  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 823  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 835  | CLA  | O1D-CGD-O2D-CED |
| 14  | F     | 201  | CLA  | O1D-CGD-O2D-CED |
| 14  | K     | 101  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 817  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 824  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 824  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 836  | CLA  | O1D-CGD-O2D-CED |
| 14  | f     | 201  | CLA  | O1D-CGD-O2D-CED |
| 14  | k     | 101  | CLA  | O1D-CGD-O2D-CED |
| 14  | 1     | 1618 | CLA  | O1D-CGD-O2D-CED |
| 14  | 1     | 1625 | CLA  | O1D-CGD-O2D-CED |
| 14  | 2     | 824  | CLA  | O1D-CGD-O2D-CED |
| 14  | 2     | 836  | CLA  | O1D-CGD-O2D-CED |
| 14  | 6     | 201  | CLA  | O1D-CGD-O2D-CED |
| 14  | 9     | 101  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 812  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 822  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 834  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 812  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 823  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 835  | CLA  | O1D-CGD-O2D-CED |
| 14  | 1     | 1613 | CLA  | O1D-CGD-O2D-CED |
| 14  | 2     | 823  | CLA  | O1D-CGD-O2D-CED |
| 14  | 2     | 835  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 810  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 811  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 818  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 822  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 824  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 830  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 802  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 809  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 823  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 835  | CLA  | CBD-CGD-O2D-CED |
| 14  | F     | 204  | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | J     | 101  | CLA  | CBD-CGD-O2D-CED |
| 14  | K     | 101  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 810  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 811  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 818  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 822  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 824  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 830  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 803  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 810  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 824  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 836  | CLA  | CBD-CGD-O2D-CED |
| 14  | f     | 203  | CLA  | CBD-CGD-O2D-CED |
| 14  | j     | 1302 | CLA  | CBD-CGD-O2D-CED |
| 14  | k     | 101  | CLA  | CBD-CGD-O2D-CED |
| 14  | 1     | 1611 | CLA  | CBD-CGD-O2D-CED |
| 14  | 1     | 1612 | CLA  | CBD-CGD-O2D-CED |
| 14  | 1     | 1619 | CLA  | CBD-CGD-O2D-CED |
| 14  | 1     | 1623 | CLA  | CBD-CGD-O2D-CED |
| 14  | 1     | 1625 | CLA  | CBD-CGD-O2D-CED |
| 14  | 1     | 1631 | CLA  | CBD-CGD-O2D-CED |
| 14  | 2     | 803  | CLA  | CBD-CGD-O2D-CED |
| 14  | 2     | 810  | CLA  | CBD-CGD-O2D-CED |
| 14  | 2     | 824  | CLA  | CBD-CGD-O2D-CED |
| 14  | 2     | 836  | CLA  | CBD-CGD-O2D-CED |
| 14  | 6     | 203  | CLA  | CBD-CGD-O2D-CED |
| 14  | 8     | 1302 | CLA  | CBD-CGD-O2D-CED |
| 14  | 9     | 101  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 806  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 838  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 820  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 806  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 838  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 821  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 1     | 1607 | CLA  | O1A-CGA-O2A-C1  |
| 14  | 1     | 1639 | CLA  | O1A-CGA-O2A-C1  |
| 14  | 2     | 821  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 821  | CLA  | O1D-CGD-O2D-CED |
| 14  | F     | 204  | CLA  | O1D-CGD-O2D-CED |
| 14  | J     | 101  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 821  | CLA  | O1D-CGD-O2D-CED |
| 14  | f     | 203  | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | j     | 1302 | CLA  | O1D-CGD-O2D-CED |
| 14  | 1     | 1622 | CLA  | O1D-CGD-O2D-CED |
| 14  | 6     | 203  | CLA  | O1D-CGD-O2D-CED |
| 14  | 8     | 1302 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 810  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 803  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 810  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 823  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 804  | CLA  | O1D-CGD-O2D-CED |
| 14  | 1     | 1611 | CLA  | O1D-CGD-O2D-CED |
| 14  | 1     | 1624 | CLA  | O1D-CGD-O2D-CED |
| 14  | 2     | 804  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 806  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 838  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 806  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 838  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1607 | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1639 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 834  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 813  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 816  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 821  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 827  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 841  | CLA  | CBD-CGD-O2D-CED |
| 14  | X     | 1701 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 834  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 814  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 817  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 822  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 828  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 842  | CLA  | CBD-CGD-O2D-CED |
| 14  | x     | 1701 | CLA  | CBD-CGD-O2D-CED |
| 14  | 1     | 1635 | CLA  | CBD-CGD-O2D-CED |
| 14  | 2     | 814  | CLA  | CBD-CGD-O2D-CED |
| 14  | 2     | 817  | CLA  | CBD-CGD-O2D-CED |
| 14  | 2     | 822  | CLA  | CBD-CGD-O2D-CED |
| 14  | 2     | 828  | CLA  | CBD-CGD-O2D-CED |
| 14  | 2     | 842  | CLA  | CBD-CGD-O2D-CED |
| 14  | z     | 102  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 802  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 811  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 817  | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 818  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 833  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 819  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 830  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 802  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 811  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 817  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 818  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 833  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 820  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 831  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 1     | 1603 | CLA  | O1A-CGA-O2A-C1  |
| 14  | 1     | 1612 | CLA  | O1A-CGA-O2A-C1  |
| 14  | 1     | 1618 | CLA  | O1A-CGA-O2A-C1  |
| 14  | 1     | 1619 | CLA  | O1A-CGA-O2A-C1  |
| 14  | 1     | 1634 | CLA  | O1A-CGA-O2A-C1  |
| 14  | 2     | 820  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 2     | 831  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 823  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 829  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 819  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 829  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 820  | CLA  | O1D-CGD-O2D-CED |
| 14  | 1     | 1630 | CLA  | O1D-CGD-O2D-CED |
| 14  | 2     | 820  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 802  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 802  | CLA  | O1D-CGD-O2D-CED |
| 14  | 1     | 1603 | CLA  | O1D-CGD-O2D-CED |
| 18  | B     | 850  | LHG  | O9-C7-O7-C5     |
| 18  | b     | 851  | LHG  | O9-C7-O7-C5     |
| 18  | z     | 101  | LHG  | O9-C7-O7-C5     |
| 14  | A     | 809  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 827  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 834  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 804  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 813  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 814  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 840  | CLA  | C3-C5-C6-C7     |
| 14  | L     | 205  | CLA  | C3-C5-C6-C7     |
| 14  | a     | 809  | CLA  | C3-C5-C6-C7     |
| 14  | a     | 827  | CLA  | C3-C5-C6-C7     |
| 14  | a     | 834  | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 14  | a     | 838  | CLA  | C3-C5-C6-C7    |
| 14  | b     | 805  | CLA  | C3-C5-C6-C7    |
| 14  | b     | 814  | CLA  | C3-C5-C6-C7    |
| 14  | b     | 815  | CLA  | C3-C5-C6-C7    |
| 14  | b     | 841  | CLA  | C3-C5-C6-C7    |
| 14  | l     | 206  | CLA  | C3-C5-C6-C7    |
| 14  | 1     | 1610 | CLA  | C3-C5-C6-C7    |
| 14  | 1     | 1628 | CLA  | C3-C5-C6-C7    |
| 14  | 1     | 1635 | CLA  | C3-C5-C6-C7    |
| 14  | 2     | 805  | CLA  | C3-C5-C6-C7    |
| 14  | 2     | 814  | CLA  | C3-C5-C6-C7    |
| 14  | 2     | 815  | CLA  | C3-C5-C6-C7    |
| 14  | 2     | 841  | CLA  | C3-C5-C6-C7    |
| 14  | 0     | 207  | CLA  | C3-C5-C6-C7    |
| 14  | A     | 802  | CLA  | CBA-CGA-O2A-C1 |
| 14  | A     | 818  | CLA  | CBA-CGA-O2A-C1 |
| 14  | B     | 819  | CLA  | CBA-CGA-O2A-C1 |
| 14  | B     | 820  | CLA  | CBA-CGA-O2A-C1 |
| 14  | a     | 802  | CLA  | CBA-CGA-O2A-C1 |
| 14  | a     | 818  | CLA  | CBA-CGA-O2A-C1 |
| 14  | b     | 820  | CLA  | CBA-CGA-O2A-C1 |
| 14  | b     | 821  | CLA  | CBA-CGA-O2A-C1 |
| 14  | 1     | 1603 | CLA  | CBA-CGA-O2A-C1 |
| 14  | 1     | 1619 | CLA  | CBA-CGA-O2A-C1 |
| 14  | 2     | 820  | CLA  | CBA-CGA-O2A-C1 |
| 14  | 2     | 821  | CLA  | CBA-CGA-O2A-C1 |
| 18  | L     | 208  | LHG  | C24-C23-O8-C6  |
| 18  | l     | 201  | LHG  | C24-C23-O8-C6  |
| 18  | 0     | 202  | LHG  | C24-C23-O8-C6  |
| 14  | A     | 806  | CLA  | C4-C3-C5-C6    |
| 14  | A     | 833  | CLA  | C4-C3-C5-C6    |
| 14  | B     | 817  | CLA  | C4-C3-C5-C6    |
| 14  | a     | 806  | CLA  | C4-C3-C5-C6    |
| 14  | a     | 833  | CLA  | C4-C3-C5-C6    |
| 14  | b     | 818  | CLA  | C4-C3-C5-C6    |
| 14  | 1     | 1607 | CLA  | C4-C3-C5-C6    |
| 14  | 1     | 1634 | CLA  | C4-C3-C5-C6    |
| 14  | 2     | 818  | CLA  | C4-C3-C5-C6    |
| 14  | A     | 806  | CLA  | C2-C3-C5-C6    |
| 14  | B     | 817  | CLA  | C2-C3-C5-C6    |
| 14  | a     | 806  | CLA  | C2-C3-C5-C6    |
| 14  | b     | 818  | CLA  | C2-C3-C5-C6    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | 1     | 1607 | CLA  | C2-C3-C5-C6     |
| 14  | 2     | 818  | CLA  | C2-C3-C5-C6     |
| 14  | B     | 811  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 812  | CLA  | CBD-CGD-O2D-CED |
| 14  | 2     | 812  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 813  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 818  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 830  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 835  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 855  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 840  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 813  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 818  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 830  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 835  | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 802  | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 841  | CLA  | C2A-CAA-CBA-CGA |
| 14  | 1     | 1614 | CLA  | C2A-CAA-CBA-CGA |
| 14  | 1     | 1619 | CLA  | C2A-CAA-CBA-CGA |
| 14  | 1     | 1631 | CLA  | C2A-CAA-CBA-CGA |
| 14  | 1     | 1636 | CLA  | C2A-CAA-CBA-CGA |
| 14  | 2     | 802  | CLA  | C2A-CAA-CBA-CGA |
| 14  | 2     | 841  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 810  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 811  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 2     | 811  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 819  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 838  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 811  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 820  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 822  | CLA  | C3-C5-C6-C7     |
| 14  | F     | 201  | CLA  | C3-C5-C6-C7     |
| 14  | a     | 819  | CLA  | C3-C5-C6-C7     |
| 14  | a     | 833  | CLA  | C3-C5-C6-C7     |
| 14  | b     | 812  | CLA  | C3-C5-C6-C7     |
| 14  | b     | 821  | CLA  | C3-C5-C6-C7     |
| 14  | b     | 823  | CLA  | C3-C5-C6-C7     |
| 14  | f     | 201  | CLA  | C3-C5-C6-C7     |
| 14  | 1     | 1620 | CLA  | C3-C5-C6-C7     |
| 14  | 1     | 1634 | CLA  | C3-C5-C6-C7     |
| 14  | 1     | 1639 | CLA  | C3-C5-C6-C7     |
| 14  | 2     | 812  | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | 2     | 821  | CLA  | C3-C5-C6-C7     |
| 14  | 2     | 823  | CLA  | C3-C5-C6-C7     |
| 14  | 6     | 201  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 805  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 811  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 817  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 820  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 833  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 815  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 818  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 824  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 830  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 805  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 811  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 817  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 820  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 833  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 816  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 819  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 825  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 831  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1606 | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1612 | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1618 | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1621 | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1634 | CLA  | CBA-CGA-O2A-C1  |
| 14  | 2     | 816  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 2     | 819  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 2     | 825  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 2     | 831  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 803  | CLA  | C2C-C3C-CAC-CBC |
| 14  | b     | 804  | CLA  | C2C-C3C-CAC-CBC |
| 14  | 2     | 804  | CLA  | C2C-C3C-CAC-CBC |
| 14  | B     | 802  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 803  | CLA  | O1D-CGD-O2D-CED |
| 14  | 2     | 803  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 820  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 815  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 817  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 818  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 824  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 825  | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 820  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 816  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 818  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 819  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 825  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 826  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 1     | 1621 | CLA  | O1A-CGA-O2A-C1  |
| 14  | 2     | 816  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 2     | 818  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 2     | 819  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 2     | 825  | CLA  | O1A-CGA-O2A-C1  |
| 18  | L     | 208  | LHG  | O10-C23-O8-C6   |
| 18  | l     | 201  | LHG  | O10-C23-O8-C6   |
| 18  | 0     | 202  | LHG  | O10-C23-O8-C6   |
| 14  | A     | 811  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 811  | CLA  | O1D-CGD-O2D-CED |
| 14  | 1     | 1612 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 830  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 831  | CLA  | CBD-CGD-O2D-CED |
| 14  | 2     | 831  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 818  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 830  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 818  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 830  | CLA  | O1D-CGD-O2D-CED |
| 14  | 1     | 1619 | CLA  | O1D-CGD-O2D-CED |
| 14  | 1     | 1631 | CLA  | O1D-CGD-O2D-CED |
| 18  | L     | 208  | LHG  | O2-C2-C3-O3     |
| 18  | l     | 201  | LHG  | O2-C2-C3-O3     |
| 18  | 0     | 202  | LHG  | O2-C2-C3-O3     |
| 14  | A     | 833  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 808  | CLA  | C3-C5-C6-C7     |
| 14  | b     | 809  | CLA  | C3-C5-C6-C7     |
| 14  | 2     | 809  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 809  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 809  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 810  | CLA  | CBA-CGA-O2A-C1  |
| 14  | L     | 205  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 809  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 810  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 811  | CLA  | CBA-CGA-O2A-C1  |
| 14  | l     | 206  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1610 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | 2     | 810  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 2     | 811  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 0     | 207  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 2     | 826  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 809  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 810  | CLA  | O1D-CGD-O2D-CED |
| 14  | 2     | 810  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 837  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 841  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 831  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 837  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 841  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 832  | CLA  | CBD-CGD-O2D-CED |
| 14  | 1     | 1638 | CLA  | CBD-CGD-O2D-CED |
| 14  | 1     | 1642 | CLA  | CBD-CGD-O2D-CED |
| 14  | 2     | 832  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 805  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 805  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 1     | 1606 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 840  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 841  | CLA  | C3-C5-C6-C7     |
| 14  | a     | 840  | CLA  | C3-C5-C6-C7     |
| 14  | a     | 841  | CLA  | C3-C5-C6-C7     |
| 14  | 1     | 1641 | CLA  | C3-C5-C6-C7     |
| 14  | 1     | 1642 | CLA  | C3-C5-C6-C7     |
| 14  | B     | 817  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 825  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 818  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 826  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 2     | 818  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 2     | 826  | CLA  | CBA-CGA-O2A-C1  |
| 20  | B     | 849  | LMG  | O6-C5-C6-O5     |
| 20  | b     | 850  | LMG  | O6-C5-C6-O5     |
| 20  | 2     | 850  | LMG  | O6-C5-C6-O5     |
| 14  | A     | 855  | CLA  | C4-C3-C5-C6     |
| 14  | B     | 818  | CLA  | C4-C3-C5-C6     |
| 14  | b     | 802  | CLA  | C4-C3-C5-C6     |
| 14  | b     | 819  | CLA  | C4-C3-C5-C6     |
| 14  | 2     | 802  | CLA  | C4-C3-C5-C6     |
| 14  | 2     | 819  | CLA  | C4-C3-C5-C6     |
| 14  | A     | 833  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 855  | CLA  | C2-C3-C5-C6     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 818  | CLA  | C2-C3-C5-C6     |
| 14  | a     | 833  | CLA  | C2-C3-C5-C6     |
| 14  | b     | 802  | CLA  | C2-C3-C5-C6     |
| 14  | b     | 819  | CLA  | C2-C3-C5-C6     |
| 14  | 1     | 1634 | CLA  | C2-C3-C5-C6     |
| 14  | 2     | 802  | CLA  | C2-C3-C5-C6     |
| 14  | 2     | 819  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 802  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 814  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 802  | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 815  | CLA  | C2A-CAA-CBA-CGA |
| 14  | 1     | 1603 | CLA  | C2A-CAA-CBA-CGA |
| 14  | 2     | 815  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 809  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 809  | CLA  | O1A-CGA-O2A-C1  |
| 14  | L     | 205  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 809  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 810  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 1     | 206  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 1     | 1610 | CLA  | O1A-CGA-O2A-C1  |
| 14  | 2     | 810  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 0     | 207  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 822  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 822  | CLA  | O1D-CGD-O2D-CED |
| 14  | 1     | 1623 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 821  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 822  | CLA  | O1D-CGD-O2D-CED |
| 14  | 2     | 822  | CLA  | O1D-CGD-O2D-CED |
| 14  | X     | 1701 | CLA  | O1D-CGD-O2D-CED |
| 14  | x     | 1701 | CLA  | O1D-CGD-O2D-CED |
| 14  | z     | 102  | CLA  | O1D-CGD-O2D-CED |
| 14  | L     | 204  | CLA  | C3-C5-C6-C7     |
| 14  | 1     | 205  | CLA  | C3-C5-C6-C7     |
| 14  | 0     | 206  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 841  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 842  | CLA  | O1D-CGD-O2D-CED |
| 14  | 2     | 842  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 812  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 825  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 805  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 816  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 835  | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | L     | 203  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 812  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 825  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 806  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 817  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 836  | CLA  | CBA-CGA-O2A-C1  |
| 14  | l     | 204  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1613 | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1626 | CLA  | CBA-CGA-O2A-C1  |
| 14  | 2     | 806  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 2     | 817  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 2     | 836  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 0     | 205  | CLA  | CBA-CGA-O2A-C1  |
| 18  | m     | 101  | LHG  | C28-C29-C30-C31 |
| 14  | B     | 828  | CLA  | C13-C15-C16-C17 |
| 14  | B     | 838  | CLA  | C5-C6-C7-C8     |
| 14  | b     | 839  | CLA  | C5-C6-C7-C8     |
| 14  | 2     | 839  | CLA  | C5-C6-C7-C8     |
| 18  | A     | 853  | LHG  | O2-C2-C3-O3     |
| 18  | a     | 853  | LHG  | O2-C2-C3-O3     |
| 18  | 1     | 1654 | LHG  | O2-C2-C3-O3     |
| 18  | M     | 101  | LHG  | C28-C29-C30-C31 |
| 18  | y     | 101  | LHG  | C28-C29-C30-C31 |
| 14  | A     | 805  | CLA  | C6-C7-C8-C9     |
| 14  | A     | 806  | CLA  | C14-C13-C15-C16 |
| 14  | A     | 817  | CLA  | C14-C13-C15-C16 |
| 14  | A     | 833  | CLA  | C11-C12-C13-C14 |
| 14  | A     | 834  | CLA  | C11-C12-C13-C14 |
| 14  | A     | 839  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 803  | CLA  | C11-C12-C13-C14 |
| 14  | B     | 807  | CLA  | C11-C12-C13-C14 |
| 14  | B     | 813  | CLA  | C11-C12-C13-C14 |
| 14  | B     | 816  | CLA  | C14-C13-C15-C16 |
| 14  | L     | 204  | CLA  | C6-C7-C8-C9     |
| 14  | a     | 805  | CLA  | C6-C7-C8-C9     |
| 14  | a     | 806  | CLA  | C14-C13-C15-C16 |
| 14  | a     | 817  | CLA  | C14-C13-C15-C16 |
| 14  | a     | 833  | CLA  | C11-C12-C13-C14 |
| 14  | a     | 834  | CLA  | C11-C12-C13-C14 |
| 14  | a     | 839  | CLA  | C6-C7-C8-C9     |
| 14  | b     | 804  | CLA  | C11-C12-C13-C14 |
| 14  | b     | 808  | CLA  | C11-C12-C13-C14 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 814  | CLA  | C11-C12-C13-C14 |
| 14  | b     | 817  | CLA  | C14-C13-C15-C16 |
| 14  | l     | 205  | CLA  | C6-C7-C8-C9     |
| 14  | 1     | 1604 | CLA  | C6-C7-C8-C9     |
| 14  | 1     | 1606 | CLA  | C6-C7-C8-C9     |
| 14  | 1     | 1607 | CLA  | C14-C13-C15-C16 |
| 14  | 1     | 1618 | CLA  | C14-C13-C15-C16 |
| 14  | 1     | 1634 | CLA  | C11-C12-C13-C14 |
| 14  | 1     | 1635 | CLA  | C11-C12-C13-C14 |
| 14  | 1     | 1640 | CLA  | C6-C7-C8-C9     |
| 14  | 2     | 804  | CLA  | C11-C12-C13-C14 |
| 14  | 2     | 808  | CLA  | C11-C12-C13-C14 |
| 14  | 2     | 814  | CLA  | C11-C12-C13-C14 |
| 14  | 2     | 817  | CLA  | C14-C13-C15-C16 |
| 14  | 0     | 206  | CLA  | C6-C7-C8-C9     |
| 14  | A     | 834  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 816  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 834  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 817  | CLA  | O1D-CGD-O2D-CED |
| 14  | 1     | 1635 | CLA  | O1D-CGD-O2D-CED |
| 14  | 2     | 817  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 807  | CLA  | C15-C16-C17-C18 |
| 14  | b     | 808  | CLA  | C15-C16-C17-C18 |
| 14  | b     | 829  | CLA  | C13-C15-C16-C17 |
| 14  | 2     | 808  | CLA  | C15-C16-C17-C18 |
| 14  | 2     | 829  | CLA  | C13-C15-C16-C17 |
| 14  | A     | 843  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 843  | CLA  | C2A-CAA-CBA-CGA |
| 14  | 1     | 1644 | CLA  | C2A-CAA-CBA-CGA |
| 17  | A     | 848  | BCR  | C37-C22-C23-C24 |
| 17  | B     | 843  | BCR  | C7-C8-C9-C34    |
| 17  | B     | 846  | BCR  | C11-C12-C13-C35 |
| 17  | B     | 847  | BCR  | C7-C8-C9-C34    |
| 17  | L     | 201  | BCR  | C11-C12-C13-C35 |
| 17  | M     | 103  | BCR  | C37-C22-C23-C24 |
| 17  | a     | 848  | BCR  | C37-C22-C23-C24 |
| 17  | b     | 844  | BCR  | C7-C8-C9-C34    |
| 17  | b     | 847  | BCR  | C11-C12-C13-C35 |
| 17  | b     | 848  | BCR  | C7-C8-C9-C34    |
| 17  | m     | 102  | BCR  | C37-C22-C23-C24 |
| 17  | 1     | 1648 | BCR  | C11-C12-C13-C35 |
| 17  | 1     | 1649 | BCR  | C37-C22-C23-C24 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | 2     | 844  | BCR  | C7-C8-C9-C34    |
| 17  | 2     | 847  | BCR  | C11-C12-C13-C35 |
| 17  | 2     | 848  | BCR  | C7-C8-C9-C34    |
| 17  | y     | 102  | BCR  | C37-C22-C23-C24 |
| 14  | B     | 805  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 835  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 806  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 836  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 2     | 806  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 2     | 836  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 802  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 826  | CLA  | C13-C15-C16-C17 |
| 14  | B     | 840  | CLA  | C8-C10-C11-C12  |
| 14  | a     | 807  | CLA  | C8-C10-C11-C12  |
| 14  | b     | 803  | CLA  | C15-C16-C17-C18 |
| 14  | b     | 827  | CLA  | C13-C15-C16-C17 |
| 14  | b     | 841  | CLA  | C8-C10-C11-C12  |
| 14  | 1     | 1608 | CLA  | C8-C10-C11-C12  |
| 14  | 2     | 803  | CLA  | C15-C16-C17-C18 |
| 14  | 2     | 827  | CLA  | C13-C15-C16-C17 |
| 14  | 2     | 841  | CLA  | C8-C10-C11-C12  |
| 14  | A     | 842  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 842  | CLA  | CBD-CGD-O2D-CED |
| 14  | 1     | 1643 | CLA  | CBD-CGD-O2D-CED |
| 20  | B     | 849  | LMG  | C4-C5-C6-O5     |
| 20  | b     | 850  | LMG  | C4-C5-C6-O5     |
| 20  | 2     | 850  | LMG  | C4-C5-C6-O5     |
| 18  | A     | 854  | LHG  | C29-C30-C31-C32 |
| 14  | B     | 825  | CLA  | C3-C5-C6-C7     |
| 14  | b     | 826  | CLA  | C3-C5-C6-C7     |
| 14  | 2     | 826  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 802  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 828  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 831  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 803  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 829  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 832  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 2     | 803  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 2     | 829  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 2     | 832  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 807  | CLA  | C5-C6-C7-C8     |
| 14  | A     | 807  | CLA  | C8-C10-C11-C12  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 841  | CLA  | C8-C10-C11-C12  |
| 14  | B     | 808  | CLA  | C13-C15-C16-C17 |
| 14  | B     | 813  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 824  | CLA  | C15-C16-C17-C18 |
| 14  | L     | 205  | CLA  | C5-C6-C7-C8     |
| 14  | a     | 807  | CLA  | C5-C6-C7-C8     |
| 14  | a     | 841  | CLA  | C8-C10-C11-C12  |
| 14  | b     | 809  | CLA  | C13-C15-C16-C17 |
| 14  | b     | 814  | CLA  | C15-C16-C17-C18 |
| 14  | b     | 825  | CLA  | C15-C16-C17-C18 |
| 14  | l     | 206  | CLA  | C5-C6-C7-C8     |
| 14  | 1     | 1608 | CLA  | C5-C6-C7-C8     |
| 14  | 1     | 1642 | CLA  | C8-C10-C11-C12  |
| 14  | 2     | 809  | CLA  | C13-C15-C16-C17 |
| 14  | 2     | 814  | CLA  | C15-C16-C17-C18 |
| 14  | 2     | 825  | CLA  | C15-C16-C17-C18 |
| 14  | 0     | 207  | CLA  | C5-C6-C7-C8     |
| 18  | a     | 854  | LHG  | C29-C30-C31-C32 |
| 18  | 1     | 1655 | LHG  | C29-C30-C31-C32 |
| 14  | F     | 203  | CLA  | CBD-CGD-O2D-CED |
| 14  | j     | 1301 | CLA  | CBD-CGD-O2D-CED |
| 14  | 8     | 1301 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 807  | CLA  | C13-C15-C16-C17 |
| 14  | A     | 828  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 839  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 855  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 814  | CLA  | C10-C11-C12-C13 |
| 14  | B     | 817  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 834  | CLA  | C8-C10-C11-C12  |
| 14  | a     | 807  | CLA  | C13-C15-C16-C17 |
| 14  | a     | 828  | CLA  | C15-C16-C17-C18 |
| 14  | a     | 839  | CLA  | C15-C16-C17-C18 |
| 14  | b     | 802  | CLA  | C15-C16-C17-C18 |
| 14  | b     | 815  | CLA  | C10-C11-C12-C13 |
| 14  | b     | 818  | CLA  | C5-C6-C7-C8     |
| 14  | b     | 835  | CLA  | C8-C10-C11-C12  |
| 14  | 1     | 1608 | CLA  | C13-C15-C16-C17 |
| 14  | 1     | 1629 | CLA  | C15-C16-C17-C18 |
| 14  | 1     | 1640 | CLA  | C15-C16-C17-C18 |
| 14  | 2     | 802  | CLA  | C15-C16-C17-C18 |
| 14  | 2     | 815  | CLA  | C10-C11-C12-C13 |
| 14  | 2     | 818  | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | 2     | 835  | CLA  | C8-C10-C11-C12  |
| 18  | A     | 853  | LHG  | O1-C1-C2-O2     |
| 18  | B     | 850  | LHG  | O1-C1-C2-O2     |
| 18  | L     | 208  | LHG  | O1-C1-C2-O2     |
| 18  | a     | 853  | LHG  | O1-C1-C2-O2     |
| 18  | b     | 851  | LHG  | O1-C1-C2-O2     |
| 18  | l     | 201  | LHG  | O1-C1-C2-O2     |
| 18  | 1     | 1654 | LHG  | O1-C1-C2-O2     |
| 18  | 0     | 202  | LHG  | O1-C1-C2-O2     |
| 18  | z     | 101  | LHG  | O1-C1-C2-O2     |
| 14  | L     | 203  | CLA  | O1A-CGA-O2A-C1  |
| 14  | l     | 204  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 2     | 817  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 0     | 205  | CLA  | O1A-CGA-O2A-C1  |
| 13  | A     | 801  | CL0  | C8-C10-C11-C12  |
| 13  | a     | 801  | CL0  | C8-C10-C11-C12  |
| 13  | 1     | 1602 | CL0  | C8-C10-C11-C12  |
| 14  | A     | 810  | CLA  | C8-C10-C11-C12  |
| 14  | A     | 818  | CLA  | C5-C6-C7-C8     |
| 14  | A     | 828  | CLA  | C5-C6-C7-C8     |
| 14  | A     | 836  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 829  | CLA  | C13-C15-C16-C17 |
| 14  | B     | 833  | CLA  | C13-C15-C16-C17 |
| 14  | a     | 810  | CLA  | C8-C10-C11-C12  |
| 14  | a     | 818  | CLA  | C5-C6-C7-C8     |
| 14  | a     | 828  | CLA  | C5-C6-C7-C8     |
| 14  | a     | 836  | CLA  | C15-C16-C17-C18 |
| 14  | b     | 830  | CLA  | C13-C15-C16-C17 |
| 14  | b     | 834  | CLA  | C13-C15-C16-C17 |
| 14  | 1     | 1611 | CLA  | C8-C10-C11-C12  |
| 14  | 1     | 1619 | CLA  | C5-C6-C7-C8     |
| 14  | 1     | 1629 | CLA  | C5-C6-C7-C8     |
| 14  | 1     | 1637 | CLA  | C15-C16-C17-C18 |
| 14  | 2     | 830  | CLA  | C13-C15-C16-C17 |
| 14  | 2     | 834  | CLA  | C13-C15-C16-C17 |
| 14  | A     | 829  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 829  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1630 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 813  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 827  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 828  | CLA  | O1D-CGD-O2D-CED |
| 14  | 2     | 828  | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 825  | CLA  | C13-C15-C16-C17 |
| 14  | a     | 825  | CLA  | C13-C15-C16-C17 |
| 14  | 1     | 1626 | CLA  | C13-C15-C16-C17 |
| 14  | b     | 817  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 804  | CLA  | C5-C6-C7-C8     |
| 14  | a     | 804  | CLA  | C5-C6-C7-C8     |
| 14  | 1     | 1605 | CLA  | C5-C6-C7-C8     |
| 13  | A     | 801  | CL0  | C11-C12-C13-C15 |
| 13  | a     | 801  | CL0  | C11-C12-C13-C15 |
| 13  | 1     | 1602 | CL0  | C11-C12-C13-C15 |
| 14  | A     | 822  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 840  | CLA  | C6-C7-C8-C10    |
| 14  | B     | 810  | CLA  | C6-C7-C8-C10    |
| 14  | a     | 822  | CLA  | C6-C7-C8-C10    |
| 14  | a     | 840  | CLA  | C6-C7-C8-C10    |
| 14  | b     | 811  | CLA  | C6-C7-C8-C10    |
| 14  | 1     | 1623 | CLA  | C6-C7-C8-C10    |
| 14  | 1     | 1641 | CLA  | C6-C7-C8-C10    |
| 14  | 2     | 811  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 825  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 816  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 825  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 1     | 1626 | CLA  | O1A-CGA-O2A-C1  |
| 17  | A     | 848  | BCR  | C15-C16-C17-C18 |
| 17  | a     | 848  | BCR  | C15-C16-C17-C18 |
| 17  | 1     | 1649 | BCR  | C15-C16-C17-C18 |
| 14  | A     | 803  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 822  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 825  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 827  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 822  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 825  | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 828  | CLA  | C2A-CAA-CBA-CGA |
| 14  | 1     | 1604 | CLA  | C2A-CAA-CBA-CGA |
| 14  | 1     | 1623 | CLA  | C2A-CAA-CBA-CGA |
| 14  | 1     | 1626 | CLA  | C2A-CAA-CBA-CGA |
| 14  | 2     | 828  | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 814  | CLA  | O1D-CGD-O2D-CED |
| 14  | 2     | 814  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 812  | CLA  | C10-C11-C12-C13 |
| 14  | A     | 828  | CLA  | C8-C10-C11-C12  |
| 14  | a     | 812  | CLA  | C10-C11-C12-C13 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 828  | CLA  | C8-C10-C11-C12  |
| 14  | 1     | 1613 | CLA  | C10-C11-C12-C13 |
| 14  | 1     | 1629 | CLA  | C8-C10-C11-C12  |
| 14  | B     | 803  | CLA  | C4C-C3C-CAC-CBC |
| 14  | b     | 804  | CLA  | C4C-C3C-CAC-CBC |
| 14  | 2     | 804  | CLA  | C4C-C3C-CAC-CBC |
| 17  | L     | 206  | BCR  | C22-C23-C24-C25 |
| 17  | M     | 103  | BCR  | C22-C23-C24-C25 |
| 17  | l     | 207  | BCR  | C22-C23-C24-C25 |
| 17  | m     | 102  | BCR  | C22-C23-C24-C25 |
| 17  | 0     | 208  | BCR  | C22-C23-C24-C25 |
| 17  | y     | 102  | BCR  | C22-C23-C24-C25 |
| 14  | A     | 812  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 812  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 1     | 1613 | CLA  | O1A-CGA-O2A-C1  |
| 20  | B     | 849  | LMG  | O6-C1-O1-C7     |
| 20  | b     | 850  | LMG  | O6-C1-O1-C7     |
| 20  | 2     | 850  | LMG  | O6-C1-O1-C7     |
| 17  | B     | 845  | BCR  | C18-C19-C20-C21 |
| 17  | B     | 847  | BCR  | C10-C11-C12-C13 |
| 17  | K     | 102  | BCR  | C10-C11-C12-C13 |
| 17  | M     | 103  | BCR  | C18-C19-C20-C21 |
| 17  | b     | 846  | BCR  | C18-C19-C20-C21 |
| 17  | b     | 848  | BCR  | C10-C11-C12-C13 |
| 17  | k     | 102  | BCR  | C10-C11-C12-C13 |
| 17  | m     | 102  | BCR  | C18-C19-C20-C21 |
| 17  | 2     | 846  | BCR  | C18-C19-C20-C21 |
| 17  | 2     | 848  | BCR  | C10-C11-C12-C13 |
| 17  | 9     | 102  | BCR  | C10-C11-C12-C13 |
| 17  | y     | 102  | BCR  | C18-C19-C20-C21 |
| 14  | A     | 843  | CLA  | C3-C5-C6-C7     |
| 14  | a     | 843  | CLA  | C3-C5-C6-C7     |
| 14  | 1     | 1644 | CLA  | C3-C5-C6-C7     |
| 14  | A     | 841  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 804  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 810  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 824  | CLA  | C13-C15-C16-C17 |
| 14  | B     | 834  | CLA  | C15-C16-C17-C18 |
| 14  | a     | 841  | CLA  | C5-C6-C7-C8     |
| 14  | b     | 805  | CLA  | C15-C16-C17-C18 |
| 14  | b     | 811  | CLA  | C15-C16-C17-C18 |
| 14  | b     | 825  | CLA  | C13-C15-C16-C17 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 835  | CLA  | C15-C16-C17-C18 |
| 14  | 1     | 1642 | CLA  | C5-C6-C7-C8     |
| 14  | 2     | 805  | CLA  | C15-C16-C17-C18 |
| 14  | 2     | 811  | CLA  | C15-C16-C17-C18 |
| 14  | 2     | 825  | CLA  | C13-C15-C16-C17 |
| 14  | 2     | 835  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 831  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 2     | 832  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 802  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 818  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 829  | CLA  | C10-C11-C12-C13 |
| 14  | A     | 840  | CLA  | C13-C15-C16-C17 |
| 14  | B     | 811  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 816  | CLA  | C13-C15-C16-C17 |
| 14  | B     | 819  | CLA  | C8-C10-C11-C12  |
| 14  | B     | 825  | CLA  | C8-C10-C11-C12  |
| 14  | a     | 802  | CLA  | C15-C16-C17-C18 |
| 14  | a     | 818  | CLA  | C15-C16-C17-C18 |
| 14  | a     | 829  | CLA  | C10-C11-C12-C13 |
| 14  | a     | 840  | CLA  | C13-C15-C16-C17 |
| 14  | b     | 812  | CLA  | C15-C16-C17-C18 |
| 14  | b     | 817  | CLA  | C13-C15-C16-C17 |
| 14  | b     | 820  | CLA  | C8-C10-C11-C12  |
| 14  | b     | 826  | CLA  | C8-C10-C11-C12  |
| 14  | 1     | 1603 | CLA  | C15-C16-C17-C18 |
| 14  | 1     | 1619 | CLA  | C15-C16-C17-C18 |
| 14  | 1     | 1630 | CLA  | C10-C11-C12-C13 |
| 14  | 1     | 1641 | CLA  | C13-C15-C16-C17 |
| 14  | 2     | 812  | CLA  | C15-C16-C17-C18 |
| 14  | 2     | 817  | CLA  | C13-C15-C16-C17 |
| 14  | 2     | 820  | CLA  | C8-C10-C11-C12  |
| 14  | 2     | 826  | CLA  | C8-C10-C11-C12  |
| 14  | B     | 802  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 829  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 803  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 832  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 2     | 803  | CLA  | O1A-CGA-O2A-C1  |
| 18  | M     | 101  | LHG  | C32-C33-C34-C35 |
| 18  | m     | 101  | LHG  | C32-C33-C34-C35 |
| 18  | y     | 101  | LHG  | C32-C33-C34-C35 |
| 14  | A     | 824  | CLA  | C13-C15-C16-C17 |
| 14  | B     | 805  | CLA  | C13-C15-C16-C17 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 805  | CLA  | C15-C16-C17-C18 |
| 14  | a     | 824  | CLA  | C13-C15-C16-C17 |
| 14  | b     | 806  | CLA  | C13-C15-C16-C17 |
| 14  | b     | 806  | CLA  | C15-C16-C17-C18 |
| 14  | 1     | 1625 | CLA  | C13-C15-C16-C17 |
| 14  | 2     | 806  | CLA  | C13-C15-C16-C17 |
| 14  | 2     | 806  | CLA  | C15-C16-C17-C18 |
| 18  | A     | 853  | LHG  | C3-O3-P-O6      |
| 18  | L     | 208  | LHG  | C3-O3-P-O6      |
| 18  | L     | 208  | LHG  | C4-O6-P-O3      |
| 18  | M     | 101  | LHG  | C4-O6-P-O3      |
| 18  | a     | 853  | LHG  | C3-O3-P-O6      |
| 18  | l     | 201  | LHG  | C3-O3-P-O6      |
| 18  | l     | 201  | LHG  | C4-O6-P-O3      |
| 18  | m     | 101  | LHG  | C4-O6-P-O3      |
| 18  | 1     | 1654 | LHG  | C3-O3-P-O6      |
| 18  | 0     | 202  | LHG  | C3-O3-P-O6      |
| 18  | 0     | 202  | LHG  | C4-O6-P-O3      |
| 18  | y     | 101  | LHG  | C4-O6-P-O3      |
| 14  | B     | 834  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 835  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 2     | 835  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 829  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 1     | 1630 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 811  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 812  | CLA  | O1D-CGD-O2D-CED |
| 14  | 2     | 812  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 829  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 2     | 829  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 814  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 823  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 821  | CLA  | C2A-CAA-CBA-CGA |
| 14  | X     | 1701 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 803  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 814  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 823  | CLA  | C2A-CAA-CBA-CGA |
| 14  | x     | 1701 | CLA  | C2A-CAA-CBA-CGA |
| 14  | 1     | 1615 | CLA  | C2A-CAA-CBA-CGA |
| 14  | 1     | 1624 | CLA  | C2A-CAA-CBA-CGA |
| 14  | 2     | 822  | CLA  | C2A-CAA-CBA-CGA |
| 14  | z     | 102  | CLA  | C2A-CAA-CBA-CGA |
| 14  | K     | 103  | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | k     | 103  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 9     | 103  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 827  | CLA  | C10-C11-C12-C13 |
| 14  | b     | 828  | CLA  | C10-C11-C12-C13 |
| 14  | 2     | 828  | CLA  | C10-C11-C12-C13 |
| 17  | A     | 852  | BCR  | C9-C10-C11-C12  |
| 17  | B     | 843  | BCR  | C15-C16-C17-C18 |
| 17  | a     | 852  | BCR  | C9-C10-C11-C12  |
| 17  | 1     | 1653 | BCR  | C9-C10-C11-C12  |
| 18  | b     | 851  | LHG  | C32-C33-C34-C35 |
| 17  | A     | 847  | BCR  | C20-C21-C22-C37 |
| 17  | A     | 850  | BCR  | C16-C17-C18-C36 |
| 17  | A     | 851  | BCR  | C35-C13-C14-C15 |
| 17  | A     | 856  | BCR  | C35-C13-C14-C15 |
| 17  | A     | 856  | BCR  | C20-C21-C22-C37 |
| 17  | B     | 846  | BCR  | C16-C17-C18-C36 |
| 17  | B     | 851  | BCR  | C16-C17-C18-C36 |
| 17  | F     | 202  | BCR  | C11-C10-C9-C34  |
| 17  | F     | 202  | BCR  | C35-C13-C14-C15 |
| 17  | F     | 202  | BCR  | C20-C21-C22-C37 |
| 17  | F     | 205  | BCR  | C35-C13-C14-C15 |
| 17  | I     | 101  | BCR  | C35-C13-C14-C15 |
| 17  | L     | 201  | BCR  | C35-C13-C14-C15 |
| 17  | L     | 206  | BCR  | C20-C21-C22-C37 |
| 17  | M     | 103  | BCR  | C35-C13-C14-C15 |
| 17  | M     | 103  | BCR  | C20-C21-C22-C37 |
| 17  | a     | 847  | BCR  | C20-C21-C22-C37 |
| 17  | a     | 850  | BCR  | C16-C17-C18-C36 |
| 17  | a     | 851  | BCR  | C35-C13-C14-C15 |
| 17  | b     | 847  | BCR  | C16-C17-C18-C36 |
| 17  | b     | 852  | BCR  | C16-C17-C18-C36 |
| 17  | f     | 202  | BCR  | C11-C10-C9-C34  |
| 17  | f     | 202  | BCR  | C35-C13-C14-C15 |
| 17  | f     | 202  | BCR  | C20-C21-C22-C37 |
| 17  | f     | 204  | BCR  | C35-C13-C14-C15 |
| 17  | i     | 101  | BCR  | C35-C13-C14-C15 |
| 17  | j     | 1305 | BCR  | C35-C13-C14-C15 |
| 17  | j     | 1305 | BCR  | C20-C21-C22-C37 |
| 17  | l     | 202  | BCR  | C35-C13-C14-C15 |
| 17  | l     | 207  | BCR  | C20-C21-C22-C37 |
| 17  | m     | 102  | BCR  | C35-C13-C14-C15 |
| 17  | m     | 102  | BCR  | C20-C21-C22-C37 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | 1     | 1648 | BCR  | C20-C21-C22-C37 |
| 17  | 1     | 1651 | BCR  | C16-C17-C18-C36 |
| 17  | 1     | 1652 | BCR  | C35-C13-C14-C15 |
| 17  | 2     | 847  | BCR  | C16-C17-C18-C36 |
| 17  | 6     | 202  | BCR  | C11-C10-C9-C34  |
| 17  | 6     | 202  | BCR  | C35-C13-C14-C15 |
| 17  | 6     | 202  | BCR  | C20-C21-C22-C37 |
| 17  | 6     | 204  | BCR  | C35-C13-C14-C15 |
| 17  | 7     | 101  | BCR  | C35-C13-C14-C15 |
| 17  | 8     | 1305 | BCR  | C35-C13-C14-C15 |
| 17  | 8     | 1305 | BCR  | C20-C21-C22-C37 |
| 17  | 0     | 203  | BCR  | C35-C13-C14-C15 |
| 17  | 0     | 208  | BCR  | C20-C21-C22-C37 |
| 17  | y     | 102  | BCR  | C35-C13-C14-C15 |
| 17  | y     | 102  | BCR  | C20-C21-C22-C37 |
| 18  | B     | 850  | LHG  | C32-C33-C34-C35 |
| 18  | L     | 208  | LHG  | C15-C16-C17-C18 |
| 18  | l     | 201  | LHG  | C15-C16-C17-C18 |
| 18  | 0     | 202  | LHG  | C15-C16-C17-C18 |
| 18  | z     | 101  | LHG  | C32-C33-C34-C35 |
| 14  | B     | 828  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 819  | CLA  | C16-C17-C18-C20 |
| 14  | A     | 821  | CLA  | C16-C17-C18-C19 |
| 14  | B     | 824  | CLA  | C16-C17-C18-C20 |
| 14  | a     | 819  | CLA  | C16-C17-C18-C20 |
| 14  | a     | 821  | CLA  | C16-C17-C18-C19 |
| 14  | b     | 825  | CLA  | C16-C17-C18-C20 |
| 14  | 1     | 1620 | CLA  | C16-C17-C18-C20 |
| 14  | 1     | 1622 | CLA  | C16-C17-C18-C19 |
| 14  | 2     | 825  | CLA  | C16-C17-C18-C20 |
| 14  | b     | 805  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 819  | CLA  | C8-C10-C11-C12  |
| 14  | B     | 833  | CLA  | C10-C11-C12-C13 |
| 14  | a     | 819  | CLA  | C8-C10-C11-C12  |
| 14  | 1     | 1620 | CLA  | C8-C10-C11-C12  |
| 14  | 2     | 834  | CLA  | C10-C11-C12-C13 |
| 18  | B     | 850  | LHG  | C11-C10-C9-C8   |
| 18  | b     | 851  | LHG  | C11-C10-C9-C8   |
| 18  | M     | 101  | LHG  | C30-C31-C32-C33 |
| 18  | m     | 101  | LHG  | C30-C31-C32-C33 |
| 18  | y     | 101  | LHG  | C30-C31-C32-C33 |
| 18  | z     | 101  | LHG  | C11-C10-C9-C8   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 20  | B     | 849  | LMG  | C18-C19-C20-C21 |
| 20  | b     | 850  | LMG  | C18-C19-C20-C21 |
| 20  | 2     | 850  | LMG  | C18-C19-C20-C21 |
| 14  | b     | 834  | CLA  | C10-C11-C12-C13 |
| 18  | A     | 853  | LHG  | C24-C25-C26-C27 |
| 18  | a     | 853  | LHG  | C24-C25-C26-C27 |
| 18  | 1     | 1654 | LHG  | C24-C25-C26-C27 |
| 14  | B     | 824  | CLA  | C3-C5-C6-C7     |
| 14  | b     | 825  | CLA  | C3-C5-C6-C7     |
| 14  | 2     | 825  | CLA  | C3-C5-C6-C7     |
| 17  | A     | 848  | BCR  | C20-C21-C22-C23 |
| 17  | A     | 850  | BCR  | C20-C21-C22-C23 |
| 17  | A     | 851  | BCR  | C11-C10-C9-C8   |
| 17  | A     | 851  | BCR  | C16-C17-C18-C19 |
| 17  | B     | 843  | BCR  | C16-C17-C18-C19 |
| 17  | B     | 845  | BCR  | C11-C10-C9-C8   |
| 17  | B     | 851  | BCR  | C20-C21-C22-C23 |
| 17  | K     | 104  | BCR  | C11-C10-C9-C8   |
| 17  | a     | 848  | BCR  | C20-C21-C22-C23 |
| 17  | a     | 850  | BCR  | C20-C21-C22-C23 |
| 17  | a     | 851  | BCR  | C11-C10-C9-C8   |
| 17  | a     | 851  | BCR  | C16-C17-C18-C19 |
| 17  | b     | 844  | BCR  | C16-C17-C18-C19 |
| 17  | b     | 846  | BCR  | C11-C10-C9-C8   |
| 17  | b     | 852  | BCR  | C20-C21-C22-C23 |
| 17  | k     | 104  | BCR  | C11-C10-C9-C8   |
| 17  | 1     | 1649 | BCR  | C20-C21-C22-C23 |
| 17  | 1     | 1651 | BCR  | C20-C21-C22-C23 |
| 17  | 1     | 1652 | BCR  | C11-C10-C9-C8   |
| 17  | 1     | 1652 | BCR  | C16-C17-C18-C19 |
| 17  | 2     | 844  | BCR  | C16-C17-C18-C19 |
| 17  | 2     | 846  | BCR  | C11-C10-C9-C8   |
| 17  | 8     | 1306 | BCR  | C20-C21-C22-C23 |
| 17  | 9     | 104  | BCR  | C11-C10-C9-C8   |
| 20  | B     | 849  | LMG  | C2-C1-O1-C7     |
| 20  | b     | 850  | LMG  | C2-C1-O1-C7     |
| 20  | 2     | 850  | LMG  | C2-C1-O1-C7     |
| 14  | B     | 804  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 2     | 805  | CLA  | CBA-CGA-O2A-C1  |
| 18  | A     | 853  | LHG  | C11-C10-C9-C8   |
| 18  | B     | 850  | LHG  | C15-C16-C17-C18 |
| 18  | L     | 208  | LHG  | C12-C13-C14-C15 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | a     | 853  | LHG  | C11-C10-C9-C8   |
| 18  | l     | 201  | LHG  | C12-C13-C14-C15 |
| 18  | 1     | 1654 | LHG  | C11-C10-C9-C8   |
| 14  | A     | 831  | CLA  | C5-C6-C7-C8     |
| 14  | a     | 831  | CLA  | C5-C6-C7-C8     |
| 14  | 1     | 1632 | CLA  | C5-C6-C7-C8     |
| 14  | B     | 834  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 835  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 2     | 835  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 810  | CLA  | C16-C17-C18-C19 |
| 14  | B     | 810  | CLA  | C16-C17-C18-C20 |
| 14  | B     | 818  | CLA  | C16-C17-C18-C20 |
| 14  | B     | 824  | CLA  | C16-C17-C18-C19 |
| 14  | b     | 811  | CLA  | C16-C17-C18-C19 |
| 14  | b     | 811  | CLA  | C16-C17-C18-C20 |
| 14  | b     | 819  | CLA  | C16-C17-C18-C20 |
| 14  | b     | 825  | CLA  | C16-C17-C18-C19 |
| 14  | 2     | 811  | CLA  | C16-C17-C18-C20 |
| 14  | 2     | 819  | CLA  | C16-C17-C18-C20 |
| 14  | b     | 831  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 820  | CLA  | C4-C3-C5-C6     |
| 14  | A     | 822  | CLA  | C4-C3-C5-C6     |
| 14  | a     | 820  | CLA  | C4-C3-C5-C6     |
| 14  | a     | 822  | CLA  | C4-C3-C5-C6     |
| 14  | 1     | 1621 | CLA  | C4-C3-C5-C6     |
| 14  | 1     | 1623 | CLA  | C4-C3-C5-C6     |
| 18  | a     | 853  | LHG  | C32-C33-C34-C35 |
| 18  | b     | 851  | LHG  | C15-C16-C17-C18 |
| 18  | 0     | 202  | LHG  | C12-C13-C14-C15 |
| 18  | z     | 101  | LHG  | C15-C16-C17-C18 |
| 14  | A     | 812  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 822  | CLA  | C2-C3-C5-C6     |
| 14  | B     | 814  | CLA  | C2-C3-C5-C6     |
| 14  | a     | 812  | CLA  | C2-C3-C5-C6     |
| 14  | a     | 822  | CLA  | C2-C3-C5-C6     |
| 14  | b     | 815  | CLA  | C2-C3-C5-C6     |
| 14  | 1     | 1613 | CLA  | C2-C3-C5-C6     |
| 14  | 1     | 1623 | CLA  | C2-C3-C5-C6     |
| 14  | 2     | 815  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 804  | CLA  | C6-C7-C8-C9     |
| 14  | A     | 816  | CLA  | C11-C12-C13-C14 |
| 14  | A     | 830  | CLA  | C11-C12-C13-C14 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 810  | CLA  | C11-C12-C13-C14 |
| 14  | a     | 804  | CLA  | C6-C7-C8-C9     |
| 14  | a     | 816  | CLA  | C11-C12-C13-C14 |
| 14  | a     | 830  | CLA  | C11-C12-C13-C14 |
| 14  | b     | 811  | CLA  | C11-C12-C13-C14 |
| 14  | 1     | 1605 | CLA  | C6-C7-C8-C9     |
| 14  | 1     | 1617 | CLA  | C11-C12-C13-C14 |
| 14  | 1     | 1631 | CLA  | C11-C12-C13-C14 |
| 14  | 2     | 811  | CLA  | C11-C12-C13-C14 |
| 14  | B     | 830  | CLA  | O1D-CGD-O2D-CED |
| 14  | 2     | 831  | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 853  | LHG  | C32-C33-C34-C35 |
| 18  | 1     | 1654 | LHG  | C32-C33-C34-C35 |
| 20  | B     | 849  | LMG  | C12-C13-C14-C15 |
| 20  | b     | 850  | LMG  | C12-C13-C14-C15 |
| 20  | 2     | 850  | LMG  | C12-C13-C14-C15 |
| 14  | A     | 834  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 809  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 823  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 834  | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 810  | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 822  | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 824  | CLA  | C2A-CAA-CBA-CGA |
| 14  | 1     | 1635 | CLA  | C2A-CAA-CBA-CGA |
| 14  | 2     | 810  | CLA  | C2A-CAA-CBA-CGA |
| 14  | 2     | 824  | CLA  | C2A-CAA-CBA-CGA |
| 17  | B     | 843  | BCR  | C37-C22-C23-C24 |
| 17  | b     | 844  | BCR  | C37-C22-C23-C24 |
| 17  | 1     | 202  | BCR  | C11-C12-C13-C35 |
| 17  | 2     | 844  | BCR  | C37-C22-C23-C24 |
| 17  | 0     | 203  | BCR  | C11-C12-C13-C35 |
| 18  | A     | 853  | LHG  | O1-C1-C2-C3     |
| 18  | B     | 850  | LHG  | O1-C1-C2-C3     |
| 18  | M     | 101  | LHG  | O1-C1-C2-C3     |
| 18  | a     | 853  | LHG  | O1-C1-C2-C3     |
| 18  | b     | 851  | LHG  | O1-C1-C2-C3     |
| 18  | m     | 101  | LHG  | O1-C1-C2-C3     |
| 18  | 1     | 1654 | LHG  | O1-C1-C2-C3     |
| 18  | y     | 101  | LHG  | O1-C1-C2-C3     |
| 18  | z     | 101  | LHG  | O1-C1-C2-C3     |
| 14  | B     | 814  | CLA  | CBD-CGD-O2D-CED |
| 20  | B     | 849  | LMG  | C35-C36-C37-C38 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 20  | 2     | 850  | LMG  | C35-C36-C37-C38 |
| 14  | A     | 816  | CLA  | C16-C17-C18-C19 |
| 14  | B     | 828  | CLA  | C16-C17-C18-C19 |
| 14  | B     | 830  | CLA  | C6-C7-C8-C10    |
| 14  | a     | 816  | CLA  | C16-C17-C18-C19 |
| 14  | a     | 816  | CLA  | C16-C17-C18-C20 |
| 14  | b     | 829  | CLA  | C16-C17-C18-C19 |
| 14  | b     | 831  | CLA  | C6-C7-C8-C10    |
| 14  | 1     | 1617 | CLA  | C16-C17-C18-C19 |
| 14  | 2     | 811  | CLA  | C16-C17-C18-C19 |
| 14  | 2     | 825  | CLA  | C16-C17-C18-C19 |
| 14  | 2     | 829  | CLA  | C16-C17-C18-C19 |
| 14  | 2     | 831  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 804  | CLA  | C10-C11-C12-C13 |
| 14  | a     | 804  | CLA  | C10-C11-C12-C13 |
| 14  | 1     | 1605 | CLA  | C10-C11-C12-C13 |
| 18  | A     | 853  | LHG  | C10-C11-C12-C13 |
| 18  | M     | 101  | LHG  | C34-C35-C36-C37 |
| 18  | a     | 853  | LHG  | C10-C11-C12-C13 |
| 18  | m     | 101  | LHG  | C34-C35-C36-C37 |
| 18  | 1     | 1654 | LHG  | C10-C11-C12-C13 |
| 18  | y     | 101  | LHG  | C34-C35-C36-C37 |
| 20  | b     | 850  | LMG  | C35-C36-C37-C38 |
| 14  | a     | 820  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 815  | CLA  | CBD-CGD-O2D-CED |
| 14  | 2     | 815  | CLA  | CBD-CGD-O2D-CED |
| 20  | B     | 849  | LMG  | O10-C28-O8-C9   |
| 20  | b     | 850  | LMG  | O10-C28-O8-C9   |
| 20  | 2     | 850  | LMG  | O10-C28-O8-C9   |
| 18  | A     | 854  | LHG  | C24-C25-C26-C27 |
| 18  | a     | 854  | LHG  | C24-C25-C26-C27 |
| 18  | 1     | 1655 | LHG  | C24-C25-C26-C27 |
| 13  | A     | 801  | CL0  | C3-C5-C6-C7     |
| 13  | a     | 801  | CL0  | C3-C5-C6-C7     |
| 13  | 1     | 1602 | CL0  | C3-C5-C6-C7     |
| 14  | A     | 832  | CLA  | C3-C5-C6-C7     |
| 14  | a     | 832  | CLA  | C3-C5-C6-C7     |
| 14  | 1     | 1633 | CLA  | C3-C5-C6-C7     |
| 18  | A     | 853  | LHG  | C9-C10-C11-C12  |
| 18  | a     | 853  | LHG  | C9-C10-C11-C12  |
| 18  | 1     | 1654 | LHG  | C9-C10-C11-C12  |
| 14  | A     | 804  | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 806  | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 813  | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 825  | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 836  | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 804  | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 806  | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 814  | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 826  | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 837  | CLA  | C3A-C2A-CAA-CBA |
| 14  | 1     | 1605 | CLA  | C3A-C2A-CAA-CBA |
| 14  | 1     | 1607 | CLA  | C3A-C2A-CAA-CBA |
| 14  | 2     | 814  | CLA  | C3A-C2A-CAA-CBA |
| 14  | 2     | 826  | CLA  | C3A-C2A-CAA-CBA |
| 14  | 2     | 837  | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 838  | CLA  | C13-C15-C16-C17 |
| 14  | b     | 839  | CLA  | C13-C15-C16-C17 |
| 14  | 2     | 839  | CLA  | C13-C15-C16-C17 |
| 17  | b     | 844  | BCR  | C15-C16-C17-C18 |
| 17  | 2     | 844  | BCR  | C15-C16-C17-C18 |
| 18  | M     | 101  | LHG  | C11-C10-C9-C8   |
| 18  | m     | 101  | LHG  | C11-C10-C9-C8   |
| 14  | A     | 816  | CLA  | C16-C17-C18-C20 |
| 14  | A     | 821  | CLA  | C16-C17-C18-C20 |
| 14  | A     | 839  | CLA  | C16-C17-C18-C20 |
| 14  | B     | 828  | CLA  | C16-C17-C18-C20 |
| 14  | a     | 821  | CLA  | C16-C17-C18-C20 |
| 14  | a     | 839  | CLA  | C16-C17-C18-C20 |
| 14  | b     | 829  | CLA  | C16-C17-C18-C20 |
| 14  | 1     | 1617 | CLA  | C16-C17-C18-C20 |
| 14  | 1     | 1622 | CLA  | C16-C17-C18-C20 |
| 14  | 1     | 1640 | CLA  | C16-C17-C18-C20 |
| 14  | 2     | 829  | CLA  | C16-C17-C18-C20 |
| 14  | 2     | 831  | CLA  | C6-C7-C8-C9     |
| 18  | y     | 101  | LHG  | C11-C10-C9-C8   |
| 14  | A     | 820  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 840  | CLA  | CBD-CGD-O2D-CED |
| 14  | 1     | 1621 | CLA  | CBD-CGD-O2D-CED |
| 14  | 2     | 840  | CLA  | CBD-CGD-O2D-CED |
| 17  | 6     | 202  | BCR  | C14-C15-C16-C17 |
| 14  | A     | 812  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 826  | CLA  | C3-C5-C6-C7     |
| 14  | a     | 826  | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | 1     | 1627 | CLA  | C3-C5-C6-C7     |
| 18  | M     | 101  | LHG  | C7-C8-C9-C10    |
| 18  | m     | 101  | LHG  | C7-C8-C9-C10    |
| 18  | y     | 101  | LHG  | C7-C8-C9-C10    |
| 14  | A     | 804  | CLA  | C8-C10-C11-C12  |
| 14  | a     | 804  | CLA  | C8-C10-C11-C12  |
| 14  | 1     | 1605 | CLA  | C8-C10-C11-C12  |
| 14  | A     | 812  | CLA  | C4-C3-C5-C6     |
| 14  | A     | 825  | CLA  | C4-C3-C5-C6     |
| 14  | B     | 814  | CLA  | C4-C3-C5-C6     |
| 14  | a     | 812  | CLA  | C4-C3-C5-C6     |
| 14  | a     | 825  | CLA  | C4-C3-C5-C6     |
| 14  | b     | 815  | CLA  | C4-C3-C5-C6     |
| 14  | 1     | 1613 | CLA  | C4-C3-C5-C6     |
| 14  | 1     | 1626 | CLA  | C4-C3-C5-C6     |
| 14  | 2     | 815  | CLA  | C4-C3-C5-C6     |
| 14  | a     | 825  | CLA  | C2-C3-C5-C6     |
| 14  | 1     | 1626 | CLA  | C2-C3-C5-C6     |
| 14  | B     | 839  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 835  | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 836  | CLA  | C2A-CAA-CBA-CGA |
| 14  | 2     | 836  | CLA  | C2A-CAA-CBA-CGA |
| 14  | K     | 103  | CLA  | O1A-CGA-O2A-C1  |
| 14  | k     | 103  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 9     | 103  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 830  | CLA  | C6-C7-C8-C9     |
| 14  | b     | 831  | CLA  | C6-C7-C8-C9     |
| 14  | A     | 812  | CLA  | C8-C10-C11-C12  |
| 14  | A     | 832  | CLA  | C5-C6-C7-C8     |
| 14  | a     | 812  | CLA  | C8-C10-C11-C12  |
| 14  | a     | 832  | CLA  | C5-C6-C7-C8     |
| 14  | 1     | 1613 | CLA  | C8-C10-C11-C12  |
| 14  | a     | 812  | CLA  | C3-C5-C6-C7     |
| 14  | 1     | 1613 | CLA  | C3-C5-C6-C7     |
| 14  | A     | 819  | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 819  | CLA  | C2-C1-O2A-CGA   |
| 14  | a     | 819  | CLA  | C2-C1-O2A-CGA   |
| 14  | b     | 820  | CLA  | C2-C1-O2A-CGA   |
| 14  | 1     | 1620 | CLA  | C2-C1-O2A-CGA   |
| 14  | 2     | 820  | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 838  | CLA  | C2C-C3C-CAC-CBC |
| 14  | a     | 838  | CLA  | C2C-C3C-CAC-CBC |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | 1     | 1639 | CLA  | C2C-C3C-CAC-CBC |
| 18  | L     | 208  | LHG  | C14-C15-C16-C17 |
| 18  | l     | 201  | LHG  | C14-C15-C16-C17 |
| 18  | 0     | 202  | LHG  | C14-C15-C16-C17 |
| 14  | A     | 816  | CLA  | C8-C10-C11-C12  |
| 14  | A     | 825  | CLA  | C15-C16-C17-C18 |
| 14  | a     | 816  | CLA  | C8-C10-C11-C12  |
| 14  | a     | 825  | CLA  | C15-C16-C17-C18 |
| 14  | 1     | 1617 | CLA  | C8-C10-C11-C12  |
| 14  | 1     | 1626 | CLA  | C15-C16-C17-C18 |
| 14  | 1     | 1633 | CLA  | C5-C6-C7-C8     |
| 14  | B     | 804  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 805  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 2     | 805  | CLA  | O1A-CGA-O2A-C1  |
| 18  | A     | 853  | LHG  | C27-C28-C29-C30 |
| 18  | A     | 854  | LHG  | C32-C33-C34-C35 |
| 18  | a     | 853  | LHG  | C27-C28-C29-C30 |
| 18  | a     | 854  | LHG  | C32-C33-C34-C35 |
| 18  | 1     | 1654 | LHG  | C27-C28-C29-C30 |
| 17  | A     | 847  | BCR  | C23-C24-C25-C26 |
| 17  | A     | 849  | BCR  | C23-C24-C25-C26 |
| 17  | A     | 849  | BCR  | C23-C24-C25-C30 |
| 17  | A     | 851  | BCR  | C5-C6-C7-C8     |
| 17  | A     | 856  | BCR  | C1-C6-C7-C8     |
| 17  | A     | 856  | BCR  | C5-C6-C7-C8     |
| 17  | A     | 856  | BCR  | C23-C24-C25-C26 |
| 17  | A     | 856  | BCR  | C23-C24-C25-C30 |
| 17  | B     | 844  | BCR  | C5-C6-C7-C8     |
| 17  | B     | 845  | BCR  | C1-C6-C7-C8     |
| 17  | B     | 847  | BCR  | C23-C24-C25-C26 |
| 17  | B     | 847  | BCR  | C23-C24-C25-C30 |
| 17  | B     | 851  | BCR  | C1-C6-C7-C8     |
| 17  | B     | 851  | BCR  | C5-C6-C7-C8     |
| 17  | F     | 205  | BCR  | C5-C6-C7-C8     |
| 17  | F     | 205  | BCR  | C23-C24-C25-C26 |
| 17  | J     | 103  | BCR  | C5-C6-C7-C8     |
| 17  | L     | 206  | BCR  | C23-C24-C25-C26 |
| 17  | L     | 206  | BCR  | C23-C24-C25-C30 |
| 17  | M     | 103  | BCR  | C1-C6-C7-C8     |
| 17  | M     | 103  | BCR  | C5-C6-C7-C8     |
| 17  | a     | 847  | BCR  | C23-C24-C25-C26 |
| 17  | a     | 849  | BCR  | C23-C24-C25-C26 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | a     | 849  | BCR  | C23-C24-C25-C30 |
| 17  | a     | 851  | BCR  | C5-C6-C7-C8     |
| 17  | b     | 845  | BCR  | C5-C6-C7-C8     |
| 17  | b     | 846  | BCR  | C1-C6-C7-C8     |
| 17  | b     | 848  | BCR  | C23-C24-C25-C26 |
| 17  | b     | 848  | BCR  | C23-C24-C25-C30 |
| 17  | b     | 852  | BCR  | C1-C6-C7-C8     |
| 17  | b     | 852  | BCR  | C5-C6-C7-C8     |
| 17  | f     | 204  | BCR  | C5-C6-C7-C8     |
| 17  | f     | 204  | BCR  | C23-C24-C25-C26 |
| 17  | j     | 1304 | BCR  | C5-C6-C7-C8     |
| 17  | j     | 1305 | BCR  | C1-C6-C7-C8     |
| 17  | j     | 1305 | BCR  | C5-C6-C7-C8     |
| 17  | j     | 1305 | BCR  | C23-C24-C25-C26 |
| 17  | j     | 1305 | BCR  | C23-C24-C25-C30 |
| 17  | l     | 207  | BCR  | C23-C24-C25-C26 |
| 17  | l     | 207  | BCR  | C23-C24-C25-C30 |
| 17  | m     | 102  | BCR  | C1-C6-C7-C8     |
| 17  | m     | 102  | BCR  | C5-C6-C7-C8     |
| 17  | 1     | 1648 | BCR  | C23-C24-C25-C26 |
| 17  | 1     | 1650 | BCR  | C23-C24-C25-C26 |
| 17  | 1     | 1650 | BCR  | C23-C24-C25-C30 |
| 17  | 1     | 1652 | BCR  | C1-C6-C7-C8     |
| 17  | 1     | 1652 | BCR  | C5-C6-C7-C8     |
| 17  | 2     | 845  | BCR  | C5-C6-C7-C8     |
| 17  | 2     | 846  | BCR  | C1-C6-C7-C8     |
| 17  | 2     | 848  | BCR  | C23-C24-C25-C26 |
| 17  | 2     | 848  | BCR  | C23-C24-C25-C30 |
| 17  | 6     | 204  | BCR  | C5-C6-C7-C8     |
| 17  | 6     | 204  | BCR  | C23-C24-C25-C26 |
| 17  | 8     | 1304 | BCR  | C5-C6-C7-C8     |
| 17  | 8     | 1305 | BCR  | C1-C6-C7-C8     |
| 17  | 8     | 1305 | BCR  | C5-C6-C7-C8     |
| 17  | 8     | 1305 | BCR  | C23-C24-C25-C26 |
| 17  | 8     | 1305 | BCR  | C23-C24-C25-C30 |
| 17  | 8     | 1306 | BCR  | C1-C6-C7-C8     |
| 17  | 8     | 1306 | BCR  | C5-C6-C7-C8     |
| 17  | 0     | 208  | BCR  | C23-C24-C25-C26 |
| 17  | 0     | 208  | BCR  | C23-C24-C25-C30 |
| 17  | y     | 102  | BCR  | C1-C6-C7-C8     |
| 17  | y     | 102  | BCR  | C5-C6-C7-C8     |
| 18  | a     | 853  | LHG  | C15-C16-C17-C18 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | 1     | 1654 | LHG  | C15-C16-C17-C18 |
| 18  | 1     | 1655 | LHG  | C32-C33-C34-C35 |
| 14  | B     | 831  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 843  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 843  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1644 | CLA  | CBA-CGA-O2A-C1  |
| 18  | L     | 208  | LHG  | C8-C7-O7-C5     |
| 18  | l     | 201  | LHG  | C8-C7-O7-C5     |
| 18  | 0     | 202  | LHG  | C8-C7-O7-C5     |
| 20  | B     | 849  | LMG  | C11-C10-O7-C8   |
| 18  | A     | 853  | LHG  | C15-C16-C17-C18 |
| 14  | b     | 832  | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 853  | LHG  | C29-C30-C31-C32 |
| 18  | a     | 853  | LHG  | C29-C30-C31-C32 |
| 18  | 1     | 1654 | LHG  | C29-C30-C31-C32 |
| 14  | A     | 839  | CLA  | C5-C6-C7-C8     |
| 14  | 2     | 832  | CLA  | O1D-CGD-O2D-CED |
| 18  | M     | 101  | LHG  | C16-C17-C18-C19 |
| 18  | m     | 101  | LHG  | C16-C17-C18-C19 |
| 18  | y     | 101  | LHG  | C16-C17-C18-C19 |
| 14  | A     | 803  | CLA  | C4-C3-C5-C6     |
| 14  | a     | 803  | CLA  | C4-C3-C5-C6     |
| 14  | 1     | 1604 | CLA  | C4-C3-C5-C6     |
| 14  | a     | 841  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 804  | CLA  | C11-C10-C8-C7   |
| 14  | A     | 805  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 806  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 820  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 825  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 830  | CLA  | C11-C12-C13-C15 |
| 14  | A     | 833  | CLA  | C11-C12-C13-C15 |
| 14  | A     | 834  | CLA  | C11-C10-C8-C7   |
| 14  | A     | 834  | CLA  | C11-C12-C13-C15 |
| 14  | A     | 836  | CLA  | C11-C10-C8-C7   |
| 14  | B     | 802  | CLA  | C11-C12-C13-C15 |
| 14  | B     | 805  | CLA  | C11-C10-C8-C7   |
| 14  | B     | 810  | CLA  | C11-C12-C13-C15 |
| 14  | B     | 827  | CLA  | C11-C12-C13-C15 |
| 14  | B     | 838  | CLA  | C12-C13-C15-C16 |
| 14  | a     | 804  | CLA  | C11-C10-C8-C7   |
| 14  | a     | 805  | CLA  | C6-C7-C8-C10    |
| 14  | a     | 806  | CLA  | C12-C13-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 820  | CLA  | C2-C3-C5-C6     |
| 14  | a     | 830  | CLA  | C11-C12-C13-C15 |
| 14  | a     | 833  | CLA  | C11-C12-C13-C15 |
| 14  | a     | 834  | CLA  | C11-C10-C8-C7   |
| 14  | a     | 834  | CLA  | C11-C12-C13-C15 |
| 14  | a     | 836  | CLA  | C11-C10-C8-C7   |
| 14  | b     | 803  | CLA  | C11-C12-C13-C15 |
| 14  | b     | 806  | CLA  | C11-C10-C8-C7   |
| 14  | b     | 811  | CLA  | C11-C12-C13-C15 |
| 14  | b     | 828  | CLA  | C11-C12-C13-C15 |
| 14  | b     | 839  | CLA  | C12-C13-C15-C16 |
| 14  | 1     | 1605 | CLA  | C11-C10-C8-C7   |
| 14  | 1     | 1606 | CLA  | C6-C7-C8-C10    |
| 14  | 1     | 1607 | CLA  | C12-C13-C15-C16 |
| 14  | 1     | 1621 | CLA  | C2-C3-C5-C6     |
| 14  | 1     | 1631 | CLA  | C11-C12-C13-C15 |
| 14  | 1     | 1634 | CLA  | C11-C12-C13-C15 |
| 14  | 1     | 1635 | CLA  | C11-C10-C8-C7   |
| 14  | 1     | 1635 | CLA  | C11-C12-C13-C15 |
| 14  | 1     | 1637 | CLA  | C11-C10-C8-C7   |
| 14  | 2     | 803  | CLA  | C11-C12-C13-C15 |
| 14  | 2     | 806  | CLA  | C11-C10-C8-C7   |
| 14  | 2     | 811  | CLA  | C11-C12-C13-C15 |
| 14  | 2     | 828  | CLA  | C11-C12-C13-C15 |
| 14  | 2     | 839  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 821  | CLA  | C3-C5-C6-C7     |
| 14  | a     | 821  | CLA  | C3-C5-C6-C7     |
| 14  | 1     | 1622 | CLA  | C3-C5-C6-C7     |
| 14  | A     | 828  | CLA  | C10-C11-C12-C13 |
| 14  | A     | 838  | CLA  | C13-C15-C16-C17 |
| 14  | B     | 825  | CLA  | C10-C11-C12-C13 |
| 14  | a     | 828  | CLA  | C10-C11-C12-C13 |
| 14  | a     | 838  | CLA  | C13-C15-C16-C17 |
| 14  | a     | 839  | CLA  | C5-C6-C7-C8     |
| 14  | b     | 826  | CLA  | C10-C11-C12-C13 |
| 14  | 1     | 1629 | CLA  | C10-C11-C12-C13 |
| 14  | 1     | 1639 | CLA  | C13-C15-C16-C17 |
| 14  | 1     | 1640 | CLA  | C5-C6-C7-C8     |
| 14  | 2     | 826  | CLA  | C10-C11-C12-C13 |
| 14  | A     | 843  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 843  | CLA  | CBD-CGD-O2D-CED |
| 14  | 1     | 1644 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 815  | CLA  | C16-C17-C18-C20 |
| 14  | b     | 816  | CLA  | C16-C17-C18-C20 |
| 14  | 2     | 816  | CLA  | C16-C17-C18-C20 |
| 14  | A     | 837  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 841  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 837  | CLA  | O1D-CGD-O2D-CED |
| 14  | 1     | 1638 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 814  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 832  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 814  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 833  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1615 | CLA  | CBA-CGA-O2A-C1  |
| 14  | 2     | 833  | CLA  | CBA-CGA-O2A-C1  |
| 18  | A     | 854  | LHG  | C24-C23-O8-C6   |
| 18  | a     | 854  | LHG  | C24-C23-O8-C6   |
| 18  | 1     | 1655 | LHG  | C24-C23-O8-C6   |
| 14  | A     | 816  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 807  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 819  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 828  | CLA  | C2A-CAA-CBA-CGA |
| 14  | J     | 101  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 816  | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 808  | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 820  | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 829  | CLA  | C2A-CAA-CBA-CGA |
| 14  | j     | 1302 | CLA  | C2A-CAA-CBA-CGA |
| 14  | 1     | 1617 | CLA  | C2A-CAA-CBA-CGA |
| 14  | 2     | 808  | CLA  | C2A-CAA-CBA-CGA |
| 14  | 2     | 820  | CLA  | C2A-CAA-CBA-CGA |
| 14  | 2     | 829  | CLA  | C2A-CAA-CBA-CGA |
| 14  | 8     | 1302 | CLA  | C2A-CAA-CBA-CGA |
| 14  | 1     | 1642 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 819  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 826  | CLA  | C5-C6-C7-C8     |
| 14  | a     | 819  | CLA  | C15-C16-C17-C18 |
| 14  | a     | 826  | CLA  | C5-C6-C7-C8     |
| 14  | 1     | 1620 | CLA  | C15-C16-C17-C18 |
| 14  | 1     | 1627 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 819  | CLA  | C5-C6-C7-C8     |
| 14  | 2     | 819  | CLA  | C5-C6-C7-C8     |
| 17  | A     | 848  | BCR  | C6-C7-C8-C9     |
| 17  | B     | 848  | BCR  | C22-C23-C24-C25 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | I     | 101  | BCR  | C22-C23-C24-C25 |
| 17  | a     | 848  | BCR  | C6-C7-C8-C9     |
| 17  | b     | 849  | BCR  | C22-C23-C24-C25 |
| 17  | i     | 101  | BCR  | C22-C23-C24-C25 |
| 17  | 1     | 1649 | BCR  | C6-C7-C8-C9     |
| 17  | 2     | 849  | BCR  | C22-C23-C24-C25 |
| 17  | 7     | 101  | BCR  | C22-C23-C24-C25 |
| 14  | B     | 811  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 818  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 825  | CLA  | C5-C6-C7-C8     |
| 14  | L     | 203  | CLA  | C8-C10-C11-C12  |
| 14  | b     | 812  | CLA  | C5-C6-C7-C8     |
| 14  | b     | 826  | CLA  | C5-C6-C7-C8     |
| 14  | l     | 204  | CLA  | C8-C10-C11-C12  |
| 14  | 2     | 812  | CLA  | C5-C6-C7-C8     |
| 14  | 2     | 826  | CLA  | C5-C6-C7-C8     |
| 14  | 0     | 205  | CLA  | C8-C10-C11-C12  |
| 18  | A     | 853  | LHG  | C8-C7-O7-C5     |
| 18  | a     | 853  | LHG  | C8-C7-O7-C5     |
| 18  | 1     | 1654 | LHG  | C8-C7-O7-C5     |
| 20  | b     | 850  | LMG  | C11-C10-O7-C8   |
| 20  | 2     | 850  | LMG  | C11-C10-O7-C8   |
| 17  | B     | 848  | BCR  | C18-C19-C20-C21 |
| 17  | L     | 206  | BCR  | C18-C19-C20-C21 |
| 17  | b     | 849  | BCR  | C18-C19-C20-C21 |
| 17  | l     | 207  | BCR  | C18-C19-C20-C21 |
| 17  | 2     | 849  | BCR  | C18-C19-C20-C21 |
| 17  | 0     | 208  | BCR  | C18-C19-C20-C21 |
| 17  | F     | 202  | BCR  | C14-C15-C16-C17 |
| 17  | L     | 206  | BCR  | C14-C15-C16-C17 |
| 17  | f     | 202  | BCR  | C14-C15-C16-C17 |
| 17  | l     | 207  | BCR  | C14-C15-C16-C17 |
| 17  | 0     | 208  | BCR  | C14-C15-C16-C17 |
| 14  | B     | 816  | CLA  | C5-C6-C7-C8     |
| 14  | b     | 817  | CLA  | C5-C6-C7-C8     |
| 14  | 1     | 1631 | CLA  | C5-C6-C7-C8     |
| 14  | 2     | 817  | CLA  | C5-C6-C7-C8     |
| 14  | A     | 806  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 806  | CLA  | CBD-CGD-O2D-CED |
| 14  | 1     | 1607 | CLA  | CBD-CGD-O2D-CED |
| 18  | A     | 854  | LHG  | C27-C28-C29-C30 |
| 18  | a     | 854  | LHG  | C27-C28-C29-C30 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | 1     | 1655 | LHG  | C27-C28-C29-C30 |
| 14  | A     | 807  | CLA  | C3-C5-C6-C7     |
| 14  | a     | 807  | CLA  | C3-C5-C6-C7     |
| 14  | 1     | 1608 | CLA  | C3-C5-C6-C7     |
| 18  | A     | 854  | LHG  | O7-C5-C6-O8     |
| 18  | a     | 854  | LHG  | O7-C5-C6-O8     |
| 18  | 1     | 1655 | LHG  | O7-C5-C6-O8     |
| 14  | a     | 843  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 1     | 1644 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 818  | CLA  | C16-C17-C18-C19 |
| 14  | b     | 819  | CLA  | C16-C17-C18-C19 |
| 14  | 2     | 819  | CLA  | C16-C17-C18-C19 |
| 14  | A     | 830  | CLA  | C5-C6-C7-C8     |
| 14  | a     | 830  | CLA  | C5-C6-C7-C8     |
| 18  | z     | 101  | LHG  | C7-C8-C9-C10    |
| 14  | A     | 803  | CLA  | C2-C3-C5-C6     |
| 14  | L     | 205  | CLA  | C2-C3-C5-C6     |
| 14  | a     | 803  | CLA  | C2-C3-C5-C6     |
| 14  | l     | 206  | CLA  | C2-C3-C5-C6     |
| 14  | 1     | 1604 | CLA  | C2-C3-C5-C6     |
| 14  | 0     | 207  | CLA  | C2-C3-C5-C6     |
| 13  | A     | 801  | CL0  | C11-C12-C13-C14 |
| 13  | a     | 801  | CL0  | C11-C12-C13-C14 |
| 13  | 1     | 1602 | CL0  | C11-C12-C13-C14 |
| 14  | A     | 804  | CLA  | C11-C10-C8-C9   |
| 14  | A     | 824  | CLA  | C11-C10-C8-C9   |
| 14  | A     | 827  | CLA  | C14-C13-C15-C16 |
| 14  | A     | 834  | CLA  | C14-C13-C15-C16 |
| 14  | B     | 805  | CLA  | C11-C10-C8-C9   |
| 14  | B     | 810  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 827  | CLA  | C11-C12-C13-C14 |
| 14  | B     | 838  | CLA  | C14-C13-C15-C16 |
| 14  | L     | 203  | CLA  | C11-C10-C8-C9   |
| 14  | L     | 203  | CLA  | C14-C13-C15-C16 |
| 14  | a     | 804  | CLA  | C11-C10-C8-C9   |
| 14  | a     | 824  | CLA  | C11-C10-C8-C9   |
| 14  | a     | 827  | CLA  | C14-C13-C15-C16 |
| 14  | a     | 834  | CLA  | C14-C13-C15-C16 |
| 14  | b     | 806  | CLA  | C11-C10-C8-C9   |
| 14  | b     | 811  | CLA  | C6-C7-C8-C9     |
| 14  | b     | 828  | CLA  | C11-C12-C13-C14 |
| 14  | b     | 839  | CLA  | C14-C13-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | l     | 204  | CLA  | C11-C10-C8-C9   |
| 14  | l     | 204  | CLA  | C14-C13-C15-C16 |
| 14  | 1     | 1605 | CLA  | C11-C10-C8-C9   |
| 14  | 1     | 1625 | CLA  | C11-C10-C8-C9   |
| 14  | 1     | 1628 | CLA  | C14-C13-C15-C16 |
| 14  | 1     | 1635 | CLA  | C14-C13-C15-C16 |
| 14  | 2     | 806  | CLA  | C11-C10-C8-C9   |
| 14  | 2     | 811  | CLA  | C6-C7-C8-C9     |
| 14  | 2     | 828  | CLA  | C11-C12-C13-C14 |
| 14  | 2     | 839  | CLA  | C14-C13-C15-C16 |
| 14  | 0     | 205  | CLA  | C11-C10-C8-C9   |
| 14  | 0     | 205  | CLA  | C14-C13-C15-C16 |
| 14  | B     | 818  | CLA  | CBD-CGD-O2D-CED |
| 14  | 2     | 819  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 843  | CLA  | O1A-CGA-O2A-C1  |
| 18  | b     | 851  | LHG  | C7-C8-C9-C10    |
| 14  | A     | 804  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 809  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 819  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 827  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 805  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 813  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 818  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 832  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 835  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 836  | CLA  | C1A-C2A-CAA-CBA |
| 14  | K     | 101  | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 804  | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 809  | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 819  | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 827  | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 806  | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 814  | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 819  | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 833  | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 836  | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 837  | CLA  | C1A-C2A-CAA-CBA |
| 14  | k     | 101  | CLA  | C1A-C2A-CAA-CBA |
| 14  | 1     | 1605 | CLA  | C1A-C2A-CAA-CBA |
| 14  | 1     | 1610 | CLA  | C1A-C2A-CAA-CBA |
| 14  | 1     | 1620 | CLA  | C1A-C2A-CAA-CBA |
| 14  | 1     | 1628 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | 2     | 806  | CLA  | C1A-C2A-CAA-CBA |
| 14  | 2     | 814  | CLA  | C1A-C2A-CAA-CBA |
| 14  | 2     | 819  | CLA  | C1A-C2A-CAA-CBA |
| 14  | 2     | 833  | CLA  | C1A-C2A-CAA-CBA |
| 14  | 2     | 836  | CLA  | C1A-C2A-CAA-CBA |
| 14  | 2     | 837  | CLA  | C1A-C2A-CAA-CBA |
| 14  | 9     | 101  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 815  | CLA  | C16-C17-C18-C19 |
| 14  | b     | 816  | CLA  | C16-C17-C18-C19 |
| 14  | 2     | 816  | CLA  | C16-C17-C18-C19 |
| 18  | B     | 850  | LHG  | C4-O6-P-O3      |
| 18  | b     | 851  | LHG  | C4-O6-P-O3      |
| 18  | z     | 101  | LHG  | C4-O6-P-O3      |
| 18  | B     | 850  | LHG  | C7-C8-C9-C10    |
| 18  | l     | 201  | LHG  | C23-C24-C25-C26 |
| 14  | b     | 819  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 812  | CLA  | C5-C6-C7-C8     |
| 14  | a     | 812  | CLA  | C5-C6-C7-C8     |
| 14  | b     | 802  | CLA  | C8-C10-C11-C12  |
| 14  | 1     | 1613 | CLA  | C5-C6-C7-C8     |
| 18  | L     | 208  | LHG  | C23-C24-C25-C26 |
| 18  | 0     | 202  | LHG  | C23-C24-C25-C26 |
| 14  | A     | 855  | CLA  | C8-C10-C11-C12  |
| 14  | 2     | 802  | CLA  | C8-C10-C11-C12  |
| 14  | A     | 819  | CLA  | C16-C17-C18-C19 |
| 14  | a     | 819  | CLA  | C16-C17-C18-C19 |
| 14  | 1     | 1620 | CLA  | C16-C17-C18-C19 |
| 14  | A     | 829  | CLA  | C3-C5-C6-C7     |
| 14  | a     | 829  | CLA  | C3-C5-C6-C7     |
| 14  | 1     | 1630 | CLA  | C3-C5-C6-C7     |
| 14  | A     | 838  | CLA  | C5-C6-C7-C8     |
| 14  | a     | 838  | CLA  | C5-C6-C7-C8     |
| 14  | 1     | 1639 | CLA  | C5-C6-C7-C8     |
| 14  | a     | 839  | CLA  | CBD-CGD-O2D-CED |
| 18  | 1     | 1655 | LHG  | C10-C11-C12-C13 |
| 14  | B     | 808  | CLA  | C8-C10-C11-C12  |
| 14  | b     | 809  | CLA  | C8-C10-C11-C12  |
| 14  | 2     | 809  | CLA  | C8-C10-C11-C12  |
| 18  | A     | 854  | LHG  | C10-C11-C12-C13 |
| 18  | a     | 854  | LHG  | C10-C11-C12-C13 |
| 18  | 1     | 1655 | LHG  | C23-C24-C25-C26 |
| 14  | A     | 814  | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 814  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 1     | 1615 | CLA  | O1A-CGA-O2A-C1  |
| 14  | j     | 1301 | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 854  | LHG  | C4-C5-C6-O8     |
| 18  | B     | 850  | LHG  | C4-C5-C6-O8     |
| 18  | M     | 101  | LHG  | C4-C5-C6-O8     |
| 18  | a     | 854  | LHG  | C4-C5-C6-O8     |
| 18  | b     | 851  | LHG  | C4-C5-C6-O8     |
| 18  | m     | 101  | LHG  | C4-C5-C6-O8     |
| 18  | 1     | 1655 | LHG  | C4-C5-C6-O8     |
| 18  | y     | 101  | LHG  | C4-C5-C6-O8     |
| 18  | z     | 101  | LHG  | C4-C5-C6-O8     |
| 14  | l     | 205  | CLA  | C2C-C3C-CAC-CBC |
| 18  | L     | 208  | LHG  | C25-C26-C27-C28 |
| 18  | l     | 201  | LHG  | C25-C26-C27-C28 |
| 18  | 0     | 202  | LHG  | C25-C26-C27-C28 |
| 14  | F     | 203  | CLA  | O1D-CGD-O2D-CED |
| 14  | 8     | 1301 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 839  | CLA  | CBD-CGD-O2D-CED |
| 14  | 1     | 1640 | CLA  | CBD-CGD-O2D-CED |
| 18  | A     | 854  | LHG  | C11-C10-C9-C8   |
| 18  | a     | 854  | LHG  | C11-C10-C9-C8   |
| 18  | 1     | 1655 | LHG  | C11-C10-C9-C8   |
| 18  | A     | 854  | LHG  | C23-C24-C25-C26 |
| 18  | a     | 854  | LHG  | C23-C24-C25-C26 |
| 14  | 2     | 833  | CLA  | O1A-CGA-O2A-C1  |
| 18  | M     | 101  | LHG  | C31-C32-C33-C34 |
| 18  | M     | 101  | LHG  | O1-C1-C2-O2     |
| 18  | m     | 101  | LHG  | O1-C1-C2-O2     |
| 18  | y     | 101  | LHG  | O1-C1-C2-O2     |
| 14  | L     | 204  | CLA  | C2C-C3C-CAC-CBC |
| 18  | m     | 101  | LHG  | C31-C32-C33-C34 |
| 18  | y     | 101  | LHG  | C31-C32-C33-C34 |
| 14  | B     | 832  | CLA  | O1A-CGA-O2A-C1  |
| 18  | M     | 101  | LHG  | C17-C18-C19-C20 |
| 18  | m     | 101  | LHG  | C17-C18-C19-C20 |
| 18  | y     | 101  | LHG  | C17-C18-C19-C20 |
| 14  | 0     | 206  | CLA  | C2C-C3C-CAC-CBC |
| 17  | B     | 851  | BCR  | C11-C10-C9-C34  |
| 17  | L     | 207  | BCR  | C16-C17-C18-C36 |
| 17  | b     | 852  | BCR  | C11-C10-C9-C34  |
| 17  | 8     | 1306 | BCR  | C11-C10-C9-C34  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | 8     | 1306 | BCR  | C16-C17-C18-C36 |
| 17  | 0     | 201  | BCR  | C16-C17-C18-C36 |
| 17  | 0     | 209  | BCR  | C16-C17-C18-C36 |
| 14  | B     | 808  | CLA  | C4-C3-C5-C6     |
| 14  | L     | 205  | CLA  | C4-C3-C5-C6     |
| 14  | b     | 809  | CLA  | C4-C3-C5-C6     |
| 14  | l     | 206  | CLA  | C4-C3-C5-C6     |
| 14  | 2     | 809  | CLA  | C4-C3-C5-C6     |
| 14  | 0     | 207  | CLA  | C4-C3-C5-C6     |
| 14  | b     | 833  | CLA  | O1A-CGA-O2A-C1  |
| 20  | B     | 849  | LMG  | C29-C28-O8-C9   |
| 20  | b     | 850  | LMG  | C29-C28-O8-C9   |
| 20  | 2     | 850  | LMG  | C29-C28-O8-C9   |
| 18  | l     | 201  | LHG  | C19-C20-C21-C22 |
| 14  | b     | 833  | CLA  | C15-C16-C17-C18 |
| 14  | 2     | 833  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 816  | CLA  | C2-C1-O2A-CGA   |
| 14  | a     | 816  | CLA  | C2-C1-O2A-CGA   |
| 14  | 1     | 1617 | CLA  | C2-C1-O2A-CGA   |
| 18  | L     | 208  | LHG  | C19-C20-C21-C22 |
| 18  | 0     | 202  | LHG  | C19-C20-C21-C22 |
| 14  | A     | 842  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 842  | CLA  | O1D-CGD-O2D-CED |
| 14  | 1     | 1643 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 832  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 840  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 840  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1641 | CLA  | CBA-CGA-O2A-C1  |
| 18  | L     | 208  | LHG  | O6-C4-C5-O7     |
| 18  | l     | 201  | LHG  | O6-C4-C5-O7     |
| 18  | 0     | 202  | LHG  | O6-C4-C5-O7     |
| 14  | A     | 824  | CLA  | C10-C11-C12-C13 |
| 14  | a     | 824  | CLA  | C10-C11-C12-C13 |
| 14  | 1     | 1625 | CLA  | C10-C11-C12-C13 |
| 17  | A     | 852  | BCR  | C12-C13-C14-C15 |
| 17  | B     | 846  | BCR  | C16-C17-C18-C19 |
| 17  | a     | 852  | BCR  | C12-C13-C14-C15 |
| 17  | b     | 847  | BCR  | C16-C17-C18-C19 |
| 17  | 1     | 1653 | BCR  | C12-C13-C14-C15 |
| 17  | 2     | 847  | BCR  | C16-C17-C18-C19 |
| 18  | A     | 853  | LHG  | O7-C5-C6-O8     |
| 18  | B     | 850  | LHG  | O7-C5-C6-O8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | a     | 853  | LHG  | O7-C5-C6-O8     |
| 18  | 1     | 1654 | LHG  | O7-C5-C6-O8     |
| 18  | z     | 101  | LHG  | O7-C5-C6-O8     |
| 14  | A     | 839  | CLA  | C16-C17-C18-C19 |
| 14  | a     | 839  | CLA  | C16-C17-C18-C19 |
| 14  | 1     | 1640 | CLA  | C16-C17-C18-C19 |
| 18  | A     | 853  | LHG  | C30-C31-C32-C33 |
| 18  | a     | 853  | LHG  | C30-C31-C32-C33 |
| 18  | 1     | 1654 | LHG  | C30-C31-C32-C33 |
| 13  | A     | 801  | CL0  | C12-C13-C15-C16 |
| 13  | a     | 801  | CL0  | C12-C13-C15-C16 |
| 13  | 1     | 1602 | CL0  | C12-C13-C15-C16 |
| 14  | A     | 807  | CLA  | C11-C12-C13-C15 |
| 14  | A     | 821  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 821  | CLA  | C11-C12-C13-C15 |
| 14  | A     | 824  | CLA  | C11-C10-C8-C7   |
| 14  | A     | 827  | CLA  | C11-C10-C8-C7   |
| 14  | A     | 827  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 832  | CLA  | C11-C10-C8-C7   |
| 14  | A     | 833  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 834  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 839  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 840  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 841  | CLA  | C11-C12-C13-C15 |
| 14  | B     | 802  | CLA  | C11-C10-C8-C7   |
| 14  | B     | 803  | CLA  | C11-C12-C13-C15 |
| 14  | B     | 804  | CLA  | C11-C12-C13-C15 |
| 14  | B     | 804  | CLA  | C12-C13-C15-C16 |
| 14  | B     | 806  | CLA  | C12-C13-C15-C16 |
| 14  | B     | 810  | CLA  | C12-C13-C15-C16 |
| 14  | B     | 819  | CLA  | C11-C12-C13-C15 |
| 14  | B     | 820  | CLA  | C11-C10-C8-C7   |
| 14  | B     | 833  | CLA  | C6-C7-C8-C10    |
| 14  | B     | 833  | CLA  | C11-C10-C8-C7   |
| 14  | B     | 841  | CLA  | C11-C12-C13-C15 |
| 14  | L     | 203  | CLA  | C11-C10-C8-C7   |
| 14  | L     | 203  | CLA  | C12-C13-C15-C16 |
| 14  | a     | 807  | CLA  | C11-C12-C13-C15 |
| 14  | a     | 821  | CLA  | C6-C7-C8-C10    |
| 14  | a     | 821  | CLA  | C11-C12-C13-C15 |
| 14  | a     | 824  | CLA  | C11-C10-C8-C7   |
| 14  | a     | 827  | CLA  | C11-C10-C8-C7   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 827  | CLA  | C12-C13-C15-C16 |
| 14  | a     | 832  | CLA  | C11-C10-C8-C7   |
| 14  | a     | 833  | CLA  | C6-C7-C8-C10    |
| 14  | a     | 834  | CLA  | C12-C13-C15-C16 |
| 14  | a     | 839  | CLA  | C12-C13-C15-C16 |
| 14  | a     | 840  | CLA  | C12-C13-C15-C16 |
| 14  | a     | 841  | CLA  | C11-C12-C13-C15 |
| 14  | b     | 803  | CLA  | C11-C10-C8-C7   |
| 14  | b     | 804  | CLA  | C11-C12-C13-C15 |
| 14  | b     | 805  | CLA  | C11-C12-C13-C15 |
| 14  | b     | 805  | CLA  | C12-C13-C15-C16 |
| 14  | b     | 807  | CLA  | C12-C13-C15-C16 |
| 14  | b     | 811  | CLA  | C12-C13-C15-C16 |
| 14  | b     | 820  | CLA  | C11-C12-C13-C15 |
| 14  | b     | 821  | CLA  | C11-C10-C8-C7   |
| 14  | b     | 834  | CLA  | C6-C7-C8-C10    |
| 14  | b     | 834  | CLA  | C11-C10-C8-C7   |
| 14  | b     | 842  | CLA  | C11-C12-C13-C15 |
| 14  | l     | 204  | CLA  | C11-C10-C8-C7   |
| 14  | l     | 204  | CLA  | C12-C13-C15-C16 |
| 14  | 1     | 1608 | CLA  | C11-C12-C13-C15 |
| 14  | 1     | 1622 | CLA  | C6-C7-C8-C10    |
| 14  | 1     | 1622 | CLA  | C11-C12-C13-C15 |
| 14  | 1     | 1625 | CLA  | C11-C10-C8-C7   |
| 14  | 1     | 1628 | CLA  | C11-C10-C8-C7   |
| 14  | 1     | 1628 | CLA  | C12-C13-C15-C16 |
| 14  | 1     | 1633 | CLA  | C11-C10-C8-C7   |
| 14  | 1     | 1634 | CLA  | C6-C7-C8-C10    |
| 14  | 1     | 1635 | CLA  | C12-C13-C15-C16 |
| 14  | 1     | 1640 | CLA  | C12-C13-C15-C16 |
| 14  | 1     | 1641 | CLA  | C12-C13-C15-C16 |
| 14  | 1     | 1642 | CLA  | C11-C12-C13-C15 |
| 14  | 2     | 803  | CLA  | C11-C10-C8-C7   |
| 14  | 2     | 804  | CLA  | C11-C12-C13-C15 |
| 14  | 2     | 805  | CLA  | C11-C12-C13-C15 |
| 14  | 2     | 805  | CLA  | C12-C13-C15-C16 |
| 14  | 2     | 807  | CLA  | C12-C13-C15-C16 |
| 14  | 2     | 811  | CLA  | C12-C13-C15-C16 |
| 14  | 2     | 820  | CLA  | C11-C12-C13-C15 |
| 14  | 2     | 821  | CLA  | C11-C10-C8-C7   |
| 14  | 2     | 834  | CLA  | C6-C7-C8-C10    |
| 14  | 2     | 834  | CLA  | C11-C10-C8-C7   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | 2     | 842 | CLA  | C11-C12-C13-C15 |
| 14  | 0     | 205 | CLA  | C11-C10-C8-C7   |
| 14  | 0     | 205 | CLA  | C12-C13-C15-C16 |
| 18  | B     | 850 | LHG  | C10-C11-C12-C13 |
| 14  | A     | 802 | CLA  | C14-C13-C15-C16 |
| 14  | A     | 806 | CLA  | C6-C7-C8-C9     |
| 14  | A     | 806 | CLA  | C11-C12-C13-C14 |
| 14  | A     | 807 | CLA  | C11-C12-C13-C14 |
| 14  | A     | 821 | CLA  | C11-C12-C13-C14 |
| 14  | A     | 822 | CLA  | C6-C7-C8-C9     |
| 14  | A     | 825 | CLA  | C11-C10-C8-C9   |
| 14  | A     | 827 | CLA  | C11-C10-C8-C9   |
| 14  | A     | 830 | CLA  | C14-C13-C15-C16 |
| 14  | A     | 832 | CLA  | C11-C10-C8-C9   |
| 14  | A     | 833 | CLA  | C6-C7-C8-C9     |
| 14  | A     | 835 | CLA  | C14-C13-C15-C16 |
| 14  | A     | 839 | CLA  | C11-C12-C13-C14 |
| 14  | A     | 840 | CLA  | C6-C7-C8-C9     |
| 14  | A     | 841 | CLA  | C11-C12-C13-C14 |
| 14  | A     | 841 | CLA  | C14-C13-C15-C16 |
| 14  | A     | 843 | CLA  | C6-C7-C8-C9     |
| 14  | A     | 843 | CLA  | C14-C13-C15-C16 |
| 14  | B     | 802 | CLA  | C11-C10-C8-C9   |
| 14  | B     | 804 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 804 | CLA  | C14-C13-C15-C16 |
| 14  | B     | 806 | CLA  | C14-C13-C15-C16 |
| 14  | B     | 811 | CLA  | C11-C12-C13-C14 |
| 14  | B     | 816 | CLA  | C11-C12-C13-C14 |
| 14  | B     | 817 | CLA  | C11-C12-C13-C14 |
| 14  | B     | 819 | CLA  | C11-C12-C13-C14 |
| 14  | B     | 832 | CLA  | C14-C13-C15-C16 |
| 14  | B     | 833 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 833 | CLA  | C11-C10-C8-C9   |
| 14  | B     | 840 | CLA  | C11-C12-C13-C14 |
| 14  | B     | 841 | CLA  | C11-C12-C13-C14 |
| 14  | L     | 205 | CLA  | C6-C7-C8-C9     |
| 14  | a     | 802 | CLA  | C14-C13-C15-C16 |
| 14  | a     | 806 | CLA  | C6-C7-C8-C9     |
| 14  | a     | 806 | CLA  | C11-C12-C13-C14 |
| 14  | a     | 807 | CLA  | C11-C12-C13-C14 |
| 14  | a     | 821 | CLA  | C11-C12-C13-C14 |
| 14  | a     | 822 | CLA  | C6-C7-C8-C9     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 825  | CLA  | C11-C10-C8-C9   |
| 14  | a     | 827  | CLA  | C11-C10-C8-C9   |
| 14  | a     | 830  | CLA  | C14-C13-C15-C16 |
| 14  | a     | 832  | CLA  | C11-C10-C8-C9   |
| 14  | a     | 833  | CLA  | C6-C7-C8-C9     |
| 14  | a     | 835  | CLA  | C14-C13-C15-C16 |
| 14  | a     | 839  | CLA  | C11-C12-C13-C14 |
| 14  | a     | 840  | CLA  | C6-C7-C8-C9     |
| 14  | a     | 841  | CLA  | C11-C12-C13-C14 |
| 14  | a     | 841  | CLA  | C14-C13-C15-C16 |
| 14  | a     | 843  | CLA  | C6-C7-C8-C9     |
| 14  | a     | 843  | CLA  | C14-C13-C15-C16 |
| 14  | b     | 803  | CLA  | C11-C10-C8-C9   |
| 14  | b     | 805  | CLA  | C6-C7-C8-C9     |
| 14  | b     | 805  | CLA  | C14-C13-C15-C16 |
| 14  | b     | 807  | CLA  | C14-C13-C15-C16 |
| 14  | b     | 812  | CLA  | C11-C12-C13-C14 |
| 14  | b     | 817  | CLA  | C11-C12-C13-C14 |
| 14  | b     | 818  | CLA  | C11-C12-C13-C14 |
| 14  | b     | 820  | CLA  | C11-C12-C13-C14 |
| 14  | b     | 833  | CLA  | C14-C13-C15-C16 |
| 14  | b     | 834  | CLA  | C6-C7-C8-C9     |
| 14  | b     | 834  | CLA  | C11-C10-C8-C9   |
| 14  | b     | 841  | CLA  | C11-C12-C13-C14 |
| 14  | b     | 842  | CLA  | C11-C12-C13-C14 |
| 14  | l     | 206  | CLA  | C6-C7-C8-C9     |
| 14  | 1     | 1603 | CLA  | C14-C13-C15-C16 |
| 14  | 1     | 1607 | CLA  | C6-C7-C8-C9     |
| 14  | 1     | 1607 | CLA  | C11-C12-C13-C14 |
| 14  | 1     | 1608 | CLA  | C11-C12-C13-C14 |
| 14  | 1     | 1622 | CLA  | C11-C12-C13-C14 |
| 14  | 1     | 1623 | CLA  | C6-C7-C8-C9     |
| 14  | 1     | 1626 | CLA  | C11-C10-C8-C9   |
| 14  | 1     | 1628 | CLA  | C11-C10-C8-C9   |
| 14  | 1     | 1631 | CLA  | C14-C13-C15-C16 |
| 14  | 1     | 1633 | CLA  | C11-C10-C8-C9   |
| 14  | 1     | 1634 | CLA  | C6-C7-C8-C9     |
| 14  | 1     | 1636 | CLA  | C14-C13-C15-C16 |
| 14  | 1     | 1640 | CLA  | C11-C12-C13-C14 |
| 14  | 1     | 1641 | CLA  | C6-C7-C8-C9     |
| 14  | 1     | 1642 | CLA  | C11-C12-C13-C14 |
| 14  | 1     | 1642 | CLA  | C14-C13-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | 1     | 1644 | CLA  | C6-C7-C8-C9     |
| 14  | 1     | 1644 | CLA  | C14-C13-C15-C16 |
| 14  | 2     | 803  | CLA  | C11-C10-C8-C9   |
| 14  | 2     | 805  | CLA  | C6-C7-C8-C9     |
| 14  | 2     | 805  | CLA  | C14-C13-C15-C16 |
| 14  | 2     | 807  | CLA  | C14-C13-C15-C16 |
| 14  | 2     | 812  | CLA  | C11-C12-C13-C14 |
| 14  | 2     | 817  | CLA  | C11-C12-C13-C14 |
| 14  | 2     | 818  | CLA  | C11-C12-C13-C14 |
| 14  | 2     | 820  | CLA  | C11-C12-C13-C14 |
| 14  | 2     | 833  | CLA  | C14-C13-C15-C16 |
| 14  | 2     | 834  | CLA  | C6-C7-C8-C9     |
| 14  | 2     | 834  | CLA  | C11-C10-C8-C9   |
| 14  | 2     | 841  | CLA  | C11-C12-C13-C14 |
| 14  | 2     | 842  | CLA  | C11-C12-C13-C14 |
| 14  | 0     | 206  | CLA  | C14-C13-C15-C16 |
| 14  | 0     | 207  | CLA  | C6-C7-C8-C9     |
| 18  | b     | 851  | LHG  | C10-C11-C12-C13 |
| 18  | z     | 101  | LHG  | C10-C11-C12-C13 |
| 14  | A     | 832  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 832  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1633 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 817  | CLA  | C5-C6-C7-C8     |
| 14  | a     | 817  | CLA  | C5-C6-C7-C8     |
| 14  | 1     | 1618 | CLA  | C5-C6-C7-C8     |
| 17  | A     | 849  | BCR  | C36-C18-C19-C20 |
| 17  | B     | 844  | BCR  | C37-C22-C23-C24 |
| 17  | a     | 849  | BCR  | C36-C18-C19-C20 |
| 17  | b     | 845  | BCR  | C37-C22-C23-C24 |
| 17  | 1     | 1650 | BCR  | C36-C18-C19-C20 |
| 17  | 2     | 845  | BCR  | C37-C22-C23-C24 |
| 14  | A     | 855  | CLA  | C3-C5-C6-C7     |
| 14  | b     | 802  | CLA  | C3-C5-C6-C7     |
| 14  | 2     | 802  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 829  | CLA  | C10-C11-C12-C13 |
| 14  | b     | 830  | CLA  | C10-C11-C12-C13 |
| 14  | 2     | 830  | CLA  | C10-C11-C12-C13 |
| 14  | B     | 841  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 842  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 2     | 842  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 826  | CLA  | C13-C15-C16-C17 |
| 14  | a     | 826  | CLA  | C13-C15-C16-C17 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | 1     | 1627 | CLA  | C13-C15-C16-C17 |
| 17  | B     | 845  | BCR  | C22-C23-C24-C25 |
| 17  | b     | 846  | BCR  | C22-C23-C24-C25 |
| 17  | 2     | 846  | BCR  | C22-C23-C24-C25 |
| 14  | A     | 838  | CLA  | C15-C16-C17-C18 |
| 15  | B     | 842  | PQN  | C18-C20-C21-C22 |
| 15  | b     | 843  | PQN  | C18-C20-C21-C22 |
| 15  | 2     | 843  | PQN  | C18-C20-C21-C22 |
| 14  | B     | 808  | CLA  | C2-C3-C5-C6     |
| 14  | b     | 809  | CLA  | C2-C3-C5-C6     |
| 14  | 2     | 809  | CLA  | C2-C3-C5-C6     |
| 14  | B     | 838  | CLA  | C8-C10-C11-C12  |
| 14  | a     | 838  | CLA  | C15-C16-C17-C18 |
| 14  | 1     | 1639 | CLA  | C15-C16-C17-C18 |
| 14  | 2     | 839  | CLA  | C8-C10-C11-C12  |
| 14  | b     | 839  | CLA  | C8-C10-C11-C12  |
| 14  | F     | 204  | CLA  | CBA-CGA-O2A-C1  |
| 14  | f     | 203  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 6     | 203  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 802  | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 803  | CLA  | CAA-CBA-CGA-O2A |
| 14  | 2     | 803  | CLA  | CAA-CBA-CGA-O2A |
| 18  | z     | 101  | LHG  | C29-C30-C31-C32 |
| 14  | b     | 815  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 815  | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 819  | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 824  | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 827  | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 830  | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 809  | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 831  | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 834  | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 815  | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 819  | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 824  | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 827  | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 830  | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 810  | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 832  | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 835  | CLA  | C3A-C2A-CAA-CBA |
| 14  | 1     | 1616 | CLA  | C3A-C2A-CAA-CBA |
| 14  | 1     | 1620 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | 1     | 1625 | CLA  | C3A-C2A-CAA-CBA |
| 14  | 1     | 1628 | CLA  | C3A-C2A-CAA-CBA |
| 14  | 1     | 1631 | CLA  | C3A-C2A-CAA-CBA |
| 14  | 2     | 810  | CLA  | C3A-C2A-CAA-CBA |
| 14  | 2     | 832  | CLA  | C3A-C2A-CAA-CBA |
| 14  | 2     | 835  | CLA  | C3A-C2A-CAA-CBA |
| 18  | b     | 851  | LHG  | C29-C30-C31-C32 |
| 18  | B     | 850  | LHG  | C29-C30-C31-C32 |
| 14  | 2     | 815  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 822  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 822  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1623 | CLA  | CBA-CGA-O2A-C1  |
| 18  | L     | 208  | LHG  | C4-C5-C6-O8     |
| 18  | l     | 201  | LHG  | C4-C5-C6-O8     |
| 18  | 0     | 202  | LHG  | C4-C5-C6-O8     |
| 14  | L     | 205  | CLA  | O2A-C1-C2-C3    |
| 14  | l     | 206  | CLA  | O2A-C1-C2-C3    |
| 14  | 0     | 207  | CLA  | O2A-C1-C2-C3    |
| 14  | B     | 814  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 843  | CLA  | C4-C3-C5-C6     |
| 14  | a     | 843  | CLA  | C4-C3-C5-C6     |
| 14  | 1     | 1644 | CLA  | C4-C3-C5-C6     |
| 18  | y     | 101  | LHG  | C10-C11-C12-C13 |
| 18  | M     | 101  | LHG  | C10-C11-C12-C13 |
| 18  | m     | 101  | LHG  | C10-C11-C12-C13 |
| 14  | A     | 827  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 827  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1628 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 820  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 843  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 840  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 840  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 1     | 1641 | CLA  | O1A-CGA-O2A-C1  |
| 14  | 1     | 1644 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 843  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 814  | CLA  | C13-C15-C16-C17 |
| 14  | b     | 815  | CLA  | C13-C15-C16-C17 |
| 14  | 2     | 815  | CLA  | C13-C15-C16-C17 |
| 18  | M     | 101  | LHG  | O7-C5-C6-O8     |
| 18  | b     | 851  | LHG  | O7-C5-C6-O8     |
| 18  | m     | 101  | LHG  | O7-C5-C6-O8     |
| 18  | y     | 101  | LHG  | O7-C5-C6-O8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | 1     | 1621 | CLA  | O1D-CGD-O2D-CED |
| 18  | L     | 208  | LHG  | C18-C19-C20-C21 |
| 18  | 0     | 202  | LHG  | C18-C19-C20-C21 |
| 14  | A     | 829  | CLA  | C16-C17-C18-C20 |
| 14  | a     | 829  | CLA  | C16-C17-C18-C20 |
| 14  | 1     | 1630 | CLA  | C16-C17-C18-C20 |
| 18  | l     | 201  | LHG  | C18-C19-C20-C21 |
| 14  | B     | 804  | CLA  | C13-C15-C16-C17 |
| 14  | A     | 810  | CLA  | C4-C3-C5-C6     |
| 14  | a     | 810  | CLA  | C4-C3-C5-C6     |
| 14  | 1     | 1611 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 817  | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 843  | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 855  | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 820  | CLA  | C2-C1-O2A-CGA   |
| 14  | a     | 817  | CLA  | C2-C1-O2A-CGA   |
| 14  | a     | 843  | CLA  | C2-C1-O2A-CGA   |
| 14  | b     | 802  | CLA  | C2-C1-O2A-CGA   |
| 14  | b     | 821  | CLA  | C2-C1-O2A-CGA   |
| 14  | 1     | 1618 | CLA  | C2-C1-O2A-CGA   |
| 14  | 1     | 1644 | CLA  | C2-C1-O2A-CGA   |
| 14  | 2     | 802  | CLA  | C2-C1-O2A-CGA   |
| 14  | 2     | 821  | CLA  | C2-C1-O2A-CGA   |
| 14  | a     | 820  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 802  | CLA  | C13-C15-C16-C17 |
| 14  | b     | 803  | CLA  | C13-C15-C16-C17 |
| 14  | 2     | 803  | CLA  | C13-C15-C16-C17 |
| 14  | 2     | 805  | CLA  | C13-C15-C16-C17 |
| 14  | A     | 815  | CLA  | C14-C13-C15-C16 |
| 14  | A     | 819  | CLA  | C14-C13-C15-C16 |
| 14  | A     | 836  | CLA  | C11-C12-C13-C14 |
| 14  | A     | 839  | CLA  | C14-C13-C15-C16 |
| 14  | A     | 841  | CLA  | C11-C10-C8-C9   |
| 14  | A     | 855  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 814  | CLA  | C11-C10-C8-C9   |
| 14  | B     | 820  | CLA  | C11-C10-C8-C9   |
| 14  | B     | 828  | CLA  | C11-C12-C13-C14 |
| 14  | L     | 204  | CLA  | C14-C13-C15-C16 |
| 14  | a     | 815  | CLA  | C14-C13-C15-C16 |
| 14  | a     | 819  | CLA  | C14-C13-C15-C16 |
| 14  | a     | 836  | CLA  | C11-C12-C13-C14 |
| 14  | a     | 839  | CLA  | C14-C13-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 841  | CLA  | C11-C10-C8-C9   |
| 14  | b     | 802  | CLA  | C6-C7-C8-C9     |
| 14  | b     | 821  | CLA  | C11-C10-C8-C9   |
| 14  | b     | 829  | CLA  | C11-C12-C13-C14 |
| 14  | l     | 205  | CLA  | C14-C13-C15-C16 |
| 14  | 1     | 1616 | CLA  | C14-C13-C15-C16 |
| 14  | 1     | 1620 | CLA  | C14-C13-C15-C16 |
| 14  | 1     | 1637 | CLA  | C11-C12-C13-C14 |
| 14  | 1     | 1640 | CLA  | C14-C13-C15-C16 |
| 14  | 1     | 1642 | CLA  | C11-C10-C8-C9   |
| 14  | 2     | 802  | CLA  | C6-C7-C8-C9     |
| 14  | 2     | 815  | CLA  | C11-C10-C8-C9   |
| 14  | 2     | 821  | CLA  | C11-C10-C8-C9   |
| 14  | 2     | 826  | CLA  | C11-C10-C8-C9   |
| 14  | 2     | 829  | CLA  | C11-C12-C13-C14 |
| 18  | L     | 208  | LHG  | C16-C17-C18-C19 |
| 18  | l     | 201  | LHG  | C16-C17-C18-C19 |
| 18  | 0     | 202  | LHG  | C16-C17-C18-C19 |
| 20  | B     | 849  | LMG  | C38-C39-C40-C41 |
| 20  | b     | 850  | LMG  | C38-C39-C40-C41 |
| 20  | 2     | 850  | LMG  | C38-C39-C40-C41 |
| 14  | A     | 814  | CLA  | C10-C11-C12-C13 |
| 14  | B     | 806  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 820  | CLA  | C15-C16-C17-C18 |
| 14  | b     | 805  | CLA  | C13-C15-C16-C17 |
| 14  | b     | 807  | CLA  | C15-C16-C17-C18 |
| 14  | b     | 821  | CLA  | C15-C16-C17-C18 |
| 14  | 2     | 807  | CLA  | C15-C16-C17-C18 |
| 14  | 2     | 821  | CLA  | C15-C16-C17-C18 |
| 18  | L     | 208  | LHG  | C5-C4-O6-P      |
| 18  | l     | 201  | LHG  | C5-C4-O6-P      |
| 18  | 0     | 202  | LHG  | C5-C4-O6-P      |
| 14  | A     | 829  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 829  | CLA  | C2A-CAA-CBA-CGA |
| 14  | 1     | 1630 | CLA  | C2A-CAA-CBA-CGA |
| 14  | L     | 204  | CLA  | C16-C17-C18-C20 |
| 14  | l     | 205  | CLA  | C16-C17-C18-C20 |
| 14  | 0     | 206  | CLA  | C16-C17-C18-C20 |
| 17  | A     | 852  | BCR  | C1-C6-C7-C8     |
| 17  | A     | 852  | BCR  | C5-C6-C7-C8     |
| 17  | B     | 846  | BCR  | C23-C24-C25-C26 |
| 17  | B     | 848  | BCR  | C1-C6-C7-C8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | B     | 848  | BCR  | C5-C6-C7-C8     |
| 17  | B     | 851  | BCR  | C23-C24-C25-C26 |
| 17  | B     | 851  | BCR  | C23-C24-C25-C30 |
| 17  | F     | 202  | BCR  | C23-C24-C25-C26 |
| 17  | F     | 202  | BCR  | C23-C24-C25-C30 |
| 17  | F     | 205  | BCR  | C1-C6-C7-C8     |
| 17  | L     | 201  | BCR  | C23-C24-C25-C26 |
| 17  | L     | 207  | BCR  | C1-C6-C7-C8     |
| 17  | L     | 207  | BCR  | C5-C6-C7-C8     |
| 17  | a     | 852  | BCR  | C1-C6-C7-C8     |
| 17  | a     | 852  | BCR  | C5-C6-C7-C8     |
| 17  | b     | 847  | BCR  | C23-C24-C25-C26 |
| 17  | b     | 849  | BCR  | C1-C6-C7-C8     |
| 17  | b     | 849  | BCR  | C5-C6-C7-C8     |
| 17  | b     | 852  | BCR  | C23-C24-C25-C26 |
| 17  | b     | 852  | BCR  | C23-C24-C25-C30 |
| 17  | f     | 202  | BCR  | C23-C24-C25-C26 |
| 17  | f     | 202  | BCR  | C23-C24-C25-C30 |
| 17  | f     | 204  | BCR  | C1-C6-C7-C8     |
| 17  | l     | 202  | BCR  | C23-C24-C25-C26 |
| 17  | 1     | 1653 | BCR  | C1-C6-C7-C8     |
| 17  | 1     | 1653 | BCR  | C5-C6-C7-C8     |
| 17  | 2     | 847  | BCR  | C23-C24-C25-C26 |
| 17  | 2     | 849  | BCR  | C1-C6-C7-C8     |
| 17  | 2     | 849  | BCR  | C5-C6-C7-C8     |
| 17  | 6     | 202  | BCR  | C23-C24-C25-C26 |
| 17  | 6     | 202  | BCR  | C23-C24-C25-C30 |
| 17  | 6     | 204  | BCR  | C1-C6-C7-C8     |
| 17  | 8     | 1306 | BCR  | C23-C24-C25-C26 |
| 17  | 8     | 1306 | BCR  | C23-C24-C25-C30 |
| 17  | 0     | 201  | BCR  | C1-C6-C7-C8     |
| 17  | 0     | 201  | BCR  | C5-C6-C7-C8     |
| 17  | 0     | 203  | BCR  | C23-C24-C25-C26 |
| 17  | 0     | 209  | BCR  | C1-C6-C7-C8     |
| 17  | 0     | 209  | BCR  | C5-C6-C7-C8     |
| 14  | a     | 814  | CLA  | C10-C11-C12-C13 |
| 17  | L     | 207  | BCR  | C37-C22-C23-C24 |
| 17  | 0     | 201  | BCR  | C37-C22-C23-C24 |
| 17  | 0     | 209  | BCR  | C37-C22-C23-C24 |
| 17  | A     | 851  | BCR  | C7-C8-C9-C10    |
| 17  | A     | 852  | BCR  | C16-C17-C18-C19 |
| 17  | A     | 856  | BCR  | C7-C8-C9-C10    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | B     | 851  | BCR  | C7-C8-C9-C10    |
| 17  | K     | 104  | BCR  | C16-C17-C18-C36 |
| 17  | a     | 851  | BCR  | C7-C8-C9-C10    |
| 17  | a     | 852  | BCR  | C16-C17-C18-C19 |
| 17  | b     | 852  | BCR  | C7-C8-C9-C10    |
| 17  | j     | 1305 | BCR  | C7-C8-C9-C10    |
| 17  | k     | 104  | BCR  | C16-C17-C18-C36 |
| 17  | 1     | 1652 | BCR  | C7-C8-C9-C10    |
| 17  | 1     | 1653 | BCR  | C16-C17-C18-C19 |
| 17  | 8     | 1305 | BCR  | C7-C8-C9-C10    |
| 17  | 8     | 1306 | BCR  | C7-C8-C9-C10    |
| 17  | 9     | 104  | BCR  | C16-C17-C18-C36 |
| 14  | 1     | 1615 | CLA  | C10-C11-C12-C13 |
| 18  | L     | 208  | LHG  | C11-C12-C13-C14 |
| 18  | l     | 201  | LHG  | C11-C12-C13-C14 |
| 18  | 0     | 202  | LHG  | C11-C12-C13-C14 |
| 14  | A     | 832  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 840  | CLA  | C16-C17-C18-C20 |
| 14  | B     | 804  | CLA  | C16-C17-C18-C20 |
| 14  | a     | 840  | CLA  | C16-C17-C18-C20 |
| 14  | b     | 805  | CLA  | C16-C17-C18-C20 |
| 14  | 1     | 1641 | CLA  | C16-C17-C18-C20 |
| 14  | 2     | 805  | CLA  | C16-C17-C18-C20 |
| 14  | a     | 832  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 1     | 1633 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 839  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 840  | CLA  | O1D-CGD-O2D-CED |
| 14  | 2     | 840  | CLA  | O1D-CGD-O2D-CED |
| 18  | L     | 208  | LHG  | O6-C4-C5-C6     |
| 18  | l     | 201  | LHG  | O6-C4-C5-C6     |
| 18  | 0     | 202  | LHG  | O6-C4-C5-C6     |
| 14  | A     | 804  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 806  | CLA  | C11-C10-C8-C7   |
| 14  | A     | 806  | CLA  | C11-C12-C13-C15 |
| 14  | A     | 810  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 810  | CLA  | C11-C12-C13-C15 |
| 14  | A     | 815  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 819  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 825  | CLA  | C11-C10-C8-C7   |
| 14  | A     | 825  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 826  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 830  | CLA  | C12-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | A     | 833 | CLA  | C12-C13-C15-C16 |
| 14  | A     | 835 | CLA  | C12-C13-C15-C16 |
| 14  | A     | 836 | CLA  | C11-C12-C13-C15 |
| 14  | A     | 839 | CLA  | C11-C12-C13-C15 |
| 14  | A     | 840 | CLA  | C11-C12-C13-C15 |
| 14  | A     | 841 | CLA  | C11-C10-C8-C7   |
| 14  | A     | 842 | CLA  | C11-C10-C8-C7   |
| 14  | A     | 843 | CLA  | C6-C7-C8-C10    |
| 14  | A     | 843 | CLA  | C12-C13-C15-C16 |
| 14  | B     | 803 | CLA  | C6-C7-C8-C10    |
| 14  | B     | 804 | CLA  | C6-C7-C8-C10    |
| 14  | B     | 811 | CLA  | C11-C12-C13-C15 |
| 14  | B     | 813 | CLA  | C11-C10-C8-C7   |
| 14  | B     | 814 | CLA  | C6-C7-C8-C10    |
| 14  | B     | 817 | CLA  | C11-C12-C13-C15 |
| 14  | B     | 819 | CLA  | C6-C7-C8-C10    |
| 14  | B     | 832 | CLA  | C12-C13-C15-C16 |
| 14  | B     | 837 | CLA  | C11-C10-C8-C7   |
| 14  | B     | 840 | CLA  | C11-C12-C13-C15 |
| 14  | L     | 204 | CLA  | C12-C13-C15-C16 |
| 14  | a     | 804 | CLA  | C6-C7-C8-C10    |
| 14  | a     | 806 | CLA  | C11-C10-C8-C7   |
| 14  | a     | 806 | CLA  | C11-C12-C13-C15 |
| 14  | a     | 810 | CLA  | C2-C3-C5-C6     |
| 14  | a     | 810 | CLA  | C11-C12-C13-C15 |
| 14  | a     | 815 | CLA  | C12-C13-C15-C16 |
| 14  | a     | 819 | CLA  | C12-C13-C15-C16 |
| 14  | a     | 825 | CLA  | C11-C10-C8-C7   |
| 14  | a     | 825 | CLA  | C12-C13-C15-C16 |
| 14  | a     | 826 | CLA  | C12-C13-C15-C16 |
| 14  | a     | 830 | CLA  | C12-C13-C15-C16 |
| 14  | a     | 833 | CLA  | C12-C13-C15-C16 |
| 14  | a     | 835 | CLA  | C12-C13-C15-C16 |
| 14  | a     | 836 | CLA  | C11-C12-C13-C15 |
| 14  | a     | 839 | CLA  | C11-C12-C13-C15 |
| 14  | a     | 840 | CLA  | C11-C12-C13-C15 |
| 14  | a     | 841 | CLA  | C11-C10-C8-C7   |
| 14  | a     | 842 | CLA  | C11-C10-C8-C7   |
| 14  | a     | 843 | CLA  | C6-C7-C8-C10    |
| 14  | a     | 843 | CLA  | C12-C13-C15-C16 |
| 14  | b     | 804 | CLA  | C6-C7-C8-C10    |
| 14  | b     | 805 | CLA  | C6-C7-C8-C10    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 812  | CLA  | C11-C12-C13-C15 |
| 14  | b     | 814  | CLA  | C11-C10-C8-C7   |
| 14  | b     | 815  | CLA  | C6-C7-C8-C10    |
| 14  | b     | 818  | CLA  | C11-C12-C13-C15 |
| 14  | b     | 820  | CLA  | C6-C7-C8-C10    |
| 14  | b     | 833  | CLA  | C12-C13-C15-C16 |
| 14  | b     | 838  | CLA  | C11-C10-C8-C7   |
| 14  | b     | 841  | CLA  | C11-C12-C13-C15 |
| 14  | l     | 205  | CLA  | C12-C13-C15-C16 |
| 14  | 1     | 1605 | CLA  | C6-C7-C8-C10    |
| 14  | 1     | 1607 | CLA  | C11-C10-C8-C7   |
| 14  | 1     | 1607 | CLA  | C11-C12-C13-C15 |
| 14  | 1     | 1611 | CLA  | C2-C3-C5-C6     |
| 14  | 1     | 1611 | CLA  | C11-C12-C13-C15 |
| 14  | 1     | 1616 | CLA  | C12-C13-C15-C16 |
| 14  | 1     | 1620 | CLA  | C12-C13-C15-C16 |
| 14  | 1     | 1626 | CLA  | C11-C10-C8-C7   |
| 14  | 1     | 1626 | CLA  | C12-C13-C15-C16 |
| 14  | 1     | 1627 | CLA  | C12-C13-C15-C16 |
| 14  | 1     | 1631 | CLA  | C12-C13-C15-C16 |
| 14  | 1     | 1634 | CLA  | C12-C13-C15-C16 |
| 14  | 1     | 1636 | CLA  | C12-C13-C15-C16 |
| 14  | 1     | 1637 | CLA  | C11-C12-C13-C15 |
| 14  | 1     | 1640 | CLA  | C11-C12-C13-C15 |
| 14  | 1     | 1641 | CLA  | C11-C12-C13-C15 |
| 14  | 1     | 1642 | CLA  | C11-C10-C8-C7   |
| 14  | 1     | 1643 | CLA  | C11-C10-C8-C7   |
| 14  | 1     | 1644 | CLA  | C6-C7-C8-C10    |
| 14  | 1     | 1644 | CLA  | C12-C13-C15-C16 |
| 14  | 2     | 804  | CLA  | C6-C7-C8-C10    |
| 14  | 2     | 805  | CLA  | C6-C7-C8-C10    |
| 14  | 2     | 812  | CLA  | C11-C12-C13-C15 |
| 14  | 2     | 814  | CLA  | C11-C10-C8-C7   |
| 14  | 2     | 815  | CLA  | C6-C7-C8-C10    |
| 14  | 2     | 818  | CLA  | C11-C12-C13-C15 |
| 14  | 2     | 820  | CLA  | C6-C7-C8-C10    |
| 14  | 2     | 833  | CLA  | C12-C13-C15-C16 |
| 14  | 2     | 838  | CLA  | C11-C10-C8-C7   |
| 14  | 2     | 841  | CLA  | C11-C12-C13-C15 |
| 14  | 0     | 206  | CLA  | C12-C13-C15-C16 |
| 14  | 1     | 1623 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 822  | CLA  | C15-C16-C17-C18 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 822  | CLA  | C15-C16-C17-C18 |
| 17  | A     | 852  | BCR  | C13-C14-C15-C16 |
| 17  | B     | 851  | BCR  | C9-C10-C11-C12  |
| 17  | K     | 102  | BCR  | C9-C10-C11-C12  |
| 17  | a     | 852  | BCR  | C13-C14-C15-C16 |
| 17  | b     | 852  | BCR  | C9-C10-C11-C12  |
| 17  | k     | 102  | BCR  | C9-C10-C11-C12  |
| 17  | 1     | 1653 | BCR  | C13-C14-C15-C16 |
| 17  | 8     | 1306 | BCR  | C9-C10-C11-C12  |
| 17  | 9     | 102  | BCR  | C9-C10-C11-C12  |
| 14  | A     | 831  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 831  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1632 | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1623 | CLA  | C15-C16-C17-C18 |
| 13  | a     | 801  | CL0  | CAA-CBA-CGA-O2A |
| 13  | 1     | 1602 | CL0  | CAA-CBA-CGA-O2A |
| 14  | A     | 822  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 841  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 822  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 842  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 811  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 831  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 811  | CLA  | C2A-CAA-CBA-CGA |
| 14  | 1     | 1612 | CLA  | C2A-CAA-CBA-CGA |
| 17  | A     | 852  | BCR  | C11-C10-C9-C34  |
| 17  | A     | 852  | BCR  | C35-C13-C14-C15 |
| 17  | A     | 856  | BCR  | C11-C10-C9-C34  |
| 17  | B     | 844  | BCR  | C20-C21-C22-C37 |
| 17  | B     | 848  | BCR  | C20-C21-C22-C37 |
| 17  | K     | 104  | BCR  | C11-C10-C9-C34  |
| 17  | a     | 852  | BCR  | C11-C10-C9-C34  |
| 17  | a     | 852  | BCR  | C35-C13-C14-C15 |
| 17  | b     | 845  | BCR  | C20-C21-C22-C37 |
| 17  | b     | 849  | BCR  | C20-C21-C22-C37 |
| 17  | j     | 1305 | BCR  | C11-C10-C9-C34  |
| 17  | k     | 104  | BCR  | C11-C10-C9-C34  |
| 17  | 1     | 1653 | BCR  | C11-C10-C9-C34  |
| 17  | 1     | 1653 | BCR  | C35-C13-C14-C15 |
| 17  | 2     | 845  | BCR  | C20-C21-C22-C37 |
| 17  | 2     | 849  | BCR  | C20-C21-C22-C37 |
| 17  | 8     | 1305 | BCR  | C11-C10-C9-C34  |
| 17  | 9     | 104  | BCR  | C11-C10-C9-C34  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | a     | 854  | LHG  | C31-C32-C33-C34 |
| 18  | 1     | 1655 | LHG  | C31-C32-C33-C34 |
| 20  | B     | 849  | LMG  | C30-C31-C32-C33 |
| 20  | b     | 850  | LMG  | C30-C31-C32-C33 |
| 20  | 2     | 850  | LMG  | C30-C31-C32-C33 |
| 14  | 2     | 842  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 807  | CLA  | C16-C17-C18-C19 |
| 14  | A     | 807  | CLA  | C16-C17-C18-C20 |
| 14  | A     | 842  | CLA  | C16-C17-C18-C20 |
| 14  | a     | 807  | CLA  | C16-C17-C18-C19 |
| 14  | a     | 807  | CLA  | C16-C17-C18-C20 |
| 14  | a     | 842  | CLA  | C16-C17-C18-C20 |
| 14  | 1     | 1608 | CLA  | C16-C17-C18-C19 |
| 14  | 1     | 1608 | CLA  | C16-C17-C18-C20 |
| 14  | 1     | 1643 | CLA  | C16-C17-C18-C20 |
| 14  | A     | 818  | CLA  | C8-C10-C11-C12  |
| 14  | B     | 834  | CLA  | C5-C6-C7-C8     |
| 14  | a     | 818  | CLA  | C8-C10-C11-C12  |
| 14  | b     | 835  | CLA  | C5-C6-C7-C8     |
| 14  | 1     | 1619 | CLA  | C8-C10-C11-C12  |
| 14  | 2     | 835  | CLA  | C5-C6-C7-C8     |
| 13  | A     | 801  | CL0  | CAA-CBA-CGA-O2A |
| 18  | A     | 854  | LHG  | C31-C32-C33-C34 |
| 14  | B     | 827  | CLA  | C8-C10-C11-C12  |
| 14  | a     | 839  | CLA  | C8-C10-C11-C12  |
| 14  | b     | 828  | CLA  | C8-C10-C11-C12  |
| 14  | 1     | 1640 | CLA  | C8-C10-C11-C12  |
| 14  | 2     | 828  | CLA  | C8-C10-C11-C12  |
| 14  | A     | 855  | CLA  | CBD-CGD-O2D-CED |
| 14  | 2     | 802  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 815  | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 840  | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 855  | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 806  | CLA  | CAD-CBD-CGD-O2D |
| 14  | K     | 101  | CLA  | CAD-CBD-CGD-O2D |
| 14  | a     | 815  | CLA  | CAD-CBD-CGD-O2D |
| 14  | a     | 840  | CLA  | CAD-CBD-CGD-O2D |
| 14  | b     | 802  | CLA  | CAD-CBD-CGD-O2D |
| 14  | b     | 807  | CLA  | CAD-CBD-CGD-O2D |
| 14  | k     | 101  | CLA  | CAD-CBD-CGD-O2D |
| 14  | 1     | 1616 | CLA  | CAD-CBD-CGD-O2D |
| 14  | 1     | 1641 | CLA  | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | 2     | 802  | CLA  | CAD-CBD-CGD-O2D |
| 14  | 2     | 807  | CLA  | CAD-CBD-CGD-O2D |
| 14  | 9     | 101  | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 839  | CLA  | C8-C10-C11-C12  |
| 17  | I     | 101  | BCR  | C6-C7-C8-C9     |
| 17  | K     | 104  | BCR  | C6-C7-C8-C9     |
| 17  | i     | 101  | BCR  | C6-C7-C8-C9     |
| 17  | k     | 104  | BCR  | C6-C7-C8-C9     |
| 17  | 7     | 101  | BCR  | C6-C7-C8-C9     |
| 17  | 9     | 104  | BCR  | C6-C7-C8-C9     |
| 14  | B     | 804  | CLA  | C10-C11-C12-C13 |
| 14  | b     | 805  | CLA  | C10-C11-C12-C13 |
| 14  | 2     | 805  | CLA  | C10-C11-C12-C13 |
| 14  | b     | 802  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 827  | CLA  | C5-C6-C7-C8     |
| 14  | L     | 203  | CLA  | C5-C6-C7-C8     |
| 14  | b     | 828  | CLA  | C5-C6-C7-C8     |
| 14  | l     | 204  | CLA  | C5-C6-C7-C8     |
| 14  | 1     | 1616 | CLA  | C10-C11-C12-C13 |
| 14  | 2     | 828  | CLA  | C5-C6-C7-C8     |
| 14  | 0     | 205  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 831  | CLA  | O2A-C1-C2-C3    |
| 14  | b     | 832  | CLA  | O2A-C1-C2-C3    |
| 14  | 2     | 832  | CLA  | O2A-C1-C2-C3    |
| 20  | b     | 850  | LMG  | C17-C18-C19-C20 |
| 14  | b     | 832  | CLA  | C2A-CAA-CBA-CGA |
| 14  | 2     | 832  | CLA  | C2A-CAA-CBA-CGA |
| 17  | B     | 843  | BCR  | C14-C15-C16-C17 |
| 17  | b     | 844  | BCR  | C14-C15-C16-C17 |
| 17  | 2     | 844  | BCR  | C14-C15-C16-C17 |
| 14  | A     | 815  | CLA  | C10-C11-C12-C13 |
| 20  | 2     | 850  | LMG  | C17-C18-C19-C20 |
| 20  | B     | 849  | LMG  | C17-C18-C19-C20 |
| 14  | A     | 806  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 811  | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 831  | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 841  | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 841  | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 802  | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 802  | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 803  | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 803  | CLA  | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | B     | 808 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 808 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 813 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 813 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 814 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 814 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 815 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 815 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 816 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 816 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 821 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 821 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 830 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 830 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 833 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 833 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 837 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 837 | CLA  | CHA-CBD-CGD-O2D |
| 14  | F     | 201 | CLA  | CHA-CBD-CGD-O2D |
| 14  | L     | 203 | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 811 | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 831 | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 841 | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 841 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 803 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 803 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 804 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 804 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 809 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 809 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 814 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 814 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 815 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 815 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 816 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 816 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 817 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 817 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 822 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 822 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 831 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 831 | CLA  | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 834  | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 834  | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 838  | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 838  | CLA  | CHA-CBD-CGD-O2D |
| 14  | f     | 201  | CLA  | CHA-CBD-CGD-O2D |
| 14  | l     | 204  | CLA  | CHA-CBD-CGD-O1D |
| 14  | 1     | 1612 | CLA  | CHA-CBD-CGD-O1D |
| 14  | 1     | 1632 | CLA  | CHA-CBD-CGD-O1D |
| 14  | 1     | 1642 | CLA  | CHA-CBD-CGD-O1D |
| 14  | 1     | 1642 | CLA  | CHA-CBD-CGD-O2D |
| 14  | 2     | 803  | CLA  | CHA-CBD-CGD-O1D |
| 14  | 2     | 803  | CLA  | CHA-CBD-CGD-O2D |
| 14  | 2     | 804  | CLA  | CHA-CBD-CGD-O1D |
| 14  | 2     | 804  | CLA  | CHA-CBD-CGD-O2D |
| 14  | 2     | 809  | CLA  | CHA-CBD-CGD-O1D |
| 14  | 2     | 809  | CLA  | CHA-CBD-CGD-O2D |
| 14  | 2     | 814  | CLA  | CHA-CBD-CGD-O1D |
| 14  | 2     | 814  | CLA  | CHA-CBD-CGD-O2D |
| 14  | 2     | 815  | CLA  | CHA-CBD-CGD-O1D |
| 14  | 2     | 815  | CLA  | CHA-CBD-CGD-O2D |
| 14  | 2     | 816  | CLA  | CHA-CBD-CGD-O1D |
| 14  | 2     | 816  | CLA  | CHA-CBD-CGD-O2D |
| 14  | 2     | 817  | CLA  | CHA-CBD-CGD-O1D |
| 14  | 2     | 817  | CLA  | CHA-CBD-CGD-O2D |
| 14  | 2     | 822  | CLA  | CHA-CBD-CGD-O1D |
| 14  | 2     | 822  | CLA  | CHA-CBD-CGD-O2D |
| 14  | 2     | 831  | CLA  | CHA-CBD-CGD-O1D |
| 14  | 2     | 831  | CLA  | CHA-CBD-CGD-O2D |
| 14  | 2     | 834  | CLA  | CHA-CBD-CGD-O1D |
| 14  | 2     | 834  | CLA  | CHA-CBD-CGD-O2D |
| 14  | 2     | 838  | CLA  | CHA-CBD-CGD-O1D |
| 14  | 2     | 838  | CLA  | CHA-CBD-CGD-O2D |
| 14  | 6     | 201  | CLA  | CHA-CBD-CGD-O2D |
| 14  | 0     | 205  | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 815  | CLA  | C10-C11-C12-C13 |
| 20  | B     | 849  | LMG  | C11-C12-C13-C14 |
| 20  | b     | 850  | LMG  | C11-C12-C13-C14 |
| 14  | F     | 204  | CLA  | O1A-CGA-O2A-C1  |
| 20  | 2     | 850  | LMG  | C11-C12-C13-C14 |
| 14  | b     | 819  | CLA  | O1D-CGD-O2D-CED |
| 14  | 1     | 1607 | CLA  | O1D-CGD-O2D-CED |
| 17  | J     | 103  | BCR  | C11-C10-C9-C8   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | j     | 1304 | BCR  | C11-C10-C9-C8   |
| 17  | 8     | 1304 | BCR  | C11-C10-C9-C8   |
| 14  | a     | 806  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 827  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 827  | CLA  | O1A-CGA-O2A-C1  |
| 14  | f     | 203  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 6     | 203  | CLA  | O1A-CGA-O2A-C1  |
| 14  | l     | 205  | CLA  | C16-C17-C18-C19 |
| 14  | B     | 818  | CLA  | O1D-CGD-O2D-CED |
| 14  | 2     | 819  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 810  | CLA  | C11-C12-C13-C14 |
| 14  | A     | 840  | CLA  | C11-C12-C13-C14 |
| 14  | B     | 814  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 825  | CLA  | C11-C10-C8-C9   |
| 14  | B     | 837  | CLA  | C11-C10-C8-C9   |
| 14  | a     | 810  | CLA  | C11-C12-C13-C14 |
| 14  | a     | 840  | CLA  | C11-C12-C13-C14 |
| 14  | b     | 815  | CLA  | C6-C7-C8-C9     |
| 14  | b     | 815  | CLA  | C11-C10-C8-C9   |
| 14  | b     | 826  | CLA  | C11-C10-C8-C9   |
| 14  | b     | 838  | CLA  | C11-C10-C8-C9   |
| 14  | 1     | 1611 | CLA  | C11-C12-C13-C14 |
| 14  | 1     | 1641 | CLA  | C11-C12-C13-C14 |
| 14  | 2     | 815  | CLA  | C6-C7-C8-C9     |
| 14  | 2     | 838  | CLA  | C11-C10-C8-C9   |
| 14  | A     | 831  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 831  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 1     | 1628 | CLA  | O1A-CGA-O2A-C1  |
| 14  | 1     | 1632 | CLA  | O1A-CGA-O2A-C1  |
| 18  | M     | 101  | LHG  | C33-C34-C35-C36 |
| 18  | y     | 101  | LHG  | C33-C34-C35-C36 |
| 14  | L     | 204  | CLA  | C16-C17-C18-C19 |
| 14  | 0     | 206  | CLA  | C16-C17-C18-C19 |
| 18  | m     | 101  | LHG  | C33-C34-C35-C36 |
| 14  | A     | 819  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 821  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 819  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 821  | CLA  | C2A-CAA-CBA-CGA |
| 14  | 1     | 1620 | CLA  | C2A-CAA-CBA-CGA |
| 14  | 1     | 1622 | CLA  | C2A-CAA-CBA-CGA |
| 17  | F     | 202  | BCR  | C11-C12-C13-C35 |
| 17  | f     | 202  | BCR  | C11-C12-C13-C35 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | 6     | 202  | BCR  | C11-C12-C13-C35 |
| 18  | M     | 101  | LHG  | C24-C25-C26-C27 |
| 18  | m     | 101  | LHG  | C24-C25-C26-C27 |
| 17  | F     | 205  | BCR  | C21-C22-C23-C24 |
| 17  | J     | 103  | BCR  | C21-C22-C23-C24 |
| 17  | f     | 204  | BCR  | C21-C22-C23-C24 |
| 17  | j     | 1304 | BCR  | C21-C22-C23-C24 |
| 17  | 6     | 204  | BCR  | C21-C22-C23-C24 |
| 17  | 8     | 1304 | BCR  | C21-C22-C23-C24 |
| 18  | M     | 101  | LHG  | C27-C28-C29-C30 |
| 18  | m     | 101  | LHG  | C27-C28-C29-C30 |
| 18  | y     | 101  | LHG  | C24-C25-C26-C27 |
| 18  | y     | 101  | LHG  | C27-C28-C29-C30 |
| 14  | A     | 855  | CLA  | C16-C17-C18-C20 |
| 14  | b     | 802  | CLA  | C16-C17-C18-C20 |
| 14  | 2     | 802  | CLA  | C16-C17-C18-C20 |
| 14  | a     | 819  | CLA  | CBA-CGA-O2A-C1  |
| 20  | b     | 850  | LMG  | C15-C16-C17-C18 |
| 17  | B     | 847  | BCR  | C15-C16-C17-C18 |
| 18  | B     | 850  | LHG  | C3-O3-P-O6      |
| 18  | b     | 851  | LHG  | C3-O3-P-O6      |
| 18  | z     | 101  | LHG  | C3-O3-P-O6      |
| 20  | B     | 849  | LMG  | C15-C16-C17-C18 |
| 20  | 2     | 850  | LMG  | C15-C16-C17-C18 |
| 18  | A     | 853  | LHG  | C3-O3-P-O5      |
| 18  | L     | 208  | LHG  | C3-O3-P-O5      |
| 18  | L     | 208  | LHG  | C4-O6-P-O5      |
| 18  | M     | 101  | LHG  | C4-O6-P-O4      |
| 18  | a     | 853  | LHG  | C3-O3-P-O5      |
| 18  | l     | 201  | LHG  | C3-O3-P-O5      |
| 18  | l     | 201  | LHG  | C4-O6-P-O5      |
| 18  | m     | 101  | LHG  | C4-O6-P-O4      |
| 18  | 1     | 1654 | LHG  | C3-O3-P-O5      |
| 18  | 0     | 202  | LHG  | C3-O3-P-O5      |
| 18  | 0     | 202  | LHG  | C4-O6-P-O5      |
| 18  | y     | 101  | LHG  | C4-O6-P-O4      |
| 14  | A     | 814  | CLA  | C16-C17-C18-C20 |
| 14  | A     | 829  | CLA  | C16-C17-C18-C19 |
| 14  | a     | 814  | CLA  | C16-C17-C18-C20 |
| 14  | 1     | 1615 | CLA  | C16-C17-C18-C20 |
| 14  | a     | 842  | CLA  | C5-C6-C7-C8     |
| 14  | 1     | 1643 | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 807  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 819  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 855  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 807  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 802  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1608 | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1620 | CLA  | CBA-CGA-O2A-C1  |
| 14  | 2     | 802  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 855  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 842  | CLA  | C5-C6-C7-C8     |
| 14  | A     | 810  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 810  | CLA  | C2A-CAA-CBA-CGA |
| 14  | 1     | 1611 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 810  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 806  | CLA  | C3-C5-C6-C7     |
| 14  | a     | 810  | CLA  | C3-C5-C6-C7     |
| 14  | b     | 807  | CLA  | C3-C5-C6-C7     |
| 14  | 1     | 1611 | CLA  | C3-C5-C6-C7     |
| 14  | 2     | 807  | CLA  | C3-C5-C6-C7     |
| 14  | 2     | 802  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 813  | CLA  | C16-C17-C18-C20 |
| 14  | L     | 203  | CLA  | C16-C17-C18-C20 |
| 14  | a     | 829  | CLA  | C16-C17-C18-C19 |
| 14  | b     | 814  | CLA  | C16-C17-C18-C20 |
| 14  | l     | 204  | CLA  | C16-C17-C18-C20 |
| 14  | 1     | 1630 | CLA  | C16-C17-C18-C19 |
| 14  | 2     | 814  | CLA  | C16-C17-C18-C20 |
| 14  | 0     | 205  | CLA  | C16-C17-C18-C20 |
| 14  | A     | 810  | CLA  | CAD-CBD-CGD-O1D |
| 14  | A     | 829  | CLA  | CAD-CBD-CGD-O1D |
| 14  | A     | 844  | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 811  | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 813  | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 815  | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 822  | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 826  | CLA  | CAD-CBD-CGD-O1D |
| 14  | L     | 203  | CLA  | CAD-CBD-CGD-O1D |
| 14  | a     | 810  | CLA  | CAD-CBD-CGD-O1D |
| 14  | a     | 829  | CLA  | CAD-CBD-CGD-O1D |
| 14  | a     | 844  | CLA  | CAD-CBD-CGD-O1D |
| 14  | b     | 812  | CLA  | CAD-CBD-CGD-O1D |
| 14  | b     | 814  | CLA  | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 816  | CLA  | CAD-CBD-CGD-O1D |
| 14  | b     | 823  | CLA  | CAD-CBD-CGD-O1D |
| 14  | b     | 827  | CLA  | CAD-CBD-CGD-O1D |
| 14  | l     | 204  | CLA  | CAD-CBD-CGD-O1D |
| 14  | 1     | 1611 | CLA  | CAD-CBD-CGD-O1D |
| 14  | 1     | 1630 | CLA  | CAD-CBD-CGD-O1D |
| 14  | 1     | 1645 | CLA  | CAD-CBD-CGD-O1D |
| 14  | 2     | 812  | CLA  | CAD-CBD-CGD-O1D |
| 14  | 2     | 814  | CLA  | CAD-CBD-CGD-O1D |
| 14  | 2     | 816  | CLA  | CAD-CBD-CGD-O1D |
| 14  | 2     | 823  | CLA  | CAD-CBD-CGD-O1D |
| 14  | 2     | 827  | CLA  | CAD-CBD-CGD-O1D |
| 14  | 0     | 205  | CLA  | CAD-CBD-CGD-O1D |
| 14  | K     | 101  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 802  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 833  | CLA  | C15-C16-C17-C18 |
| 14  | a     | 833  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 804  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1634 | CLA  | C15-C16-C17-C18 |
| 14  | k     | 101  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 9     | 101  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 807  | CLA  | C11-C10-C8-C7   |
| 14  | A     | 817  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 824  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 829  | CLA  | C11-C12-C13-C15 |
| 14  | A     | 831  | CLA  | C11-C10-C8-C7   |
| 14  | B     | 802  | CLA  | C12-C13-C15-C16 |
| 14  | B     | 805  | CLA  | C12-C13-C15-C16 |
| 14  | B     | 820  | CLA  | C6-C7-C8-C10    |
| 14  | B     | 820  | CLA  | C11-C12-C13-C15 |
| 14  | B     | 826  | CLA  | C6-C7-C8-C10    |
| 14  | B     | 838  | CLA  | C6-C7-C8-C10    |
| 14  | L     | 204  | CLA  | C6-C7-C8-C10    |
| 14  | a     | 807  | CLA  | C11-C10-C8-C7   |
| 14  | a     | 817  | CLA  | C12-C13-C15-C16 |
| 14  | a     | 824  | CLA  | C12-C13-C15-C16 |
| 14  | a     | 829  | CLA  | C11-C12-C13-C15 |
| 14  | a     | 831  | CLA  | C11-C10-C8-C7   |
| 14  | b     | 803  | CLA  | C12-C13-C15-C16 |
| 14  | b     | 806  | CLA  | C12-C13-C15-C16 |
| 14  | b     | 821  | CLA  | C6-C7-C8-C10    |
| 14  | b     | 821  | CLA  | C11-C12-C13-C15 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 827  | CLA  | C6-C7-C8-C10    |
| 14  | b     | 839  | CLA  | C6-C7-C8-C10    |
| 14  | l     | 205  | CLA  | C6-C7-C8-C10    |
| 14  | 1     | 1608 | CLA  | C11-C10-C8-C7   |
| 14  | 1     | 1618 | CLA  | C12-C13-C15-C16 |
| 14  | 1     | 1625 | CLA  | C12-C13-C15-C16 |
| 14  | 1     | 1630 | CLA  | C11-C12-C13-C15 |
| 14  | 1     | 1632 | CLA  | C11-C10-C8-C7   |
| 14  | 2     | 803  | CLA  | C12-C13-C15-C16 |
| 14  | 2     | 806  | CLA  | C12-C13-C15-C16 |
| 14  | 2     | 821  | CLA  | C6-C7-C8-C10    |
| 14  | 2     | 821  | CLA  | C11-C12-C13-C15 |
| 14  | 2     | 827  | CLA  | C6-C7-C8-C10    |
| 14  | 2     | 839  | CLA  | C6-C7-C8-C10    |
| 14  | 0     | 206  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 816  | CLA  | C3-C5-C6-C7     |
| 14  | a     | 816  | CLA  | C3-C5-C6-C7     |
| 14  | 1     | 1617 | CLA  | C3-C5-C6-C7     |
| 17  | b     | 848  | BCR  | C15-C16-C17-C18 |
| 17  | 2     | 848  | BCR  | C15-C16-C17-C18 |
| 14  | B     | 802  | CLA  | C10-C11-C12-C13 |
| 14  | b     | 803  | CLA  | C10-C11-C12-C13 |
| 14  | 2     | 803  | CLA  | C10-C11-C12-C13 |
| 20  | B     | 849  | LMG  | C31-C32-C33-C34 |
| 20  | b     | 850  | LMG  | C31-C32-C33-C34 |
| 20  | 2     | 850  | LMG  | C31-C32-C33-C34 |
| 14  | A     | 807  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 807  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 1     | 1608 | CLA  | O1A-CGA-O2A-C1  |
| 14  | 2     | 809  | CLA  | C5-C6-C7-C8     |
| 14  | A     | 841  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 841  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 842  | CLA  | C2A-CAA-CBA-CGA |
| 14  | 1     | 1642 | CLA  | C2A-CAA-CBA-CGA |
| 14  | 1     | 1643 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 804  | CLA  | C16-C17-C18-C19 |
| 14  | b     | 805  | CLA  | C16-C17-C18-C19 |
| 14  | 2     | 805  | CLA  | C16-C17-C18-C19 |
| 14  | A     | 843  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 808  | CLA  | C5-C6-C7-C8     |
| 14  | a     | 843  | CLA  | C5-C6-C7-C8     |
| 14  | b     | 809  | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | L     | 208  | LHG  | O7-C5-C6-O8     |
| 18  | l     | 201  | LHG  | O7-C5-C6-O8     |
| 18  | 0     | 202  | LHG  | O7-C5-C6-O8     |
| 14  | a     | 804  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 818  | CLA  | O2A-C1-C2-C3    |
| 14  | b     | 819  | CLA  | O2A-C1-C2-C3    |
| 14  | 2     | 819  | CLA  | O2A-C1-C2-C3    |
| 14  | A     | 819  | CLA  | C13-C15-C16-C17 |
| 14  | a     | 819  | CLA  | C13-C15-C16-C17 |
| 14  | 1     | 1620 | CLA  | C13-C15-C16-C17 |
| 14  | 1     | 1644 | CLA  | C5-C6-C7-C8     |
| 14  | B     | 806  | CLA  | C8-C10-C11-C12  |
| 14  | b     | 807  | CLA  | C8-C10-C11-C12  |
| 14  | 2     | 807  | CLA  | C8-C10-C11-C12  |
| 14  | 1     | 1605 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 822  | CLA  | C11-C10-C8-C9   |
| 14  | A     | 826  | CLA  | C11-C12-C13-C14 |
| 14  | A     | 833  | CLA  | C14-C13-C15-C16 |
| 14  | B     | 803  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 813  | CLA  | C11-C10-C8-C9   |
| 14  | B     | 819  | CLA  | C6-C7-C8-C9     |
| 14  | a     | 822  | CLA  | C11-C10-C8-C9   |
| 14  | a     | 826  | CLA  | C11-C12-C13-C14 |
| 14  | a     | 833  | CLA  | C14-C13-C15-C16 |
| 14  | b     | 804  | CLA  | C6-C7-C8-C9     |
| 14  | b     | 814  | CLA  | C11-C10-C8-C9   |
| 14  | b     | 820  | CLA  | C6-C7-C8-C9     |
| 14  | 1     | 1607 | CLA  | C11-C10-C8-C9   |
| 14  | 1     | 1623 | CLA  | C11-C10-C8-C9   |
| 14  | 1     | 1627 | CLA  | C11-C12-C13-C14 |
| 14  | 1     | 1634 | CLA  | C14-C13-C15-C16 |
| 14  | 2     | 804  | CLA  | C6-C7-C8-C9     |
| 14  | 2     | 814  | CLA  | C11-C10-C8-C9   |
| 14  | 2     | 820  | CLA  | C6-C7-C8-C9     |
| 17  | A     | 848  | BCR  | C22-C23-C24-C25 |
| 17  | a     | 848  | BCR  | C22-C23-C24-C25 |
| 17  | 1     | 1649 | BCR  | C22-C23-C24-C25 |
| 14  | A     | 842  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 827  | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 828  | CLA  | CAA-CBA-CGA-O2A |
| 14  | 2     | 828  | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 804  | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 20  | B     | 849  | LMG  | C32-C33-C34-C35 |
| 20  | b     | 850  | LMG  | C32-C33-C34-C35 |
| 20  | 2     | 850  | LMG  | C32-C33-C34-C35 |
| 14  | A     | 804  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 838  | CLA  | C15-C16-C17-C18 |
| 14  | b     | 839  | CLA  | C15-C16-C17-C18 |
| 14  | 1     | 1605 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 813  | CLA  | C16-C17-C18-C19 |
| 14  | B     | 827  | CLA  | C16-C17-C18-C20 |
| 14  | b     | 814  | CLA  | C16-C17-C18-C19 |
| 14  | b     | 828  | CLA  | C16-C17-C18-C20 |
| 14  | 2     | 814  | CLA  | C16-C17-C18-C19 |
| 14  | 2     | 828  | CLA  | C16-C17-C18-C20 |
| 14  | 2     | 839  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 831  | CLA  | C1-C2-C3-C4     |
| 14  | b     | 832  | CLA  | C1-C2-C3-C4     |
| 14  | 2     | 832  | CLA  | C1-C2-C3-C4     |
| 14  | B     | 803  | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 804  | CLA  | C2A-CAA-CBA-CGA |
| 14  | 2     | 804  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 807  | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 828  | CLA  | C2-C1-O2A-CGA   |
| 14  | a     | 807  | CLA  | C2-C1-O2A-CGA   |
| 14  | b     | 829  | CLA  | C2-C1-O2A-CGA   |
| 14  | 1     | 1608 | CLA  | C2-C1-O2A-CGA   |
| 14  | 2     | 829  | CLA  | C2-C1-O2A-CGA   |
| 14  | 1     | 1616 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 815  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 819  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 815  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 1     | 1620 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 819  | CLA  | C16-C17-C18-C20 |
| 14  | b     | 820  | CLA  | C16-C17-C18-C20 |
| 14  | 2     | 820  | CLA  | C16-C17-C18-C20 |
| 14  | A     | 821  | CLA  | C4-C3-C5-C6     |
| 14  | a     | 821  | CLA  | C4-C3-C5-C6     |
| 14  | 1     | 1622 | CLA  | C4-C3-C5-C6     |
| 17  | A     | 847  | BCR  | C1-C6-C7-C8     |
| 17  | B     | 845  | BCR  | C5-C6-C7-C8     |
| 17  | L     | 201  | BCR  | C23-C24-C25-C30 |
| 17  | a     | 847  | BCR  | C1-C6-C7-C8     |
| 17  | b     | 846  | BCR  | C5-C6-C7-C8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | l     | 202  | BCR  | C23-C24-C25-C30 |
| 17  | 1     | 1648 | BCR  | C1-C6-C7-C8     |
| 17  | 2     | 846  | BCR  | C5-C6-C7-C8     |
| 17  | 0     | 203  | BCR  | C23-C24-C25-C30 |
| 14  | a     | 819  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 830  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 840  | CLA  | C10-C11-C12-C13 |
| 14  | 1     | 1641 | CLA  | C10-C11-C12-C13 |
| 14  | b     | 830  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 822  | CLA  | C5-C6-C7-C8     |
| 14  | a     | 840  | CLA  | C10-C11-C12-C13 |
| 14  | b     | 823  | CLA  | C5-C6-C7-C8     |
| 14  | 2     | 823  | CLA  | C5-C6-C7-C8     |
| 17  | B     | 846  | BCR  | C12-C13-C14-C15 |
| 17  | b     | 847  | BCR  | C12-C13-C14-C15 |
| 17  | 2     | 847  | BCR  | C12-C13-C14-C15 |
| 14  | L     | 204  | CLA  | C4C-C3C-CAC-CBC |
| 14  | l     | 205  | CLA  | C4C-C3C-CAC-CBC |
| 14  | 0     | 206  | CLA  | C4C-C3C-CAC-CBC |
| 20  | B     | 849  | LMG  | C24-C25-C26-C27 |
| 20  | 2     | 850  | LMG  | C24-C25-C26-C27 |
| 14  | B     | 829  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 2     | 830  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1640 | CLA  | O1D-CGD-O2D-CED |
| 20  | b     | 850  | LMG  | C24-C25-C26-C27 |
| 20  | 2     | 850  | LMG  | C16-C17-C18-C19 |
| 20  | B     | 849  | LMG  | C16-C17-C18-C19 |
| 20  | b     | 850  | LMG  | C16-C17-C18-C19 |
| 14  | A     | 839  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 839  | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 853  | LHG  | C4-C5-C6-O8     |
| 18  | a     | 853  | LHG  | C4-C5-C6-O8     |
| 18  | 1     | 1654 | LHG  | C4-C5-C6-O8     |
| 14  | A     | 838  | CLA  | C4-C3-C5-C6     |
| 14  | a     | 838  | CLA  | C4-C3-C5-C6     |
| 14  | 1     | 1639 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 802  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 828  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 838  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 843  | CLA  | C2-C3-C5-C6     |
| 14  | B     | 817  | CLA  | C6-C7-C8-C10    |
| 14  | a     | 802  | CLA  | C12-C13-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 828  | CLA  | C6-C7-C8-C10    |
| 14  | a     | 838  | CLA  | C12-C13-C15-C16 |
| 14  | a     | 843  | CLA  | C2-C3-C5-C6     |
| 14  | b     | 818  | CLA  | C6-C7-C8-C10    |
| 14  | 1     | 1603 | CLA  | C12-C13-C15-C16 |
| 14  | 1     | 1629 | CLA  | C6-C7-C8-C10    |
| 14  | 1     | 1639 | CLA  | C12-C13-C15-C16 |
| 14  | 1     | 1644 | CLA  | C2-C3-C5-C6     |
| 14  | 2     | 818  | CLA  | C6-C7-C8-C10    |
| 14  | 2     | 830  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 804  | CLA  | C14-C13-C15-C16 |
| 14  | A     | 806  | CLA  | C11-C10-C8-C9   |
| 14  | A     | 826  | CLA  | C14-C13-C15-C16 |
| 14  | A     | 831  | CLA  | C11-C10-C8-C9   |
| 14  | A     | 842  | CLA  | C11-C10-C8-C9   |
| 14  | B     | 802  | CLA  | C14-C13-C15-C16 |
| 14  | B     | 810  | CLA  | C14-C13-C15-C16 |
| 14  | B     | 820  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 826  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 838  | CLA  | C6-C7-C8-C9     |
| 14  | a     | 804  | CLA  | C14-C13-C15-C16 |
| 14  | a     | 806  | CLA  | C11-C10-C8-C9   |
| 14  | a     | 826  | CLA  | C14-C13-C15-C16 |
| 14  | a     | 831  | CLA  | C11-C10-C8-C9   |
| 14  | a     | 842  | CLA  | C11-C10-C8-C9   |
| 14  | b     | 803  | CLA  | C14-C13-C15-C16 |
| 14  | b     | 811  | CLA  | C14-C13-C15-C16 |
| 14  | b     | 821  | CLA  | C6-C7-C8-C9     |
| 14  | b     | 827  | CLA  | C6-C7-C8-C9     |
| 14  | b     | 839  | CLA  | C6-C7-C8-C9     |
| 14  | 1     | 1605 | CLA  | C14-C13-C15-C16 |
| 14  | 1     | 1627 | CLA  | C14-C13-C15-C16 |
| 14  | 1     | 1632 | CLA  | C11-C10-C8-C9   |
| 14  | 1     | 1643 | CLA  | C11-C10-C8-C9   |
| 14  | 2     | 803  | CLA  | C14-C13-C15-C16 |
| 14  | 2     | 811  | CLA  | C14-C13-C15-C16 |
| 14  | 2     | 821  | CLA  | C6-C7-C8-C9     |
| 14  | 2     | 827  | CLA  | C6-C7-C8-C9     |
| 14  | 2     | 839  | CLA  | C6-C7-C8-C9     |
| 17  | B     | 845  | BCR  | C15-C16-C17-C18 |
| 17  | b     | 846  | BCR  | C15-C16-C17-C18 |
| 17  | 2     | 846  | BCR  | C15-C16-C17-C18 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 838  | CLA  | C16-C17-C18-C20 |
| 14  | a     | 838  | CLA  | C16-C17-C18-C20 |
| 14  | 1     | 1639 | CLA  | C16-C17-C18-C20 |
| 18  | M     | 101  | LHG  | C14-C15-C16-C17 |
| 18  | m     | 101  | LHG  | C14-C15-C16-C17 |
| 18  | y     | 101  | LHG  | C14-C15-C16-C17 |
| 14  | B     | 829  | CLA  | O1A-CGA-O2A-C1  |
| 20  | B     | 849  | LMG  | C34-C35-C36-C37 |
| 20  | b     | 850  | LMG  | C34-C35-C36-C37 |
| 20  | 2     | 850  | LMG  | C34-C35-C36-C37 |
| 14  | A     | 808  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 808  | CLA  | C2A-CAA-CBA-CGA |
| 14  | 1     | 1609 | CLA  | C2A-CAA-CBA-CGA |
| 14  | 2     | 816  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 815  | CLA  | C15-C16-C17-C18 |
| 14  | b     | 816  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 814  | CLA  | C16-C17-C18-C19 |
| 14  | a     | 814  | CLA  | C16-C17-C18-C19 |
| 14  | 1     | 1615 | CLA  | C16-C17-C18-C19 |
| 14  | 2     | 812  | CLA  | C16-C17-C18-C20 |
| 20  | B     | 849  | LMG  | C42-C43-C44-C45 |
| 20  | 2     | 850  | LMG  | C42-C43-C44-C45 |
| 17  | F     | 202  | BCR  | C7-C8-C9-C10    |
| 17  | f     | 202  | BCR  | C7-C8-C9-C10    |
| 17  | 6     | 202  | BCR  | C7-C8-C9-C10    |
| 20  | b     | 850  | LMG  | C42-C43-C44-C45 |
| 14  | 1     | 1627 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 811  | CLA  | C16-C17-C18-C20 |
| 14  | b     | 812  | CLA  | C16-C17-C18-C20 |
| 14  | A     | 815  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 839  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 815  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1616 | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1640 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 826  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 826  | CLA  | CBD-CGD-O2D-CED |
| 15  | A     | 845  | PQN  | C23-C25-C26-C27 |
| 15  | a     | 845  | PQN  | C23-C25-C26-C27 |
| 15  | 1     | 1646 | PQN  | C23-C25-C26-C27 |
| 14  | a     | 839  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 838  | CLA  | C16-C17-C18-C19 |
| 14  | a     | 838  | CLA  | C16-C17-C18-C19 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | 1     | 1639 | CLA  | C16-C17-C18-C19 |
| 17  | B     | 851  | BCR  | C19-C20-C21-C22 |
| 17  | b     | 852  | BCR  | C19-C20-C21-C22 |
| 17  | 8     | 1306 | BCR  | C19-C20-C21-C22 |
| 14  | A     | 839  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 839  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 1     | 1640 | CLA  | O1A-CGA-O2A-C1  |
| 17  | A     | 856  | BCR  | C10-C11-C12-C13 |
| 17  | B     | 847  | BCR  | C18-C19-C20-C21 |
| 17  | b     | 848  | BCR  | C18-C19-C20-C21 |
| 17  | j     | 1305 | BCR  | C10-C11-C12-C13 |
| 17  | 2     | 848  | BCR  | C18-C19-C20-C21 |
| 17  | 8     | 1305 | BCR  | C10-C11-C12-C13 |
| 14  | a     | 826  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 802  | CLA  | C3-C5-C6-C7     |
| 14  | a     | 802  | CLA  | C3-C5-C6-C7     |
| 14  | 1     | 1603 | CLA  | C3-C5-C6-C7     |
| 14  | B     | 833  | CLA  | C4-C3-C5-C6     |
| 14  | L     | 203  | CLA  | C4-C3-C5-C6     |
| 14  | b     | 834  | CLA  | C4-C3-C5-C6     |
| 14  | l     | 204  | CLA  | C4-C3-C5-C6     |
| 14  | 2     | 834  | CLA  | C4-C3-C5-C6     |
| 14  | 0     | 205  | CLA  | C4-C3-C5-C6     |
| 14  | a     | 815  | CLA  | CBD-CGD-O2D-CED |
| 14  | 1     | 1616 | CLA  | CBD-CGD-O2D-CED |
| 14  | L     | 203  | CLA  | C2-C3-C5-C6     |
| 14  | l     | 204  | CLA  | C2-C3-C5-C6     |
| 14  | 0     | 205  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 826  | CLA  | O1D-CGD-O2D-CED |
| 14  | L     | 203  | CLA  | C13-C15-C16-C17 |
| 14  | l     | 204  | CLA  | C13-C15-C16-C17 |
| 14  | 0     | 205  | CLA  | C13-C15-C16-C17 |
| 14  | 1     | 1627 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 814  | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 804  | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 805  | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 818  | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 824  | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 833  | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 838  | CLA  | C2-C1-O2A-CGA   |
| 14  | a     | 814  | CLA  | C2-C1-O2A-CGA   |
| 14  | b     | 805  | CLA  | C2-C1-O2A-CGA   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 806  | CLA  | C2-C1-O2A-CGA   |
| 14  | b     | 819  | CLA  | C2-C1-O2A-CGA   |
| 14  | b     | 825  | CLA  | C2-C1-O2A-CGA   |
| 14  | b     | 834  | CLA  | C2-C1-O2A-CGA   |
| 14  | b     | 839  | CLA  | C2-C1-O2A-CGA   |
| 14  | 1     | 1615 | CLA  | C2-C1-O2A-CGA   |
| 14  | 2     | 805  | CLA  | C2-C1-O2A-CGA   |
| 14  | 2     | 806  | CLA  | C2-C1-O2A-CGA   |
| 14  | 2     | 819  | CLA  | C2-C1-O2A-CGA   |
| 14  | 2     | 834  | CLA  | C2-C1-O2A-CGA   |
| 14  | 2     | 839  | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 815  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 842  | CLA  | C2C-C3C-CAC-CBC |
| 14  | B     | 841  | CLA  | C2C-C3C-CAC-CBC |
| 14  | 2     | 842  | CLA  | C2C-C3C-CAC-CBC |
| 14  | A     | 812  | CLA  | C14-C13-C15-C16 |
| 14  | B     | 809  | CLA  | C14-C13-C15-C16 |
| 14  | B     | 819  | CLA  | C14-C13-C15-C16 |
| 14  | a     | 812  | CLA  | C14-C13-C15-C16 |
| 14  | b     | 810  | CLA  | C14-C13-C15-C16 |
| 14  | b     | 820  | CLA  | C14-C13-C15-C16 |
| 14  | 1     | 1613 | CLA  | C14-C13-C15-C16 |
| 14  | 2     | 810  | CLA  | C14-C13-C15-C16 |
| 14  | 2     | 820  | CLA  | C14-C13-C15-C16 |
| 14  | B     | 823  | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 824  | CLA  | CAA-CBA-CGA-O2A |
| 14  | 2     | 824  | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 816  | CLA  | C5-C6-C7-C8     |
| 14  | a     | 816  | CLA  | C5-C6-C7-C8     |
| 14  | 1     | 1617 | CLA  | C5-C6-C7-C8     |
| 14  | 1     | 1622 | CLA  | O1A-CGA-O2A-C1  |
| 20  | b     | 850  | LMG  | C20-C21-C22-C23 |
| 17  | A     | 851  | BCR  | C11-C10-C9-C34  |
| 17  | B     | 846  | BCR  | C35-C13-C14-C15 |
| 17  | a     | 851  | BCR  | C11-C10-C9-C34  |
| 17  | b     | 847  | BCR  | C35-C13-C14-C15 |
| 17  | 1     | 1652 | BCR  | C11-C10-C9-C34  |
| 17  | 2     | 847  | BCR  | C35-C13-C14-C15 |
| 14  | B     | 815  | CLA  | C2A-CAA-CBA-CGA |
| 14  | L     | 204  | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 816  | CLA  | C2A-CAA-CBA-CGA |
| 14  | l     | 205  | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | 0     | 206  | CLA  | C2A-CAA-CBA-CGA |
| 13  | A     | 801  | CL0  | C5-C6-C7-C8     |
| 13  | a     | 801  | CL0  | C5-C6-C7-C8     |
| 13  | 1     | 1602 | CL0  | C5-C6-C7-C8     |
| 20  | B     | 849  | LMG  | C20-C21-C22-C23 |
| 20  | 2     | 850  | LMG  | C20-C21-C22-C23 |
| 14  | A     | 821  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 821  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 802  | CLA  | C16-C17-C18-C19 |
| 14  | a     | 802  | CLA  | C16-C17-C18-C19 |
| 14  | 1     | 1603 | CLA  | C16-C17-C18-C19 |
| 14  | B     | 816  | CLA  | O2A-C1-C2-C3    |
| 14  | B     | 830  | CLA  | O2A-C1-C2-C3    |
| 14  | b     | 817  | CLA  | O2A-C1-C2-C3    |
| 14  | b     | 831  | CLA  | O2A-C1-C2-C3    |
| 14  | 2     | 817  | CLA  | O2A-C1-C2-C3    |
| 14  | 2     | 831  | CLA  | O2A-C1-C2-C3    |
| 14  | a     | 842  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1643 | CLA  | CBA-CGA-O2A-C1  |
| 20  | B     | 849  | LMG  | C14-C15-C16-C17 |
| 20  | 2     | 850  | LMG  | C14-C15-C16-C17 |
| 17  | A     | 856  | BCR  | C36-C18-C19-C20 |
| 17  | j     | 1305 | BCR  | C36-C18-C19-C20 |
| 17  | 1     | 1652 | BCR  | C11-C12-C13-C35 |
| 17  | 8     | 1305 | BCR  | C36-C18-C19-C20 |
| 20  | b     | 850  | LMG  | C14-C15-C16-C17 |
| 14  | a     | 804  | CLA  | C13-C15-C16-C17 |
| 14  | 1     | 1605 | CLA  | C13-C15-C16-C17 |
| 14  | B     | 823  | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 824  | CLA  | CAA-CBA-CGA-O1A |
| 14  | 2     | 824  | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 804  | CLA  | C13-C15-C16-C17 |
| 14  | A     | 809  | CLA  | C8-C10-C11-C12  |
| 14  | a     | 809  | CLA  | C8-C10-C11-C12  |
| 14  | 1     | 1610 | CLA  | C8-C10-C11-C12  |
| 14  | A     | 814  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 838  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 810  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 816  | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 814  | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 838  | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 811  | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 817  | CLA  | C1A-C2A-CAA-CBA |
| 14  | 1     | 1615 | CLA  | C1A-C2A-CAA-CBA |
| 14  | 1     | 1639 | CLA  | C1A-C2A-CAA-CBA |
| 14  | 2     | 811  | CLA  | C1A-C2A-CAA-CBA |
| 14  | 2     | 817  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 842  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 803  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 814  | CLA  | C11-C10-C8-C7   |
| 14  | A     | 816  | CLA  | C11-C12-C13-C15 |
| 14  | B     | 815  | CLA  | C11-C10-C8-C7   |
| 14  | B     | 832  | CLA  | C11-C10-C8-C7   |
| 14  | a     | 803  | CLA  | C6-C7-C8-C10    |
| 14  | a     | 814  | CLA  | C11-C10-C8-C7   |
| 14  | a     | 816  | CLA  | C11-C12-C13-C15 |
| 14  | b     | 816  | CLA  | C11-C10-C8-C7   |
| 14  | b     | 833  | CLA  | C11-C10-C8-C7   |
| 14  | 1     | 1604 | CLA  | C6-C7-C8-C10    |
| 14  | 1     | 1615 | CLA  | C11-C10-C8-C7   |
| 14  | 1     | 1617 | CLA  | C11-C12-C13-C15 |
| 14  | 2     | 816  | CLA  | C11-C10-C8-C7   |
| 14  | 2     | 833  | CLA  | C11-C10-C8-C7   |
| 14  | B     | 820  | CLA  | C16-C17-C18-C20 |
| 14  | A     | 839  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 839  | CLA  | C2A-CAA-CBA-CGA |
| 14  | l     | 206  | CLA  | C2A-CAA-CBA-CGA |
| 14  | 1     | 1640 | CLA  | C2A-CAA-CBA-CGA |
| 14  | 2     | 816  | CLA  | C2A-CAA-CBA-CGA |
| 14  | 0     | 207  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 810  | CLA  | C10-C11-C12-C13 |
| 14  | a     | 810  | CLA  | C10-C11-C12-C13 |
| 14  | b     | 816  | CLA  | C5-C6-C7-C8     |
| 14  | 1     | 1611 | CLA  | C10-C11-C12-C13 |
| 14  | 2     | 816  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 815  | CLA  | C5-C6-C7-C8     |
| 14  | A     | 821  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 821  | CLA  | CBA-CGA-O2A-C1  |
| 14  | 1     | 1622 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 842  | CLA  | C16-C17-C18-C19 |
| 14  | B     | 809  | CLA  | C16-C17-C18-C19 |
| 14  | a     | 802  | CLA  | C16-C17-C18-C20 |
| 14  | a     | 842  | CLA  | C16-C17-C18-C19 |
| 14  | b     | 810  | CLA  | C16-C17-C18-C19 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 821  | CLA  | C16-C17-C18-C20 |
| 14  | 1     | 1643 | CLA  | C16-C17-C18-C19 |
| 14  | 2     | 810  | CLA  | C16-C17-C18-C19 |
| 14  | 2     | 821  | CLA  | C16-C17-C18-C20 |
| 14  | B     | 806  | CLA  | C5-C6-C7-C8     |
| 14  | a     | 826  | CLA  | C8-C10-C11-C12  |
| 14  | 2     | 807  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 841  | CLA  | C4C-C3C-CAC-CBC |
| 14  | 2     | 802  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 816  | CLA  | C4-C3-C5-C6     |
| 14  | A     | 830  | CLA  | C4-C3-C5-C6     |
| 14  | B     | 827  | CLA  | C4-C3-C5-C6     |
| 14  | B     | 830  | CLA  | C4-C3-C5-C6     |
| 14  | a     | 816  | CLA  | C4-C3-C5-C6     |
| 14  | a     | 830  | CLA  | C4-C3-C5-C6     |
| 14  | b     | 828  | CLA  | C4-C3-C5-C6     |
| 14  | b     | 831  | CLA  | C4-C3-C5-C6     |
| 14  | 1     | 1617 | CLA  | C4-C3-C5-C6     |
| 14  | 1     | 1631 | CLA  | C4-C3-C5-C6     |
| 14  | 2     | 828  | CLA  | C4-C3-C5-C6     |
| 14  | 2     | 831  | CLA  | C4-C3-C5-C6     |
| 14  | A     | 826  | CLA  | C8-C10-C11-C12  |
| 14  | K     | 103  | CLA  | C5-C6-C7-C8     |
| 14  | b     | 807  | CLA  | C5-C6-C7-C8     |
| 14  | k     | 103  | CLA  | C5-C6-C7-C8     |
| 14  | 1     | 1627 | CLA  | C8-C10-C11-C12  |
| 14  | 9     | 103  | CLA  | C5-C6-C7-C8     |
| 14  | A     | 842  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 842  | CLA  | O1A-CGA-O2A-C1  |
| 20  | B     | 849  | LMG  | C13-C14-C15-C16 |
| 20  | b     | 850  | LMG  | C13-C14-C15-C16 |
| 14  | A     | 802  | CLA  | C16-C17-C18-C20 |
| 14  | A     | 840  | CLA  | C16-C17-C18-C19 |
| 14  | a     | 840  | CLA  | C16-C17-C18-C19 |
| 14  | 1     | 1603 | CLA  | C16-C17-C18-C20 |
| 14  | 1     | 1641 | CLA  | C16-C17-C18-C19 |
| 14  | 2     | 842  | CLA  | C4C-C3C-CAC-CBC |
| 20  | 2     | 850  | LMG  | C13-C14-C15-C16 |
| 14  | b     | 842  | CLA  | C4C-C3C-CAC-CBC |
| 17  | A     | 851  | BCR  | C22-C23-C24-C25 |
| 17  | B     | 851  | BCR  | C6-C7-C8-C9     |
| 17  | F     | 202  | BCR  | C6-C7-C8-C9     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | a     | 851  | BCR  | C22-C23-C24-C25 |
| 17  | b     | 852  | BCR  | C6-C7-C8-C9     |
| 17  | f     | 202  | BCR  | C6-C7-C8-C9     |
| 17  | 1     | 1652 | BCR  | C22-C23-C24-C25 |
| 17  | 6     | 202  | BCR  | C6-C7-C8-C9     |
| 17  | 8     | 1306 | BCR  | C6-C7-C8-C9     |
| 14  | 1     | 1643 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 855  | CLA  | O1D-CGD-O2D-CED |
| 14  | 1     | 1639 | CLA  | C4C-C3C-CAC-CBC |
| 14  | A     | 818  | CLA  | C2-C1-O2A-CGA   |
| 14  | F     | 201  | CLA  | C2-C1-O2A-CGA   |
| 14  | a     | 818  | CLA  | C2-C1-O2A-CGA   |
| 14  | f     | 201  | CLA  | C2-C1-O2A-CGA   |
| 14  | 1     | 1619 | CLA  | C2-C1-O2A-CGA   |
| 14  | 6     | 201  | CLA  | C2-C1-O2A-CGA   |
| 14  | b     | 802  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 838  | CLA  | C2-C3-C5-C6     |
| 14  | a     | 838  | CLA  | C2-C3-C5-C6     |
| 14  | 1     | 1639 | CLA  | C2-C3-C5-C6     |
| 14  | A     | 838  | CLA  | C4C-C3C-CAC-CBC |
| 14  | a     | 838  | CLA  | C4C-C3C-CAC-CBC |
| 14  | B     | 815  | CLA  | C6-C7-C8-C9     |
| 14  | b     | 816  | CLA  | C6-C7-C8-C9     |
| 14  | 2     | 816  | CLA  | C6-C7-C8-C9     |
| 14  | L     | 205  | CLA  | C2A-CAA-CBA-CGA |
| 18  | A     | 854  | LHG  | C9-C10-C11-C12  |
| 17  | A     | 848  | BCR  | C1-C6-C7-C8     |
| 17  | A     | 850  | BCR  | C1-C6-C7-C8     |
| 17  | A     | 850  | BCR  | C5-C6-C7-C8     |
| 17  | B     | 843  | BCR  | C1-C6-C7-C8     |
| 17  | B     | 846  | BCR  | C1-C6-C7-C8     |
| 17  | B     | 847  | BCR  | C1-C6-C7-C8     |
| 17  | I     | 101  | BCR  | C1-C6-C7-C8     |
| 17  | J     | 103  | BCR  | C23-C24-C25-C30 |
| 17  | K     | 102  | BCR  | C23-C24-C25-C30 |
| 17  | a     | 848  | BCR  | C1-C6-C7-C8     |
| 17  | a     | 850  | BCR  | C1-C6-C7-C8     |
| 17  | a     | 850  | BCR  | C5-C6-C7-C8     |
| 17  | b     | 844  | BCR  | C1-C6-C7-C8     |
| 17  | b     | 847  | BCR  | C1-C6-C7-C8     |
| 17  | b     | 848  | BCR  | C1-C6-C7-C8     |
| 17  | i     | 101  | BCR  | C1-C6-C7-C8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | j     | 1304 | BCR  | C23-C24-C25-C30 |
| 17  | k     | 102  | BCR  | C23-C24-C25-C30 |
| 17  | 1     | 1649 | BCR  | C1-C6-C7-C8     |
| 17  | 1     | 1651 | BCR  | C1-C6-C7-C8     |
| 17  | 1     | 1651 | BCR  | C5-C6-C7-C8     |
| 17  | 2     | 844  | BCR  | C1-C6-C7-C8     |
| 17  | 2     | 847  | BCR  | C1-C6-C7-C8     |
| 17  | 2     | 848  | BCR  | C1-C6-C7-C8     |
| 17  | 7     | 101  | BCR  | C1-C6-C7-C8     |
| 17  | 8     | 1304 | BCR  | C23-C24-C25-C30 |
| 17  | 9     | 102  | BCR  | C23-C24-C25-C30 |
| 14  | A     | 815  | CLA  | O1D-CGD-O2D-CED |
| 18  | a     | 854  | LHG  | C9-C10-C11-C12  |
| 18  | 1     | 1655 | LHG  | C9-C10-C11-C12  |
| 14  | B     | 810  | CLA  | C4-C3-C5-C6     |
| 14  | b     | 811  | CLA  | C4-C3-C5-C6     |
| 14  | 2     | 811  | CLA  | C4-C3-C5-C6     |
| 17  | L     | 201  | BCR  | C7-C8-C9-C10    |
| 17  | 1     | 202  | BCR  | C7-C8-C9-C10    |
| 17  | 0     | 203  | BCR  | C7-C8-C9-C10    |
| 14  | A     | 819  | CLA  | C10-C11-C12-C13 |
| 14  | 1     | 1620 | CLA  | C10-C11-C12-C13 |
| 14  | A     | 821  | CLA  | C2-C3-C5-C6     |
| 14  | a     | 821  | CLA  | C2-C3-C5-C6     |
| 14  | b     | 828  | CLA  | C2-C3-C5-C6     |
| 14  | 1     | 1622 | CLA  | C2-C3-C5-C6     |
| 14  | 2     | 828  | CLA  | C2-C3-C5-C6     |
| 14  | a     | 819  | CLA  | C10-C11-C12-C13 |
| 14  | a     | 815  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 832  | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 833  | CLA  | C2A-CAA-CBA-CGA |
| 14  | 2     | 833  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 821  | CLA  | CAA-CBA-CGA-O2A |
| 14  | 1     | 1622 | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 807  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 808  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 2     | 808  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 830  | CLA  | C2-C3-C5-C6     |
| 14  | b     | 831  | CLA  | C2-C3-C5-C6     |
| 14  | 2     | 831  | CLA  | C2-C3-C5-C6     |
| 14  | 2     | 808  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 821  | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 811  | CLA  | C16-C17-C18-C19 |
| 14  | b     | 812  | CLA  | C16-C17-C18-C19 |
| 14  | 2     | 812  | CLA  | C16-C17-C18-C19 |
| 18  | A     | 853  | LHG  | C1-C2-C3-O3     |
| 18  | a     | 853  | LHG  | C1-C2-C3-O3     |
| 18  | 1     | 1654 | LHG  | C1-C2-C3-O3     |
| 14  | B     | 807  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 808  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 802  | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 803  | CLA  | CAA-CBA-CGA-O1A |
| 14  | 2     | 803  | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 835  | CLA  | CAA-CBA-CGA-O2A |
| 14  | L     | 205  | CLA  | CAA-CBA-CGA-O2A |
| 14  | l     | 206  | CLA  | CAA-CBA-CGA-O2A |
| 14  | 0     | 207  | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 811  | CLA  | C2C-C3C-CAC-CBC |
| 14  | 1     | 1612 | CLA  | C2C-C3C-CAC-CBC |
| 17  | B     | 845  | BCR  | C11-C10-C9-C34  |
| 17  | L     | 206  | BCR  | C35-C13-C14-C15 |
| 17  | b     | 846  | BCR  | C11-C10-C9-C34  |
| 17  | l     | 207  | BCR  | C35-C13-C14-C15 |
| 17  | 2     | 846  | BCR  | C11-C10-C9-C34  |
| 17  | 0     | 208  | BCR  | C35-C13-C14-C15 |
| 14  | b     | 836  | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 811  | CLA  | C2C-C3C-CAC-CBC |
| 14  | 1     | 1616 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 828  | CLA  | C10-C11-C12-C13 |
| 14  | b     | 829  | CLA  | C10-C11-C12-C13 |
| 14  | 2     | 829  | CLA  | C10-C11-C12-C13 |
| 14  | A     | 805  | CLA  | C2-C3-C5-C6     |
| 14  | B     | 810  | CLA  | C2-C3-C5-C6     |
| 14  | B     | 827  | CLA  | C2-C3-C5-C6     |
| 14  | B     | 832  | CLA  | C2-C3-C5-C6     |
| 14  | B     | 833  | CLA  | C2-C3-C5-C6     |
| 14  | a     | 805  | CLA  | C2-C3-C5-C6     |
| 14  | b     | 811  | CLA  | C2-C3-C5-C6     |
| 14  | b     | 833  | CLA  | C2-C3-C5-C6     |
| 14  | b     | 834  | CLA  | C2-C3-C5-C6     |
| 14  | 2     | 811  | CLA  | C2-C3-C5-C6     |
| 14  | 2     | 833  | CLA  | C2-C3-C5-C6     |
| 14  | 2     | 834  | CLA  | C2-C3-C5-C6     |
| 14  | 2     | 836  | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 807  | CLA  | C11-C10-C8-C9   |
| 14  | A     | 815  | CLA  | C11-C12-C13-C14 |
| 14  | A     | 824  | CLA  | C14-C13-C15-C16 |
| 14  | A     | 828  | CLA  | C6-C7-C8-C9     |
| 14  | A     | 829  | CLA  | C11-C12-C13-C14 |
| 14  | A     | 838  | CLA  | C14-C13-C15-C16 |
| 14  | A     | 840  | CLA  | C14-C13-C15-C16 |
| 14  | B     | 805  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 805  | CLA  | C14-C13-C15-C16 |
| 14  | B     | 820  | CLA  | C11-C12-C13-C14 |
| 14  | B     | 824  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 832  | CLA  | C11-C10-C8-C9   |
| 14  | a     | 807  | CLA  | C11-C10-C8-C9   |
| 14  | a     | 815  | CLA  | C11-C12-C13-C14 |
| 14  | a     | 824  | CLA  | C14-C13-C15-C16 |
| 14  | a     | 828  | CLA  | C6-C7-C8-C9     |
| 14  | a     | 829  | CLA  | C11-C12-C13-C14 |
| 14  | a     | 838  | CLA  | C14-C13-C15-C16 |
| 14  | a     | 840  | CLA  | C14-C13-C15-C16 |
| 14  | b     | 806  | CLA  | C6-C7-C8-C9     |
| 14  | b     | 806  | CLA  | C14-C13-C15-C16 |
| 14  | b     | 821  | CLA  | C11-C12-C13-C14 |
| 14  | b     | 825  | CLA  | C6-C7-C8-C9     |
| 14  | b     | 833  | CLA  | C11-C10-C8-C9   |
| 14  | 1     | 1608 | CLA  | C11-C10-C8-C9   |
| 14  | 1     | 1616 | CLA  | C11-C12-C13-C14 |
| 14  | 1     | 1625 | CLA  | C14-C13-C15-C16 |
| 14  | 1     | 1629 | CLA  | C6-C7-C8-C9     |
| 14  | 1     | 1630 | CLA  | C11-C12-C13-C14 |
| 14  | 1     | 1639 | CLA  | C14-C13-C15-C16 |
| 14  | 1     | 1641 | CLA  | C14-C13-C15-C16 |
| 14  | 2     | 806  | CLA  | C6-C7-C8-C9     |
| 14  | 2     | 806  | CLA  | C14-C13-C15-C16 |
| 14  | 2     | 821  | CLA  | C11-C12-C13-C14 |
| 14  | 2     | 825  | CLA  | C6-C7-C8-C9     |
| 14  | 2     | 833  | CLA  | C11-C10-C8-C9   |
| 18  | b     | 851  | LHG  | C27-C28-C29-C30 |
| 18  | z     | 101  | LHG  | C27-C28-C29-C30 |
| 14  | A     | 823  | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 823  | CLA  | CAA-CBA-CGA-O2A |
| 14  | 1     | 1624 | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 814  | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 814  | CLA  | C3A-C2A-CAA-CBA |
| 14  | 1     | 1615 | CLA  | C3A-C2A-CAA-CBA |
| 18  | B     | 850  | LHG  | C27-C28-C29-C30 |
| 14  | A     | 808  | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 813  | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 818  | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 822  | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 828  | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 834  | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 820  | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 836  | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 840  | CLA  | CAD-CBD-CGD-O2D |
| 14  | L     | 205  | CLA  | CAD-CBD-CGD-O2D |
| 14  | a     | 808  | CLA  | CAD-CBD-CGD-O2D |
| 14  | a     | 813  | CLA  | CAD-CBD-CGD-O2D |
| 14  | a     | 818  | CLA  | CAD-CBD-CGD-O2D |
| 14  | a     | 822  | CLA  | CAD-CBD-CGD-O2D |
| 14  | a     | 828  | CLA  | CAD-CBD-CGD-O2D |
| 14  | a     | 834  | CLA  | CAD-CBD-CGD-O2D |
| 14  | b     | 821  | CLA  | CAD-CBD-CGD-O2D |
| 14  | b     | 837  | CLA  | CAD-CBD-CGD-O2D |
| 14  | b     | 841  | CLA  | CAD-CBD-CGD-O2D |
| 14  | l     | 206  | CLA  | CAD-CBD-CGD-O2D |
| 14  | 1     | 1609 | CLA  | CAD-CBD-CGD-O2D |
| 14  | 1     | 1614 | CLA  | CAD-CBD-CGD-O2D |
| 14  | 1     | 1619 | CLA  | CAD-CBD-CGD-O2D |
| 14  | 1     | 1623 | CLA  | CAD-CBD-CGD-O2D |
| 14  | 1     | 1629 | CLA  | CAD-CBD-CGD-O2D |
| 14  | 1     | 1635 | CLA  | CAD-CBD-CGD-O2D |
| 14  | 2     | 821  | CLA  | CAD-CBD-CGD-O2D |
| 14  | 2     | 837  | CLA  | CAD-CBD-CGD-O2D |
| 14  | 2     | 841  | CLA  | CAD-CBD-CGD-O2D |
| 14  | 0     | 207  | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 803  | CLA  | C13-C15-C16-C17 |
| 14  | a     | 803  | CLA  | C13-C15-C16-C17 |
| 14  | A     | 802  | CLA  | C2-C1-O2A-CGA   |
| 14  | a     | 802  | CLA  | C2-C1-O2A-CGA   |
| 14  | 1     | 1603 | CLA  | C2-C1-O2A-CGA   |
| 14  | 2     | 825  | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 813  | CLA  | CAA-CBA-CGA-O2A |
| 14  | K     | 103  | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 814  | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 820  | CLA  | CAA-CBA-CGA-O2A |
| 14  | 2     | 814  | CLA  | CAA-CBA-CGA-O2A |
| 14  | 1     | 1604 | CLA  | C13-C15-C16-C17 |
| 14  | A     | 816  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 830  | CLA  | C2-C3-C5-C6     |
| 14  | a     | 816  | CLA  | C2-C3-C5-C6     |
| 14  | a     | 830  | CLA  | C2-C3-C5-C6     |
| 14  | 1     | 1606 | CLA  | C2-C3-C5-C6     |
| 14  | 1     | 1617 | CLA  | C2-C3-C5-C6     |
| 14  | 1     | 1631 | CLA  | C2-C3-C5-C6     |
| 14  | B     | 806  | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 819  | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 807  | CLA  | CAA-CBA-CGA-O2A |
| 14  | k     | 103  | CLA  | CAA-CBA-CGA-O2A |
| 14  | 2     | 807  | CLA  | CAA-CBA-CGA-O2A |
| 14  | 2     | 820  | CLA  | CAA-CBA-CGA-O2A |
| 14  | 9     | 103  | CLA  | CAA-CBA-CGA-O2A |
| 17  | A     | 849  | BCR  | C21-C22-C23-C24 |
| 17  | F     | 202  | BCR  | C21-C22-C23-C24 |
| 17  | I     | 101  | BCR  | C7-C8-C9-C10    |
| 17  | K     | 102  | BCR  | C7-C8-C9-C10    |
| 17  | a     | 849  | BCR  | C21-C22-C23-C24 |
| 17  | f     | 202  | BCR  | C21-C22-C23-C24 |
| 17  | i     | 101  | BCR  | C7-C8-C9-C10    |
| 17  | k     | 102  | BCR  | C7-C8-C9-C10    |
| 17  | 1     | 1650 | BCR  | C21-C22-C23-C24 |
| 17  | 6     | 202  | BCR  | C21-C22-C23-C24 |
| 17  | 7     | 101  | BCR  | C7-C8-C9-C10    |
| 17  | 9     | 102  | BCR  | C7-C8-C9-C10    |
| 14  | X     | 1701 | CLA  | CAA-CBA-CGA-O2A |
| 14  | x     | 1701 | CLA  | CAA-CBA-CGA-O2A |
| 14  | z     | 102  | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 802  | CLA  | O2A-C1-C2-C3    |
| 14  | A     | 826  | CLA  | O2A-C1-C2-C3    |
| 14  | A     | 838  | CLA  | O2A-C1-C2-C3    |
| 14  | B     | 804  | CLA  | O2A-C1-C2-C3    |
| 14  | B     | 825  | CLA  | O2A-C1-C2-C3    |
| 14  | a     | 802  | CLA  | O2A-C1-C2-C3    |
| 14  | a     | 826  | CLA  | O2A-C1-C2-C3    |
| 14  | a     | 838  | CLA  | O2A-C1-C2-C3    |
| 14  | b     | 805  | CLA  | O2A-C1-C2-C3    |
| 14  | b     | 826  | CLA  | O2A-C1-C2-C3    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | 1     | 1603 | CLA  | O2A-C1-C2-C3    |
| 14  | 1     | 1627 | CLA  | O2A-C1-C2-C3    |
| 14  | 1     | 1639 | CLA  | O2A-C1-C2-C3    |
| 14  | 2     | 805  | CLA  | O2A-C1-C2-C3    |
| 14  | 2     | 826  | CLA  | O2A-C1-C2-C3    |
| 14  | A     | 844  | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 823  | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 844  | CLA  | CAA-CBA-CGA-O2A |
| 14  | 1     | 1624 | CLA  | CAA-CBA-CGA-O1A |
| 14  | 1     | 1645 | CLA  | CAA-CBA-CGA-O1A |
| 14  | 1     | 1645 | CLA  | CAA-CBA-CGA-O2A |
| 14  | K     | 101  | CLA  | O1A-CGA-O2A-C1  |
| 14  | k     | 101  | CLA  | O1A-CGA-O2A-C1  |
| 14  | 9     | 101  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 811  | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 815  | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 817  | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 817  | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 820  | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 820  | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 826  | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 839  | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 839  | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 840  | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 804  | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 818  | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 818  | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 824  | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 832  | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 832  | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 835  | CLA  | CHA-CBD-CGD-O2D |
| 14  | K     | 103  | CLA  | CHA-CBD-CGD-O1D |
| 14  | K     | 103  | CLA  | CHA-CBD-CGD-O2D |
| 14  | L     | 203  | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 811  | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 815  | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 817  | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 817  | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 820  | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 820  | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 826  | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 839  | CLA  | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 839  | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 840  | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 805  | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 819  | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 819  | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 825  | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 833  | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 833  | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 836  | CLA  | CHA-CBD-CGD-O2D |
| 14  | k     | 103  | CLA  | CHA-CBD-CGD-O1D |
| 14  | k     | 103  | CLA  | CHA-CBD-CGD-O2D |
| 14  | l     | 204  | CLA  | CHA-CBD-CGD-O2D |
| 14  | 1     | 1612 | CLA  | CHA-CBD-CGD-O2D |
| 14  | 1     | 1616 | CLA  | CHA-CBD-CGD-O2D |
| 14  | 1     | 1618 | CLA  | CHA-CBD-CGD-O1D |
| 14  | 1     | 1618 | CLA  | CHA-CBD-CGD-O2D |
| 14  | 1     | 1621 | CLA  | CHA-CBD-CGD-O1D |
| 14  | 1     | 1621 | CLA  | CHA-CBD-CGD-O2D |
| 14  | 1     | 1627 | CLA  | CHA-CBD-CGD-O1D |
| 14  | 1     | 1640 | CLA  | CHA-CBD-CGD-O1D |
| 14  | 1     | 1640 | CLA  | CHA-CBD-CGD-O2D |
| 14  | 1     | 1641 | CLA  | CHA-CBD-CGD-O2D |
| 14  | 2     | 805  | CLA  | CHA-CBD-CGD-O1D |
| 14  | 2     | 819  | CLA  | CHA-CBD-CGD-O1D |
| 14  | 2     | 819  | CLA  | CHA-CBD-CGD-O2D |
| 14  | 2     | 825  | CLA  | CHA-CBD-CGD-O1D |
| 14  | 2     | 833  | CLA  | CHA-CBD-CGD-O1D |
| 14  | 2     | 833  | CLA  | CHA-CBD-CGD-O2D |
| 14  | 2     | 836  | CLA  | CHA-CBD-CGD-O2D |
| 14  | 9     | 103  | CLA  | CHA-CBD-CGD-O1D |
| 14  | 9     | 103  | CLA  | CHA-CBD-CGD-O2D |
| 14  | 0     | 205  | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 823  | CLA  | CAA-CBA-CGA-O1A |
| 14  | X     | 1701 | CLA  | CAA-CBA-CGA-O1A |
| 14  | x     | 1701 | CLA  | CAA-CBA-CGA-O1A |
| 14  | z     | 102  | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 844  | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 803  | CLA  | C16-C17-C18-C20 |
| 14  | A     | 802  | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 809  | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 802  | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 809  | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | 1     | 1603 | CLA  | CAA-CBA-CGA-O2A |
| 14  | 1     | 1610 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 844  | CLA  | CAA-CBA-CGA-O1A |
| 20  | b     | 850  | LMG  | C19-C20-C21-C22 |
| 14  | B     | 802  | CLA  | C16-C17-C18-C20 |
| 20  | 2     | 850  | LMG  | C19-C20-C21-C22 |
| 14  | A     | 826  | CLA  | CAA-CBA-CGA-O2A |
| 20  | B     | 849  | LMG  | C19-C20-C21-C22 |
| 14  | A     | 839  | CLA  | C6-C7-C8-C10    |
| 14  | a     | 839  | CLA  | C6-C7-C8-C10    |
| 14  | 1     | 1640 | CLA  | C6-C7-C8-C10    |
| 14  | A     | 843  | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 826  | CLA  | CAA-CBA-CGA-O2A |
| 14  | 1     | 1627 | CLA  | CAA-CBA-CGA-O2A |
| 14  | 1     | 1644 | CLA  | CAA-CBA-CGA-O2A |
| 13  | A     | 801  | CL0  | C14-C13-C15-C16 |
| 13  | a     | 801  | CL0  | C14-C13-C15-C16 |
| 13  | 1     | 1602 | CL0  | C14-C13-C15-C16 |
| 14  | A     | 814  | CLA  | C11-C10-C8-C9   |
| 14  | A     | 821  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 802  | CLA  | C11-C12-C13-C14 |
| 14  | a     | 814  | CLA  | C11-C10-C8-C9   |
| 14  | a     | 821  | CLA  | C6-C7-C8-C9     |
| 14  | b     | 803  | CLA  | C11-C12-C13-C14 |
| 14  | 1     | 1615 | CLA  | C11-C10-C8-C9   |
| 14  | 1     | 1622 | CLA  | C6-C7-C8-C9     |
| 14  | 2     | 803  | CLA  | C11-C12-C13-C14 |
| 17  | A     | 847  | BCR  | C14-C15-C16-C17 |
| 17  | a     | 847  | BCR  | C14-C15-C16-C17 |
| 17  | 1     | 1648 | BCR  | C14-C15-C16-C17 |
| 14  | a     | 843  | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 835  | CLA  | C16-C17-C18-C20 |
| 14  | a     | 835  | CLA  | C16-C17-C18-C20 |
| 14  | 1     | 1636 | CLA  | C16-C17-C18-C20 |
| 14  | 2     | 803  | CLA  | C16-C17-C18-C20 |
| 17  | A     | 851  | BCR  | C11-C12-C13-C35 |
| 17  | a     | 851  | BCR  | C11-C12-C13-C35 |
| 14  | B     | 820  | CLA  | C16-C17-C18-C19 |
| 14  | b     | 821  | CLA  | C16-C17-C18-C19 |
| 14  | 2     | 821  | CLA  | C16-C17-C18-C19 |
| 17  | j     | 1304 | BCR  | C17-C18-C19-C20 |
| 14  | A     | 835  | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 821  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 823  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 837  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 855  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 809  | CLA  | C1A-C2A-CAA-CBA |
| 14  | J     | 101  | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 821  | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 823  | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 837  | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 802  | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 810  | CLA  | C1A-C2A-CAA-CBA |
| 14  | j     | 1302 | CLA  | C1A-C2A-CAA-CBA |
| 14  | 1     | 1622 | CLA  | C1A-C2A-CAA-CBA |
| 14  | 1     | 1624 | CLA  | C1A-C2A-CAA-CBA |
| 14  | 1     | 1638 | CLA  | C1A-C2A-CAA-CBA |
| 14  | 2     | 802  | CLA  | C1A-C2A-CAA-CBA |
| 14  | 2     | 810  | CLA  | C1A-C2A-CAA-CBA |
| 14  | 8     | 1302 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 835  | CLA  | C5-C6-C7-C8     |
| 14  | 1     | 1636 | CLA  | C5-C6-C7-C8     |
| 14  | B     | 813  | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 835  | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 836  | CLA  | CAA-CBA-CGA-O1A |
| 14  | 2     | 836  | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 813  | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 813  | CLA  | CAA-CBA-CGA-O2A |
| 14  | 1     | 1614 | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 808  | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 808  | CLA  | CAA-CBA-CGA-O2A |
| 14  | 1     | 1609 | CLA  | CAA-CBA-CGA-O2A |
| 14  | 2     | 821  | CLA  | C13-C15-C16-C17 |
| 14  | b     | 814  | CLA  | CAA-CBA-CGA-O1A |
| 14  | 2     | 814  | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 820  | CLA  | C13-C15-C16-C17 |
| 14  | b     | 821  | CLA  | C13-C15-C16-C17 |
| 14  | A     | 805  | CLA  | C4-C3-C5-C6     |
| 14  | a     | 805  | CLA  | C4-C3-C5-C6     |
| 14  | B     | 810  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 829  | CLA  | C8-C10-C11-C12  |
| 14  | b     | 811  | CLA  | C5-C6-C7-C8     |
| 14  | b     | 830  | CLA  | C8-C10-C11-C12  |
| 14  | 2     | 811  | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | 2     | 830  | CLA  | C8-C10-C11-C12  |
| 18  | A     | 853  | LHG  | C4-O6-P-O5      |
| 18  | a     | 853  | LHG  | C4-O6-P-O5      |
| 18  | 1     | 1654 | LHG  | C4-O6-P-O5      |
| 14  | B     | 806  | CLA  | CAA-CBA-CGA-O1A |
| 14  | k     | 103  | CLA  | CAA-CBA-CGA-O1A |
| 14  | 9     | 103  | CLA  | CAA-CBA-CGA-O1A |
| 18  | A     | 853  | LHG  | O9-C7-C8-C9     |
| 18  | a     | 853  | LHG  | O9-C7-C8-C9     |
| 18  | 1     | 1654 | LHG  | O9-C7-C8-C9     |
| 18  | M     | 101  | LHG  | O6-C4-C5-C6     |
| 18  | m     | 101  | LHG  | O6-C4-C5-C6     |
| 18  | y     | 101  | LHG  | O6-C4-C5-C6     |
| 17  | A     | 848  | BCR  | C5-C6-C7-C8     |
| 17  | I     | 101  | BCR  | C5-C6-C7-C8     |
| 17  | a     | 848  | BCR  | C5-C6-C7-C8     |
| 17  | i     | 101  | BCR  | C5-C6-C7-C8     |
| 17  | 1     | 1649 | BCR  | C5-C6-C7-C8     |
| 17  | 7     | 101  | BCR  | C5-C6-C7-C8     |
| 14  | K     | 103  | CLA  | CAA-CBA-CGA-O1A |
| 13  | A     | 801  | CL0  | CAA-CBA-CGA-O1A |
| 13  | a     | 801  | CL0  | CAA-CBA-CGA-O1A |
| 13  | 1     | 1602 | CL0  | CAA-CBA-CGA-O1A |
| 14  | A     | 802  | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 819  | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 802  | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 807  | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 820  | CLA  | CAA-CBA-CGA-O1A |
| 14  | 1     | 1603 | CLA  | CAA-CBA-CGA-O1A |
| 14  | 2     | 807  | CLA  | CAA-CBA-CGA-O1A |
| 14  | 2     | 821  | CLA  | C10-C11-C12-C13 |
| 14  | A     | 810  | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 810  | CLA  | CAA-CBA-CGA-O2A |
| 14  | 1     | 1611 | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 820  | CLA  | C10-C11-C12-C13 |
| 14  | b     | 821  | CLA  | C10-C11-C12-C13 |
| 14  | 2     | 820  | CLA  | CAA-CBA-CGA-O1A |
| 14  | 1     | 1606 | CLA  | C4-C3-C5-C6     |
| 17  | A     | 850  | BCR  | C19-C20-C21-C22 |
| 13  | A     | 801  | CL0  | CAD-CBD-CGD-O1D |
| 13  | a     | 801  | CL0  | CAD-CBD-CGD-O1D |
| 13  | 1     | 1602 | CL0  | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 824  | CLA  | CAD-CBD-CGD-O1D |
| 14  | A     | 830  | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 807  | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 828  | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 831  | CLA  | CAD-CBD-CGD-O1D |
| 14  | J     | 101  | CLA  | CAD-CBD-CGD-O1D |
| 14  | a     | 824  | CLA  | CAD-CBD-CGD-O1D |
| 14  | a     | 830  | CLA  | CAD-CBD-CGD-O1D |
| 14  | b     | 808  | CLA  | CAD-CBD-CGD-O1D |
| 14  | b     | 829  | CLA  | CAD-CBD-CGD-O1D |
| 14  | b     | 832  | CLA  | CAD-CBD-CGD-O1D |
| 14  | b     | 838  | CLA  | CAD-CBD-CGD-O1D |
| 14  | j     | 1302 | CLA  | CAD-CBD-CGD-O1D |
| 14  | 1     | 1625 | CLA  | CAD-CBD-CGD-O1D |
| 14  | 1     | 1631 | CLA  | CAD-CBD-CGD-O1D |
| 14  | 2     | 808  | CLA  | CAD-CBD-CGD-O1D |
| 14  | 2     | 829  | CLA  | CAD-CBD-CGD-O1D |
| 14  | 2     | 832  | CLA  | CAD-CBD-CGD-O1D |
| 14  | 2     | 838  | CLA  | CAD-CBD-CGD-O1D |
| 14  | 8     | 1302 | CLA  | CAD-CBD-CGD-O1D |
| 20  | B     | 849  | LMG  | O9-C10-C11-C12  |
| 20  | b     | 850  | LMG  | O9-C10-C11-C12  |
| 20  | 2     | 850  | LMG  | O9-C10-C11-C12  |
| 14  | A     | 830  | CLA  | C13-C15-C16-C17 |
| 14  | a     | 830  | CLA  | C13-C15-C16-C17 |
| 14  | 1     | 1631 | CLA  | C13-C15-C16-C17 |
| 14  | A     | 816  | CLA  | C11-C10-C8-C9   |
| 14  | B     | 832  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 840  | CLA  | C14-C13-C15-C16 |
| 14  | a     | 816  | CLA  | C11-C10-C8-C9   |
| 14  | b     | 833  | CLA  | C6-C7-C8-C9     |
| 14  | b     | 841  | CLA  | C14-C13-C15-C16 |
| 14  | 1     | 1617 | CLA  | C11-C10-C8-C9   |
| 14  | 2     | 833  | CLA  | C6-C7-C8-C9     |
| 14  | 2     | 841  | CLA  | C14-C13-C15-C16 |
| 18  | a     | 853  | LHG  | C14-C15-C16-C17 |
| 14  | 0     | 206  | CLA  | C13-C15-C16-C17 |
| 18  | 1     | 1654 | LHG  | C14-C15-C16-C17 |
| 18  | A     | 853  | LHG  | C14-C15-C16-C17 |
| 14  | L     | 204  | CLA  | C13-C15-C16-C17 |
| 14  | l     | 205  | CLA  | C13-C15-C16-C17 |
| 14  | B     | 827  | CLA  | C2C-C3C-CAC-CBC |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | B     | 850  | LHG  | C17-C18-C19-C20 |
| 18  | z     | 101  | LHG  | C17-C18-C19-C20 |
| 14  | A     | 816  | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 840  | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 840  | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 829  | CLA  | CAA-CBA-CGA-O2A |
| 14  | 1     | 1641 | CLA  | CAA-CBA-CGA-O2A |
| 14  | 2     | 829  | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 830  | CLA  | C8-C10-C11-C12  |
| 14  | a     | 830  | CLA  | C8-C10-C11-C12  |
| 18  | b     | 851  | LHG  | C17-C18-C19-C20 |
| 14  | B     | 832  | CLA  | C4-C3-C5-C6     |
| 14  | b     | 833  | CLA  | C4-C3-C5-C6     |
| 14  | 2     | 833  | CLA  | C4-C3-C5-C6     |
| 14  | 1     | 1631 | CLA  | C8-C10-C11-C12  |
| 14  | A     | 804  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 809  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 829  | CLA  | C6-C7-C8-C10    |
| 14  | B     | 815  | CLA  | C6-C7-C8-C10    |
| 14  | B     | 817  | CLA  | C12-C13-C15-C16 |
| 14  | B     | 824  | CLA  | C11-C10-C8-C7   |
| 14  | a     | 804  | CLA  | C12-C13-C15-C16 |
| 14  | a     | 809  | CLA  | C6-C7-C8-C10    |
| 14  | a     | 829  | CLA  | C6-C7-C8-C10    |
| 14  | b     | 816  | CLA  | C6-C7-C8-C10    |
| 14  | b     | 818  | CLA  | C12-C13-C15-C16 |
| 14  | b     | 825  | CLA  | C11-C10-C8-C7   |
| 14  | 1     | 1605 | CLA  | C12-C13-C15-C16 |
| 14  | 1     | 1610 | CLA  | C6-C7-C8-C10    |
| 14  | 1     | 1630 | CLA  | C6-C7-C8-C10    |
| 14  | 2     | 816  | CLA  | C6-C7-C8-C10    |
| 14  | 2     | 818  | CLA  | C12-C13-C15-C16 |
| 14  | 2     | 825  | CLA  | C11-C10-C8-C7   |
| 14  | A     | 809  | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 843  | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 817  | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 809  | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 843  | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 828  | CLA  | C2C-C3C-CAC-CBC |
| 14  | B     | 803  | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 817  | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 828  | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 816  | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 804  | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 818  | CLA  | CAA-CBA-CGA-O2A |
| 14  | 1     | 1617 | CLA  | CAA-CBA-CGA-O2A |
| 14  | 2     | 804  | CLA  | CAA-CBA-CGA-O2A |
| 14  | 2     | 818  | CLA  | CAA-CBA-CGA-O2A |
| 20  | B     | 849  | LMG  | C33-C34-C35-C36 |
| 20  | b     | 850  | LMG  | C33-C34-C35-C36 |
| 20  | 2     | 850  | LMG  | C33-C34-C35-C36 |
| 17  | J     | 103  | BCR  | C17-C18-C19-C20 |
| 17  | 8     | 1304 | BCR  | C17-C18-C19-C20 |
| 14  | b     | 818  | CLA  | CAA-CBA-CGA-O1A |
| 14  | 1     | 1610 | CLA  | CAA-CBA-CGA-O1A |
| 14  | 2     | 818  | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 813  | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 813  | CLA  | CAA-CBA-CGA-O1A |
| 14  | 1     | 1614 | CLA  | CAA-CBA-CGA-O1A |
| 17  | a     | 850  | BCR  | C19-C20-C21-C22 |
| 17  | 1     | 1651 | BCR  | C19-C20-C21-C22 |
| 14  | A     | 835  | CLA  | C16-C17-C18-C19 |
| 14  | a     | 835  | CLA  | C16-C17-C18-C19 |
| 14  | 1     | 1636 | CLA  | C16-C17-C18-C19 |
| 14  | a     | 841  | CLA  | CAA-CBA-CGA-O2A |
| 14  | 2     | 828  | CLA  | C2C-C3C-CAC-CBC |
| 14  | A     | 817  | CLA  | C10-C11-C12-C13 |
| 14  | a     | 817  | CLA  | C10-C11-C12-C13 |
| 14  | 1     | 1618 | CLA  | C10-C11-C12-C13 |
| 14  | A     | 808  | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 816  | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 840  | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 808  | CLA  | CAA-CBA-CGA-O1A |
| 14  | 1     | 1609 | CLA  | CAA-CBA-CGA-O1A |
| 14  | 1     | 1617 | CLA  | CAA-CBA-CGA-O1A |
| 14  | 1     | 1644 | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 841  | CLA  | CAA-CBA-CGA-O2A |
| 14  | 1     | 1642 | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 826  | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 816  | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 826  | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 840  | CLA  | CAA-CBA-CGA-O1A |
| 14  | 1     | 1627 | CLA  | CAA-CBA-CGA-O1A |
| 14  | 1     | 1641 | CLA  | CAA-CBA-CGA-O1A |

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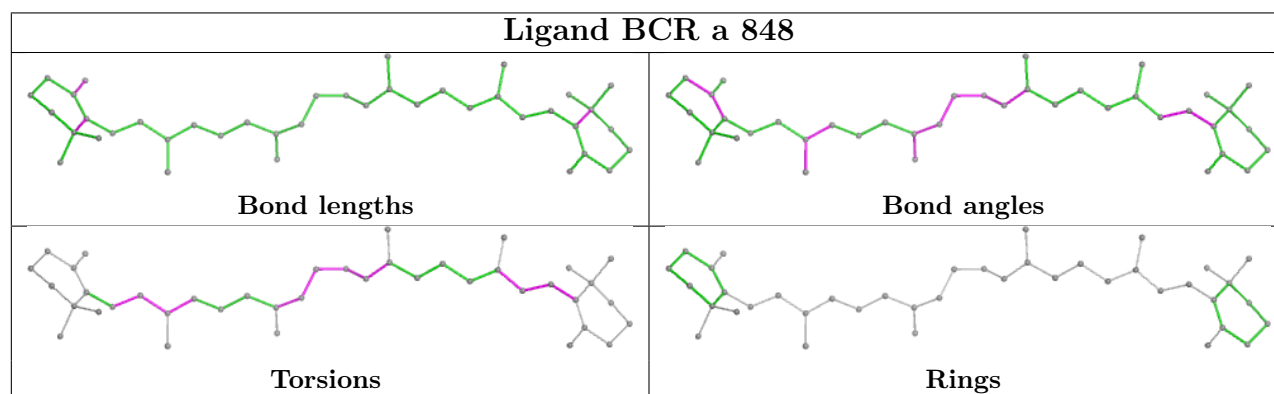
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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 820  | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 821  | CLA  | C2A-CAA-CBA-CGA |
| 14  | 2     | 821  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 806  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 817  | CLA  | C8-C10-C11-C12  |
| 14  | a     | 806  | CLA  | C15-C16-C17-C18 |
| 14  | a     | 817  | CLA  | C8-C10-C11-C12  |
| 14  | 1     | 1607 | CLA  | C15-C16-C17-C18 |
| 14  | 1     | 1618 | CLA  | C8-C10-C11-C12  |

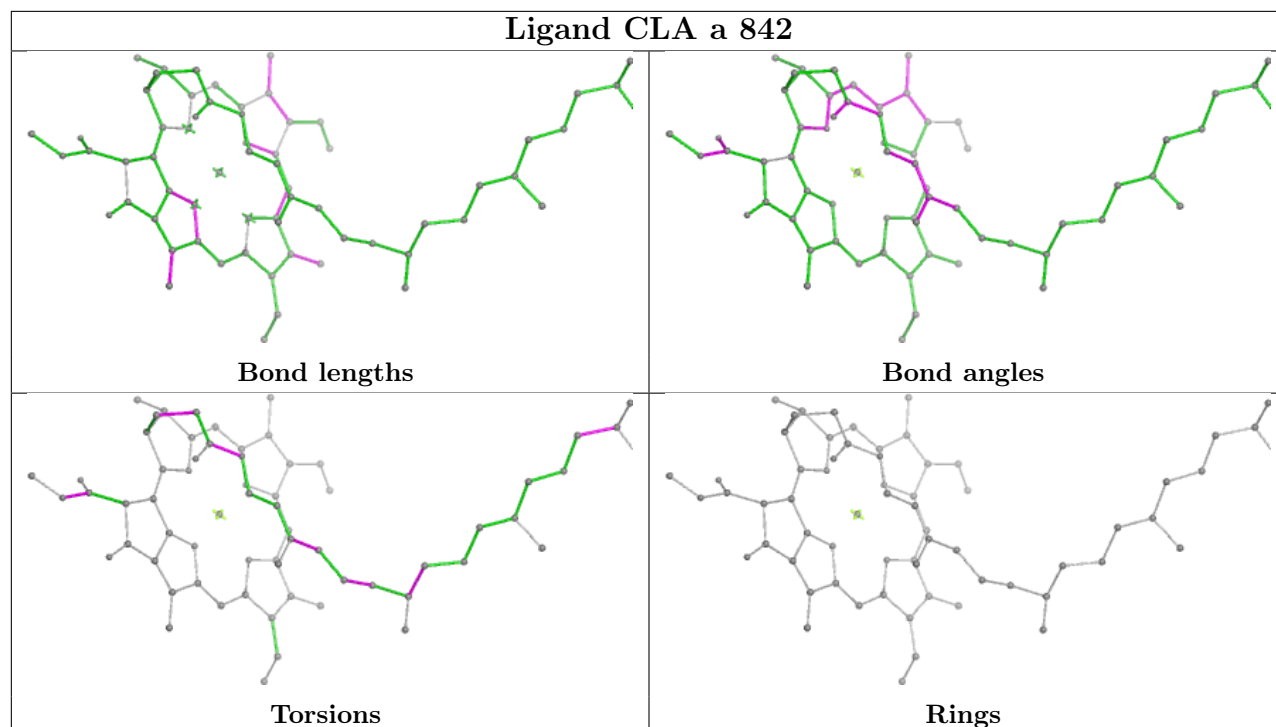
There are no ring outliers.

No monomer is involved in short contacts.

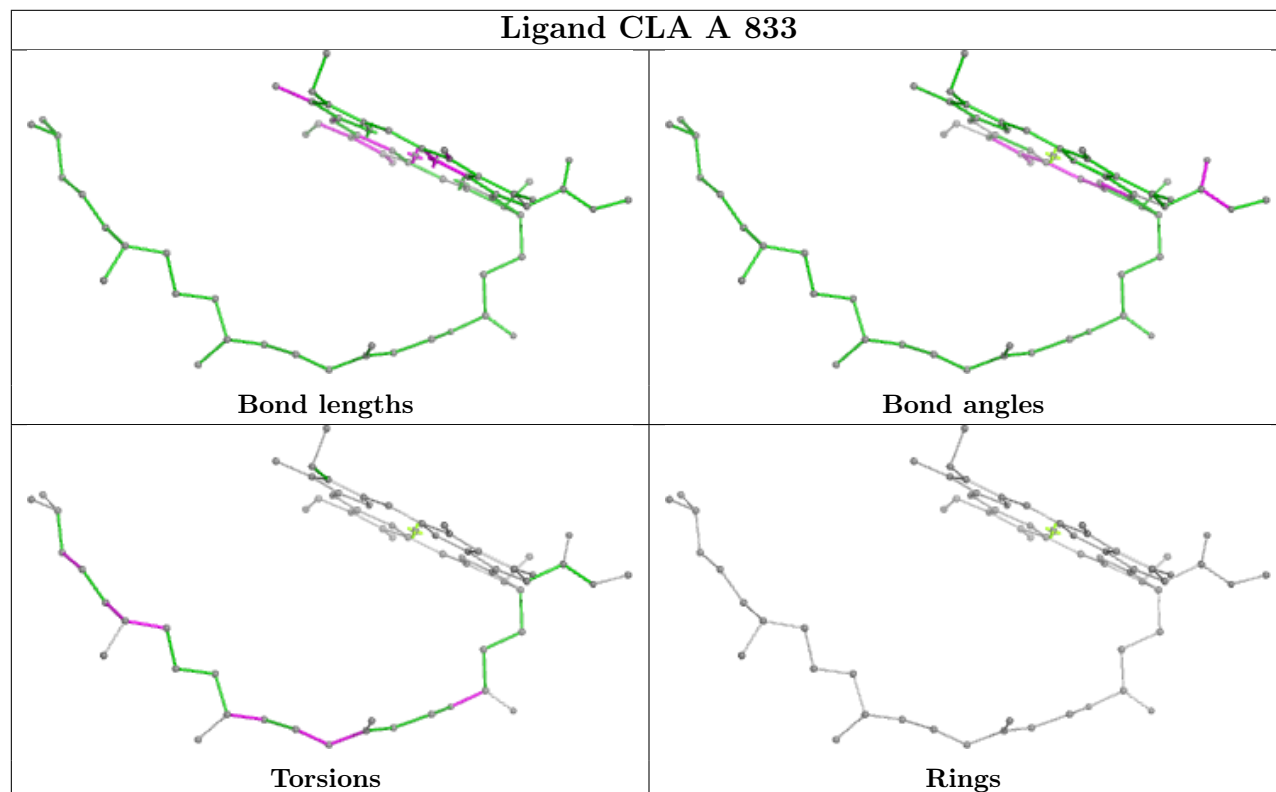
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

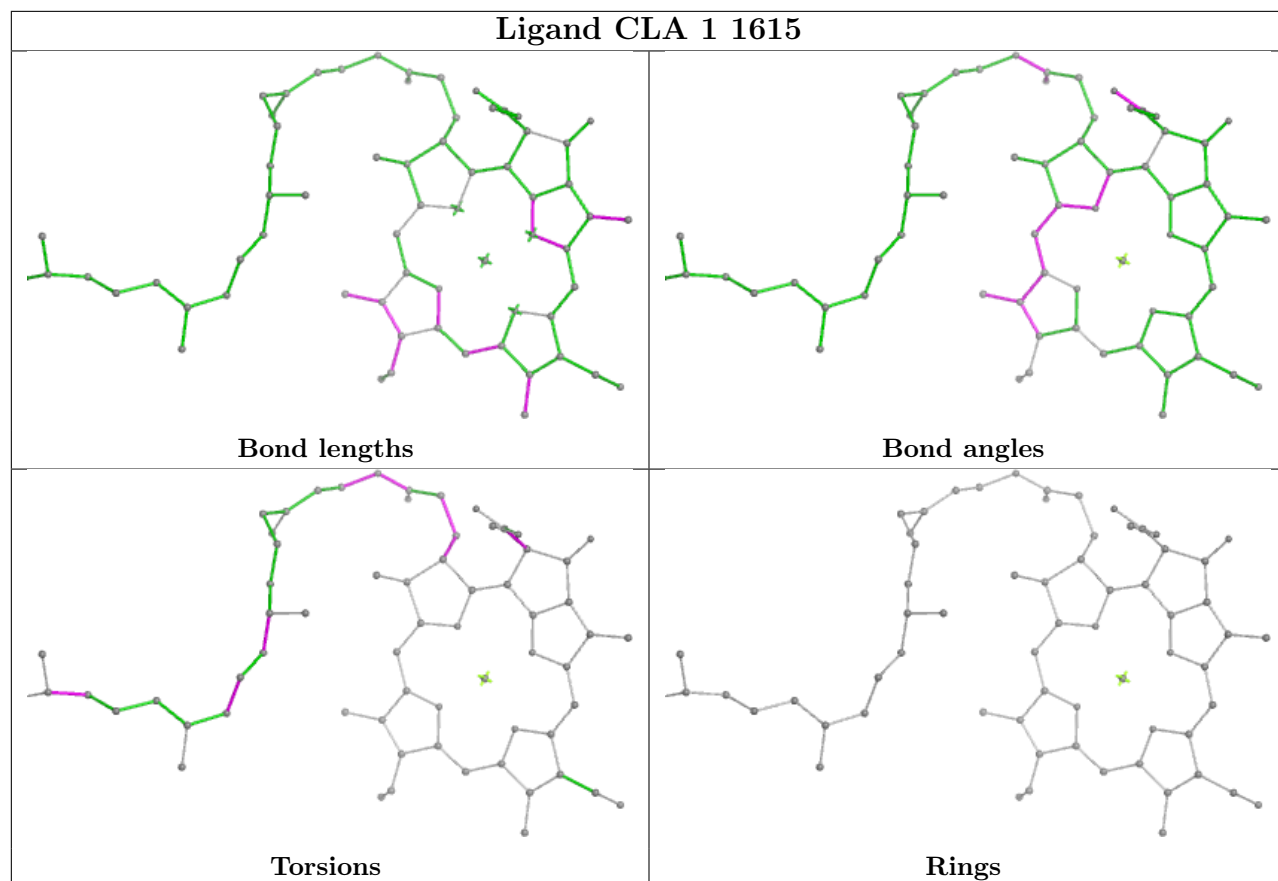


## Ligand CLA a 842

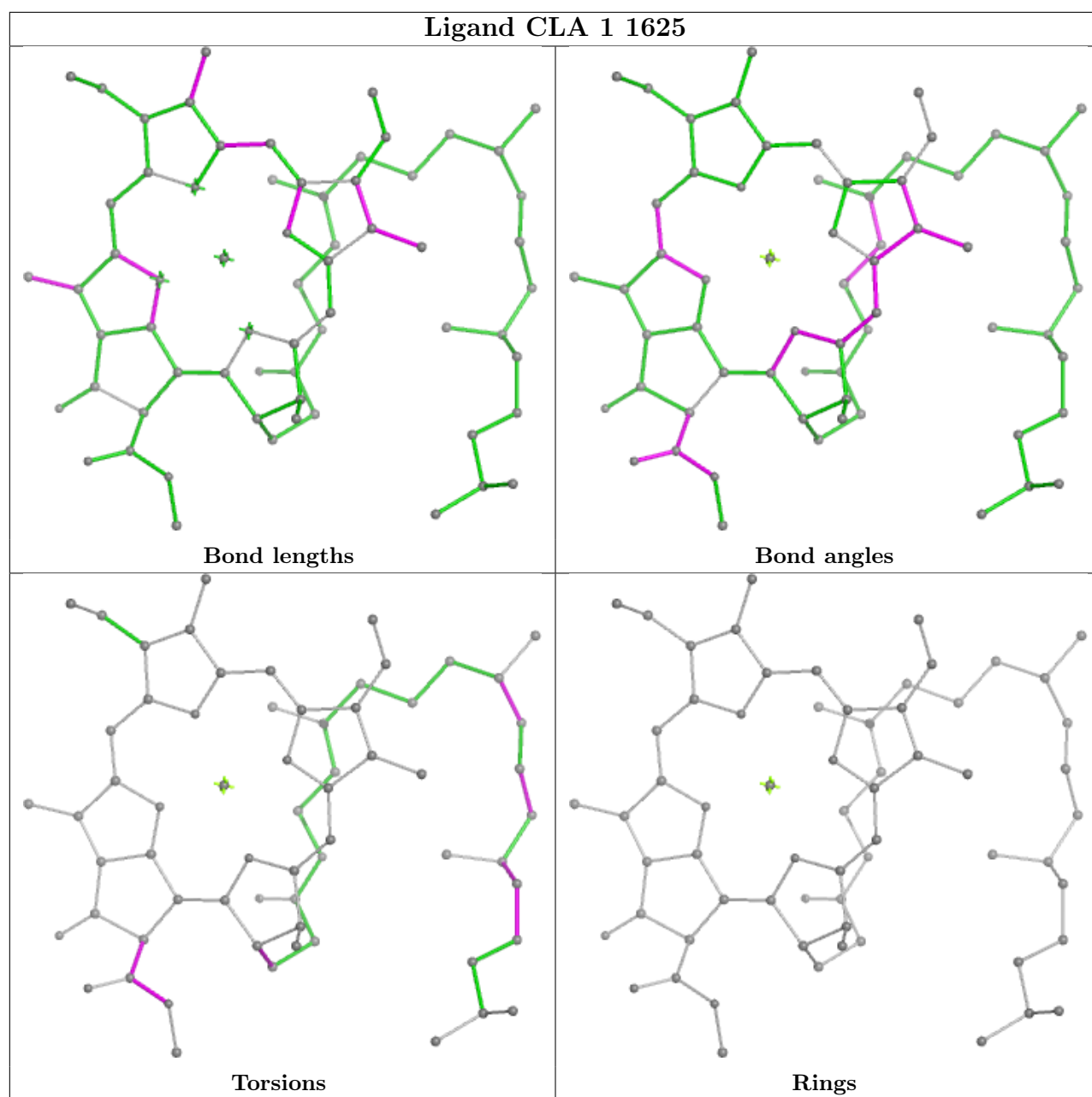


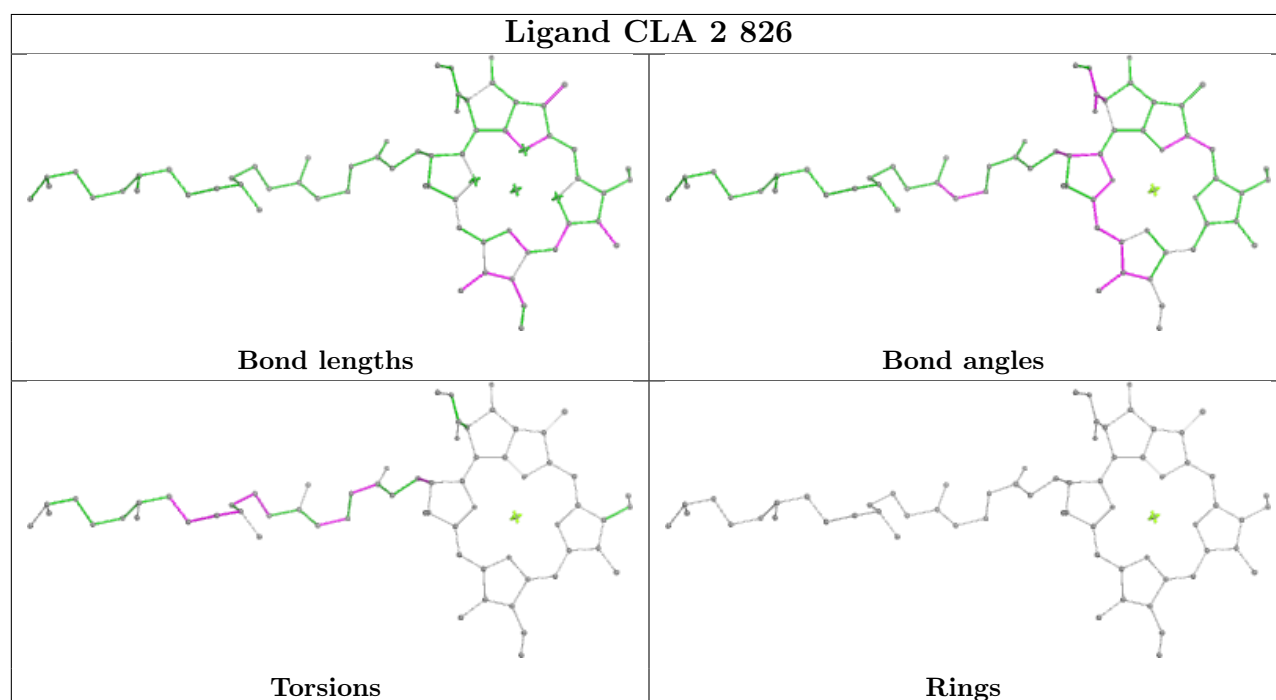
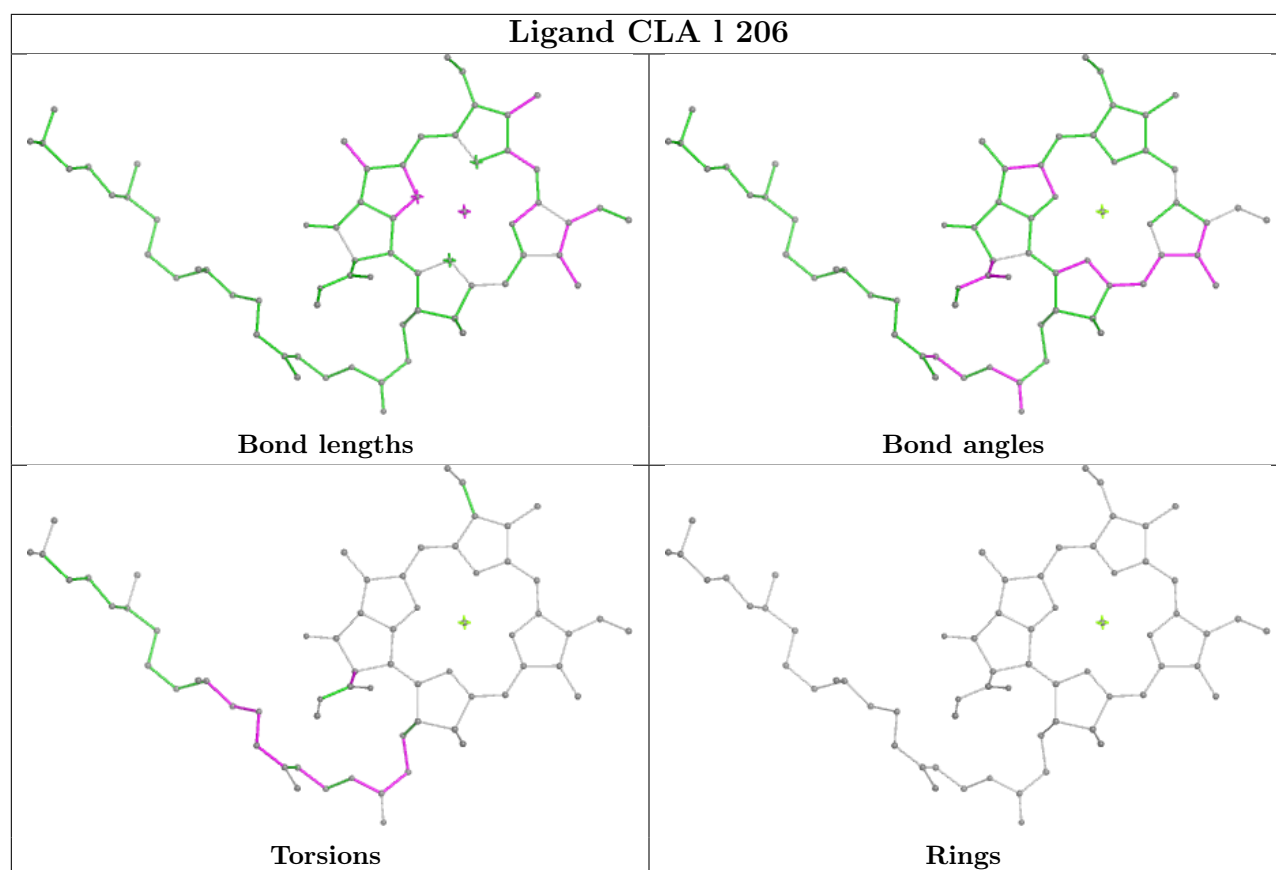
## Ligand CLA A 833

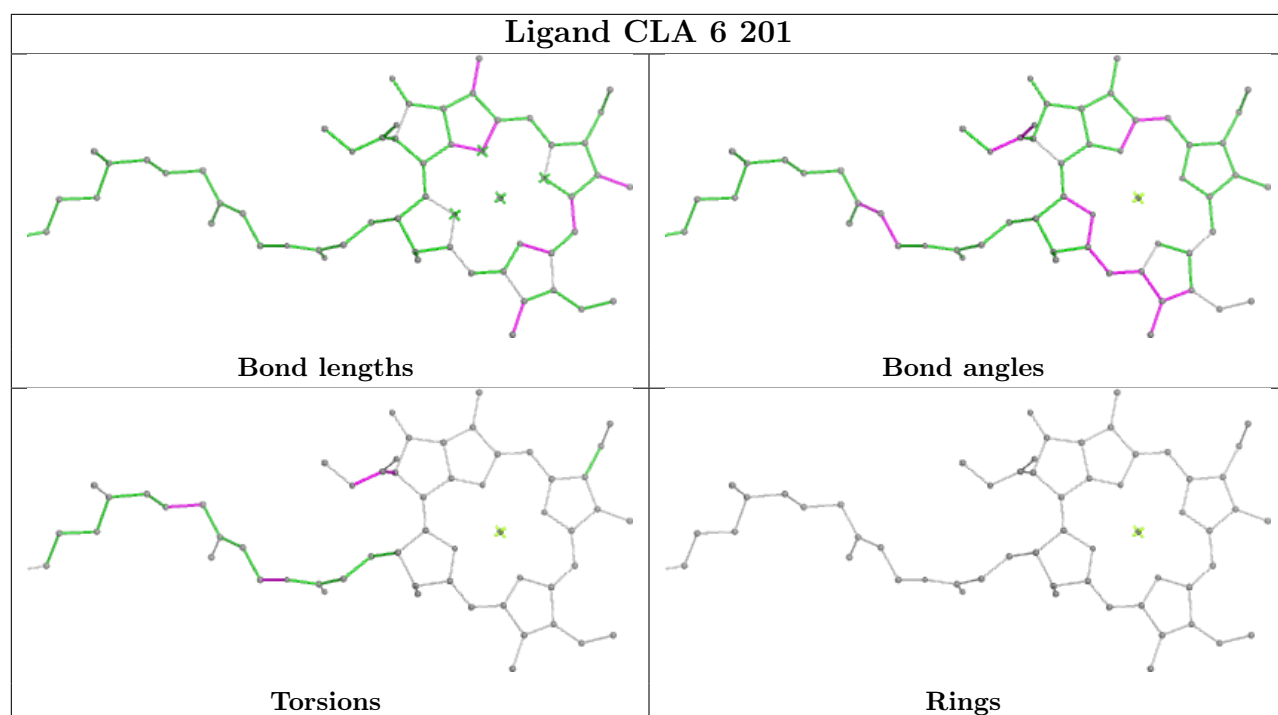




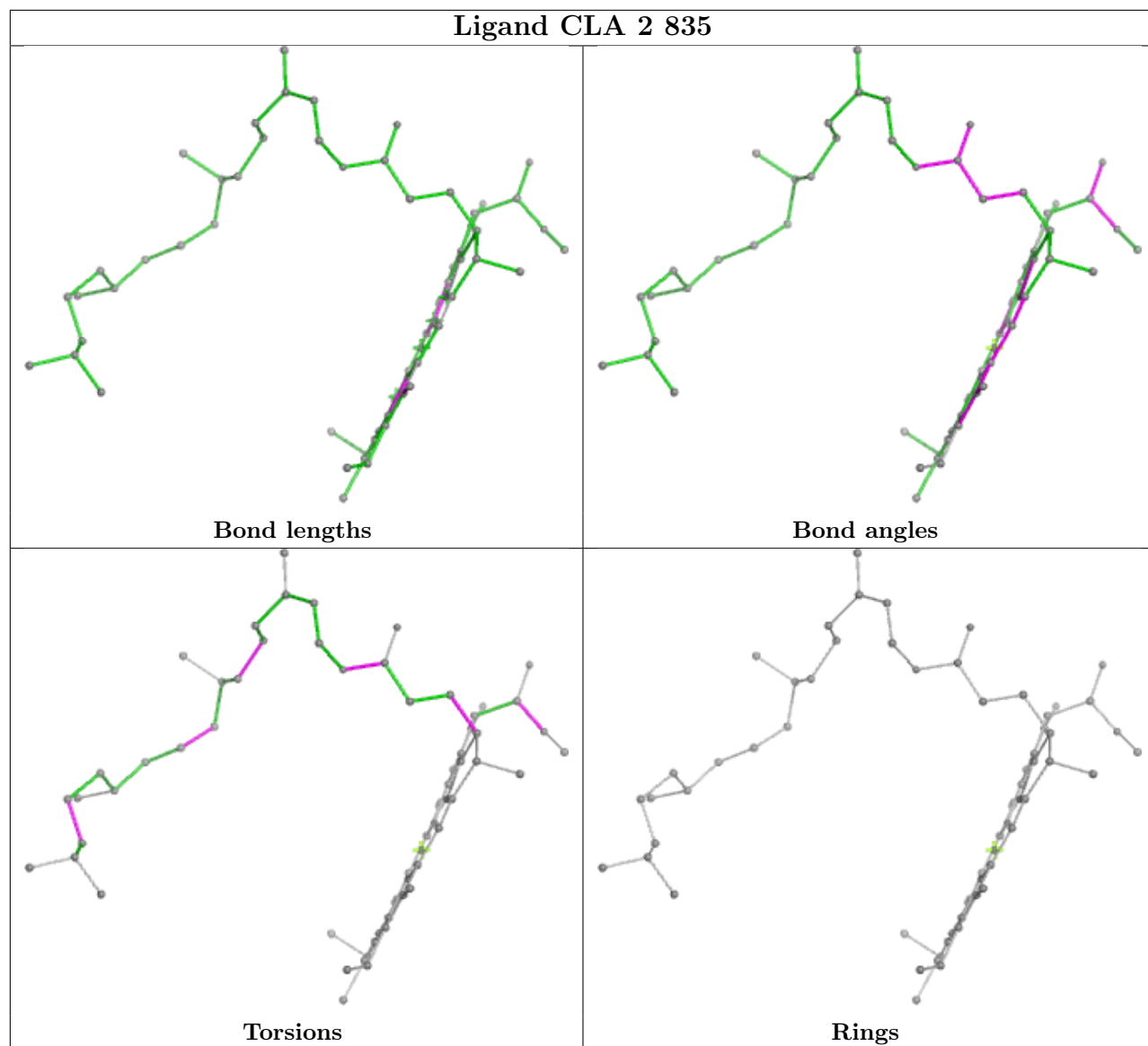


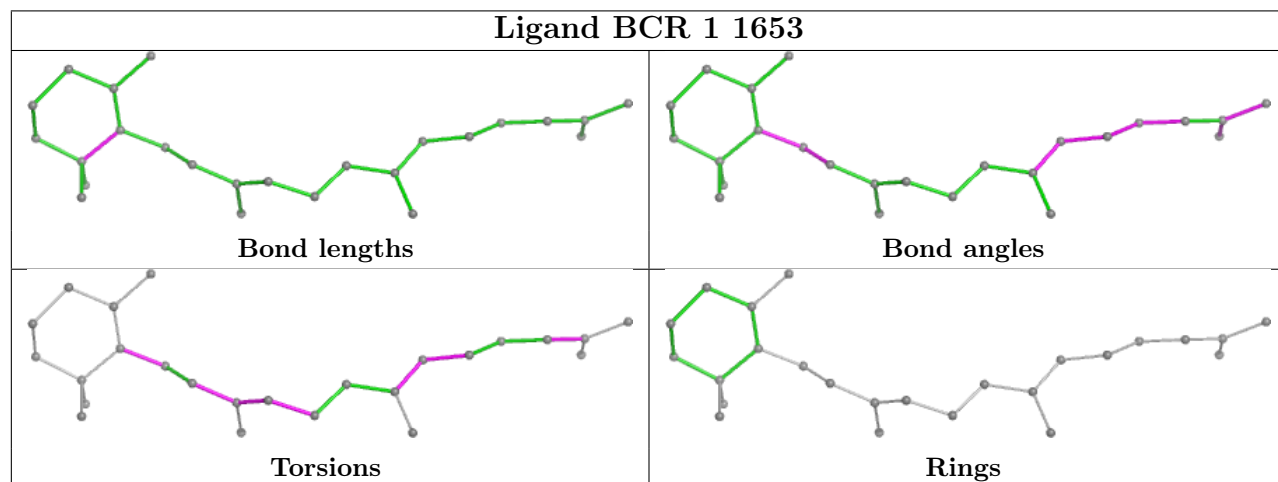
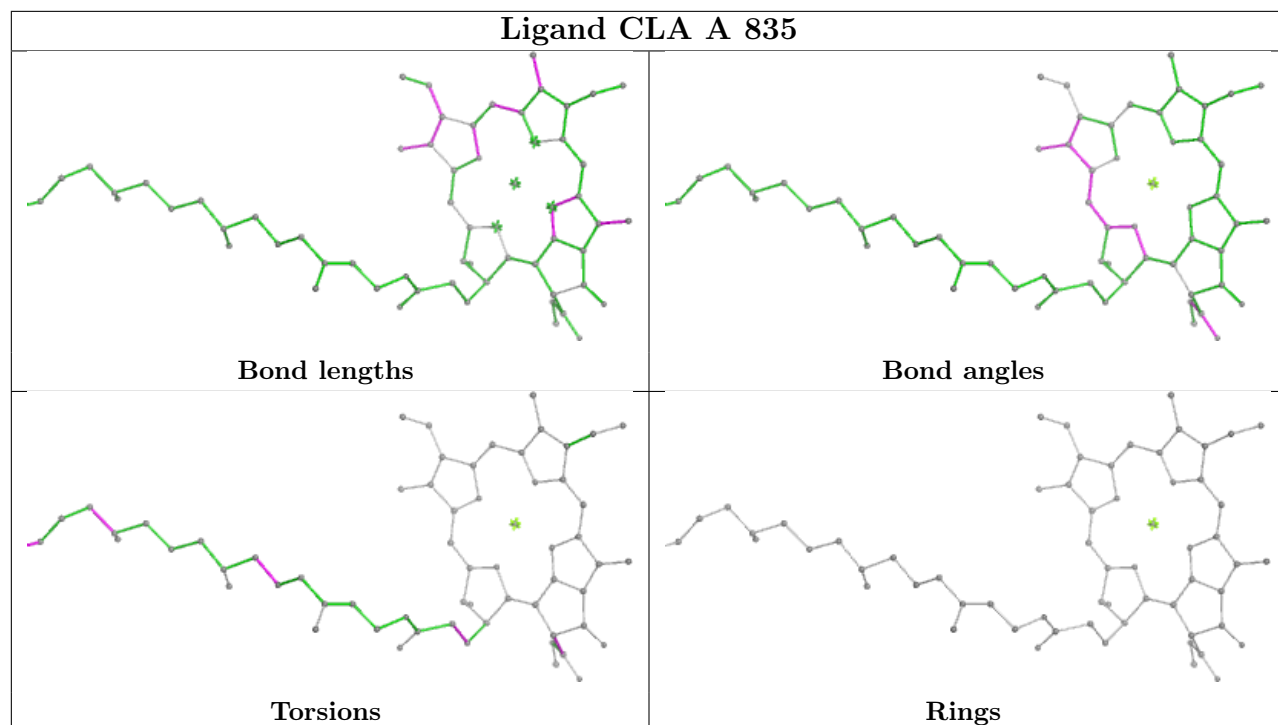




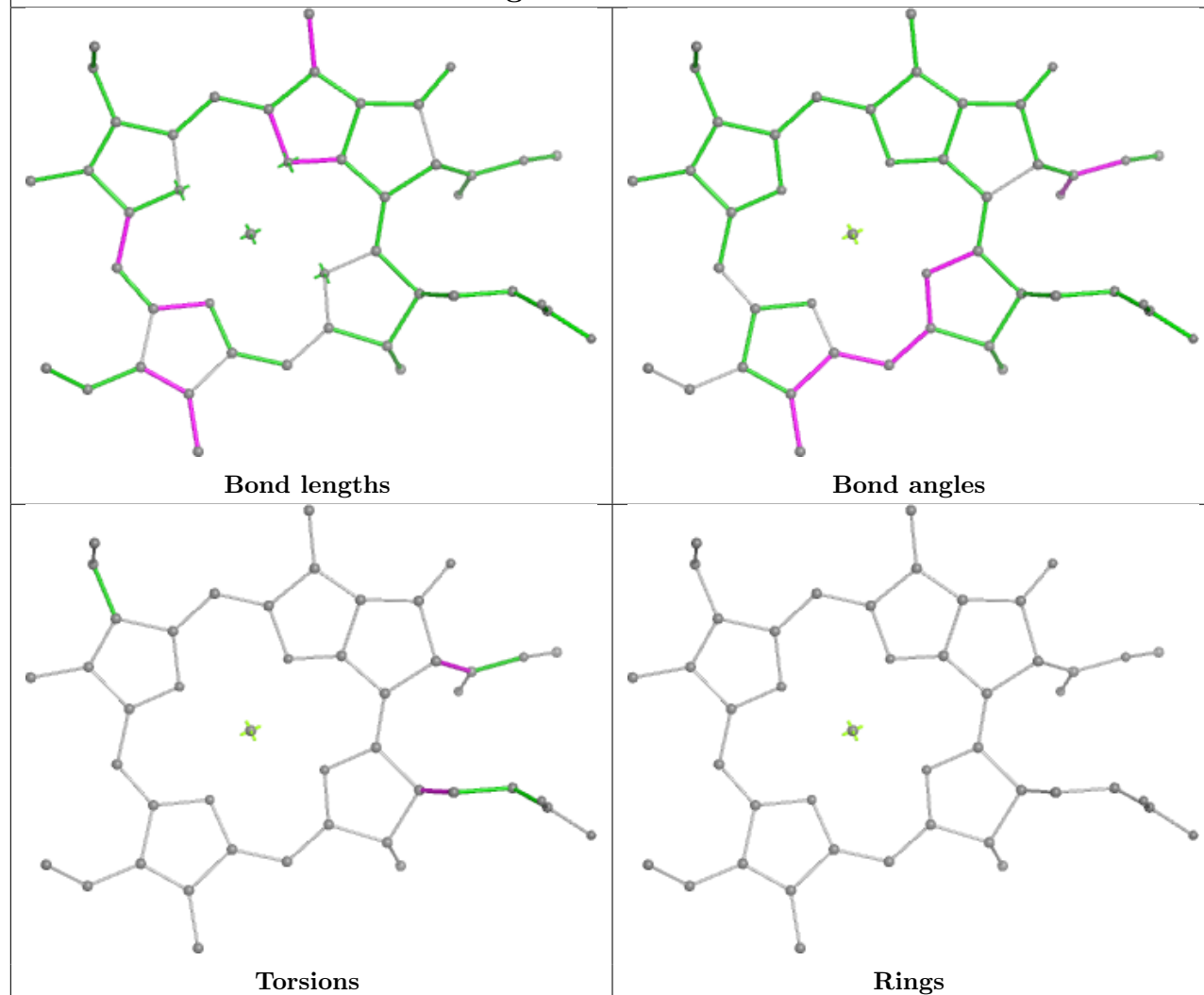


## Ligand CLA 2 835

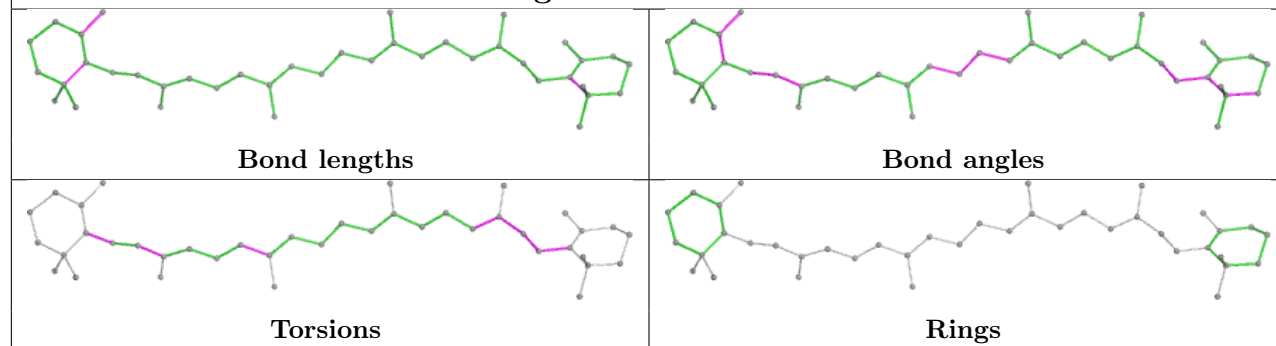




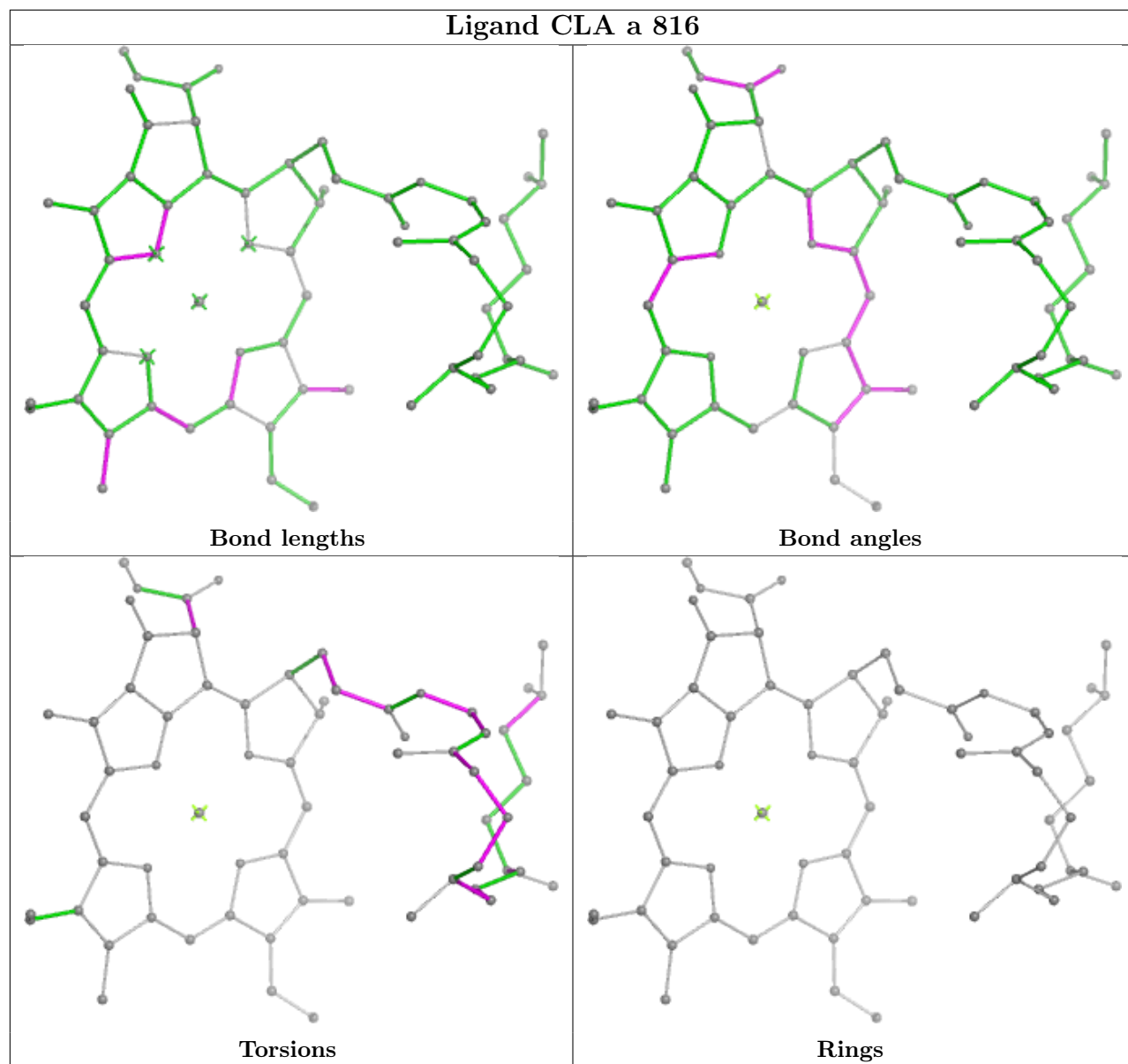
## Ligand CLA 2 837

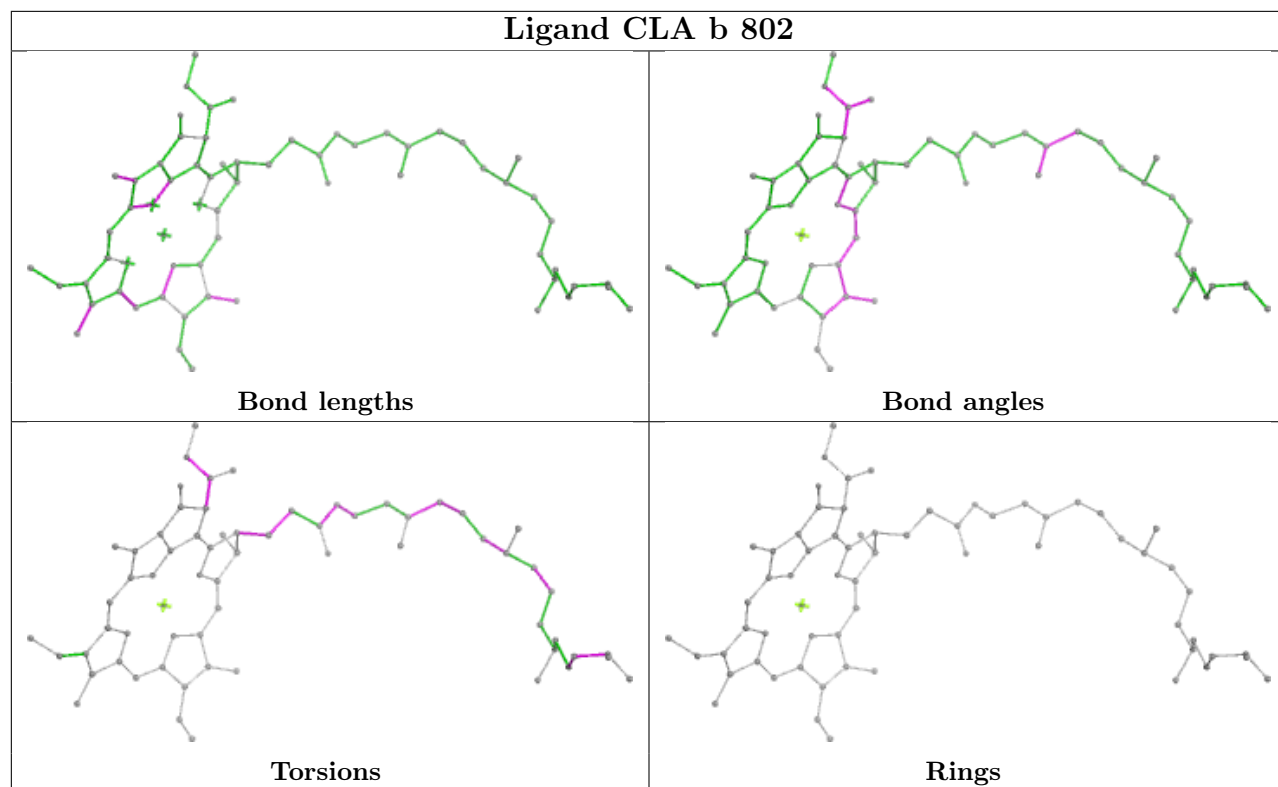


## Ligand BCR J 103



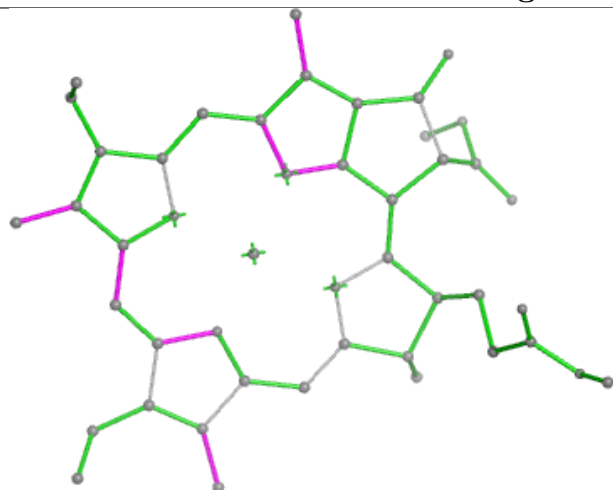
## Ligand CLA a 816



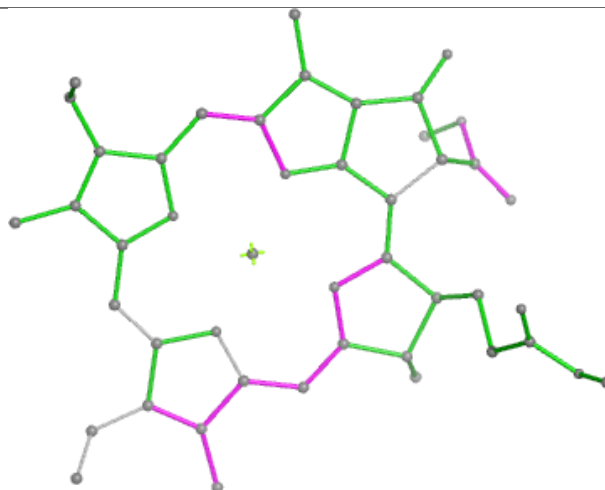




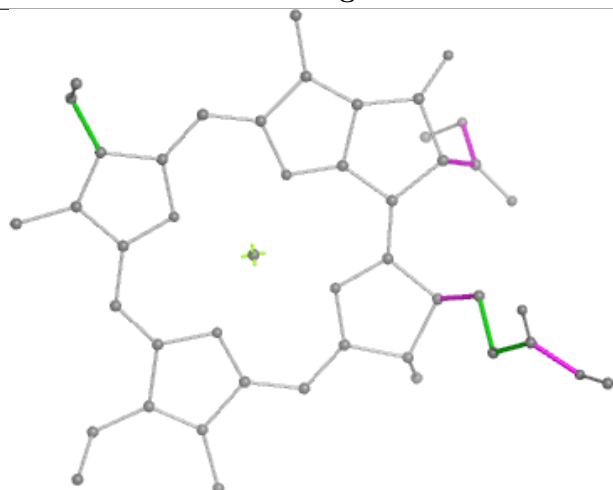
## Ligand CLA k 101



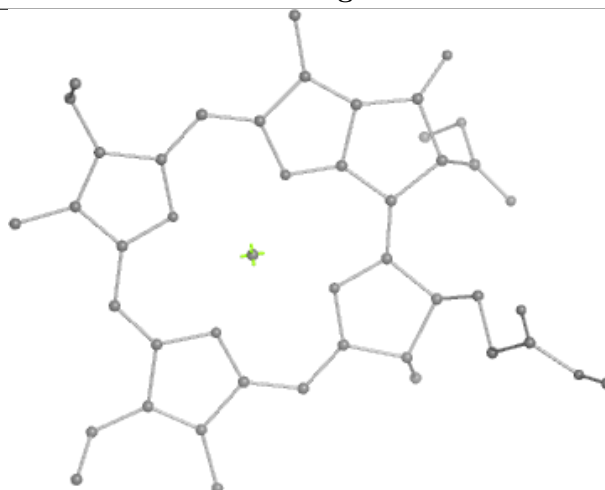
Bond lengths



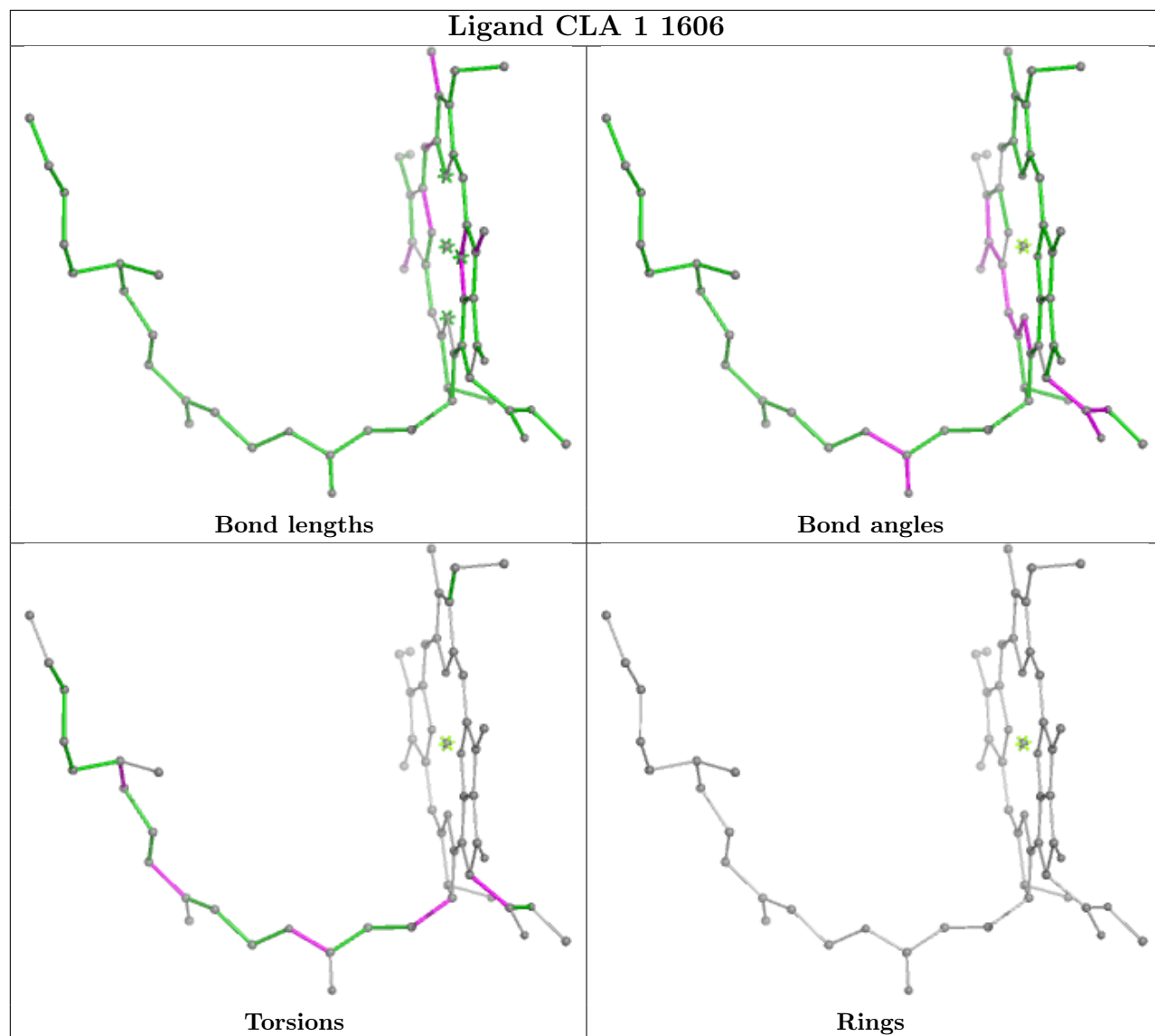
Bond angles

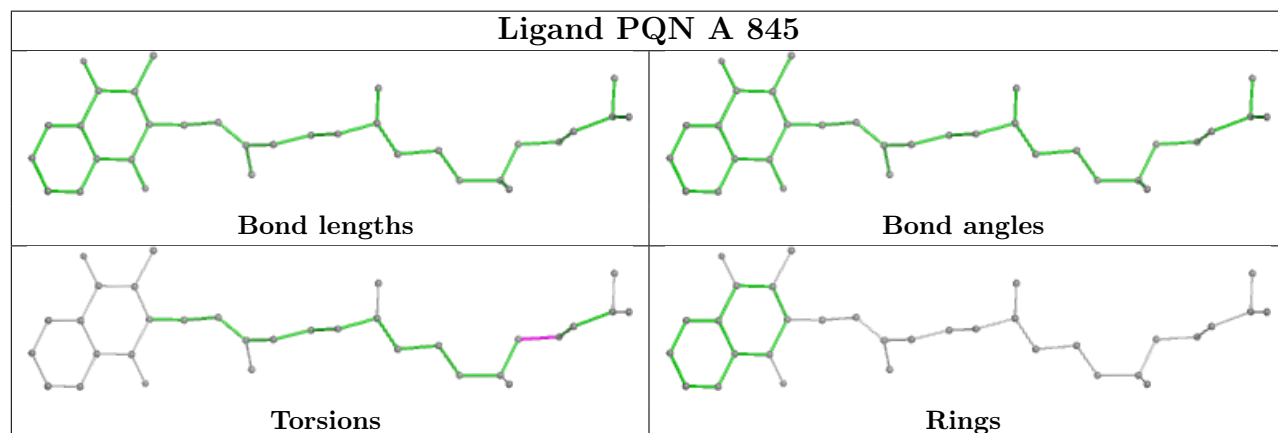
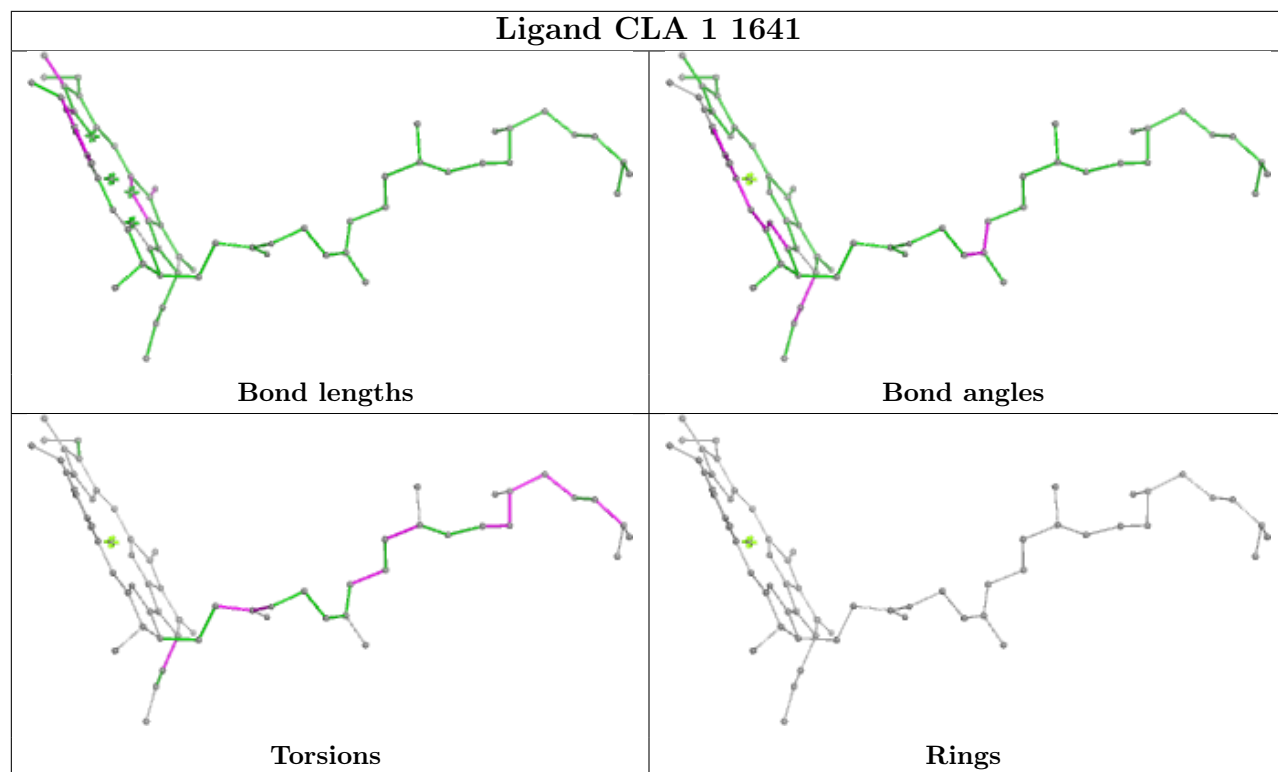


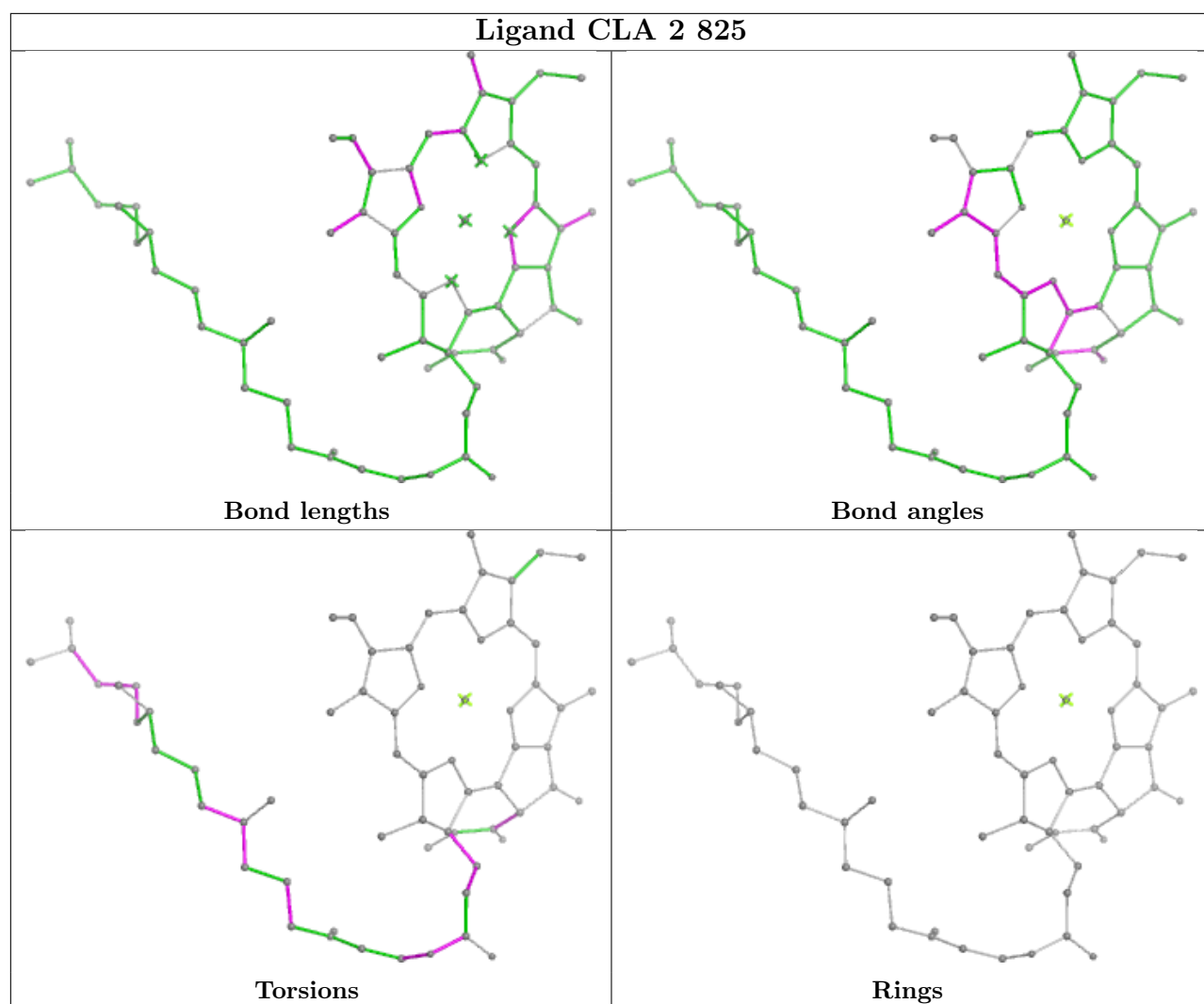
Torsions

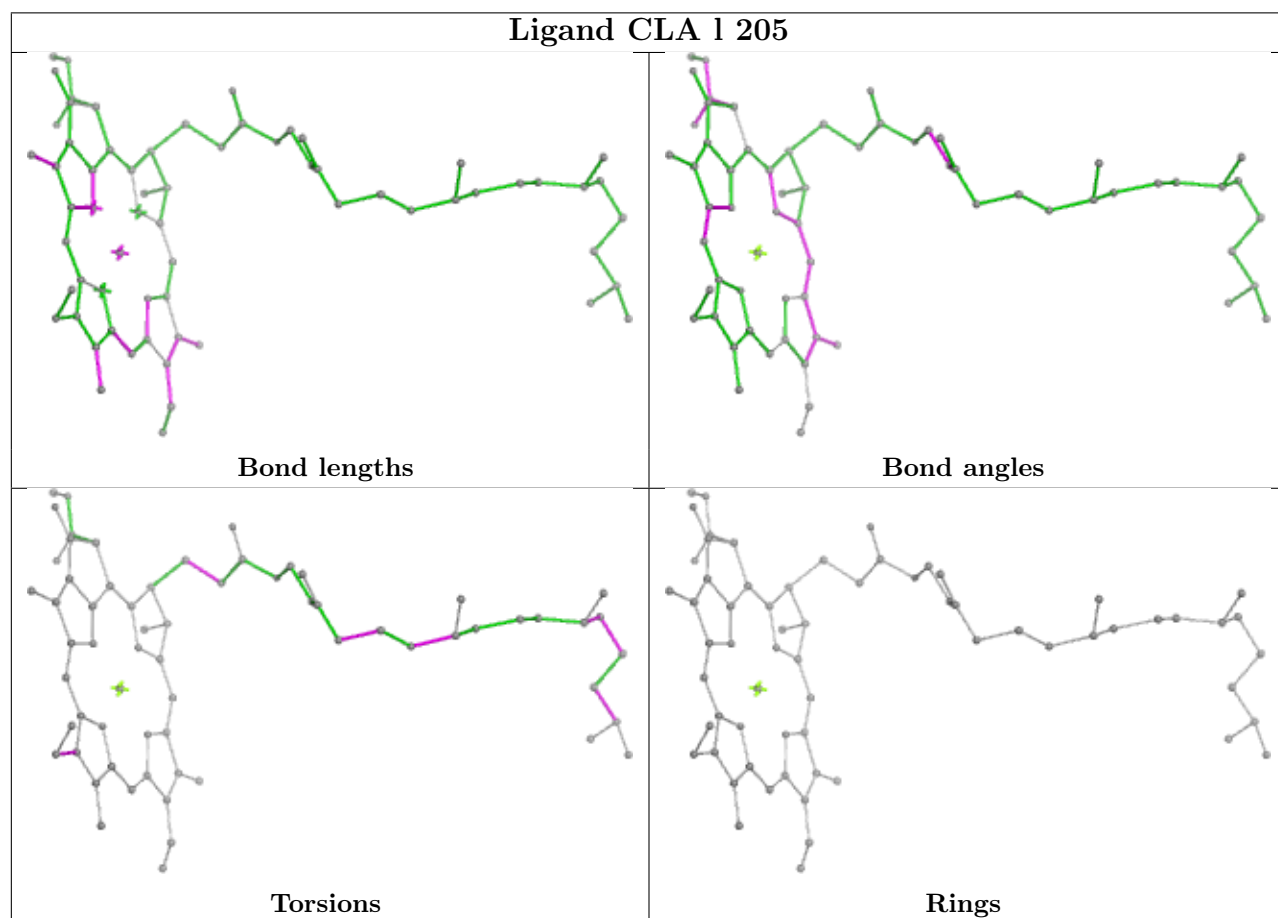
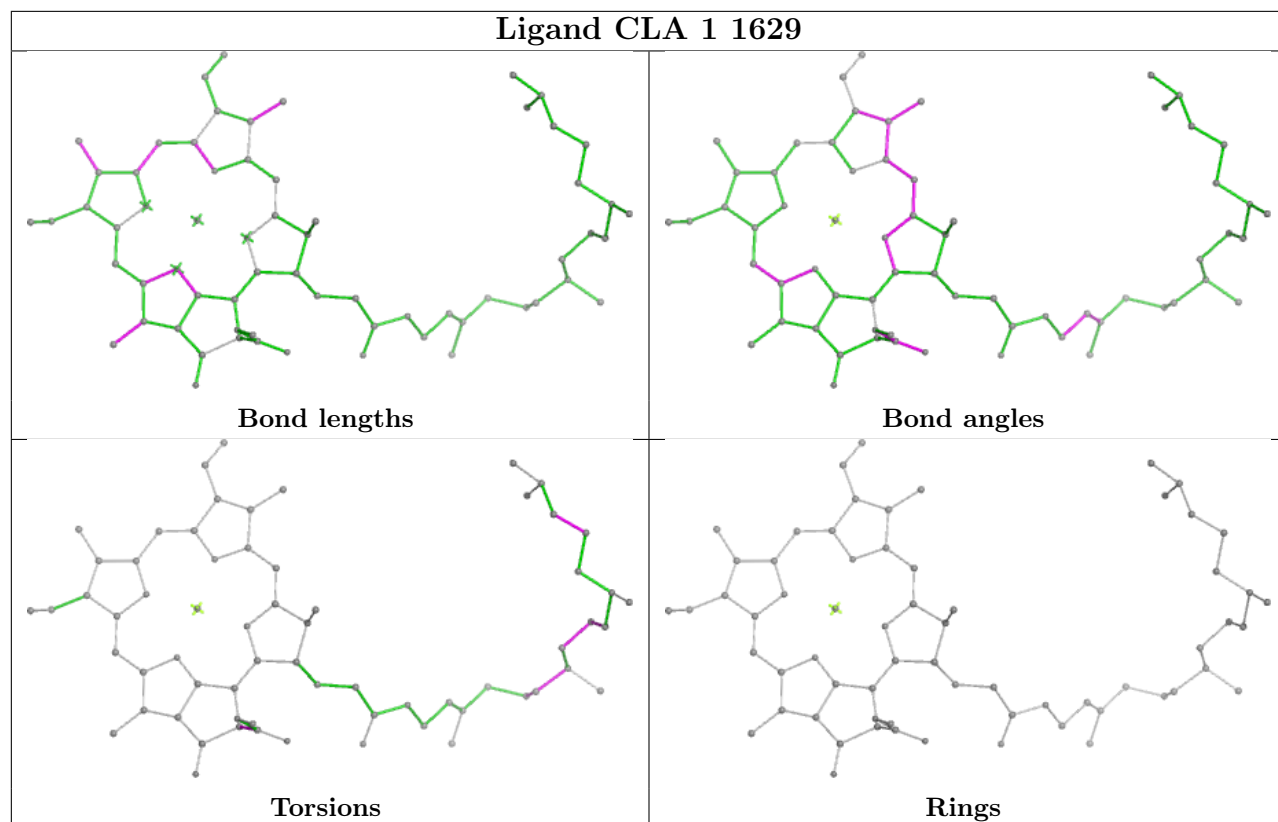


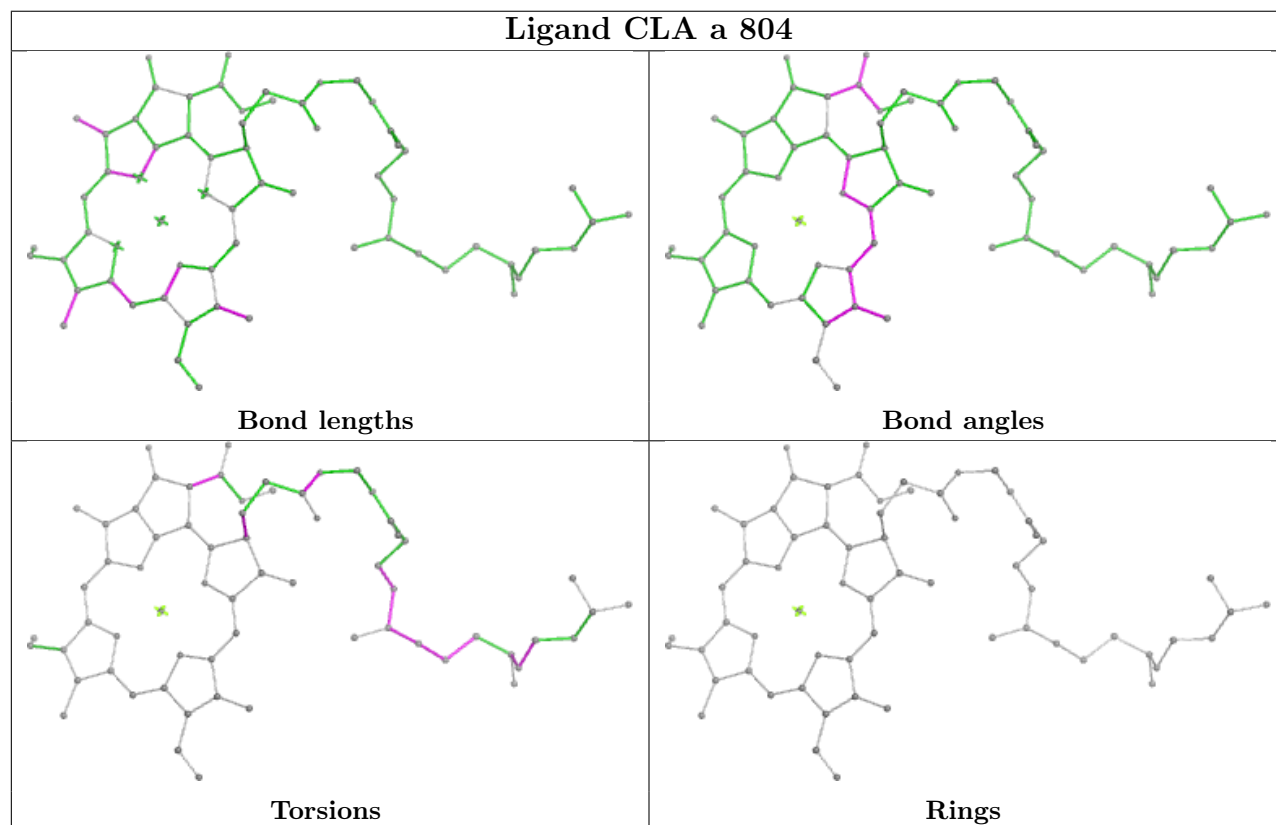
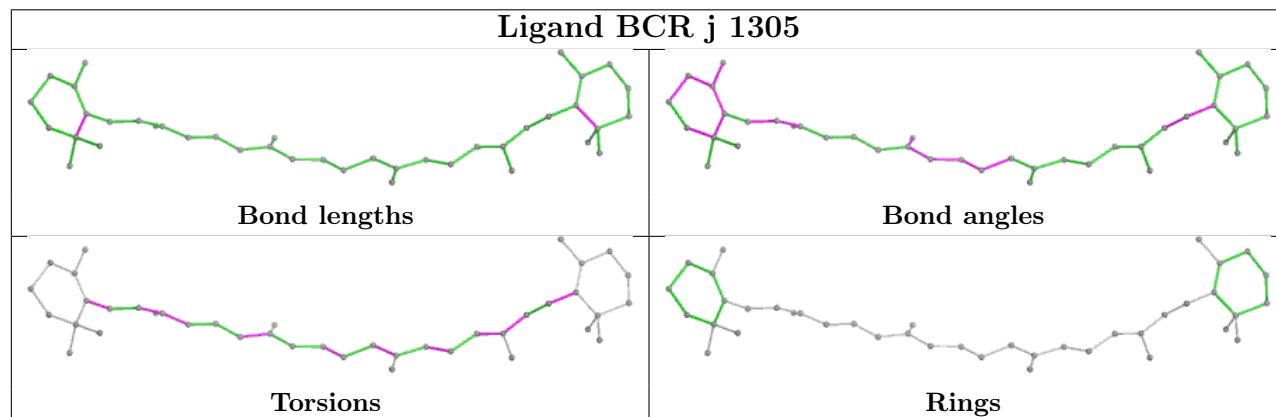
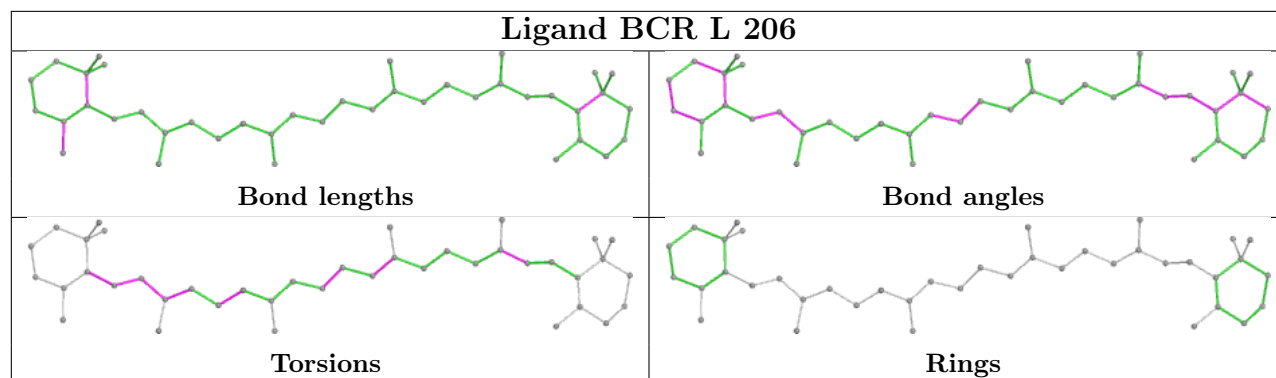
Rings



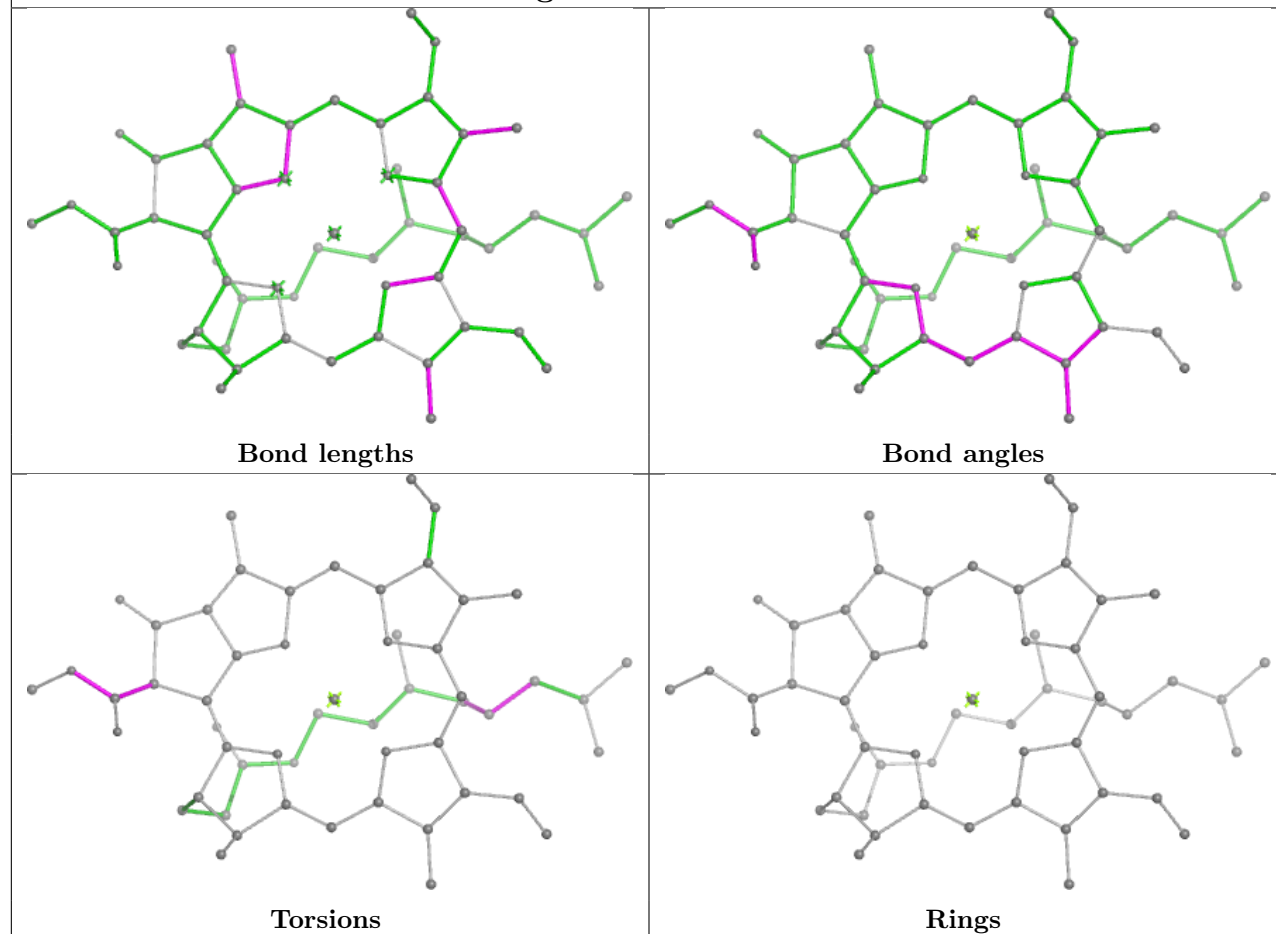




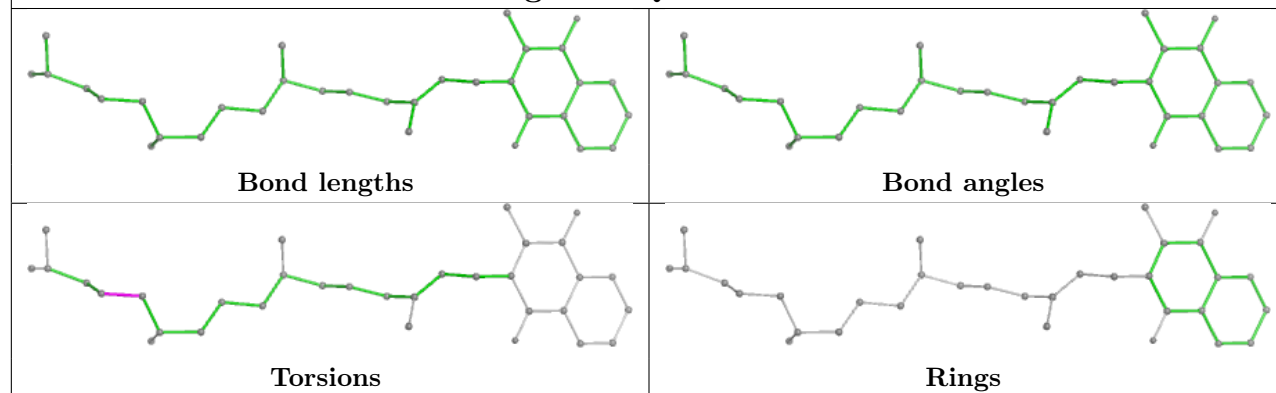




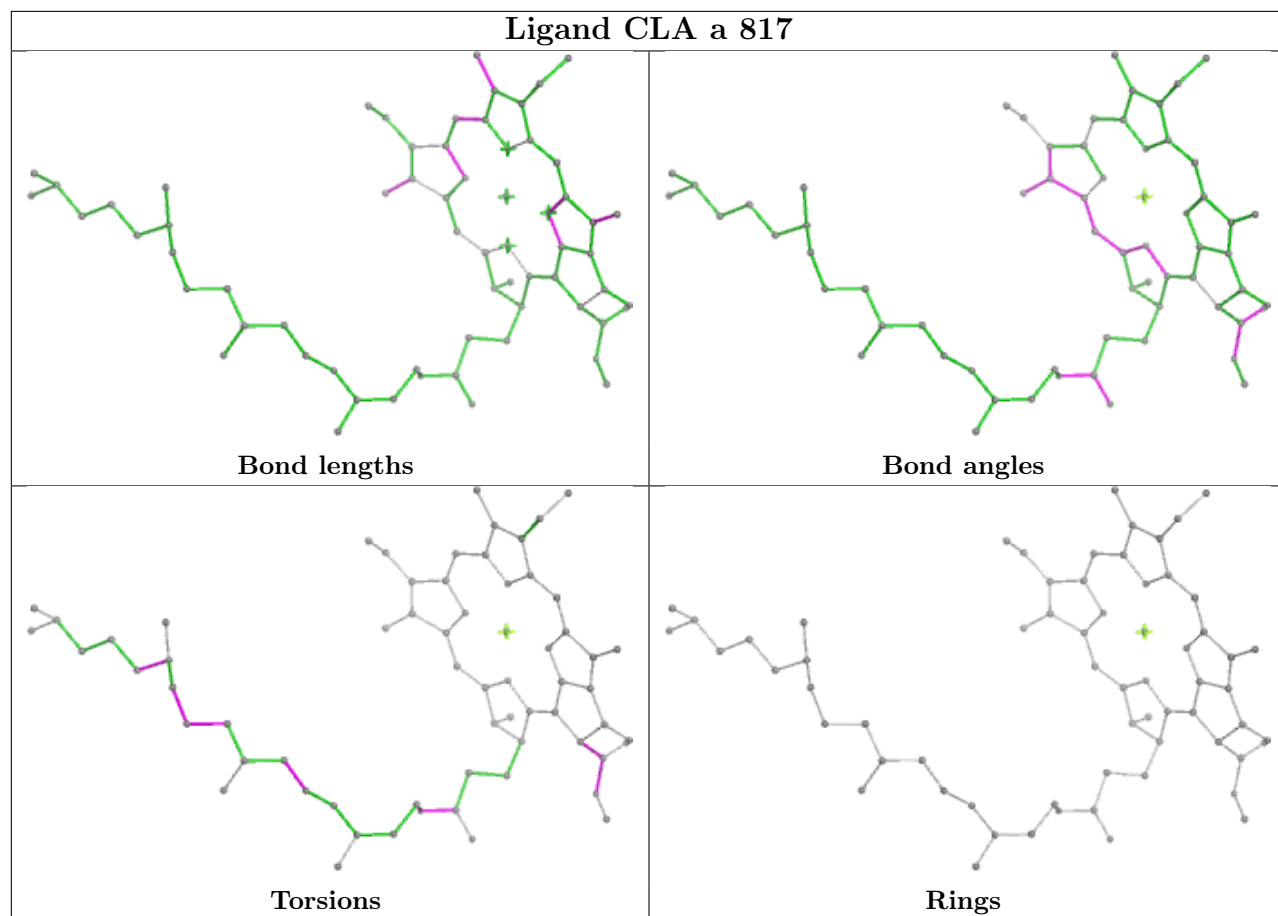
## Ligand CLA 2 823



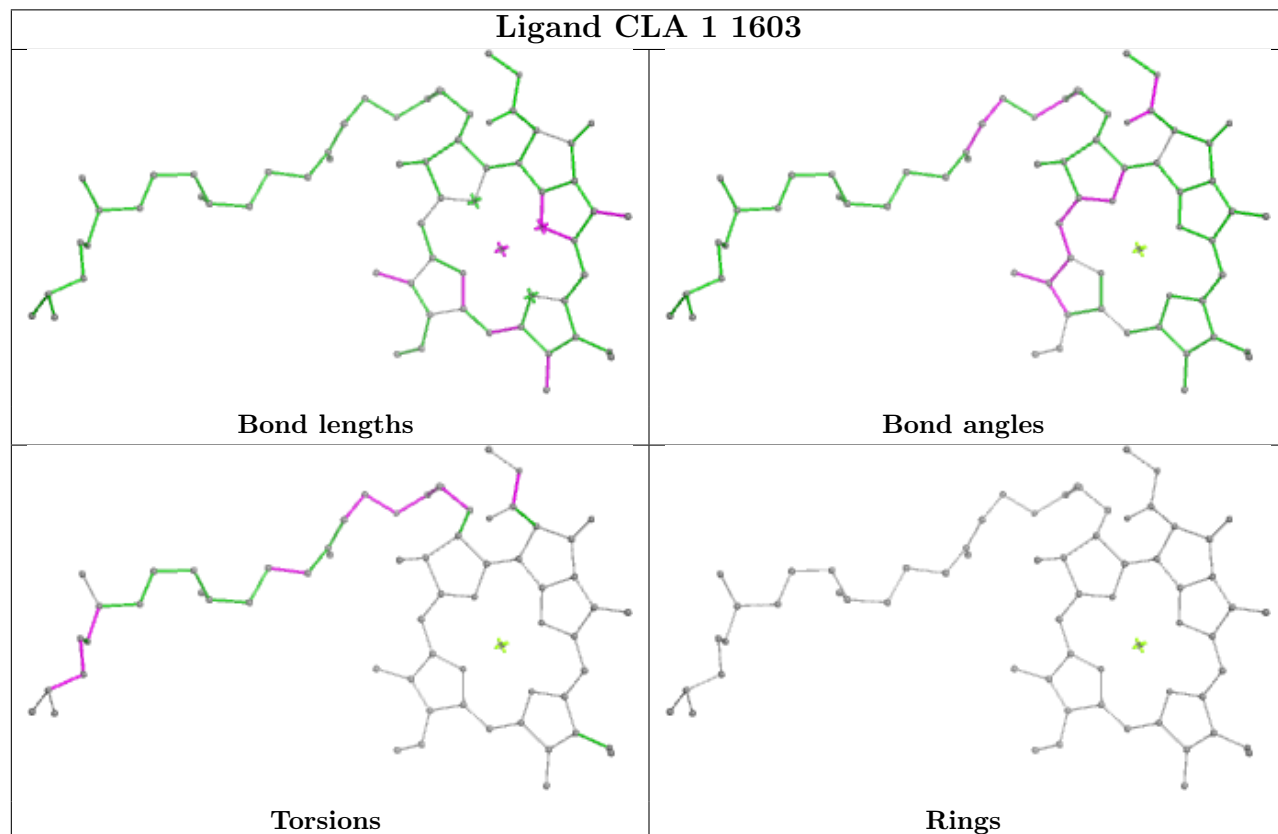
## Ligand PQN 1 1646



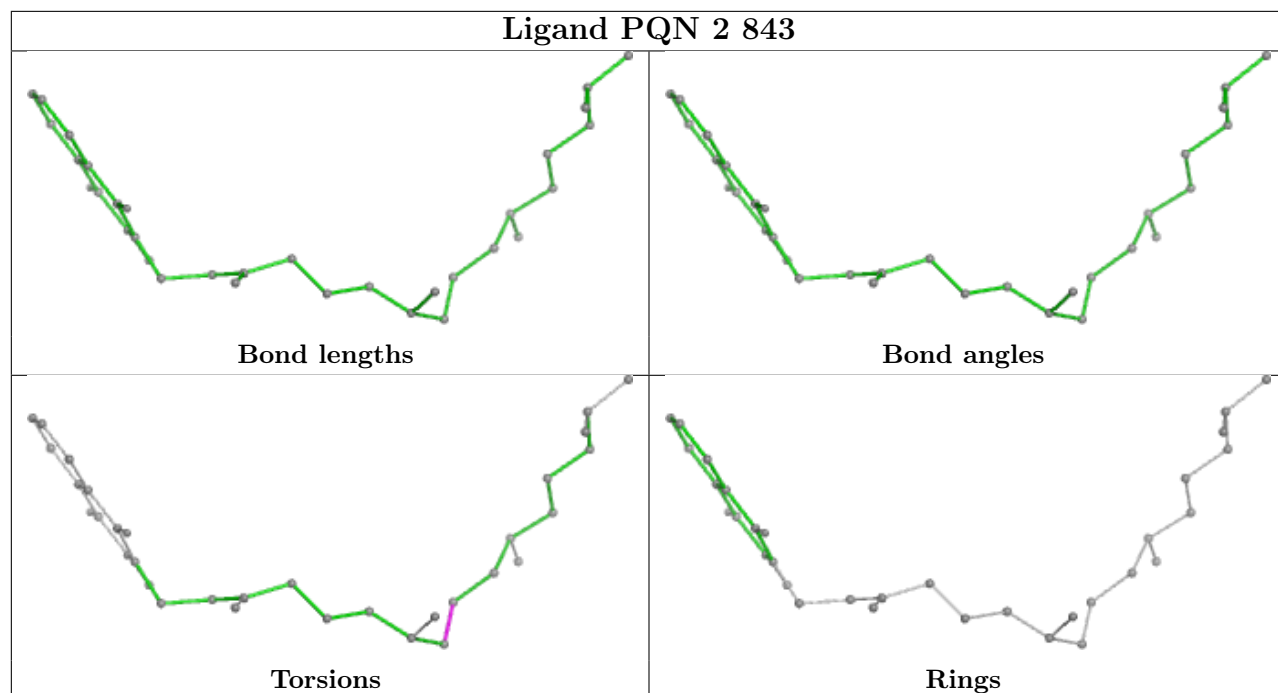
## Ligand CLA a 817

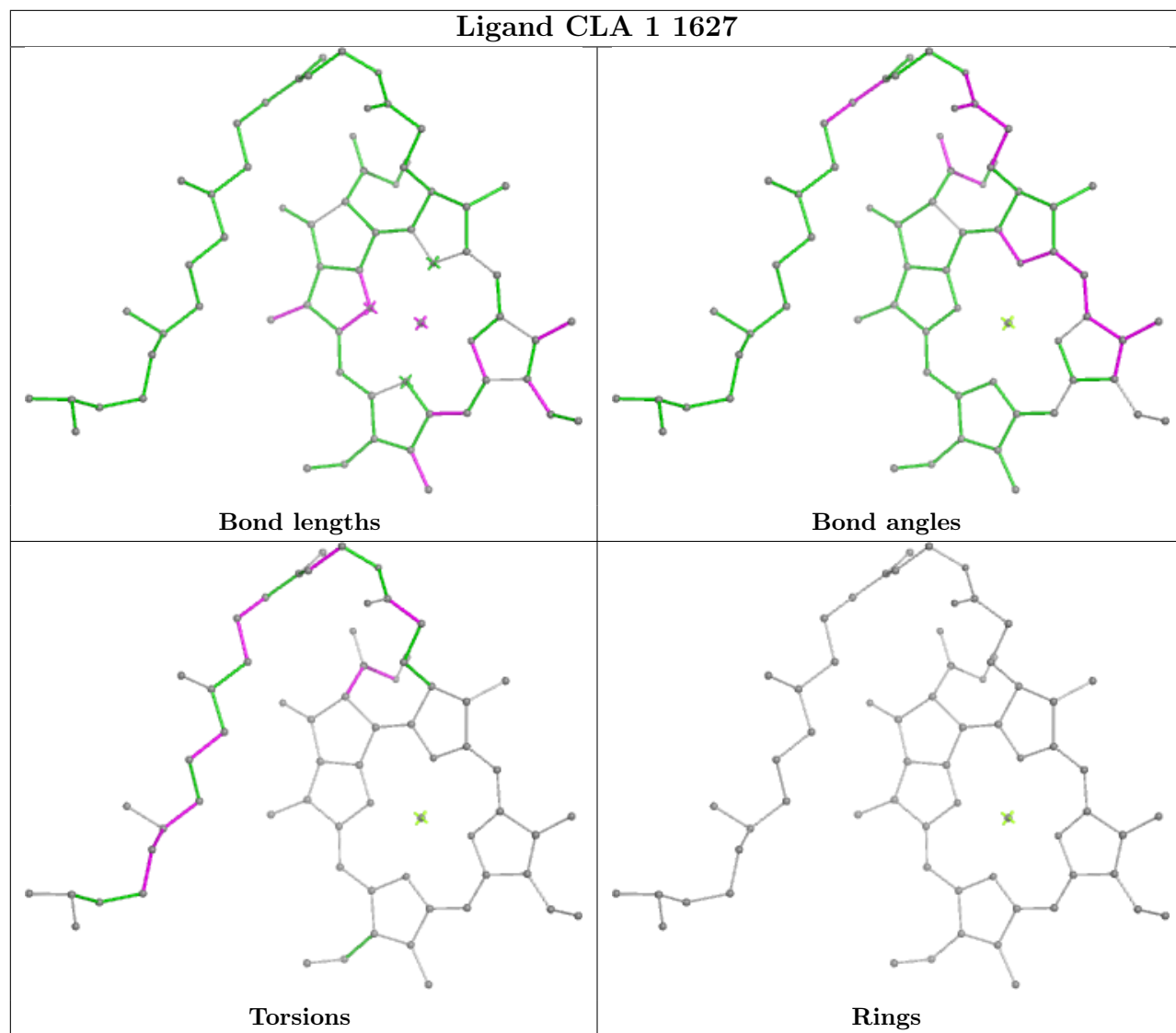


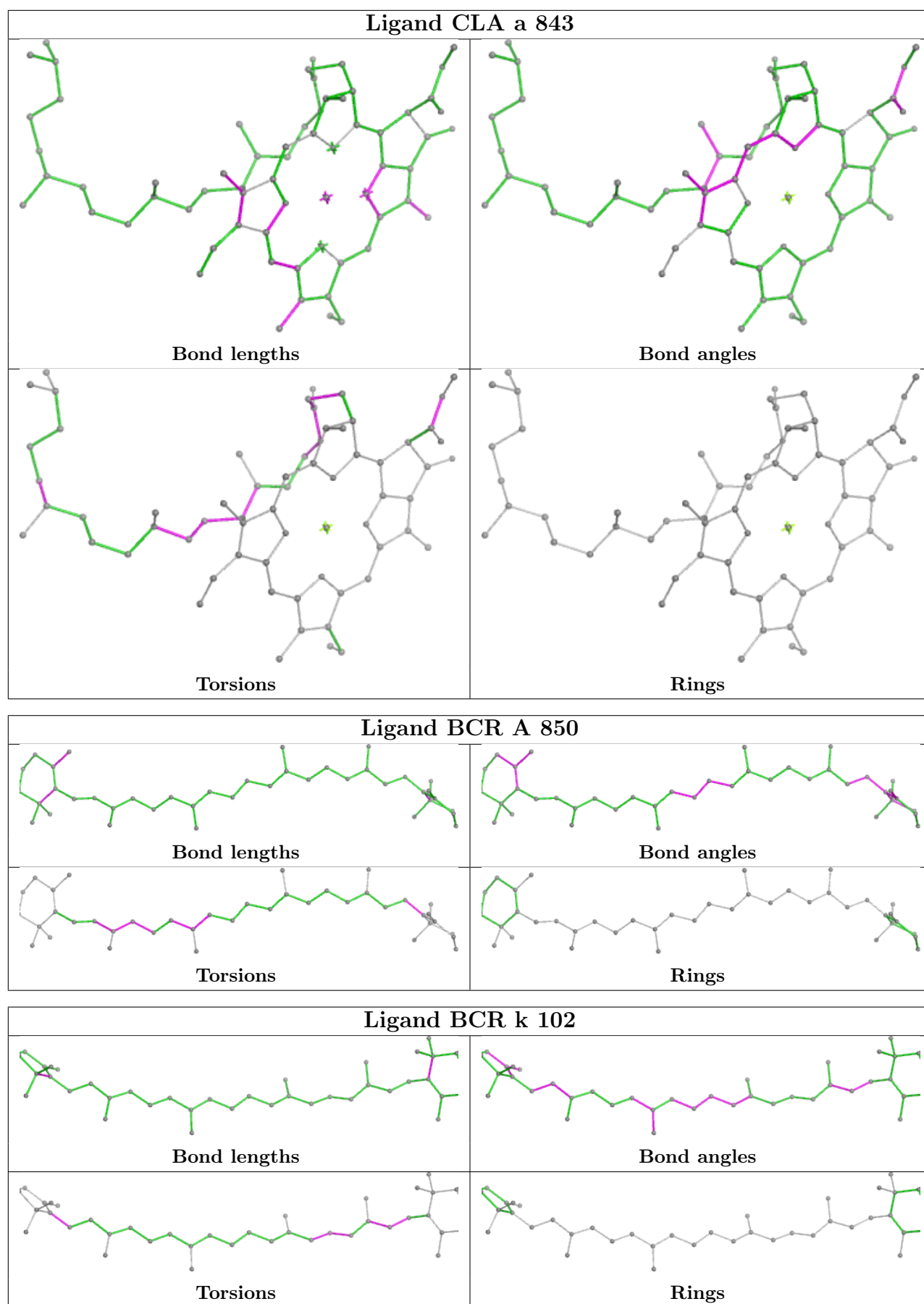
## Ligand CLA 1 1603



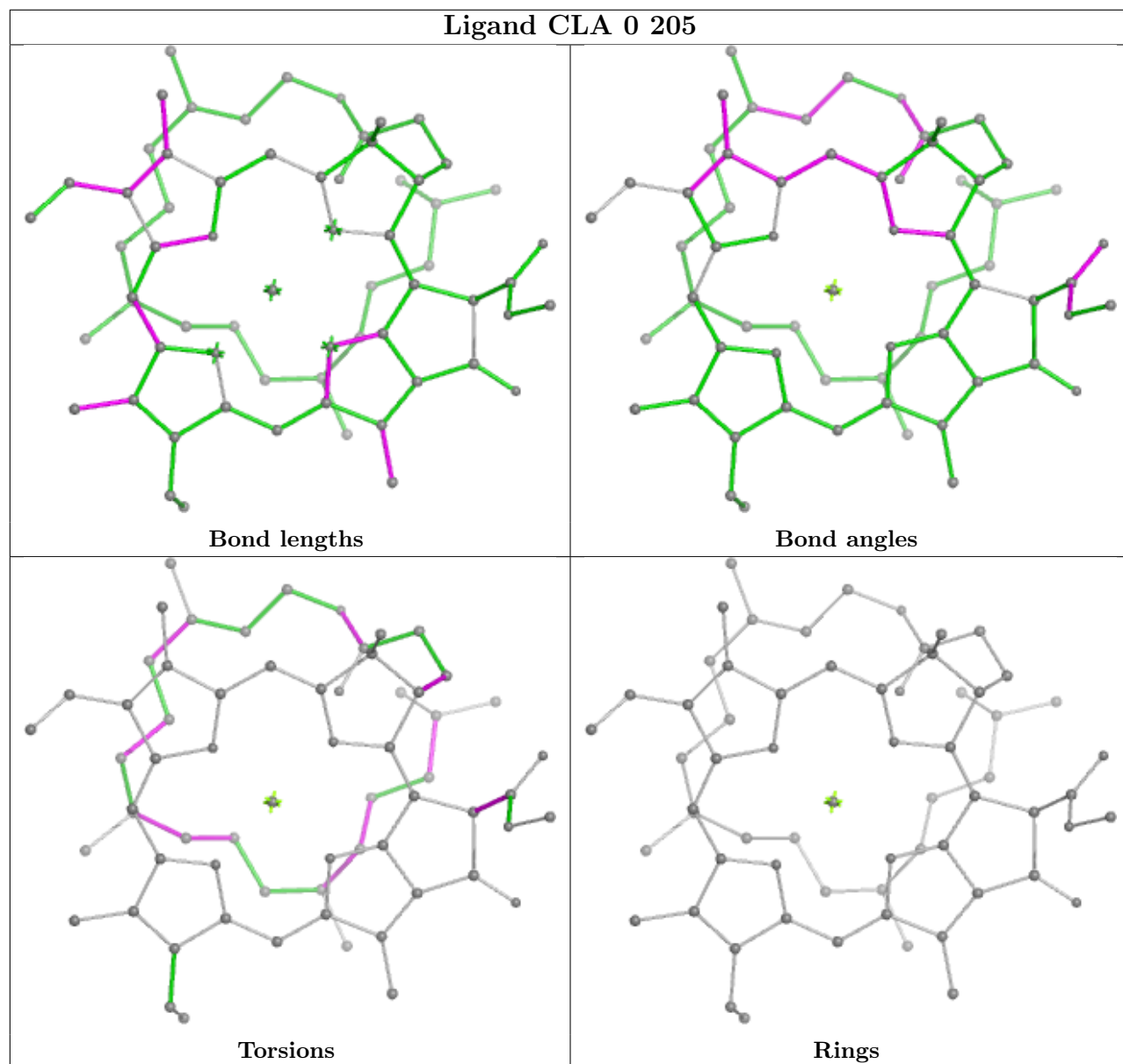




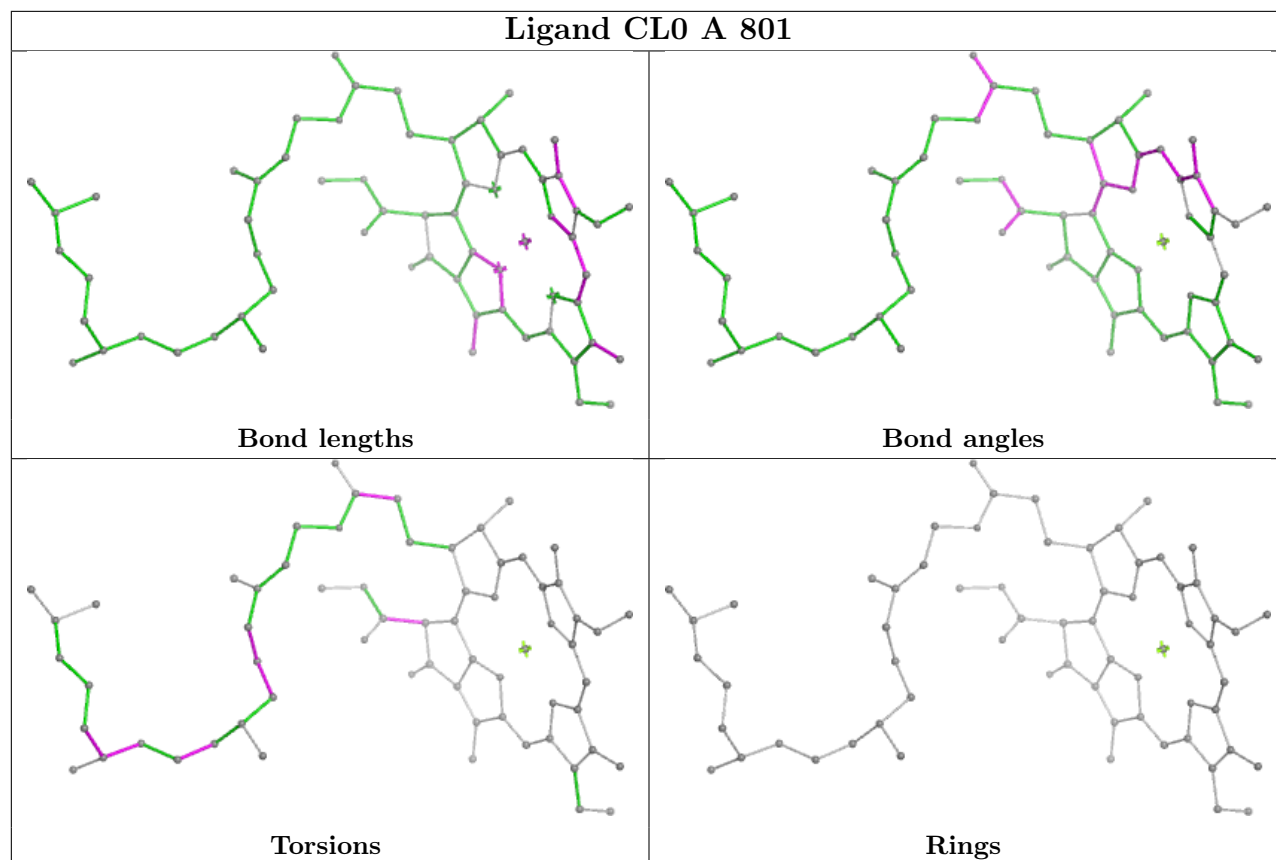




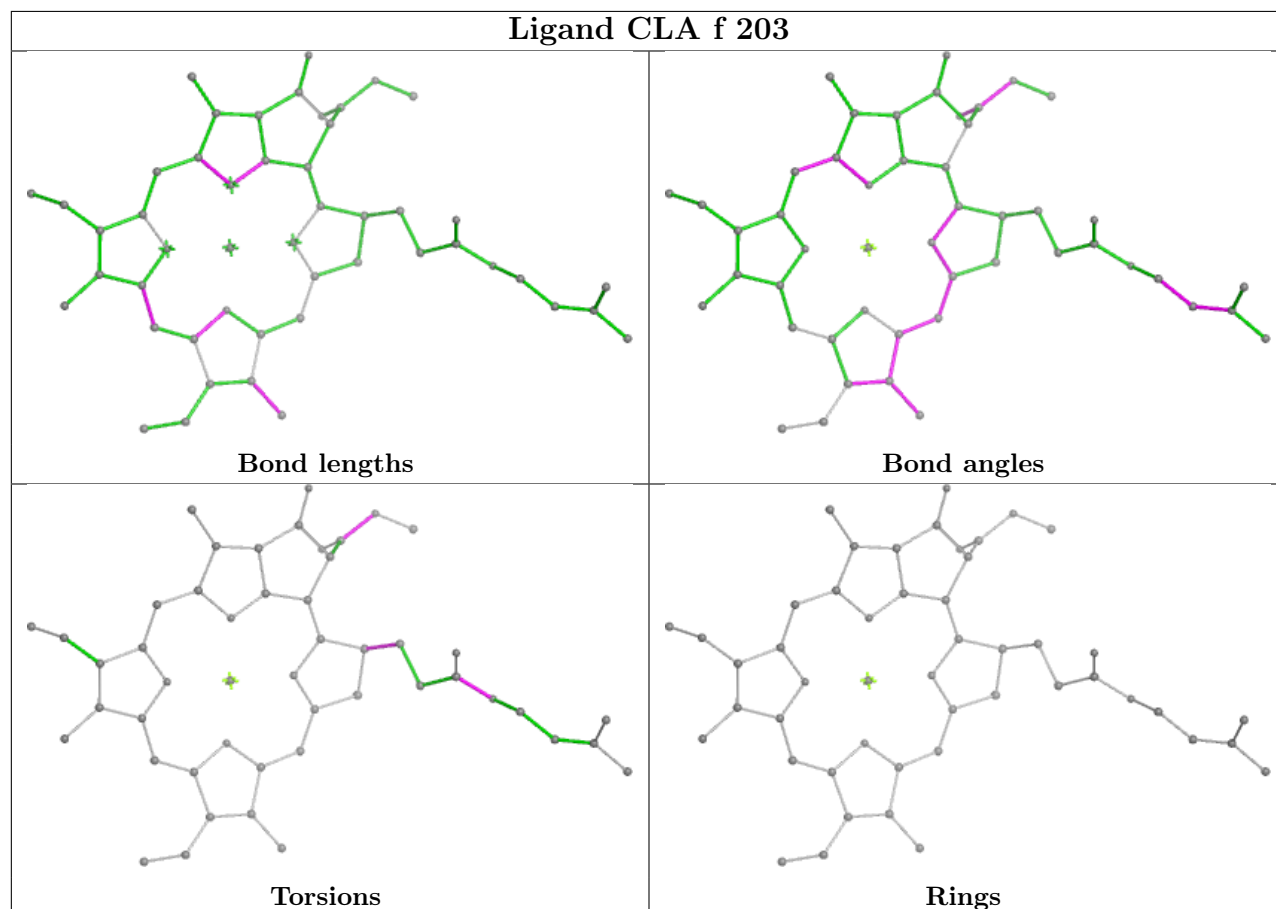
## Ligand CLA 0 205

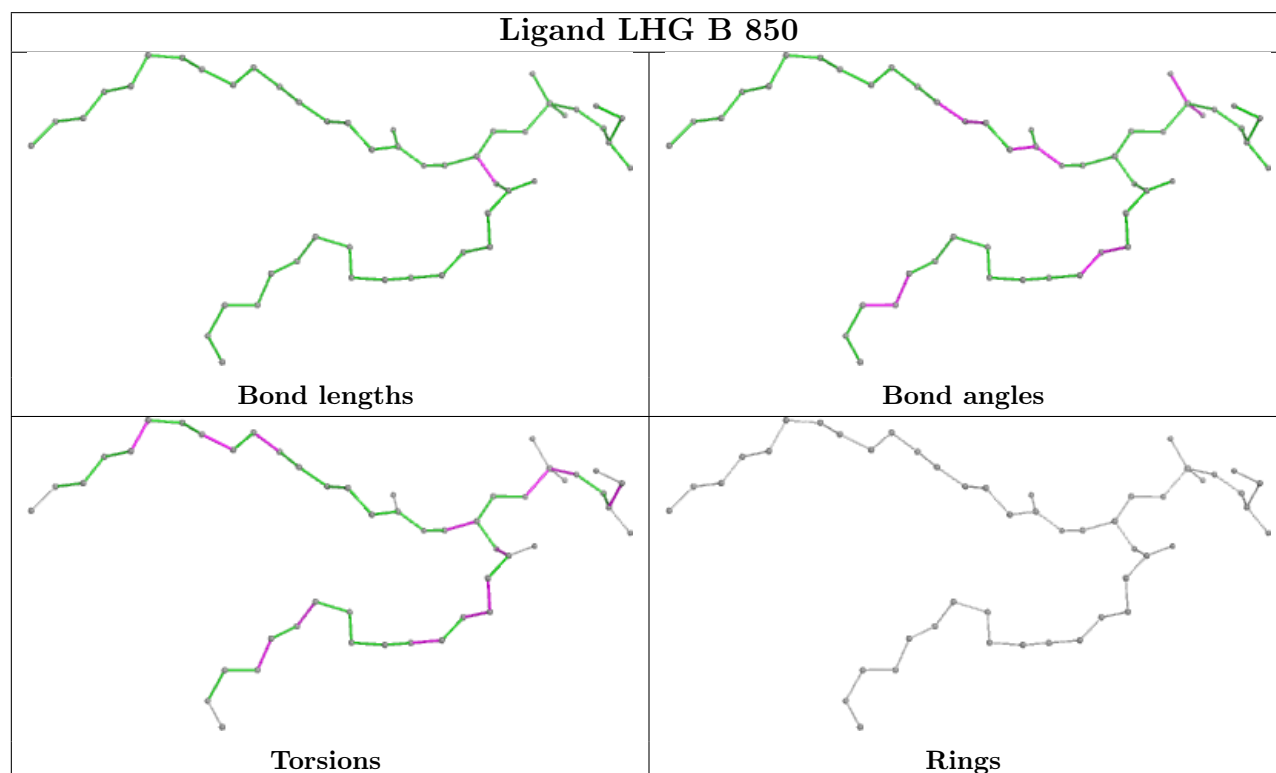
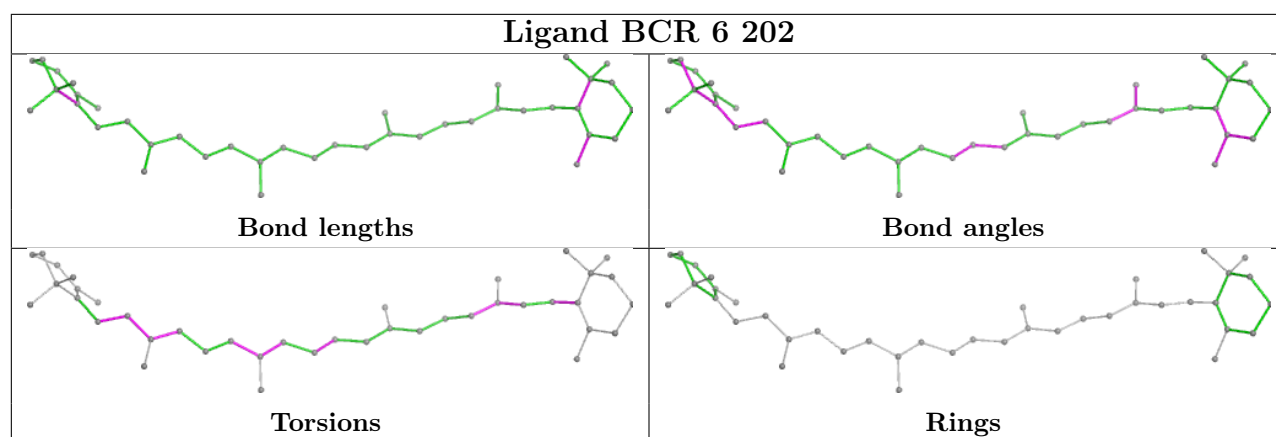


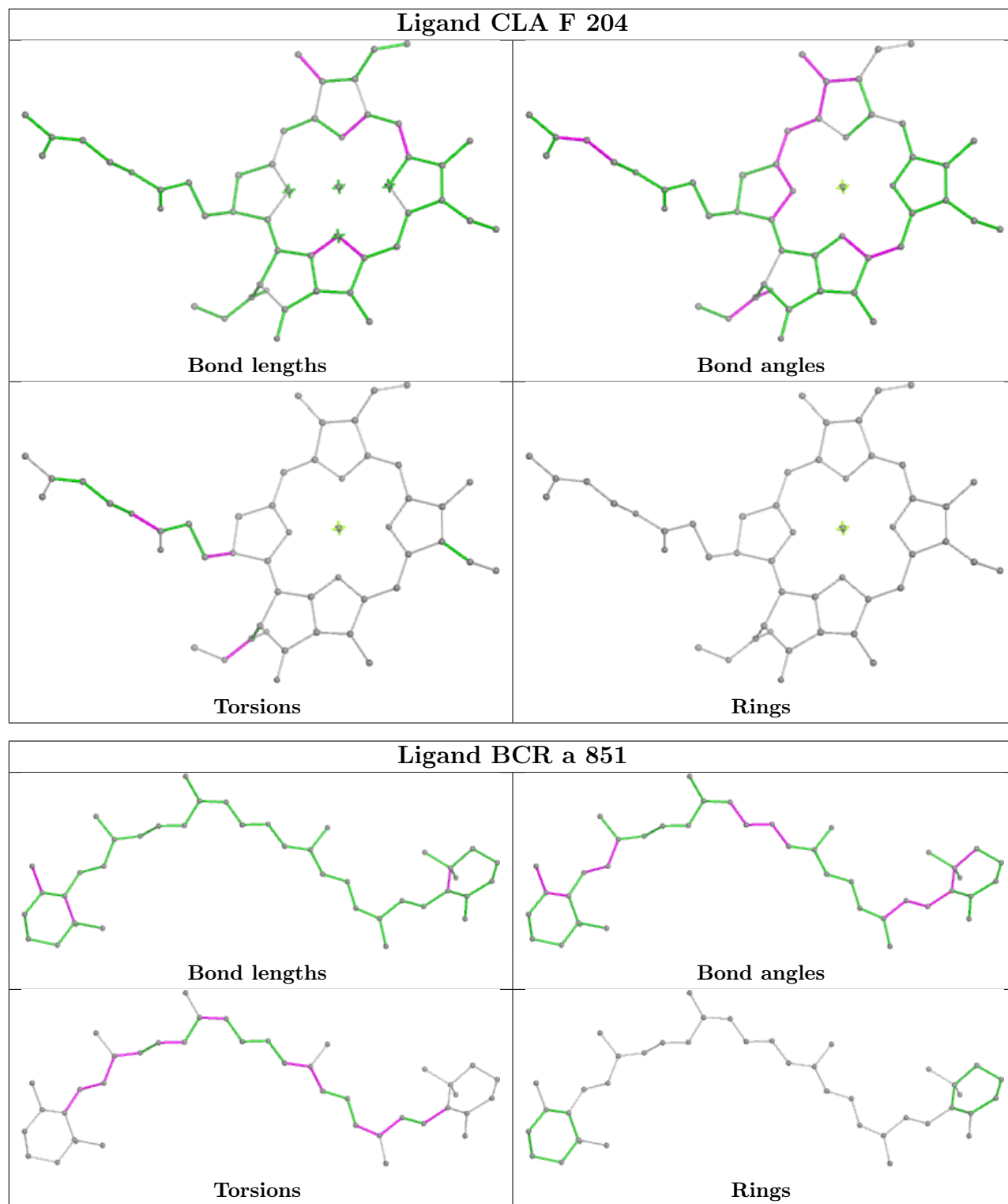
## Ligand CL0 A 801

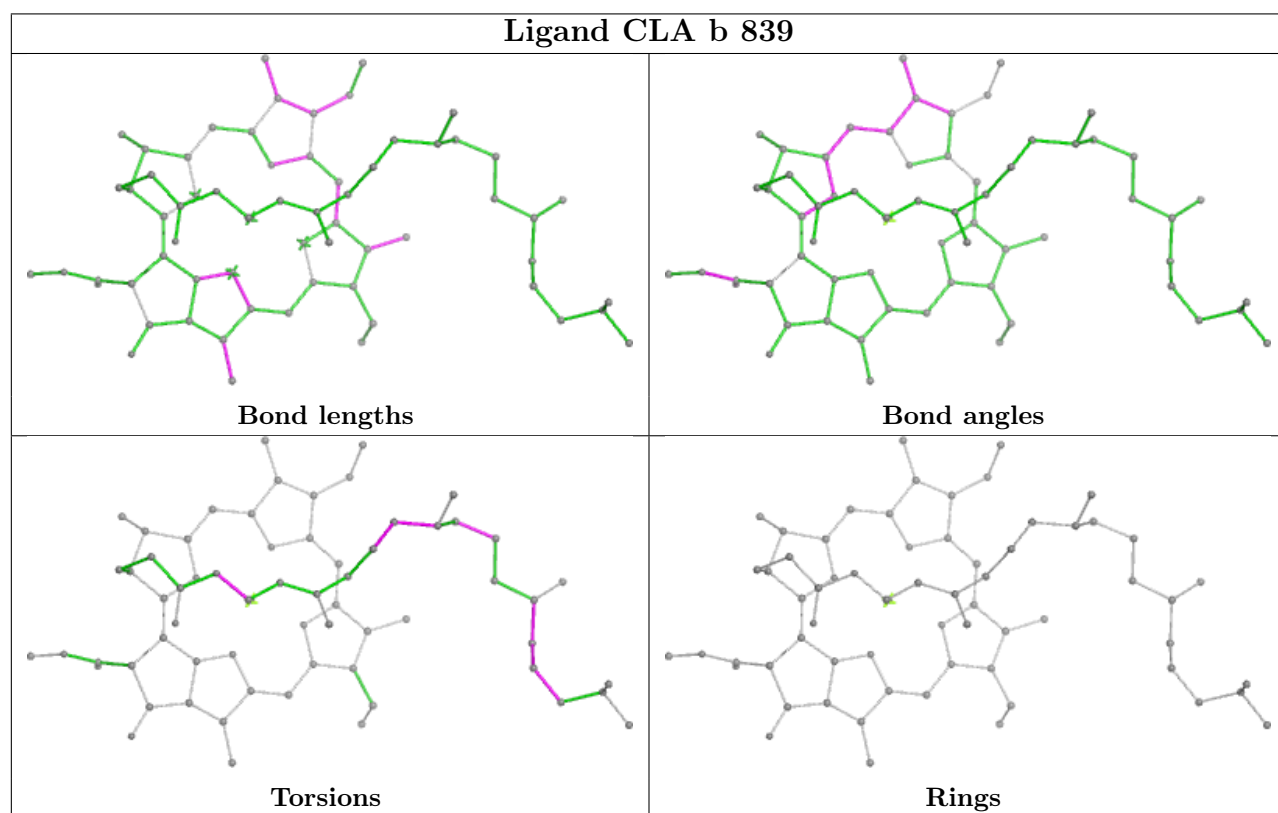
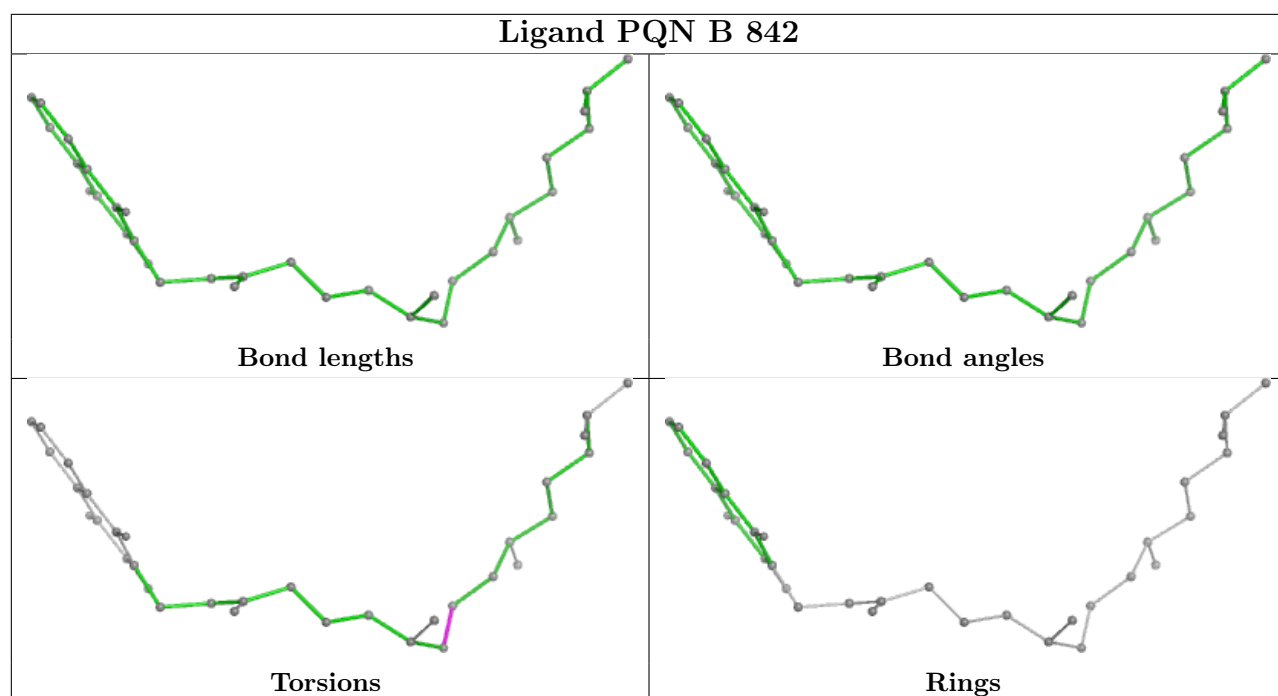


## Ligand CLA f 203

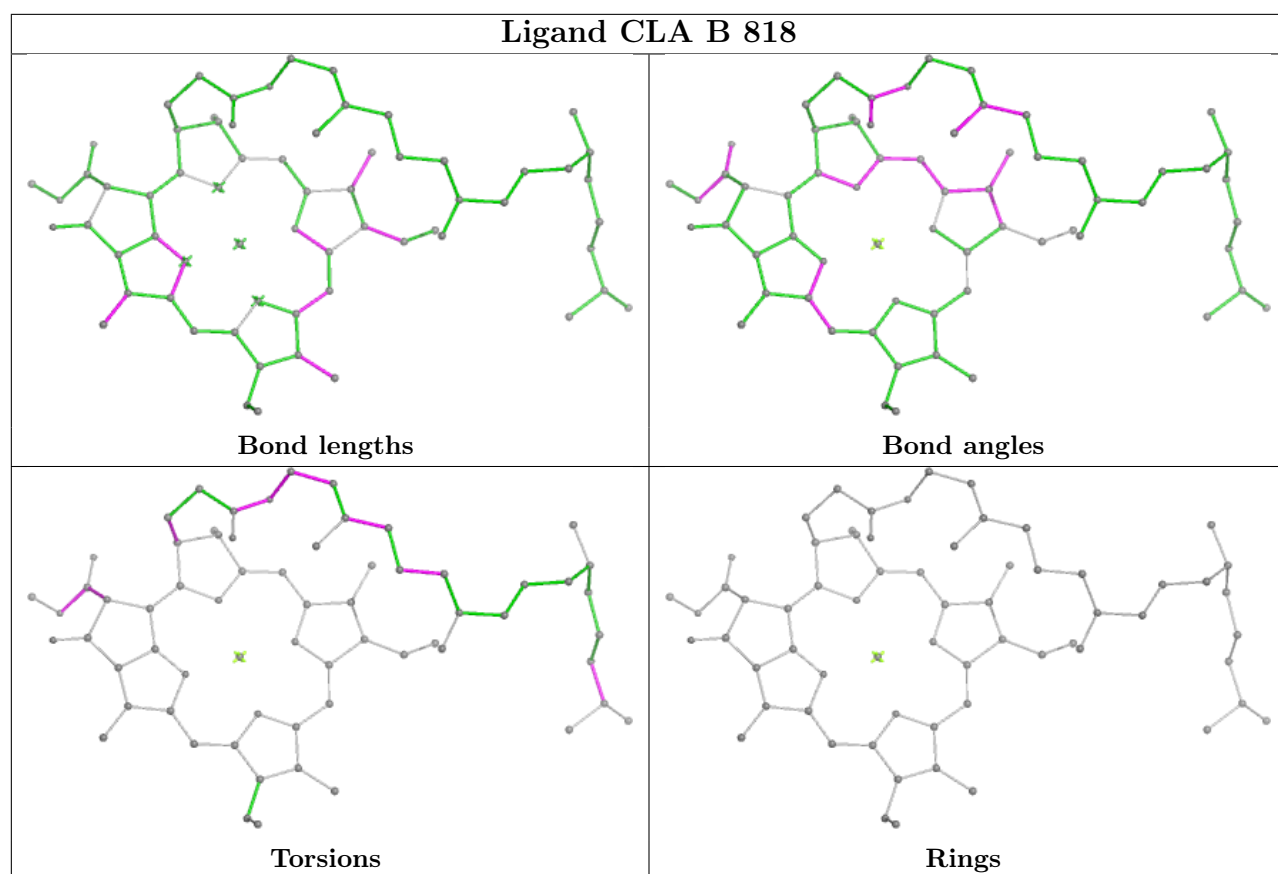




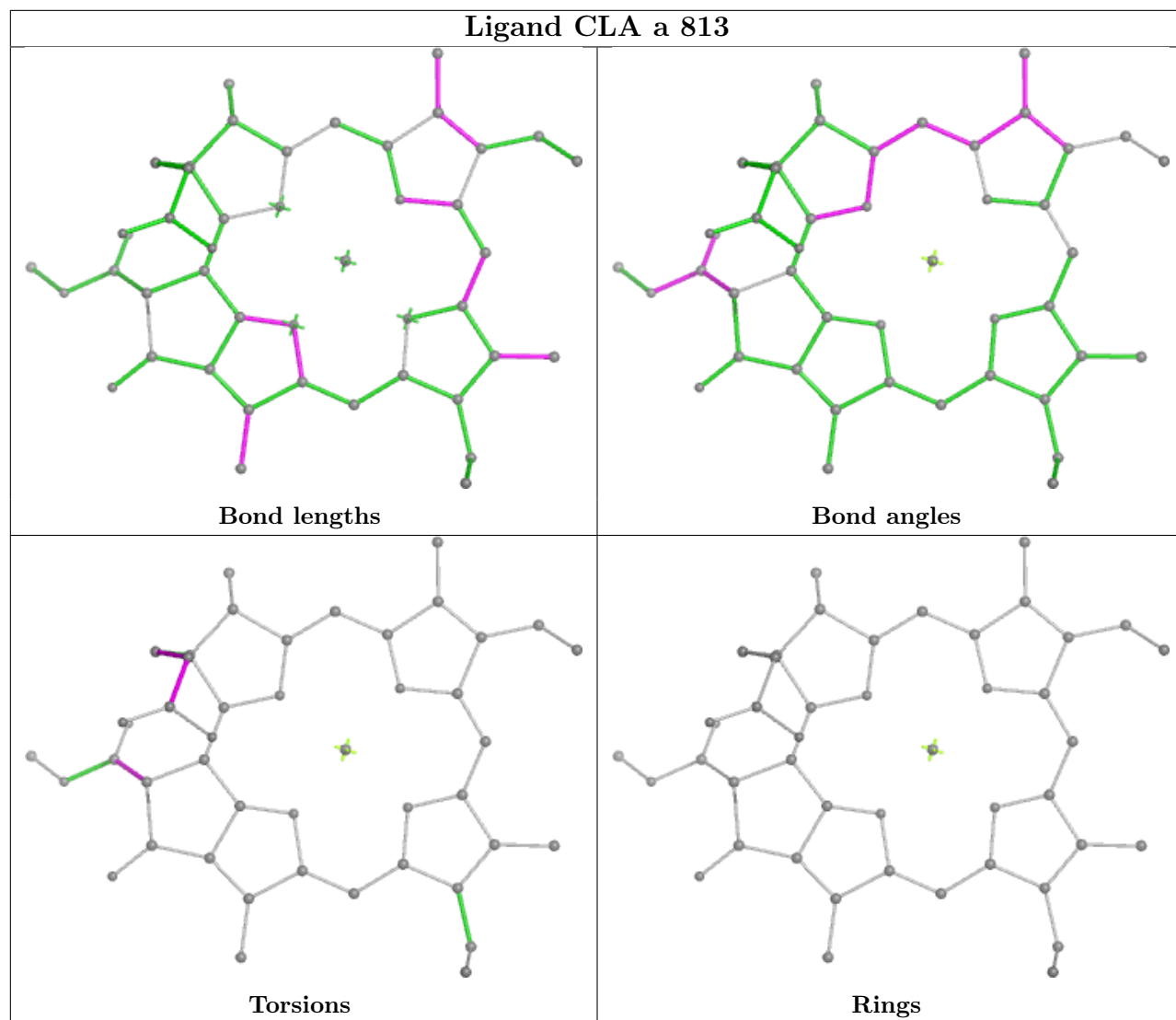


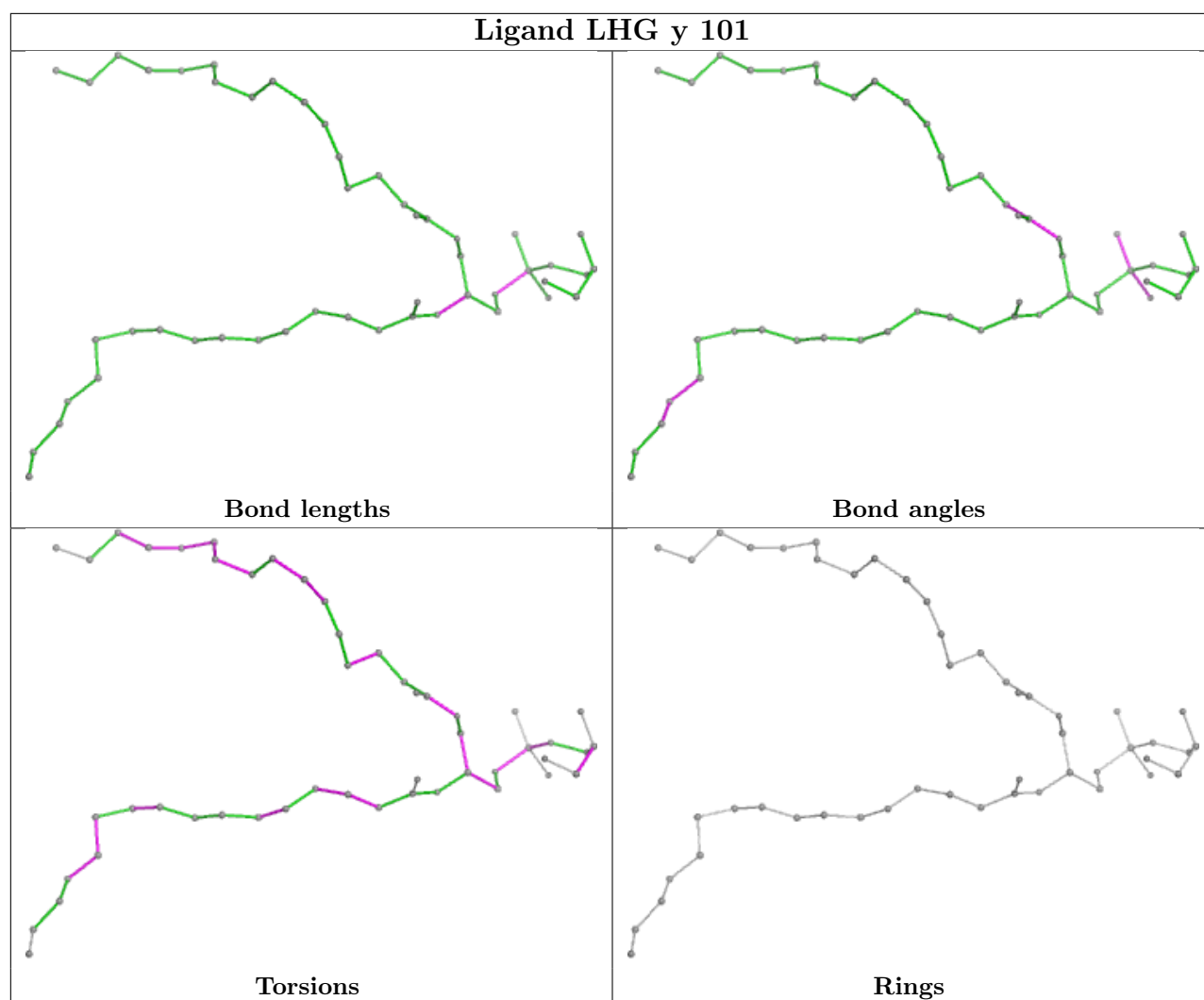


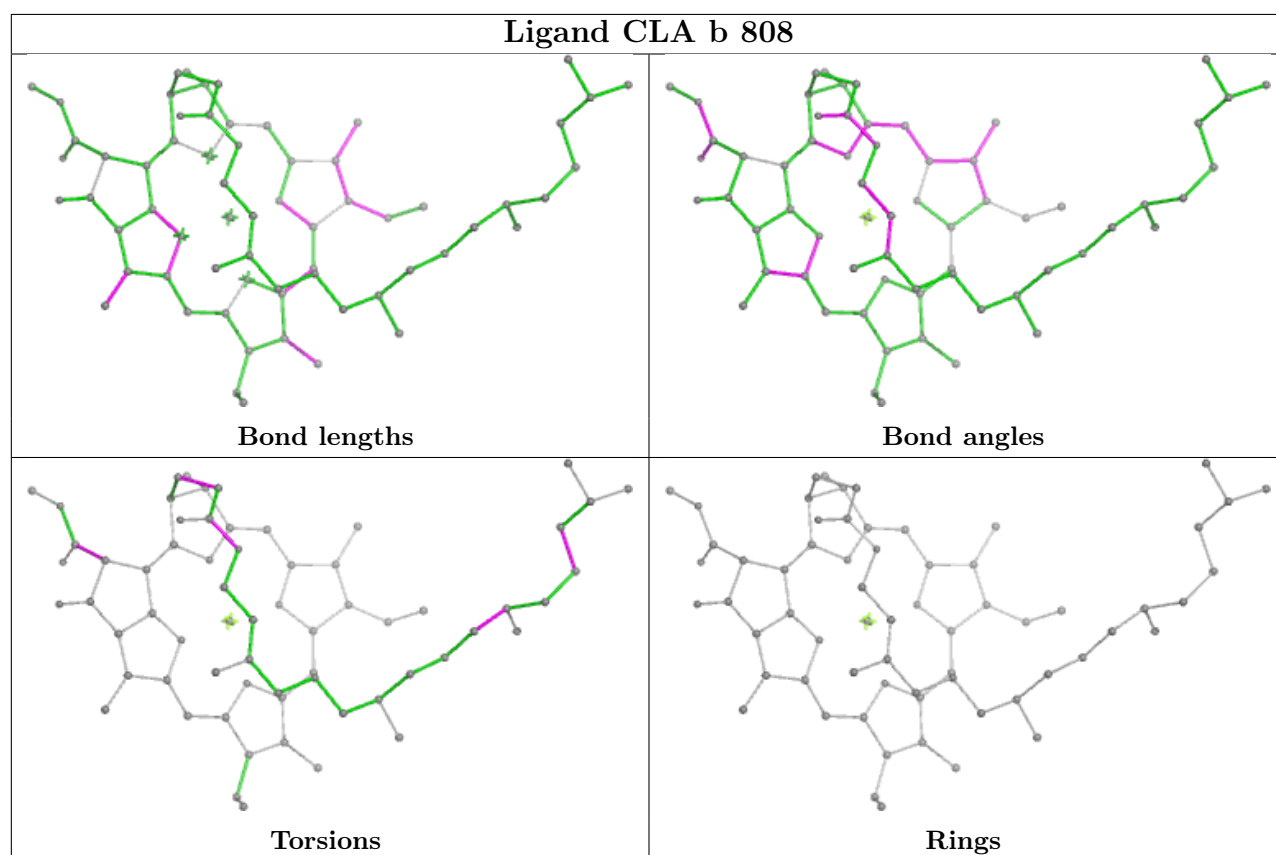
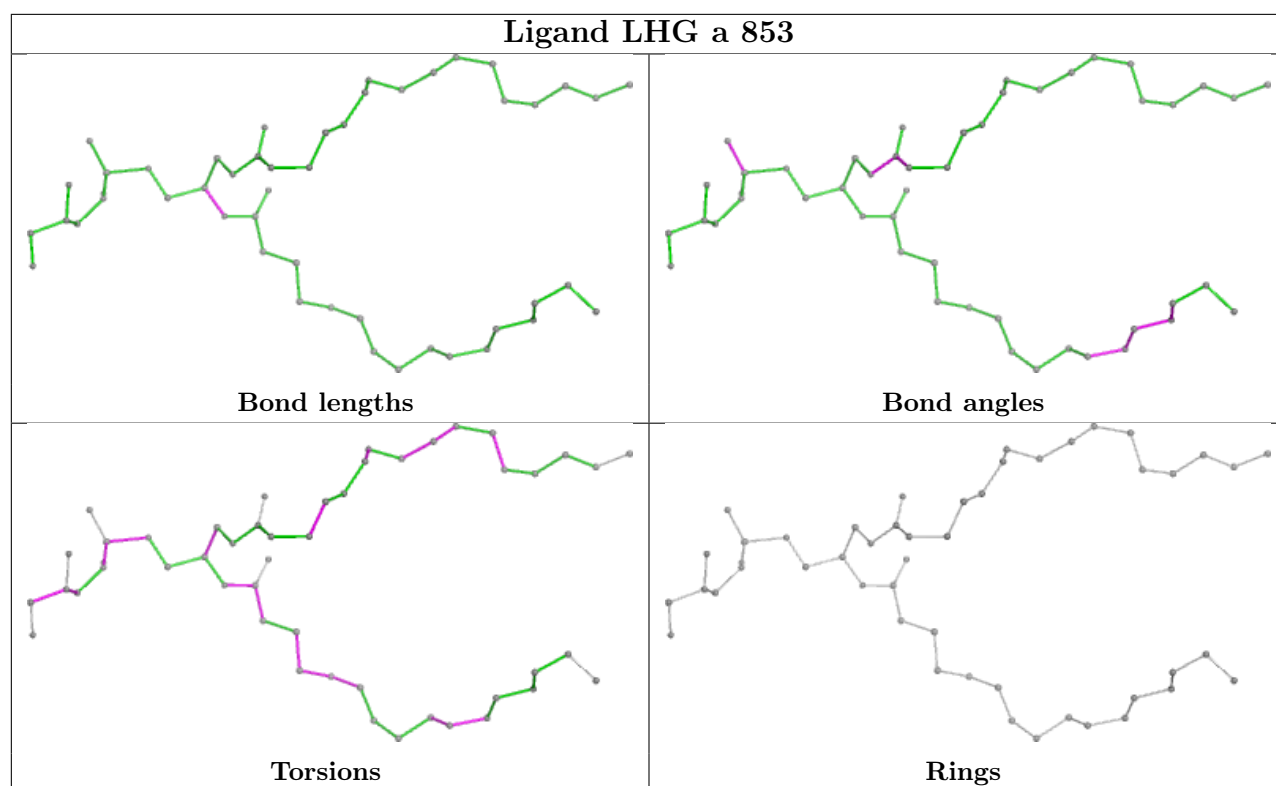


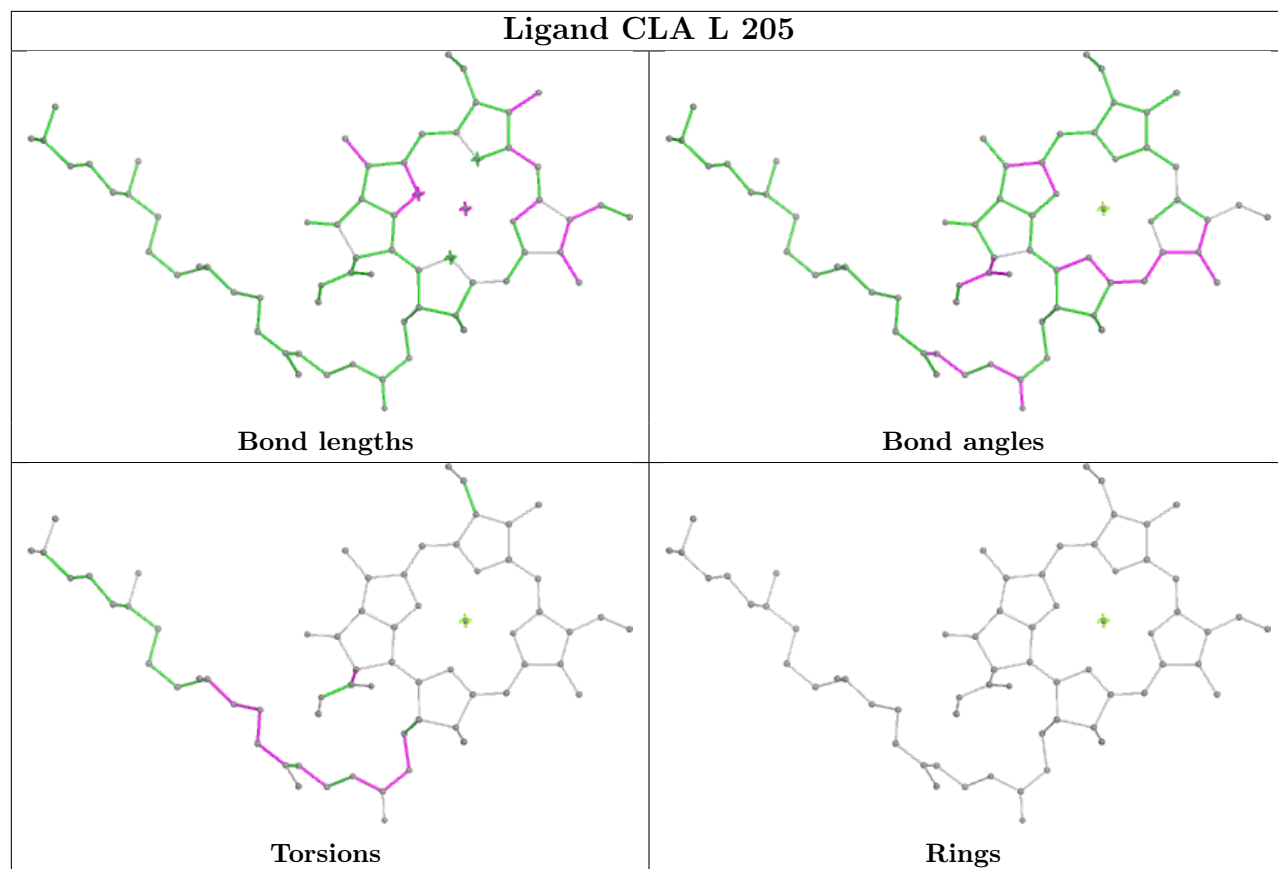


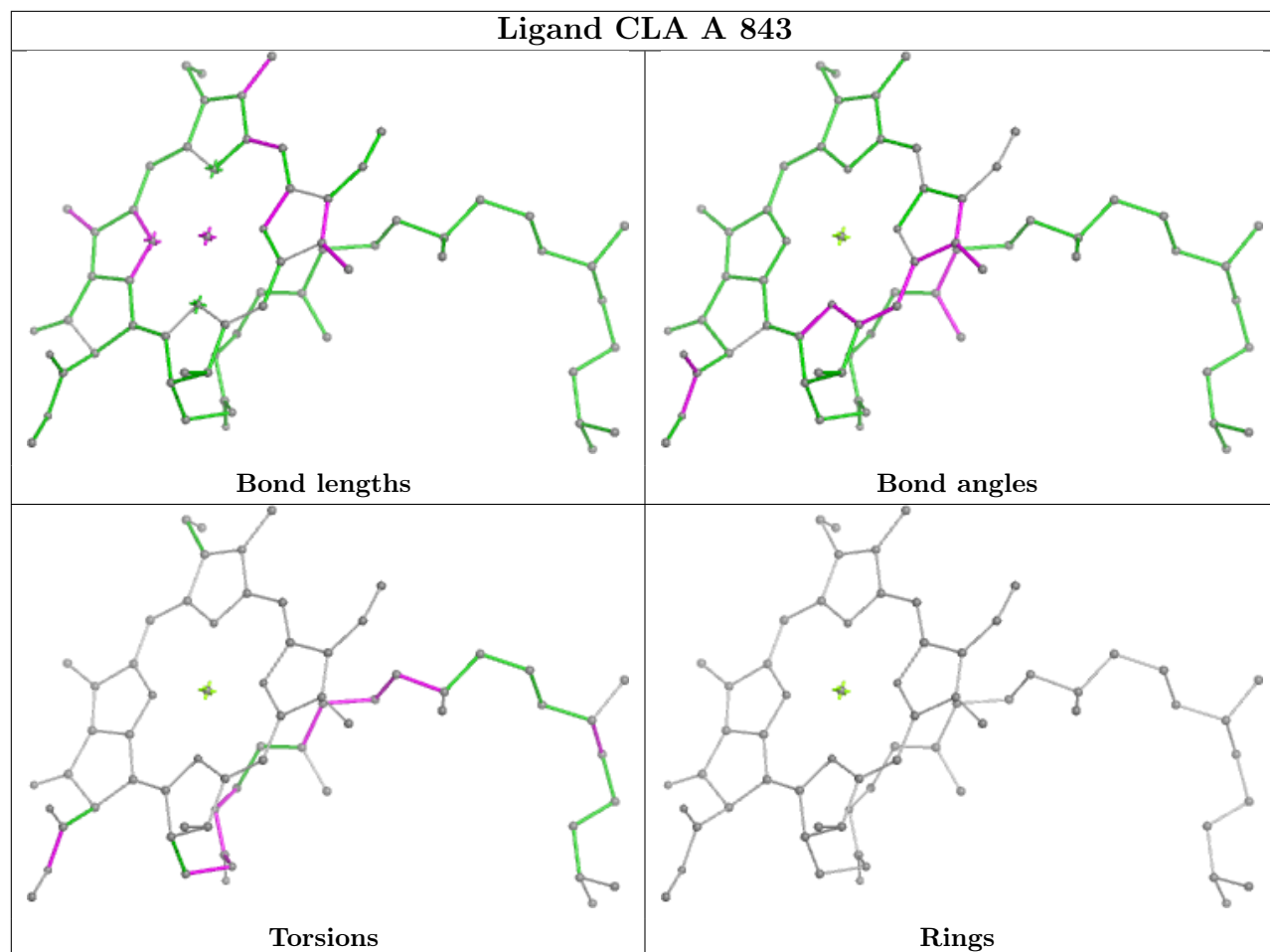
## Ligand CLA a 813



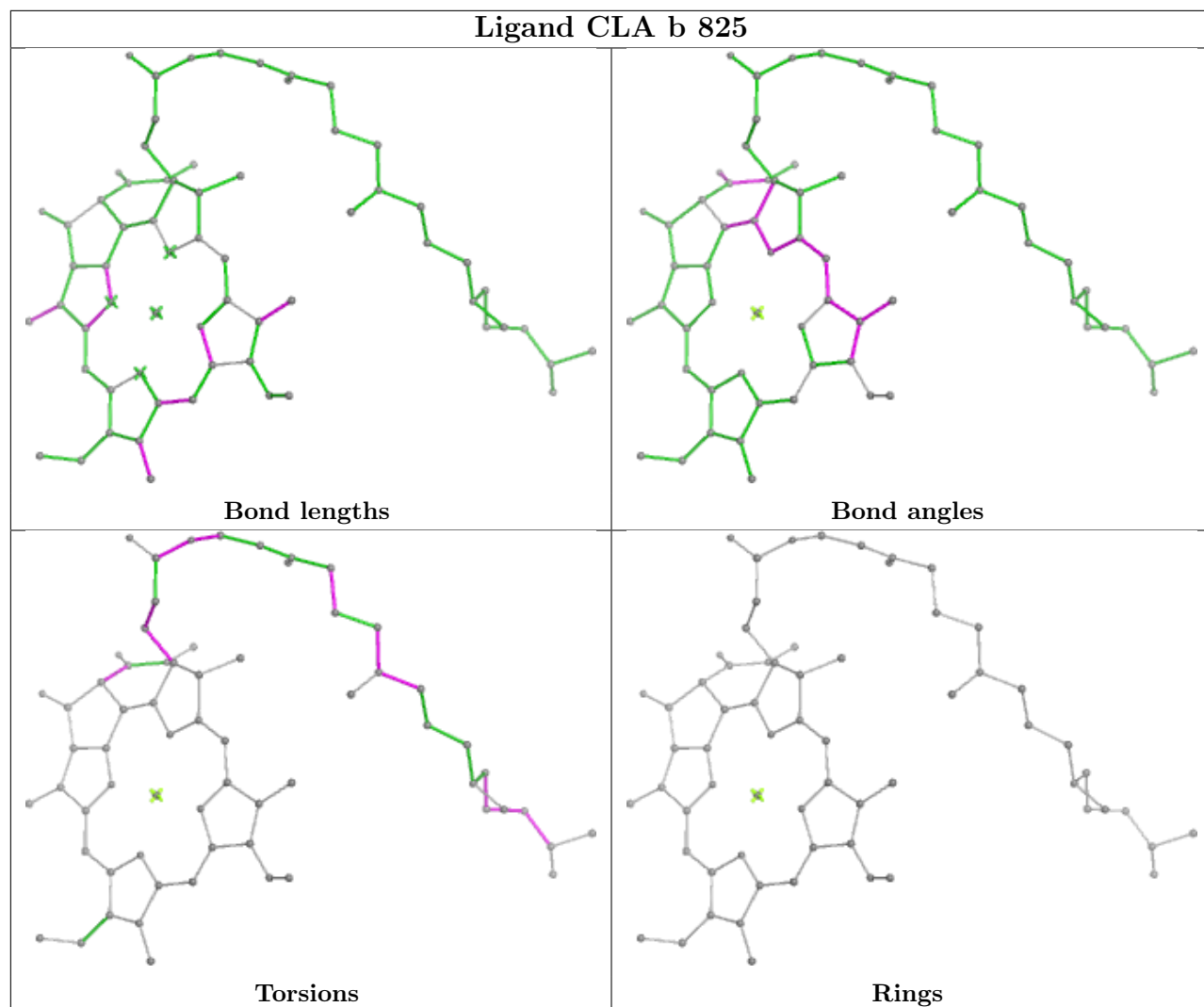




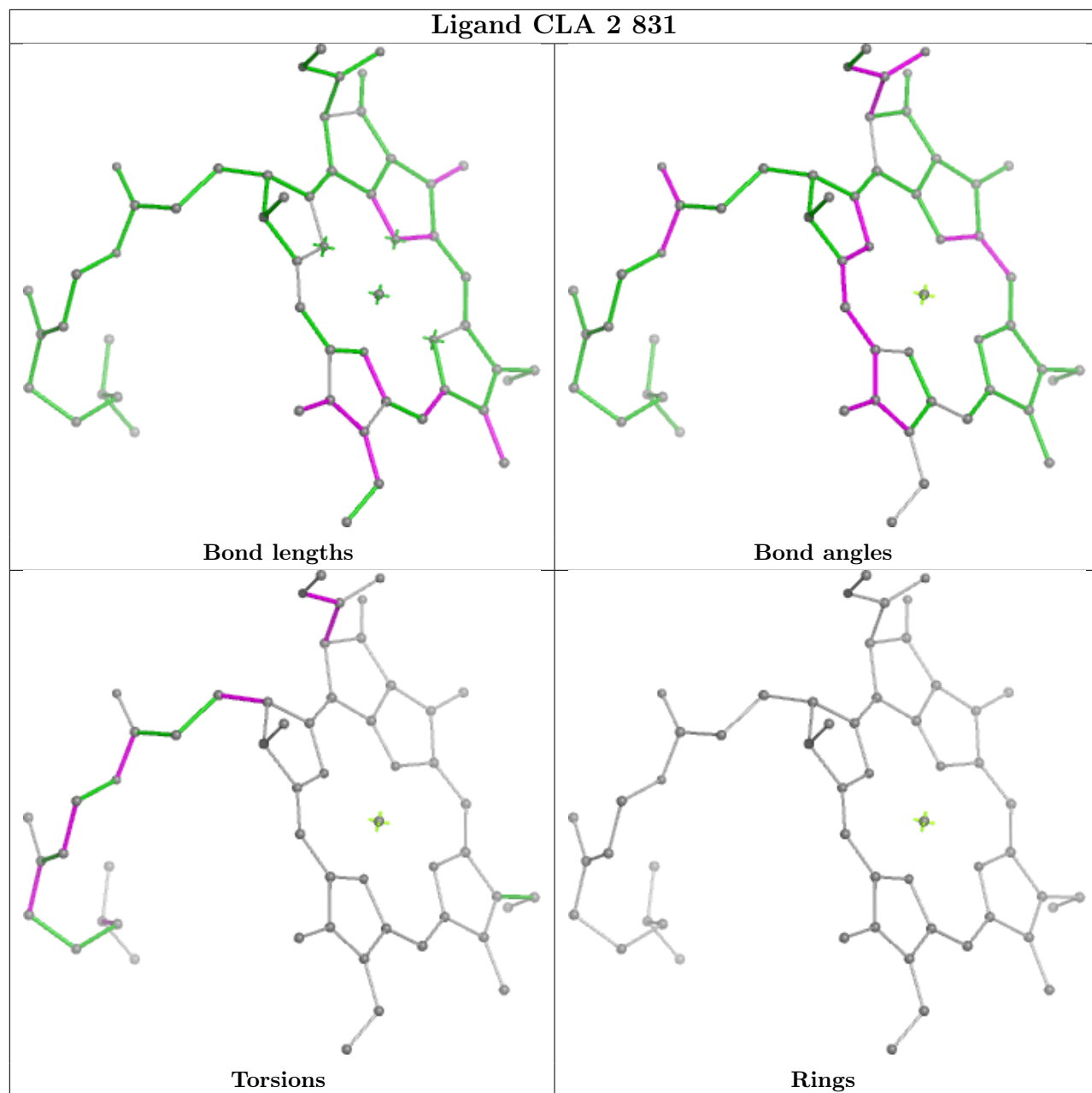




## Ligand CLA b 825

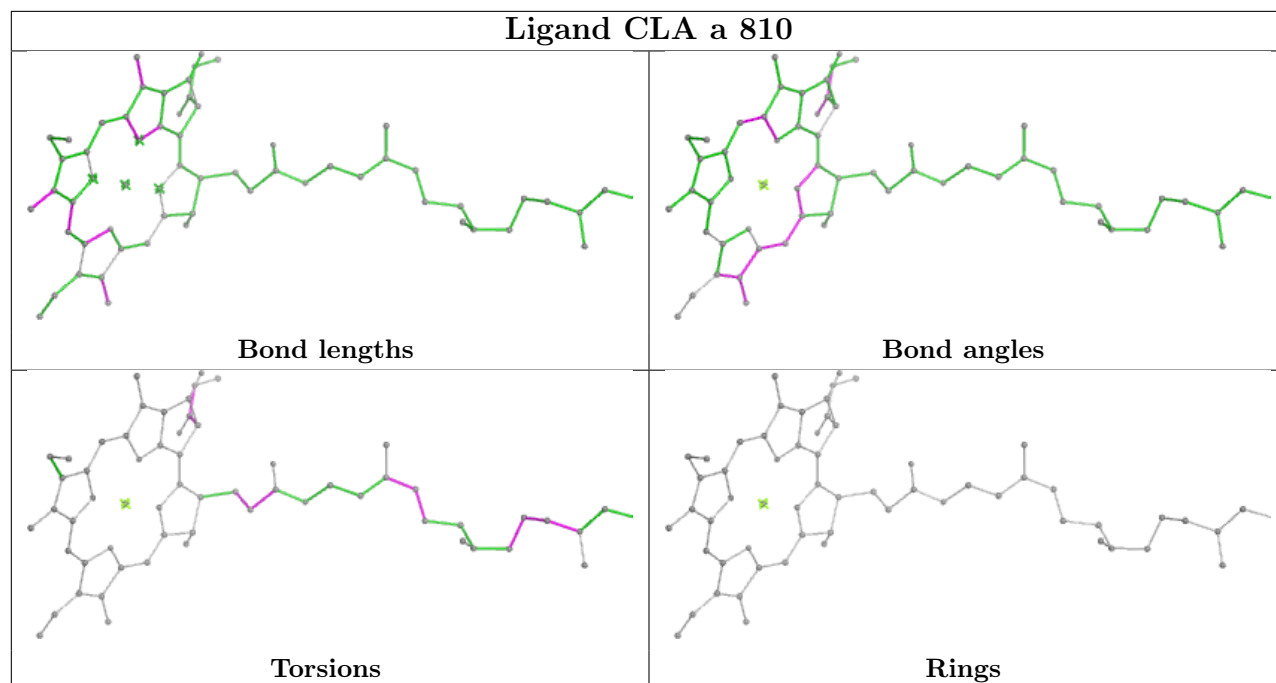


## Ligand CLA 2 831

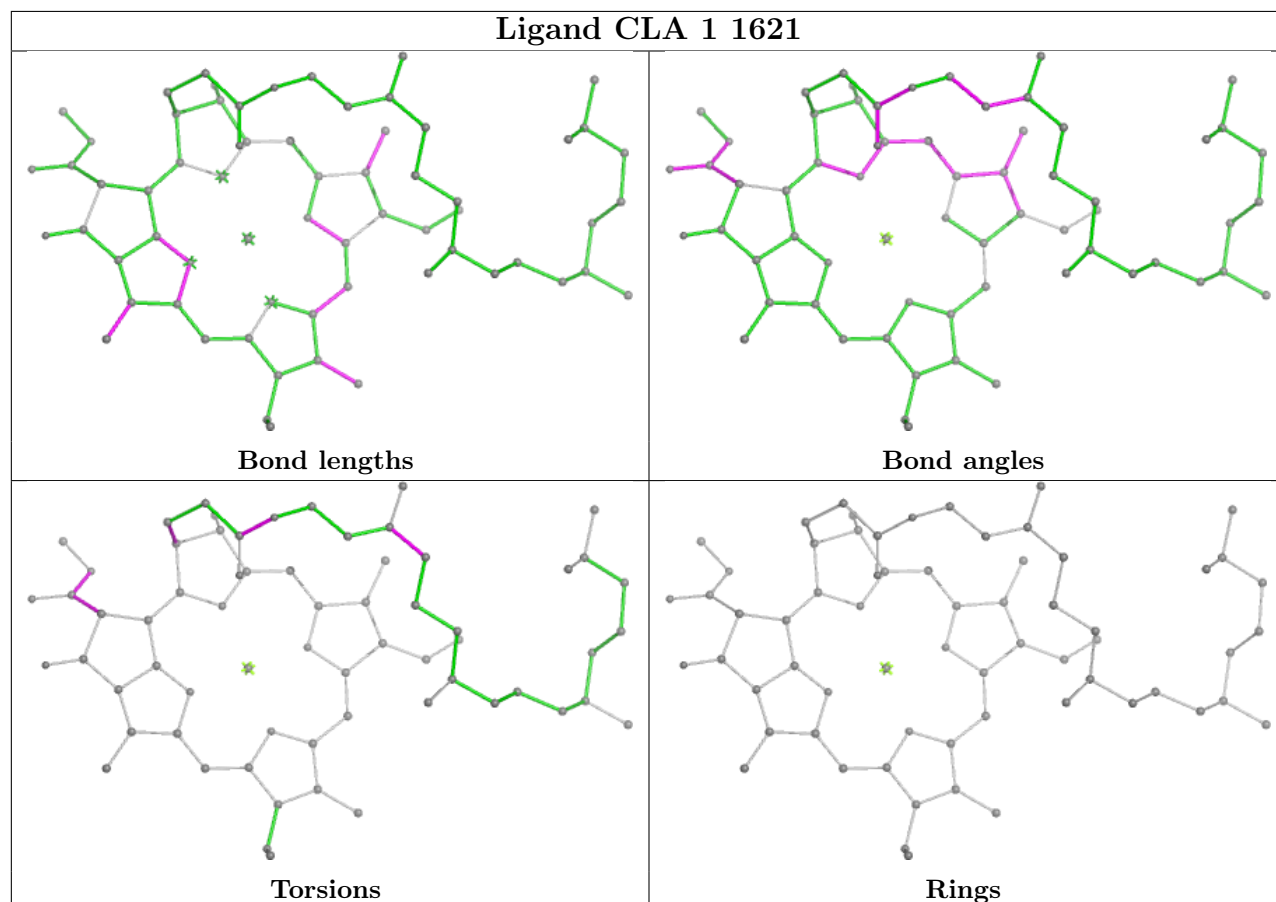


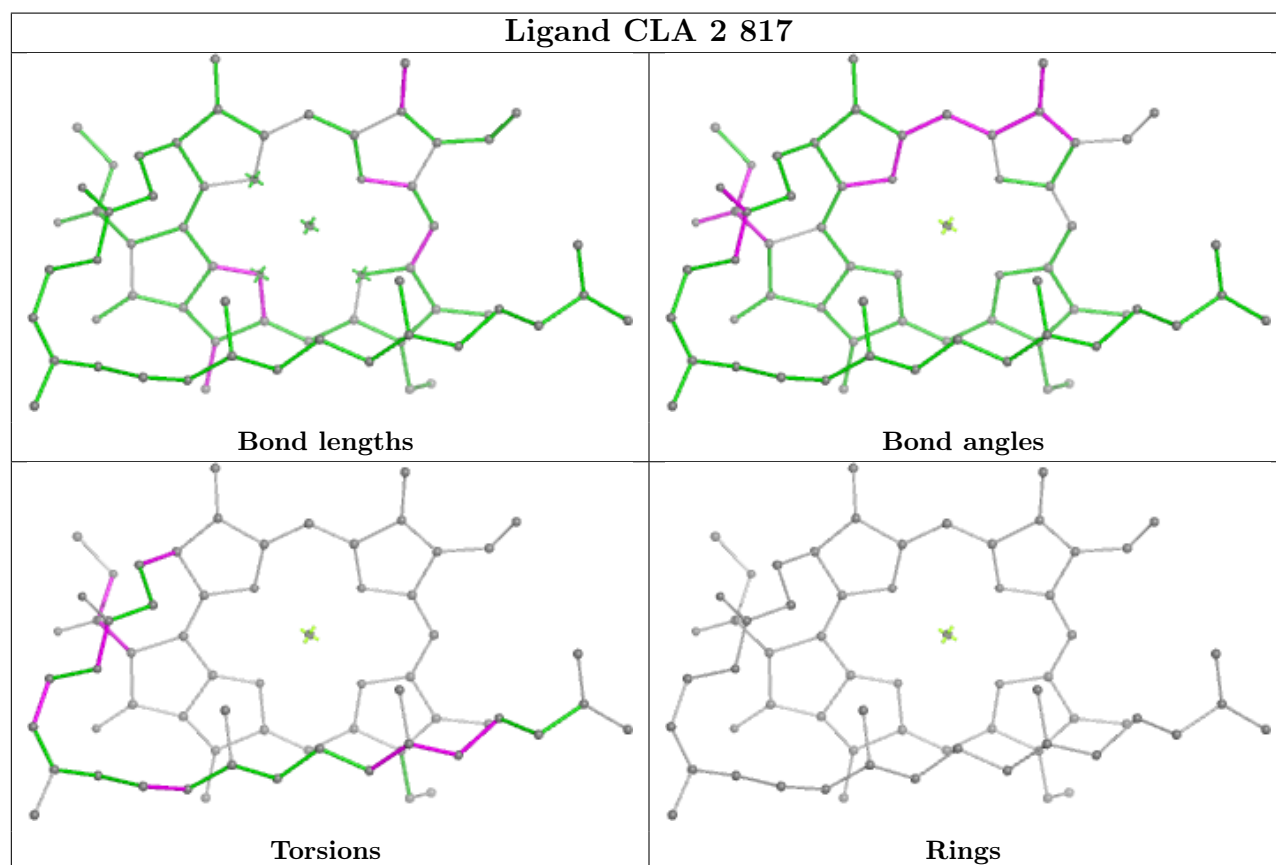
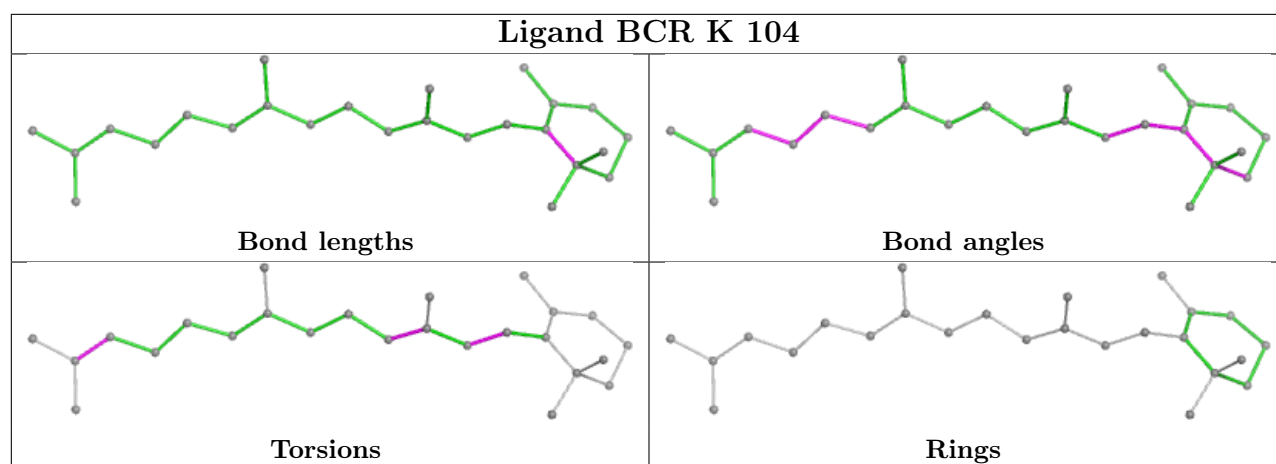


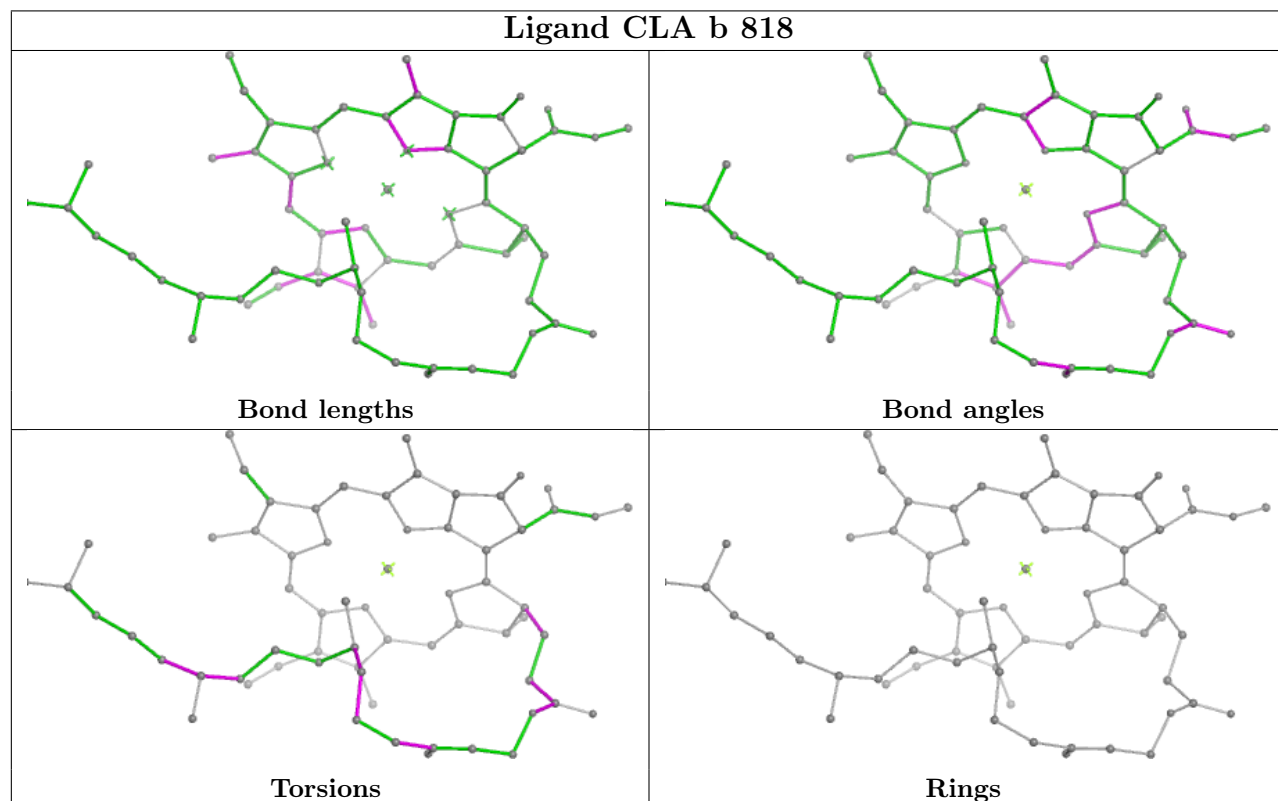
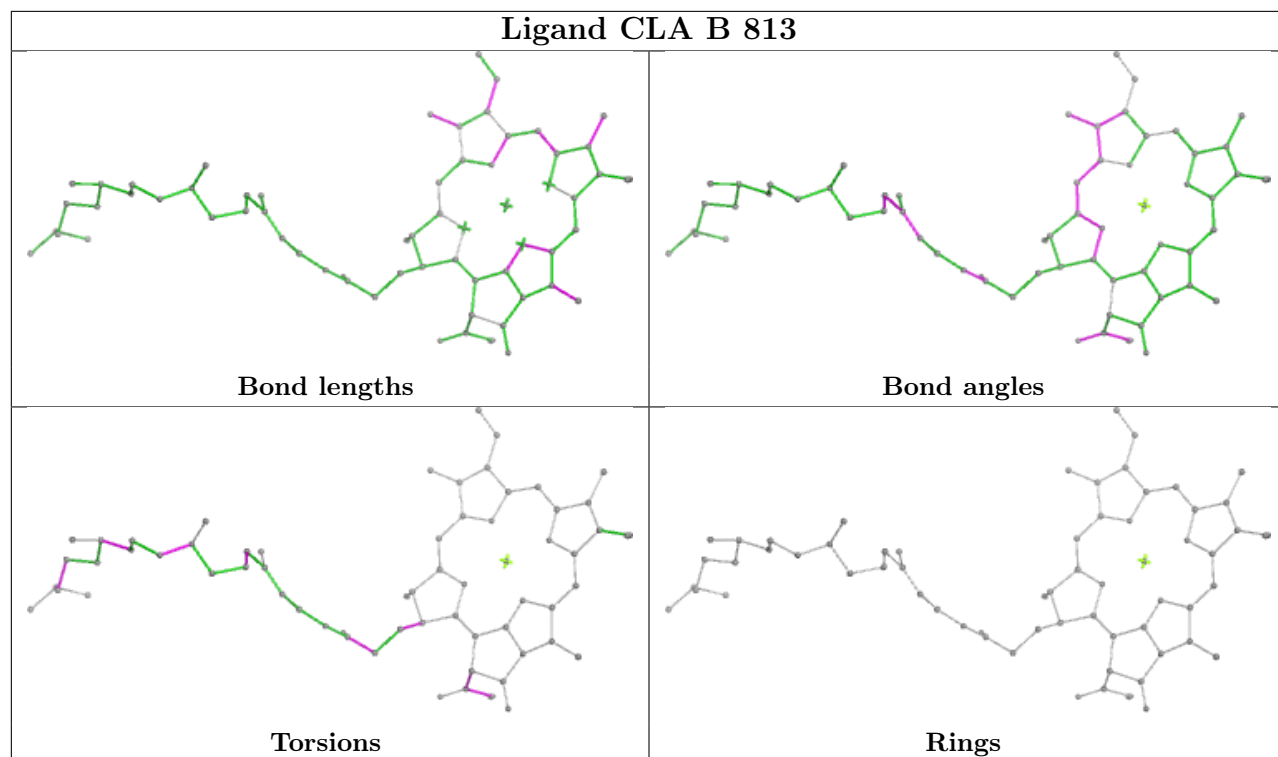
## Ligand CLA a 810

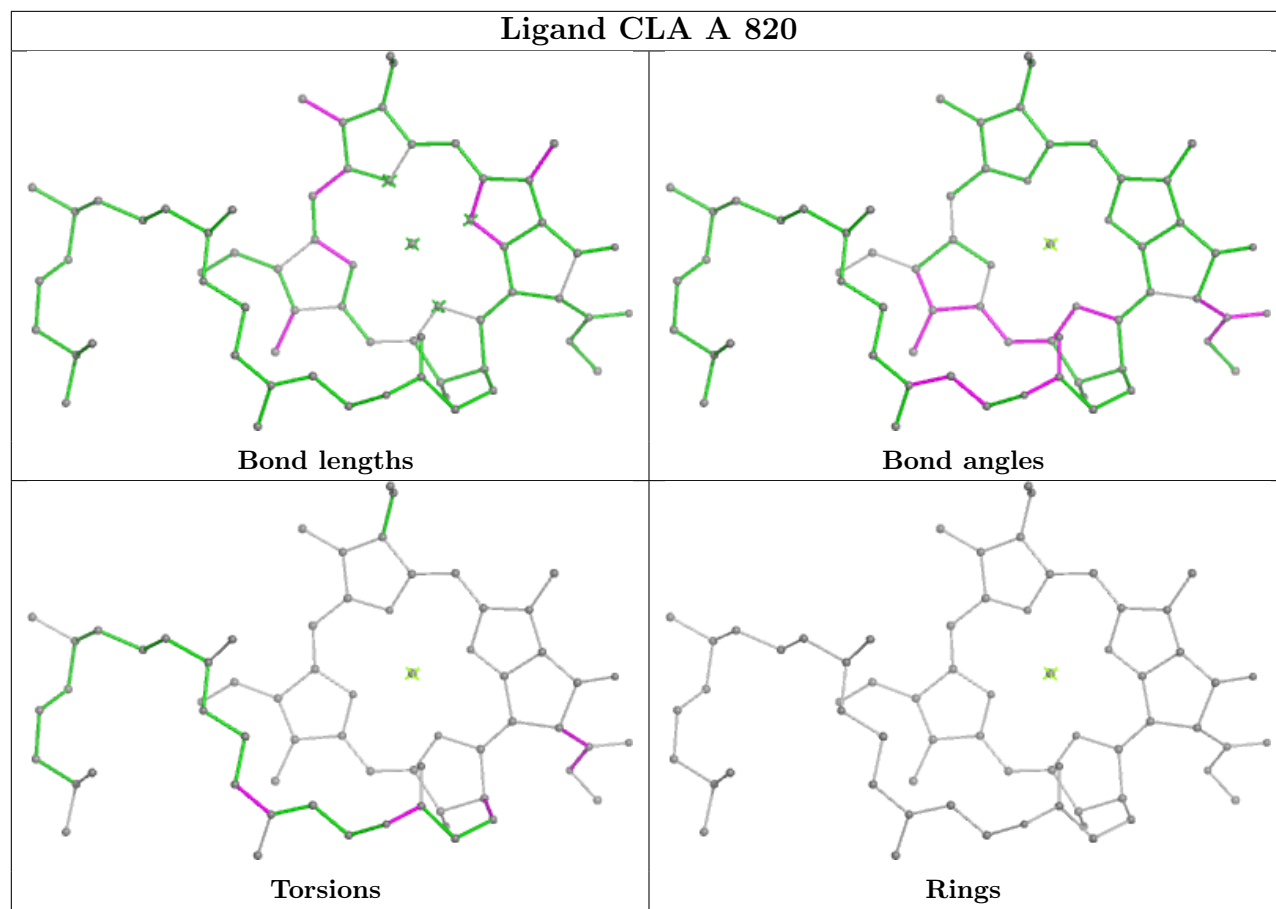


## Ligand CLA 1 1621

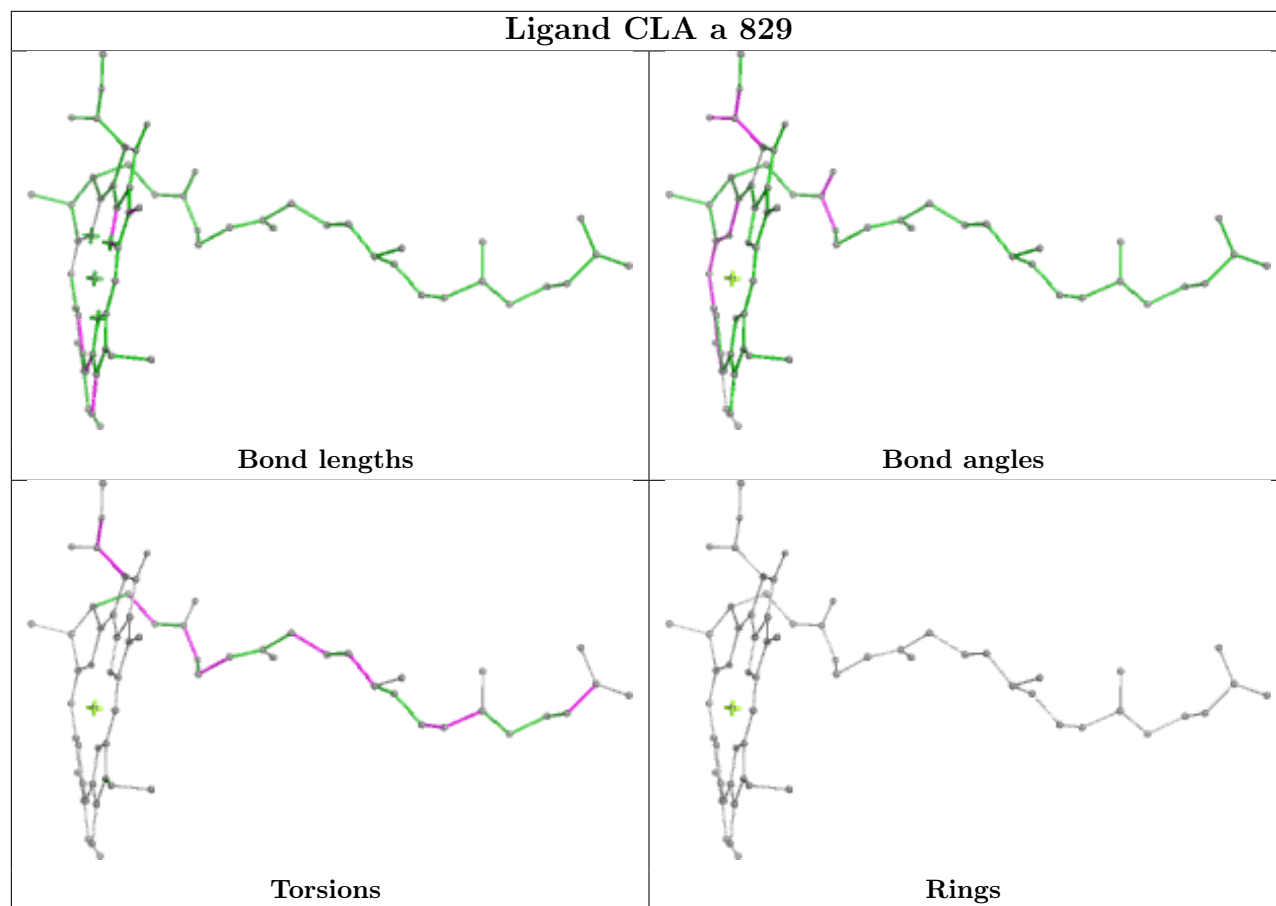




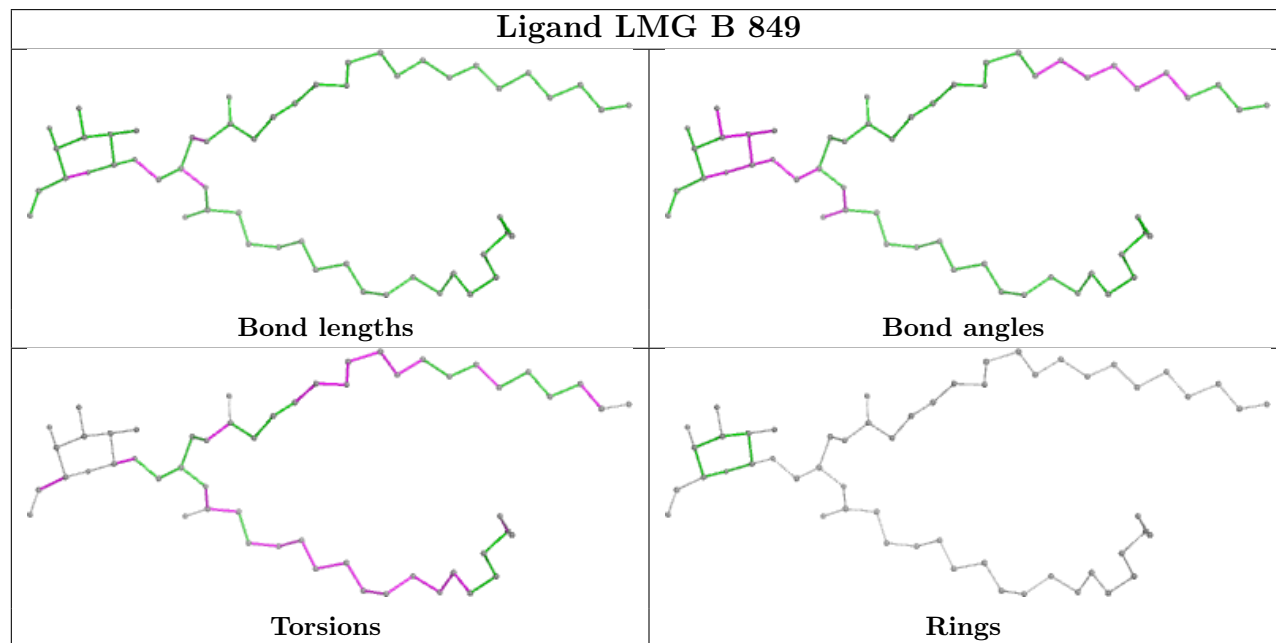


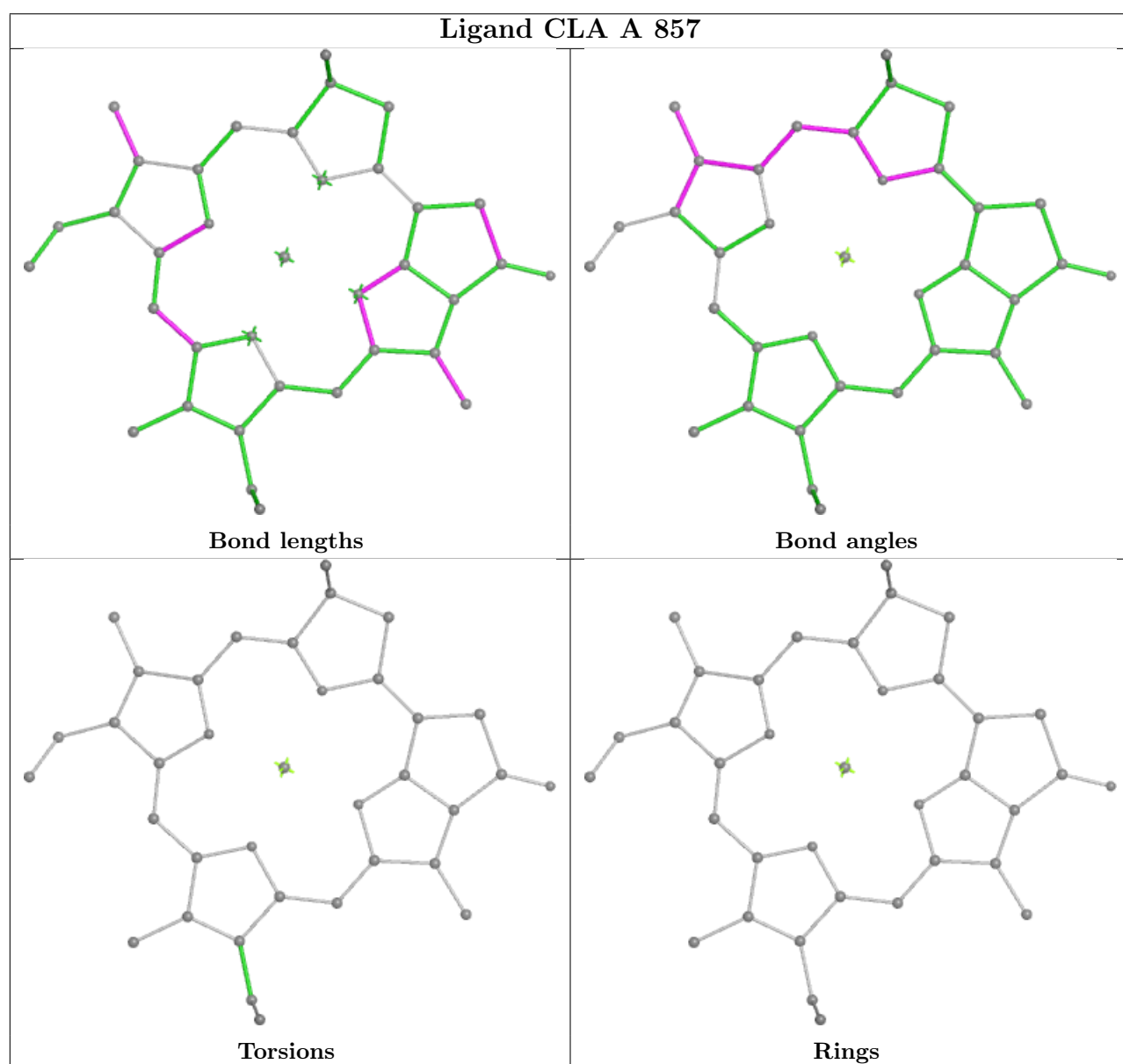
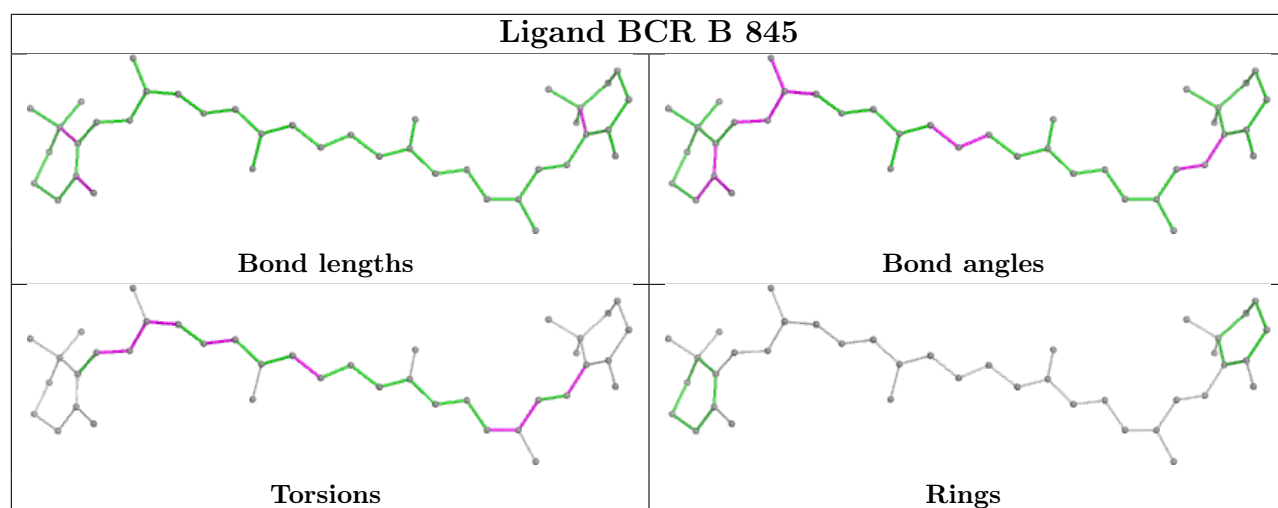


## Ligand CLA a 829

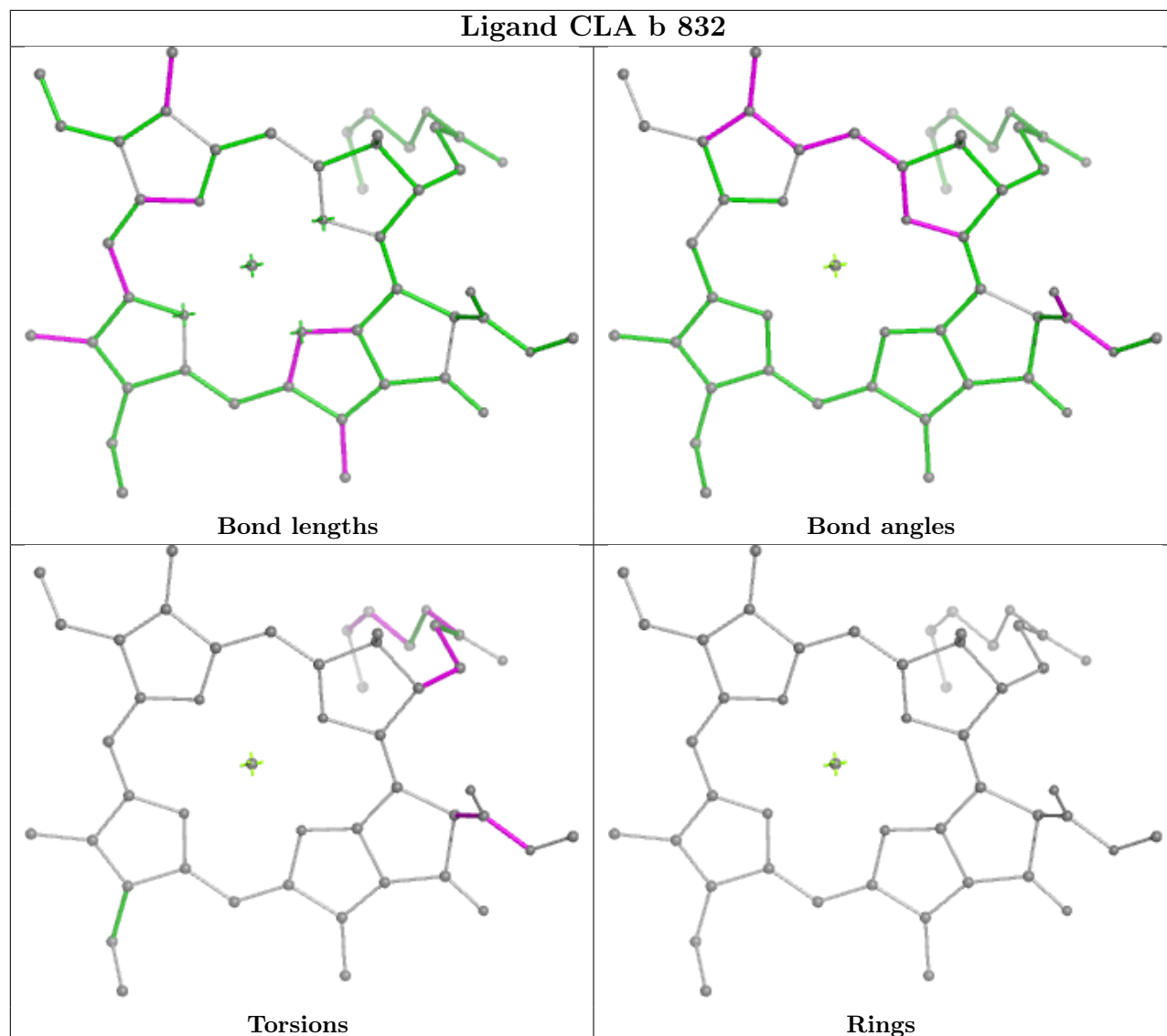


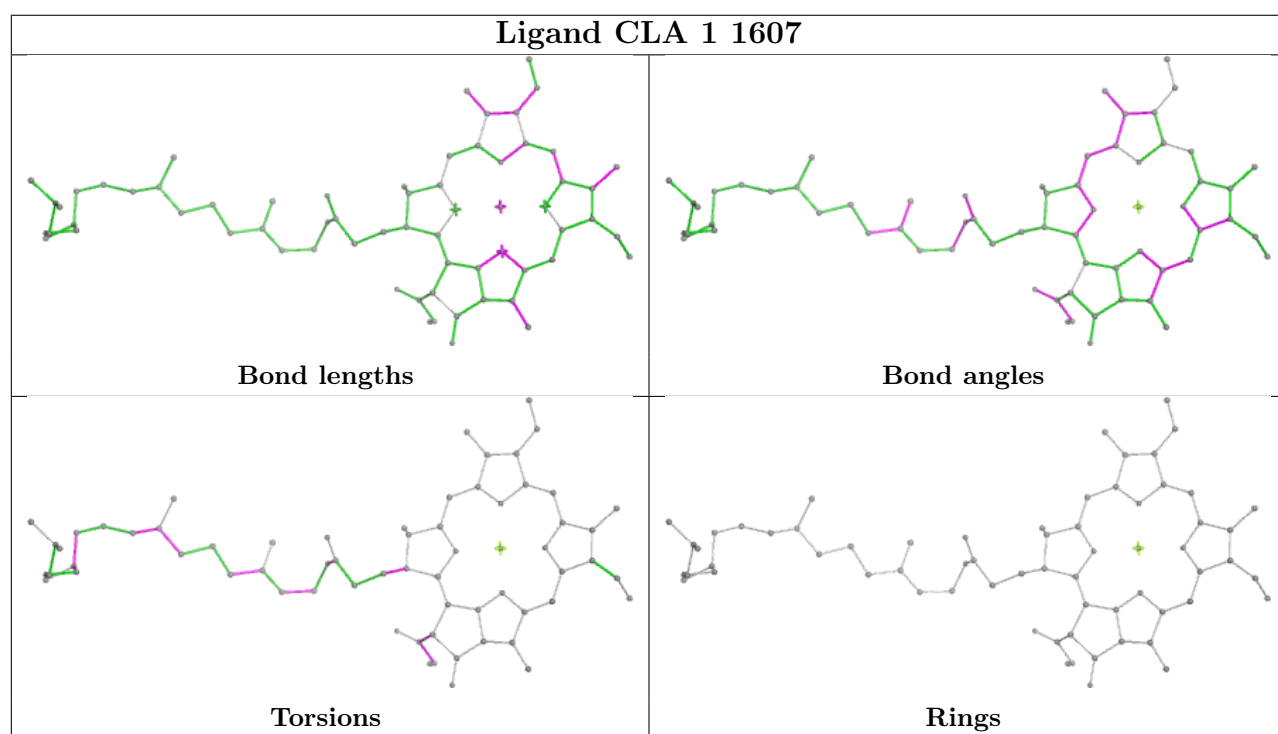
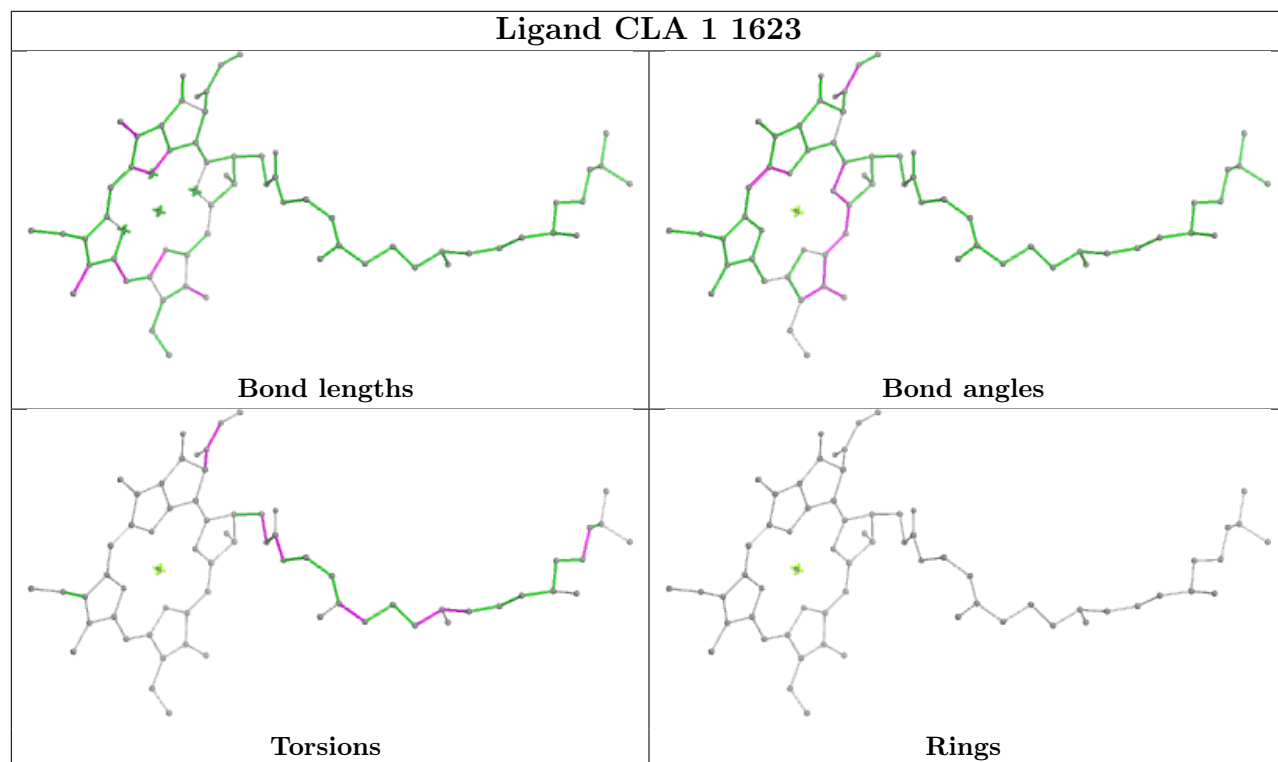
## Ligand LMG B 849



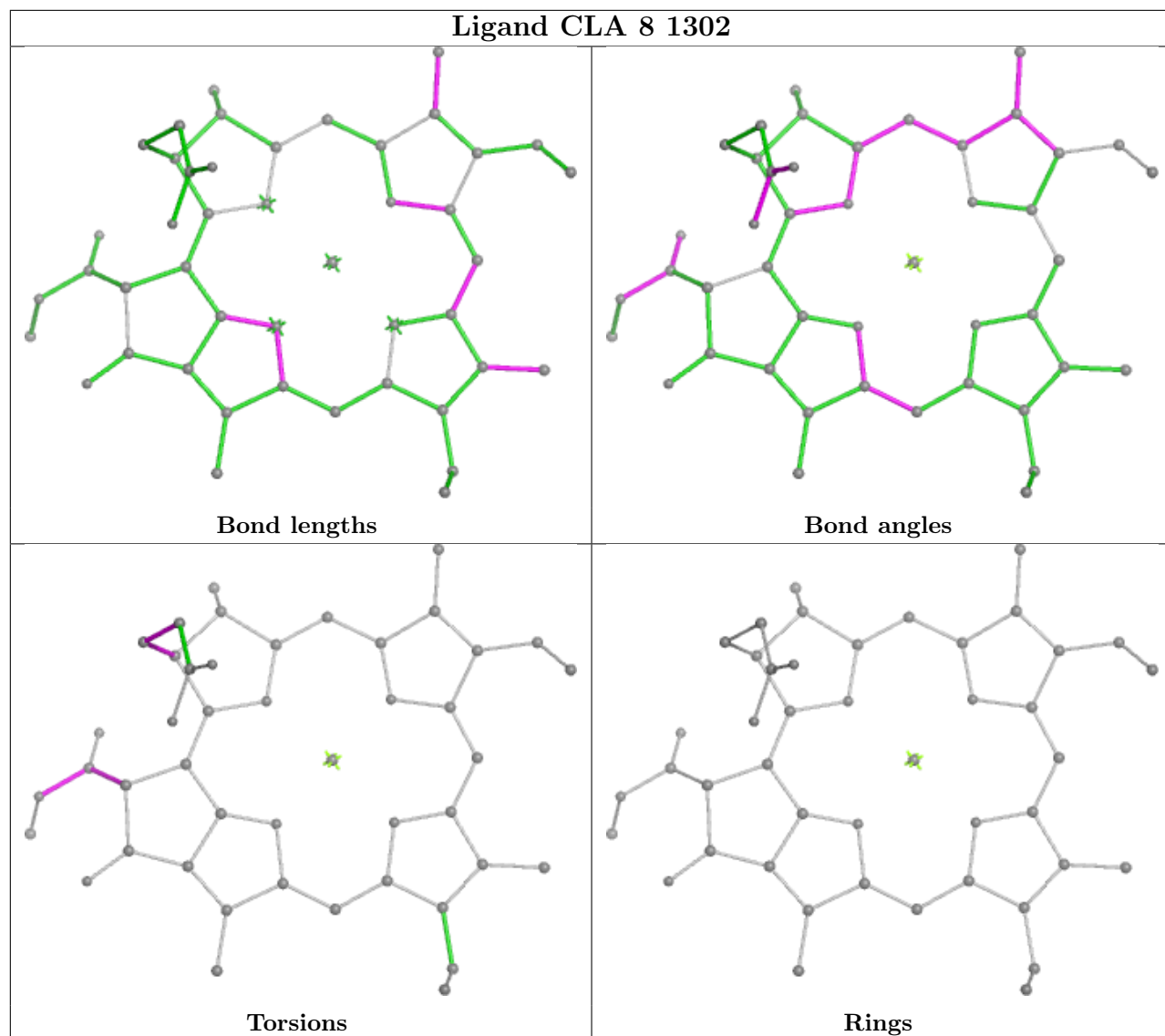


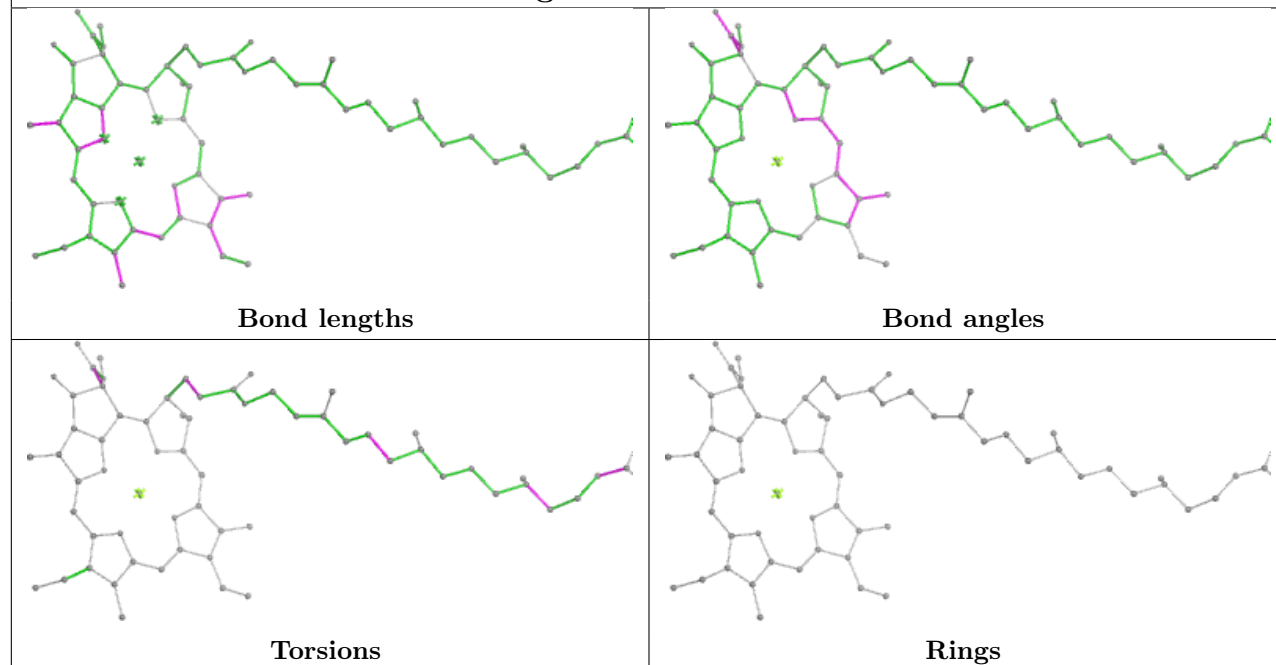
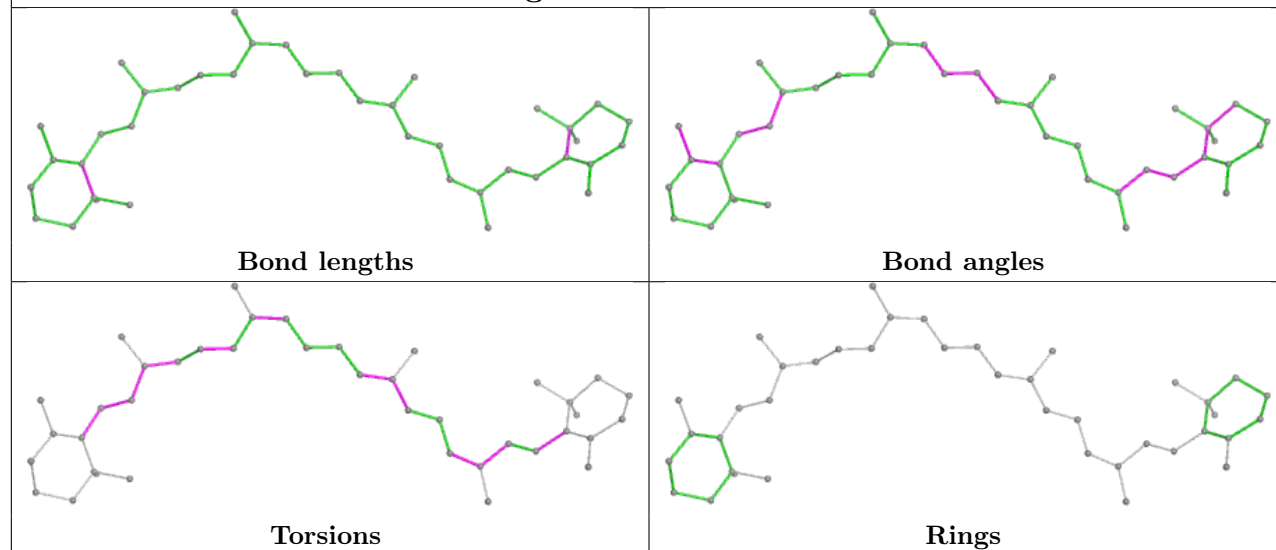
## Ligand CLA b 832

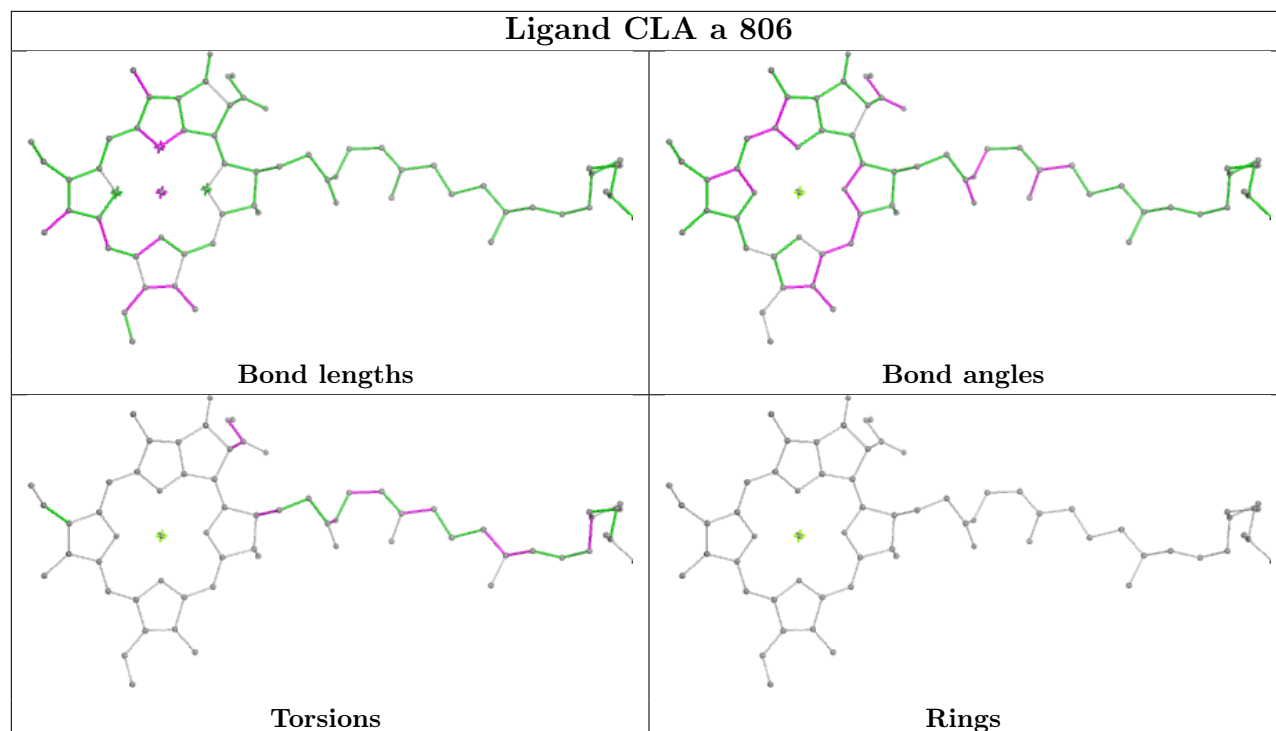
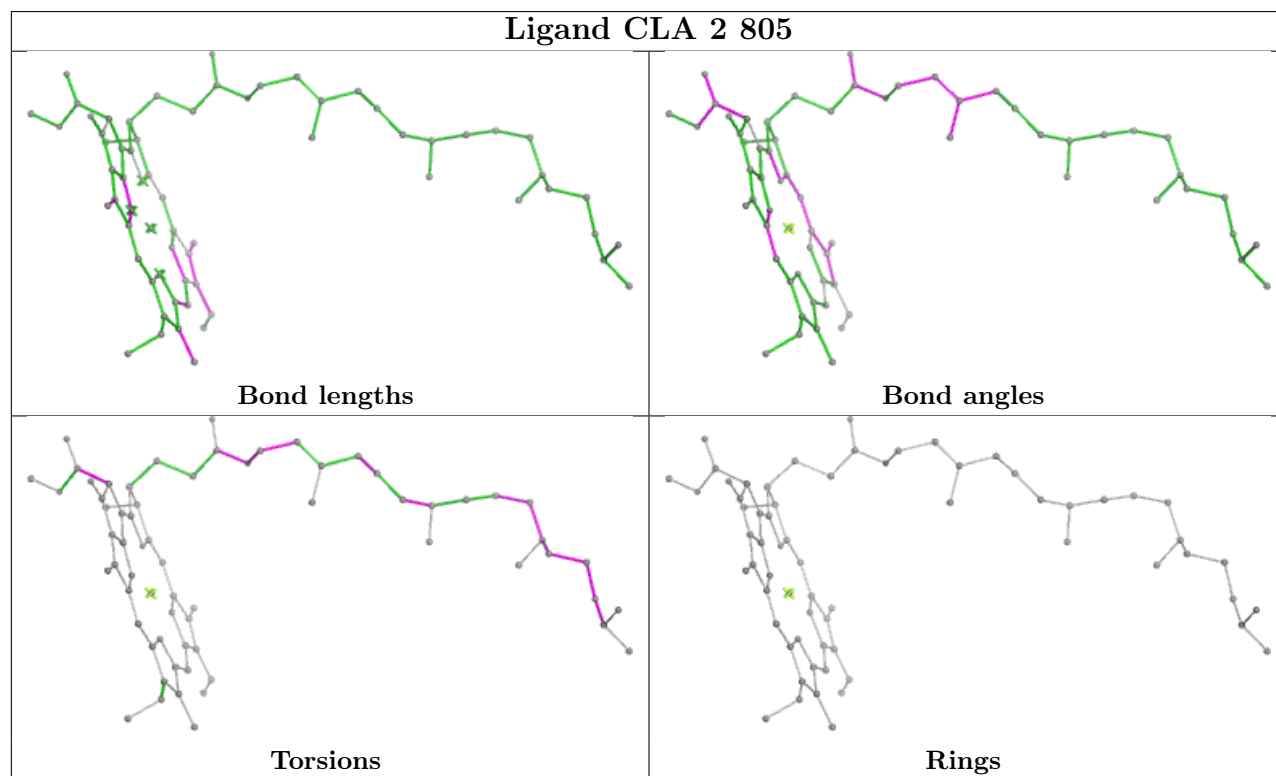


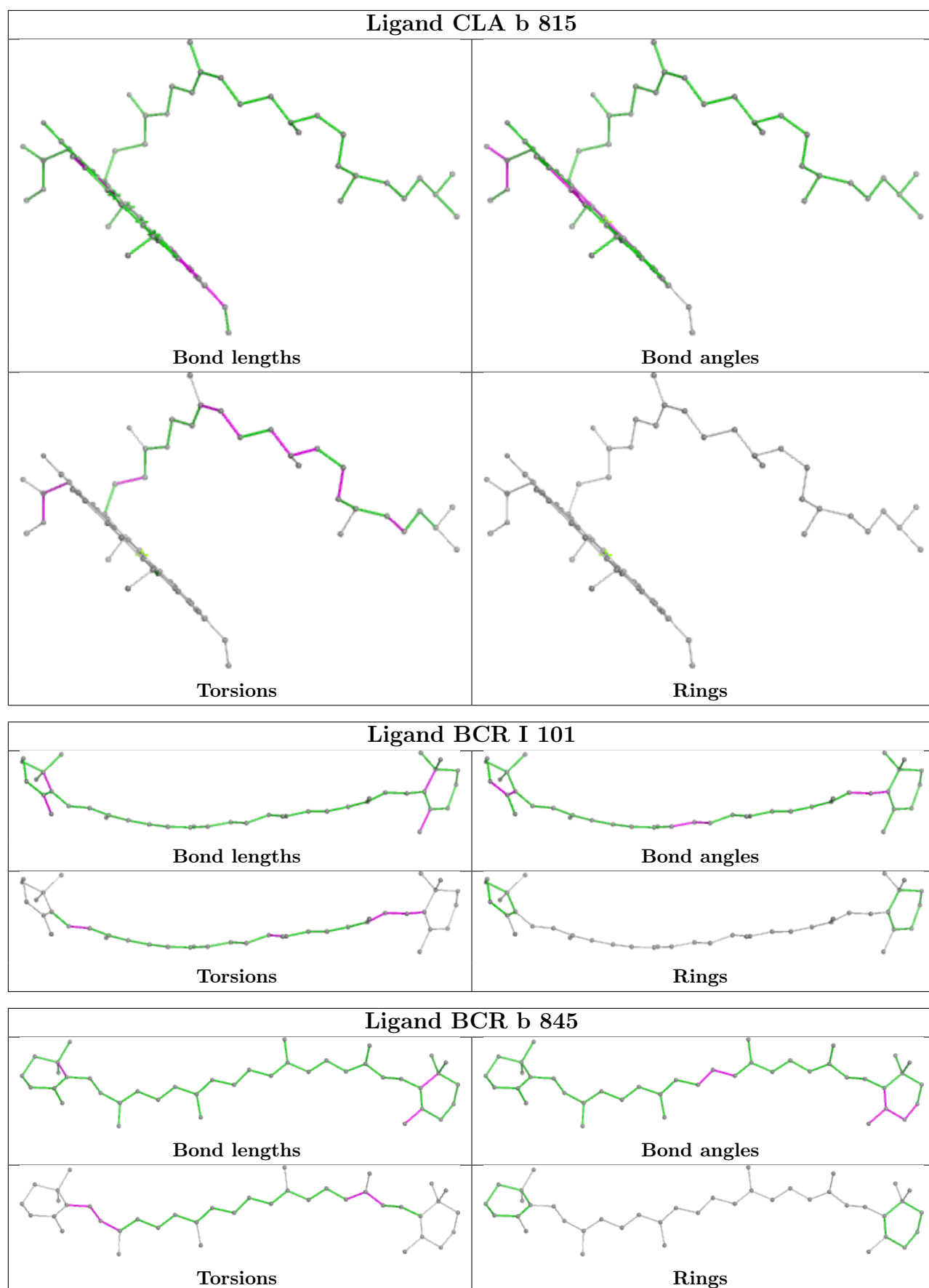




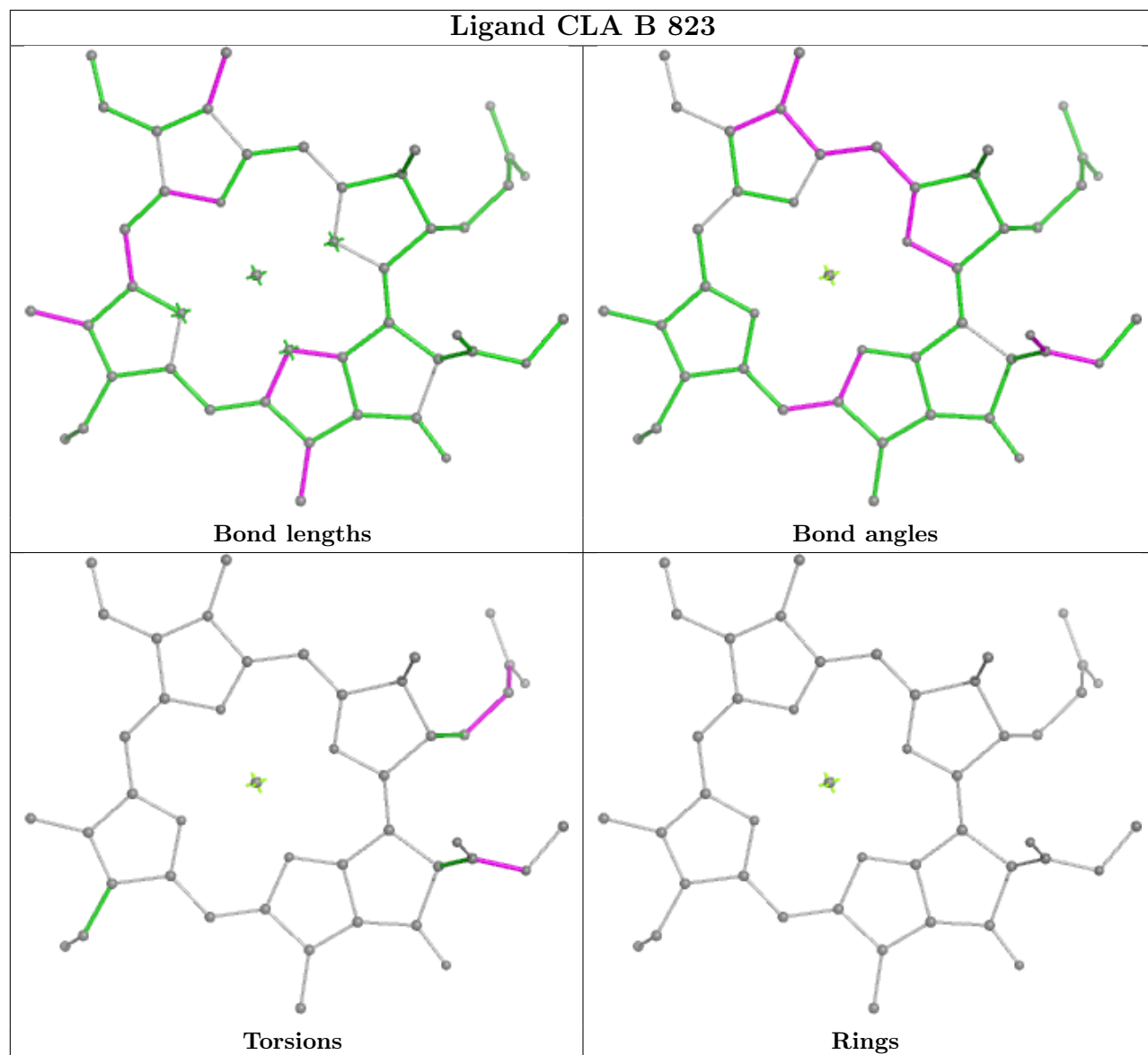


**Ligand CLA a 835****Ligand BCR 1 1652**

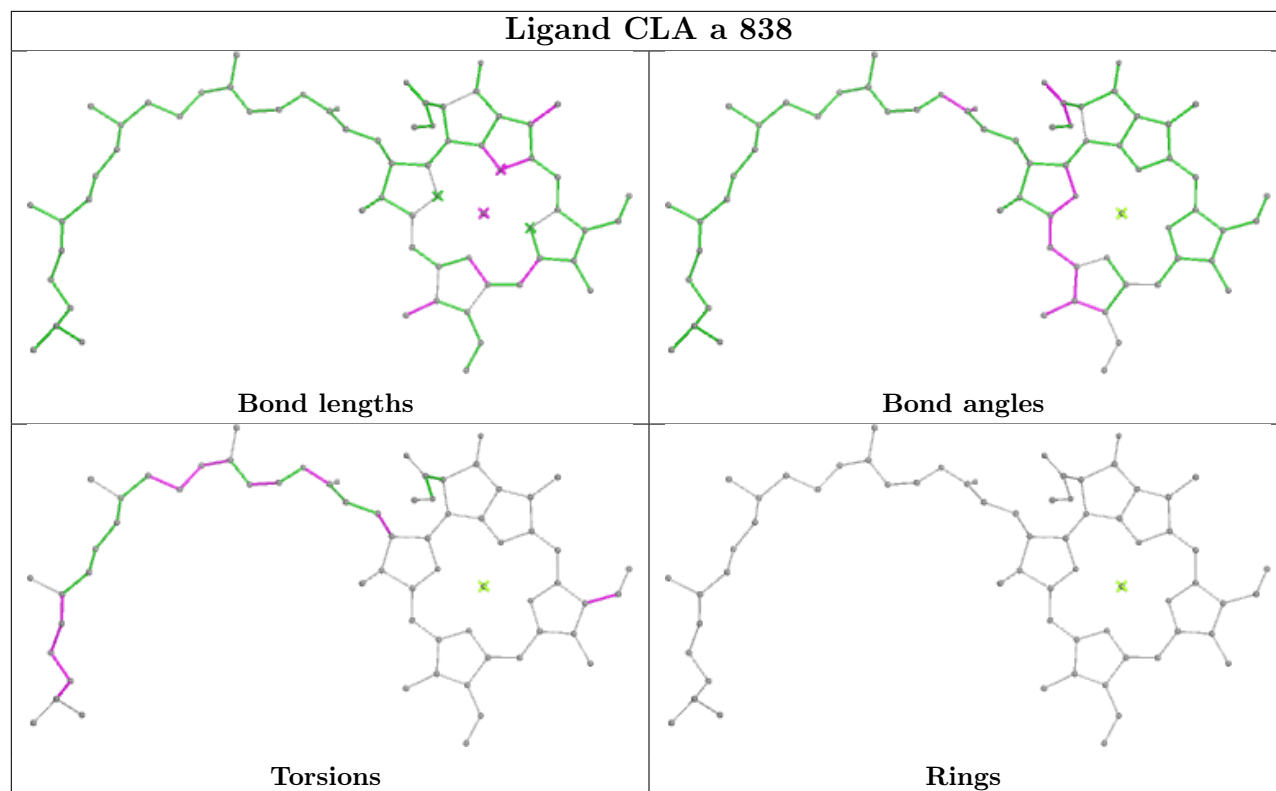
**Ligand CLA a 806****Ligand CLA 2 805**



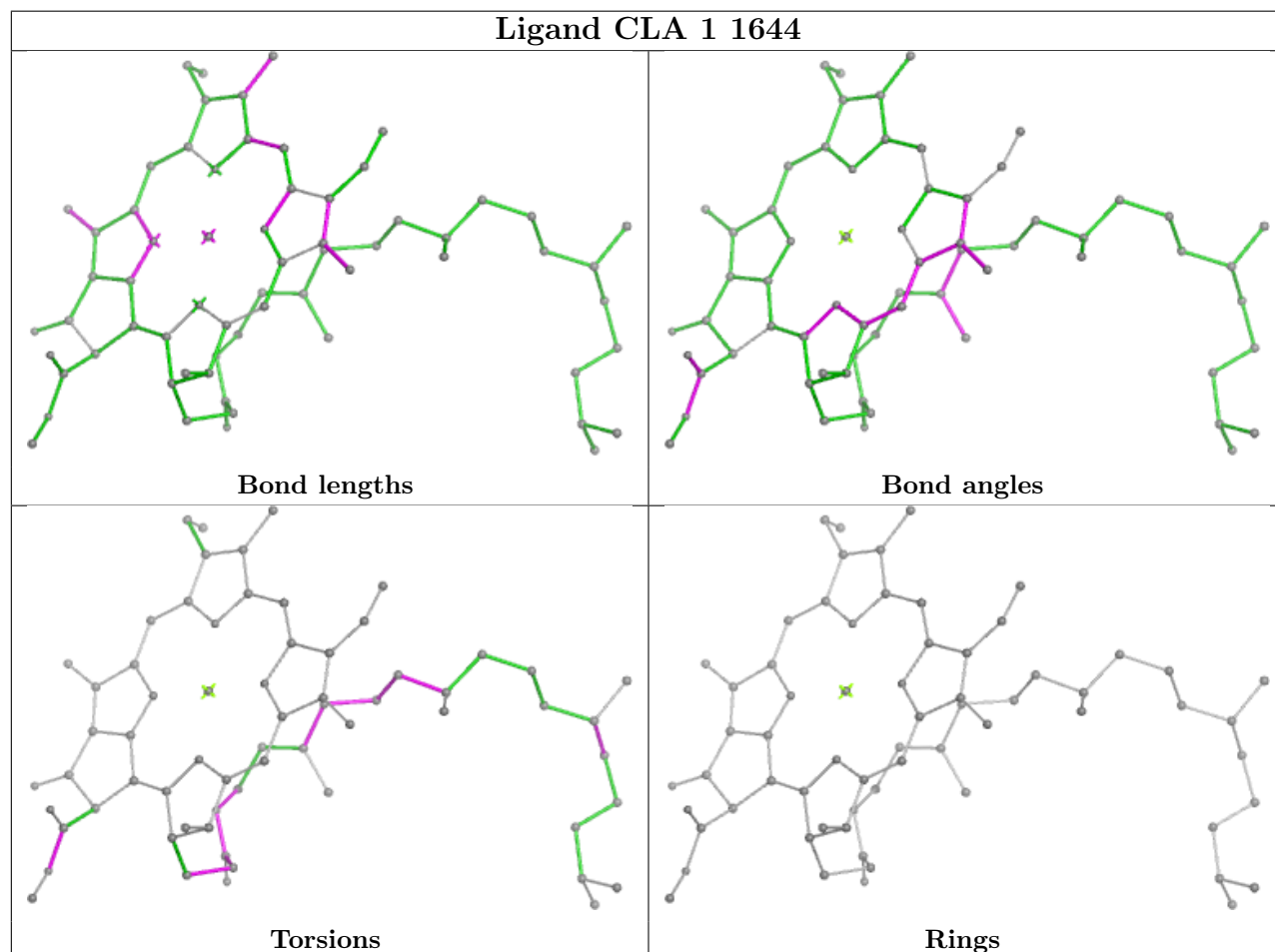
## Ligand CLA B 823

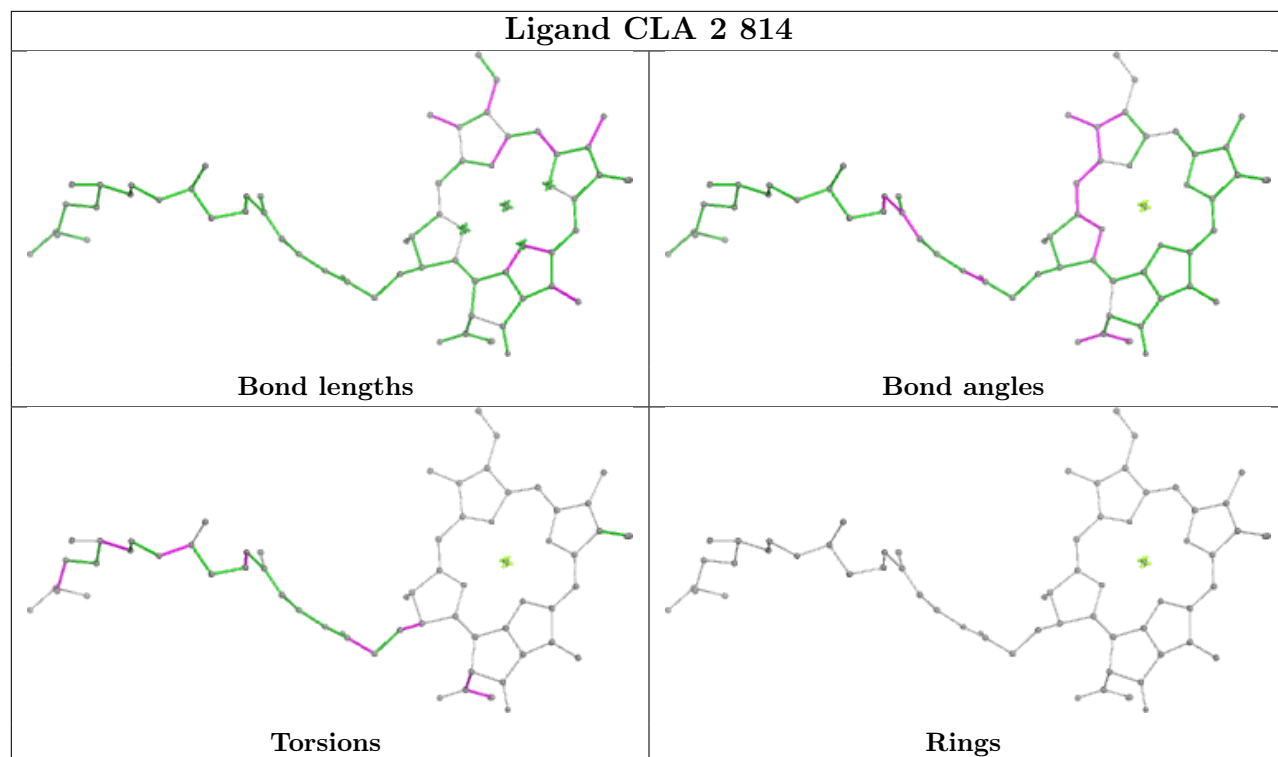


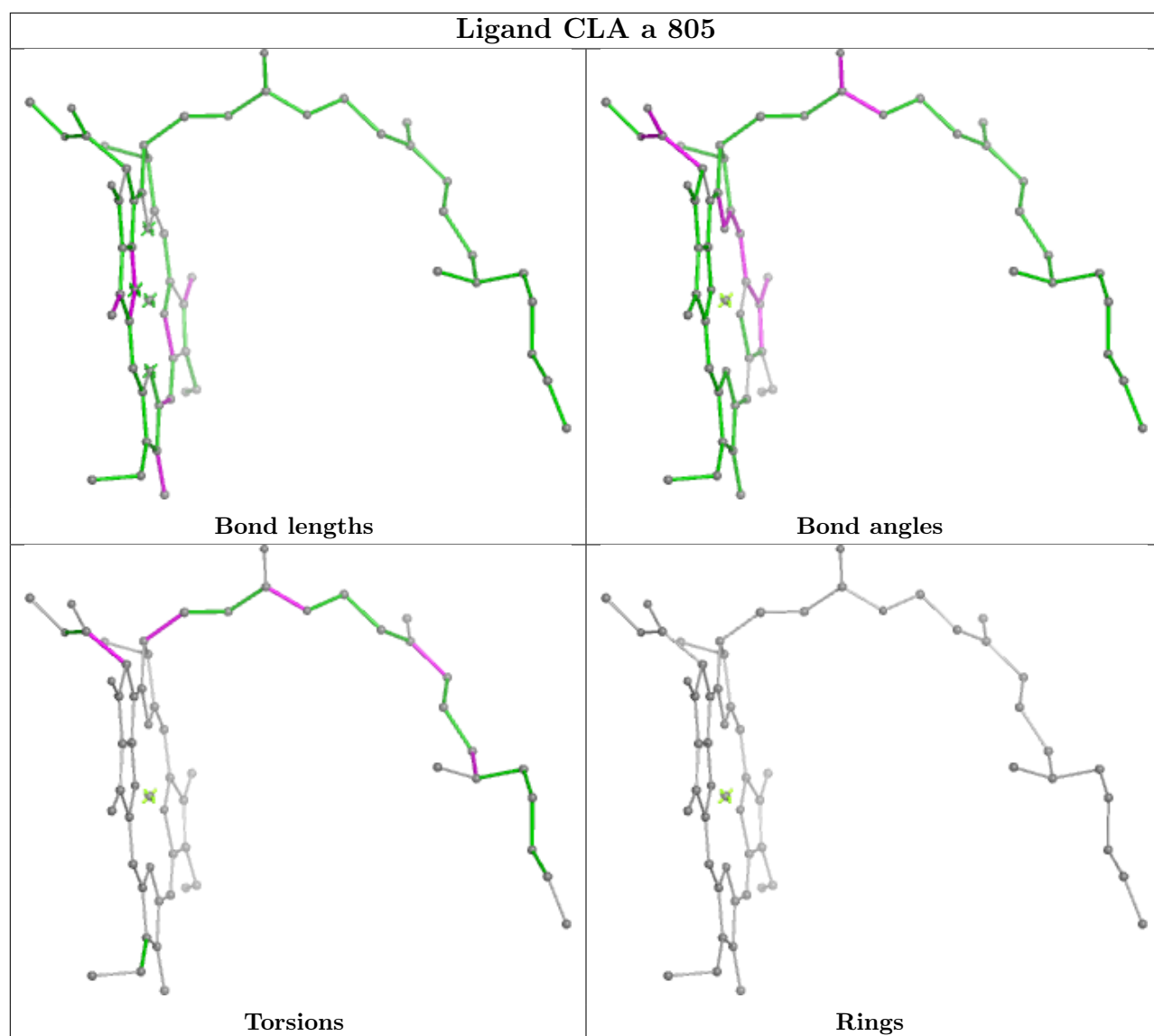
## Ligand CLA a 838



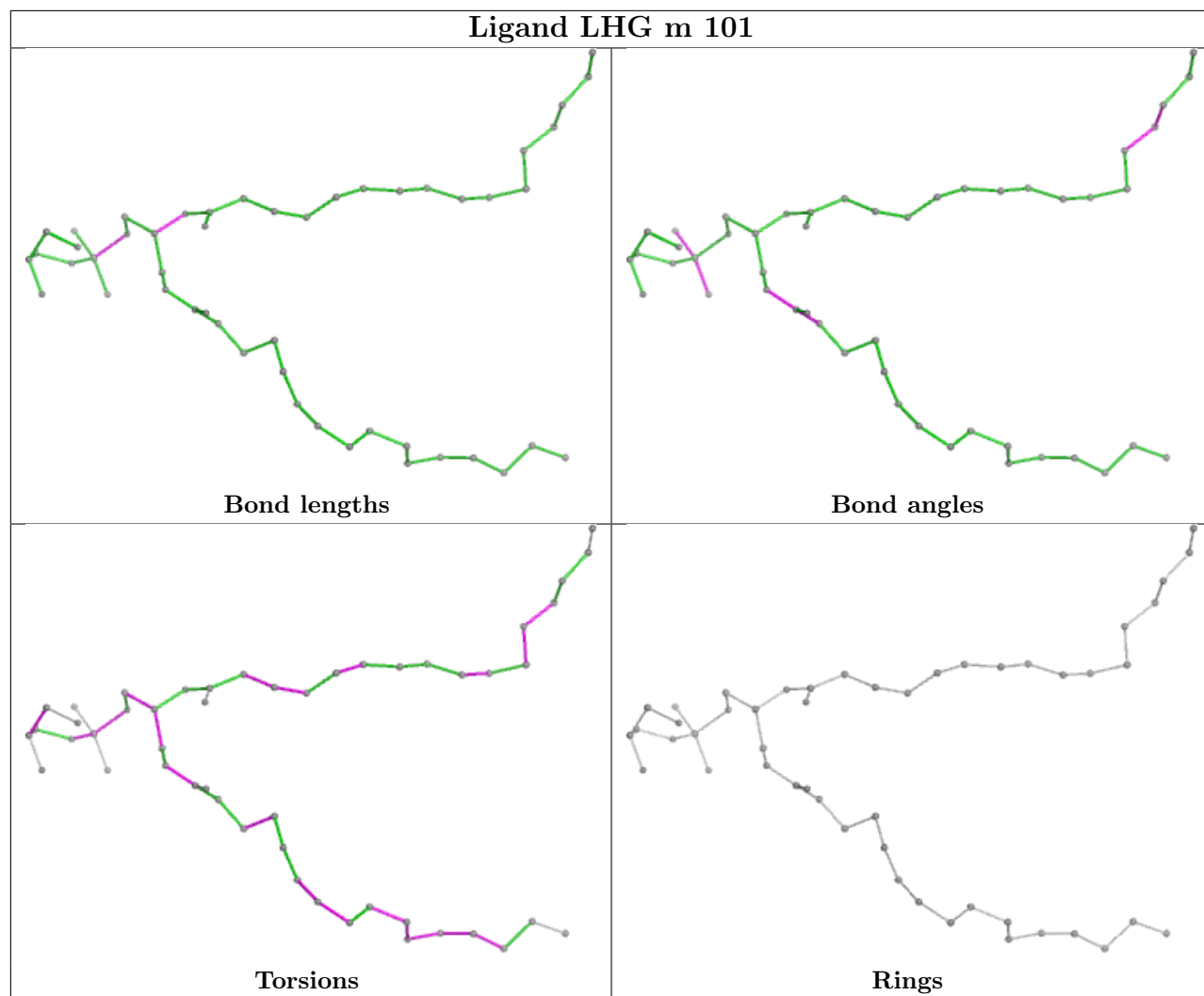
## Ligand CLA 1 1644



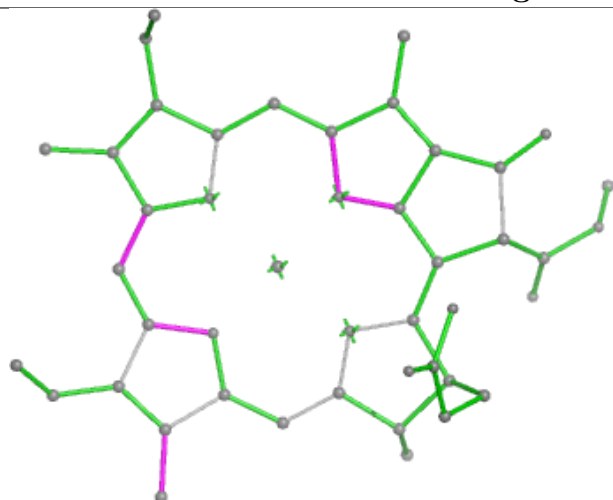




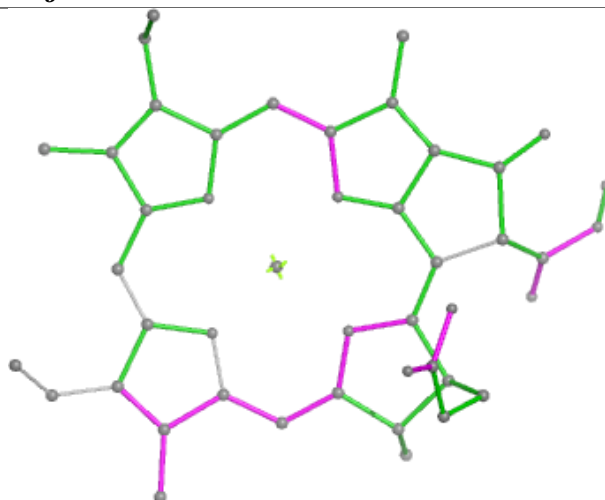




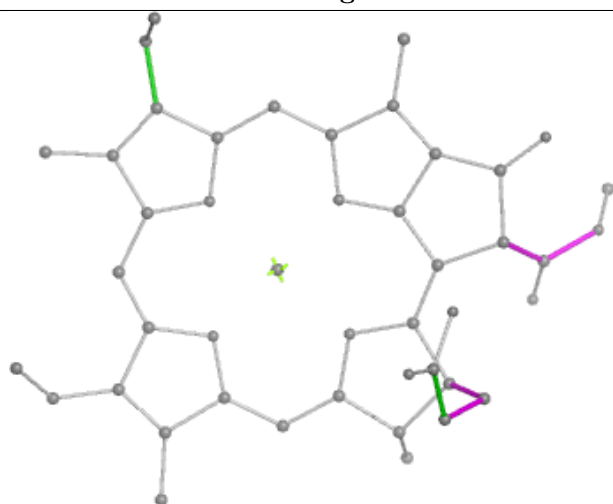
## Ligand CLA j 1302



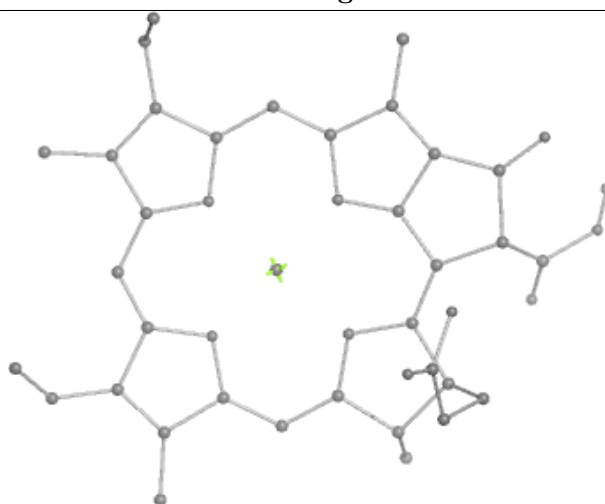
Bond lengths



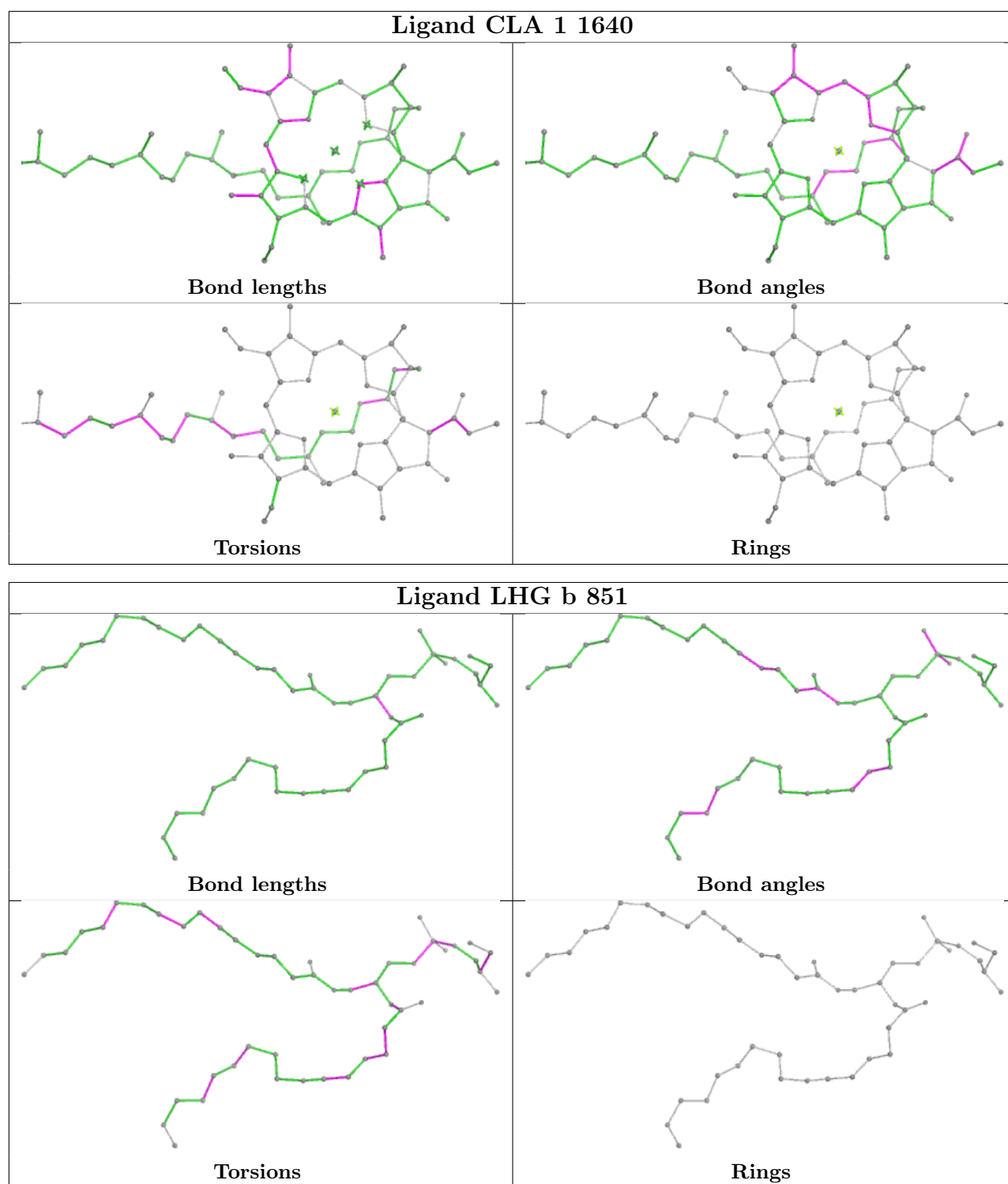
Bond angles



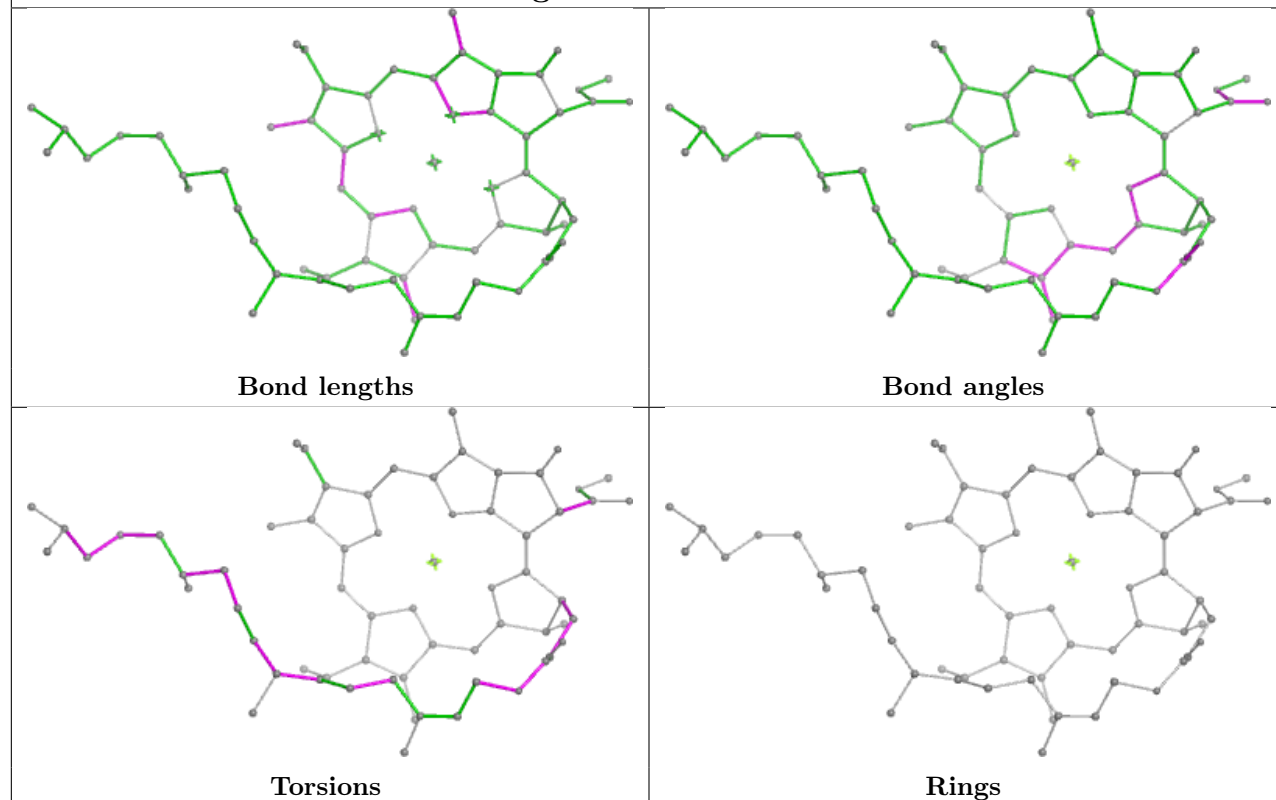
Torsions



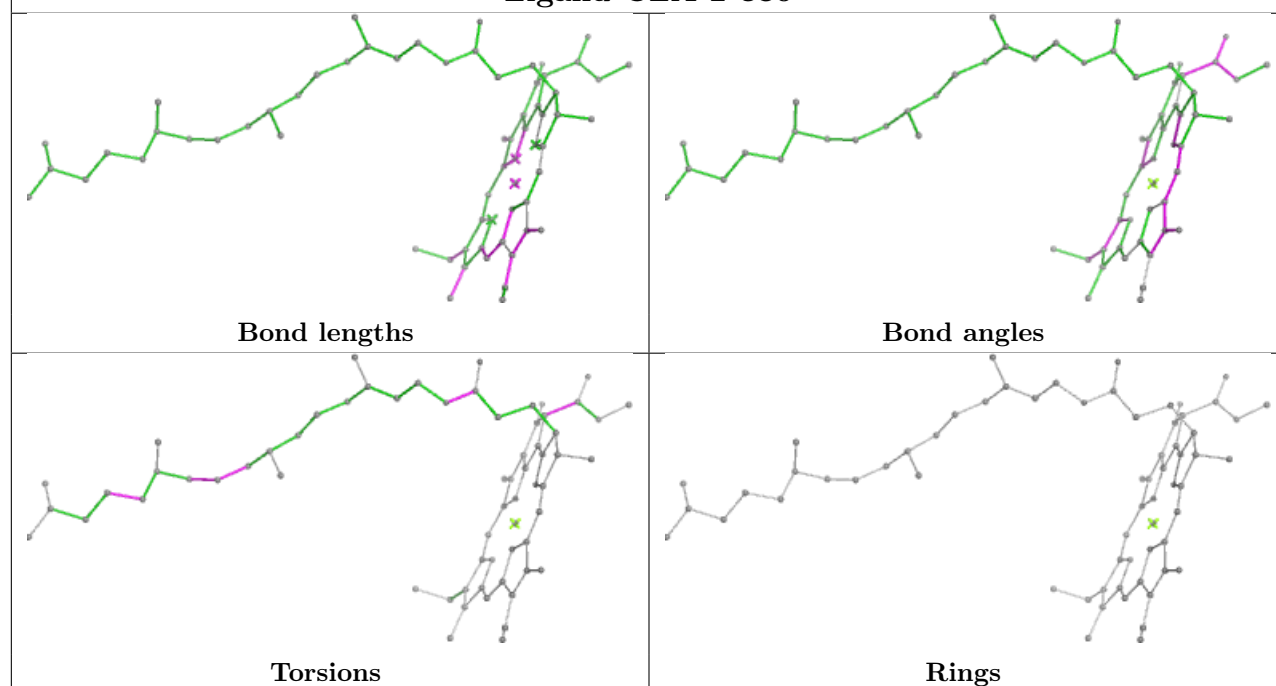
Rings



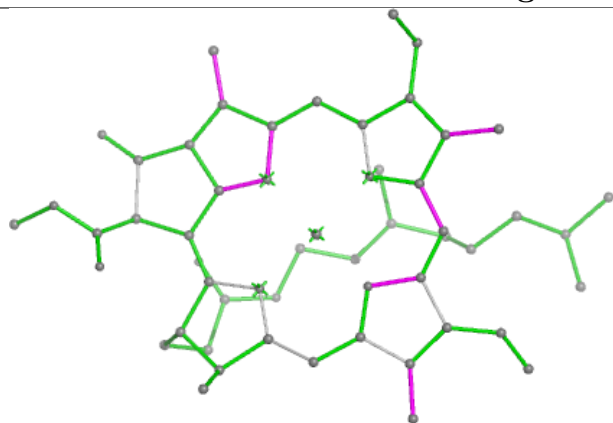
## Ligand CLA B 820



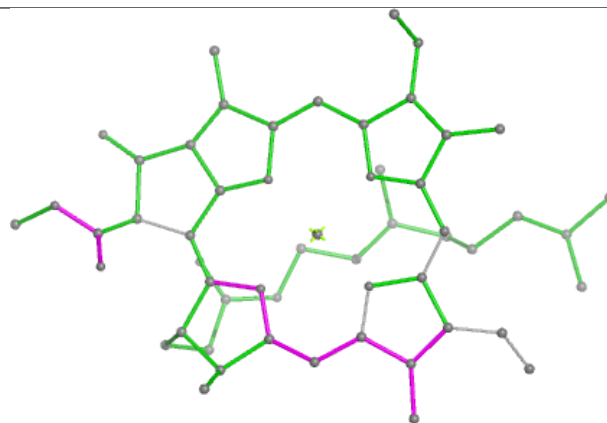
## Ligand CLA 2 830



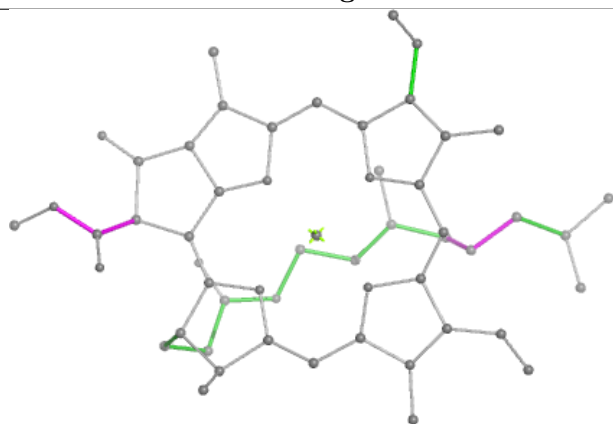
## Ligand CLA b 823



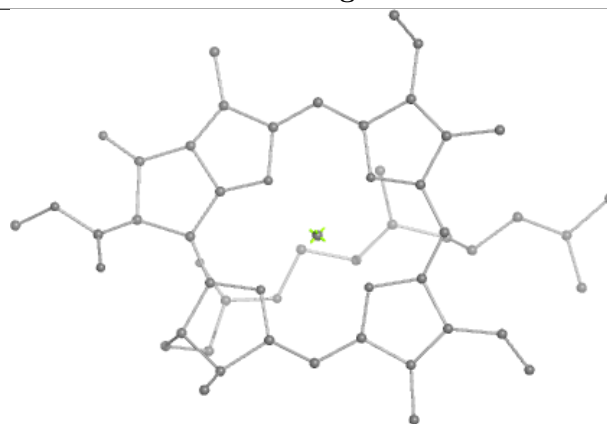
Bond lengths



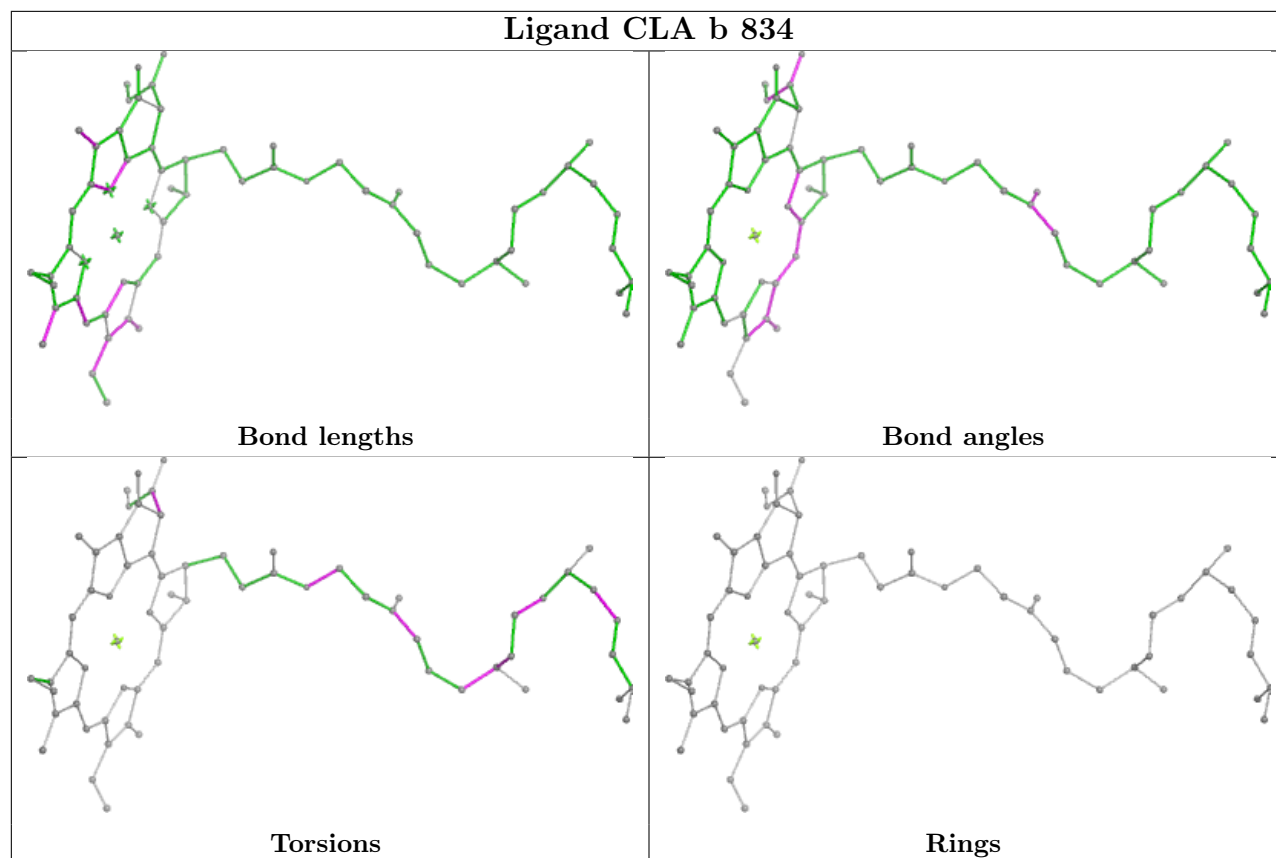
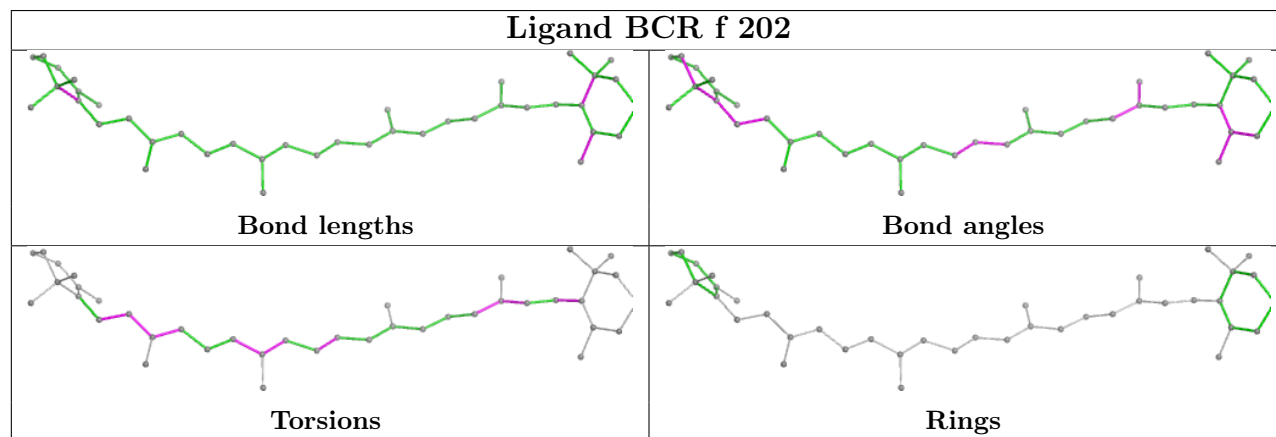
Bond angles

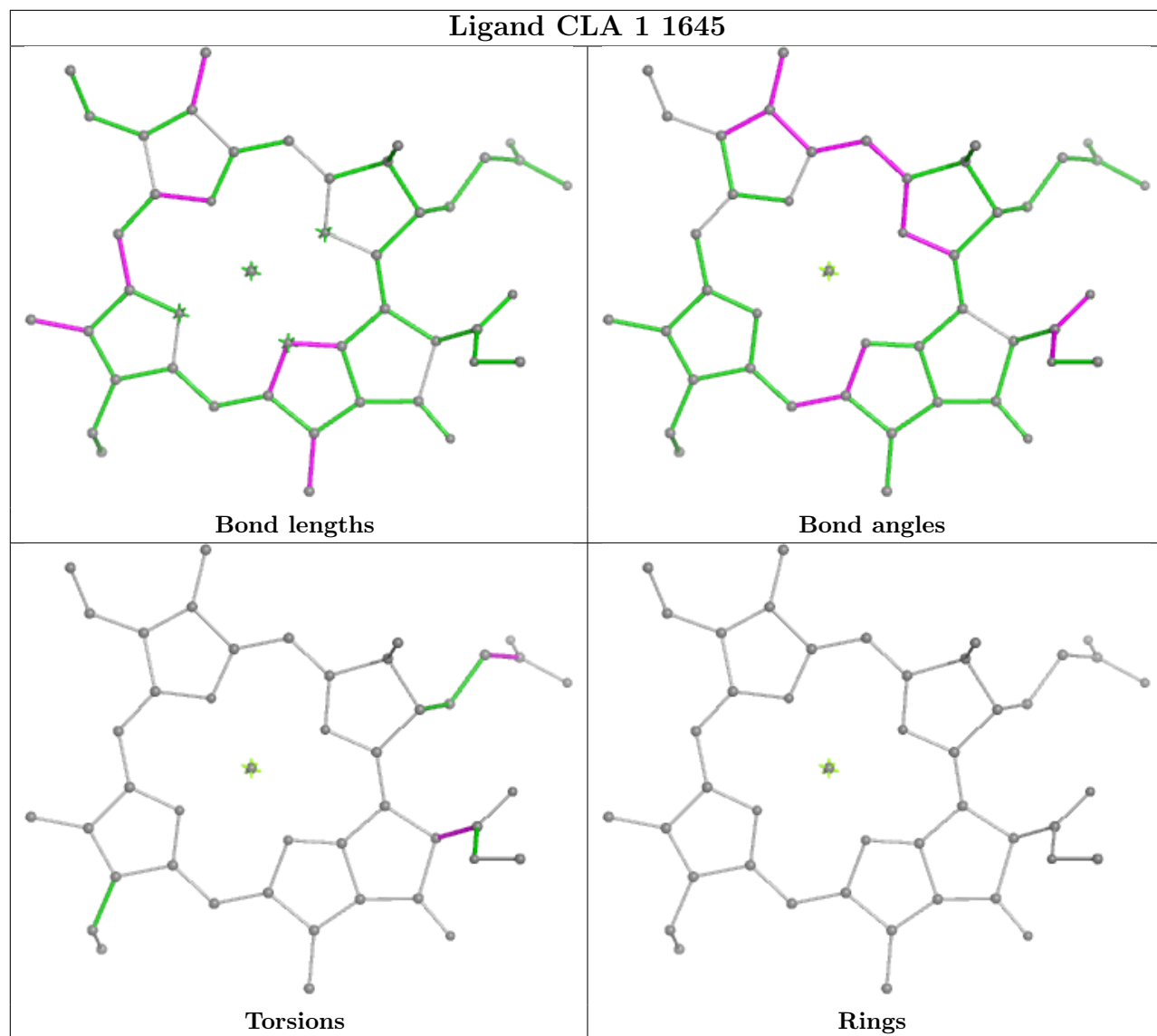


Torsions

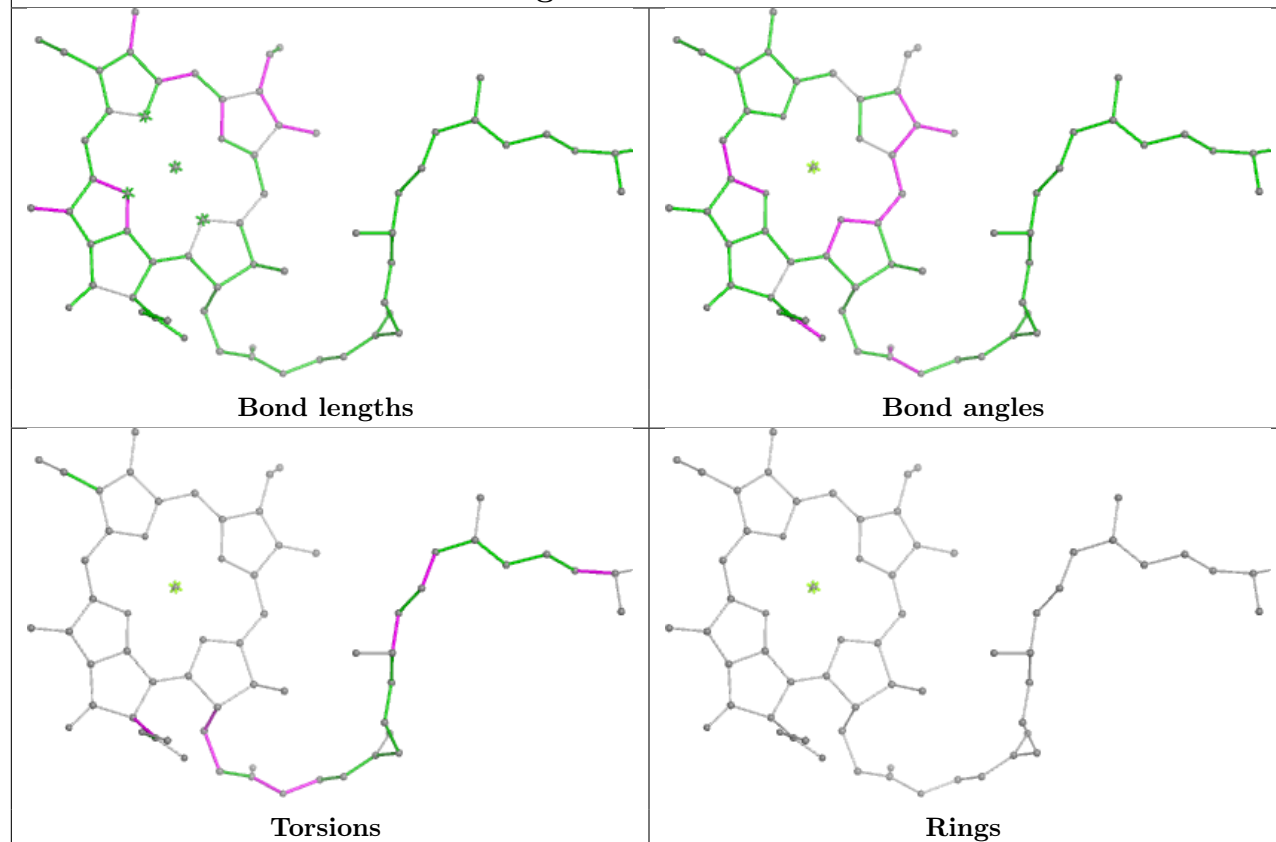


Rings

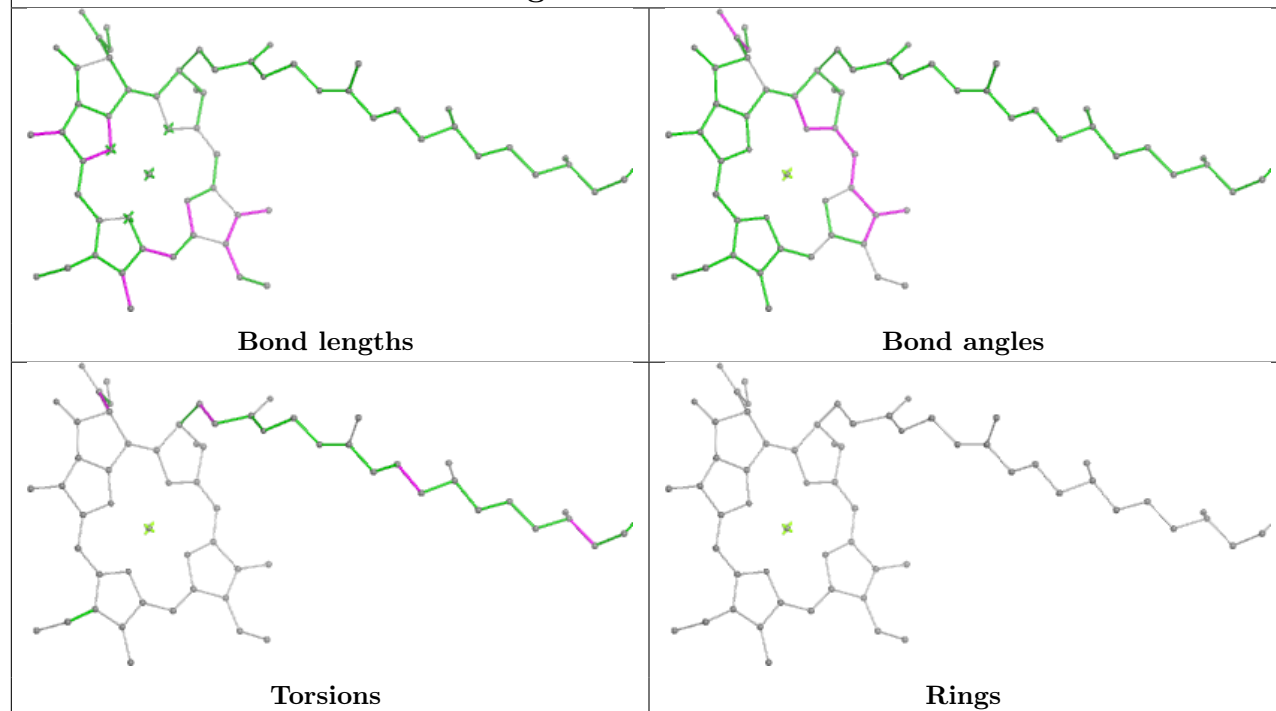
**Ligand CLA b 834****Ligand BCR f 202**



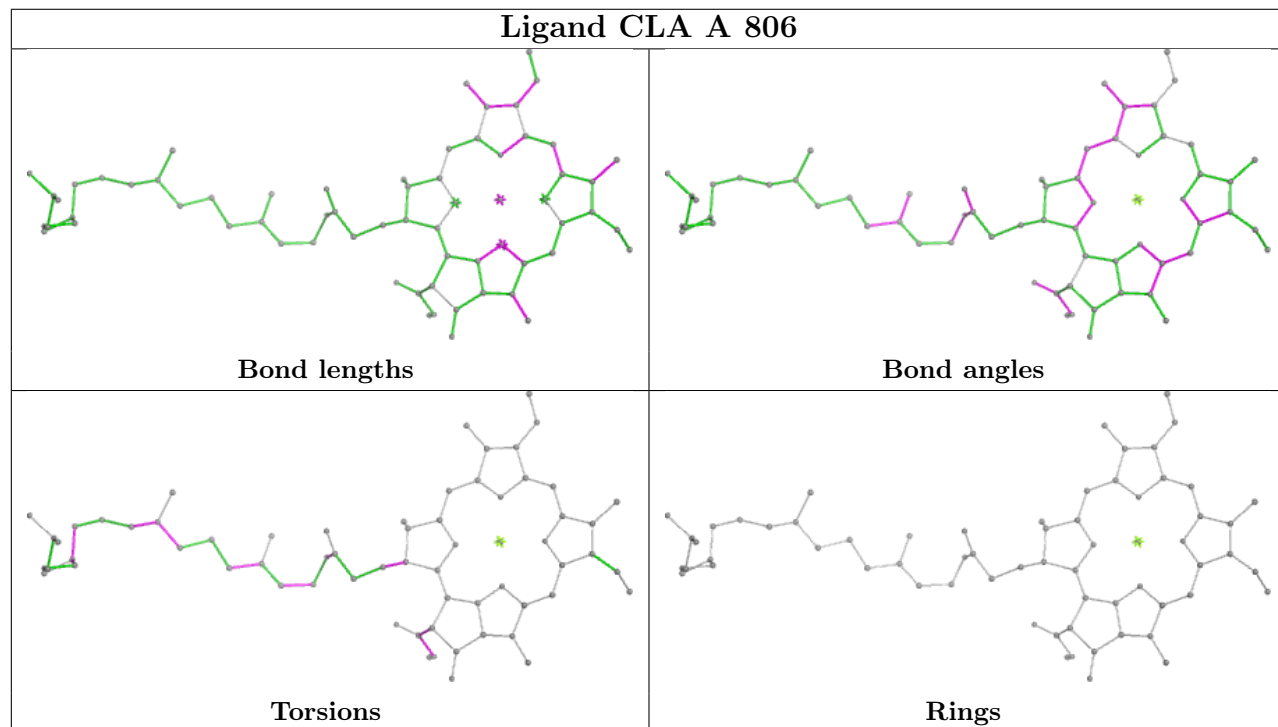
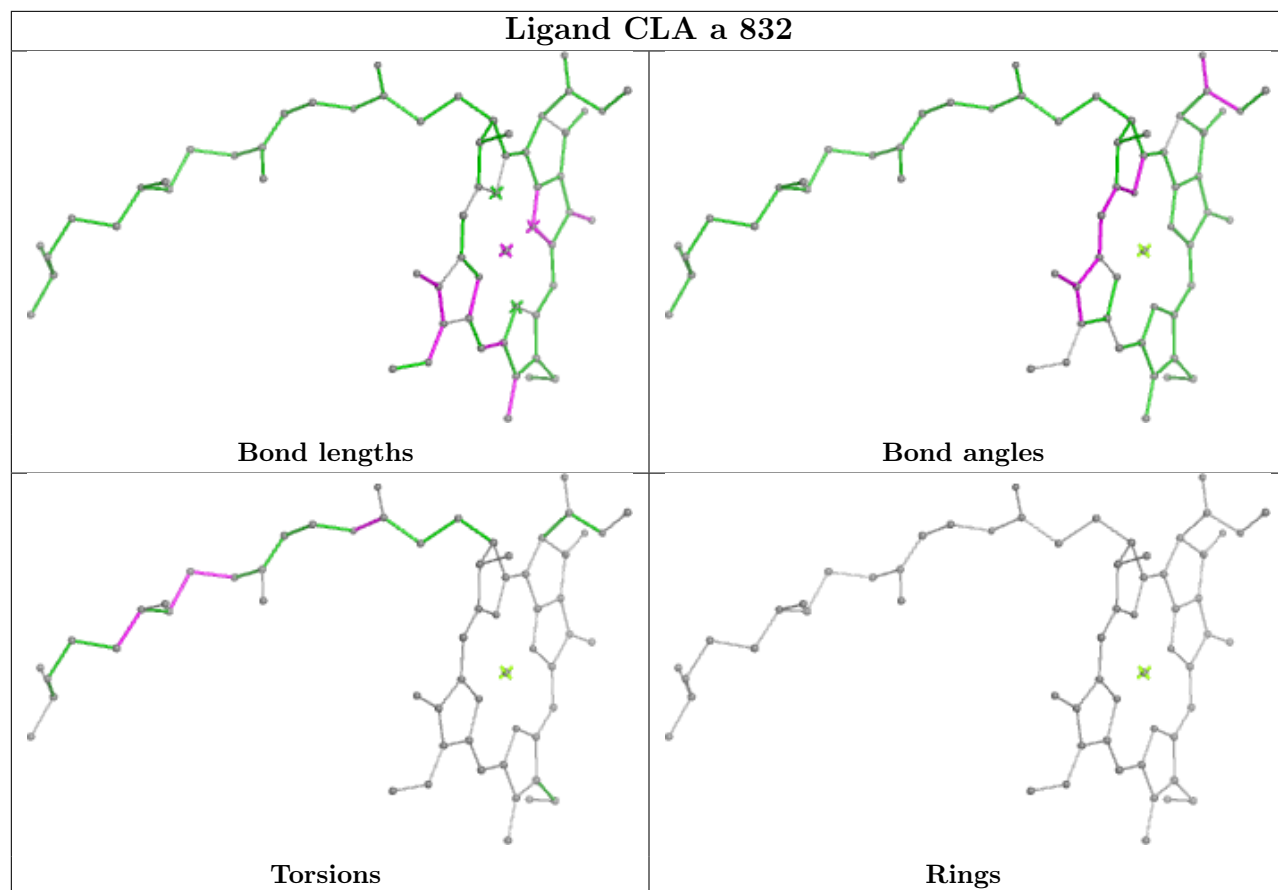
## Ligand CLA a 814

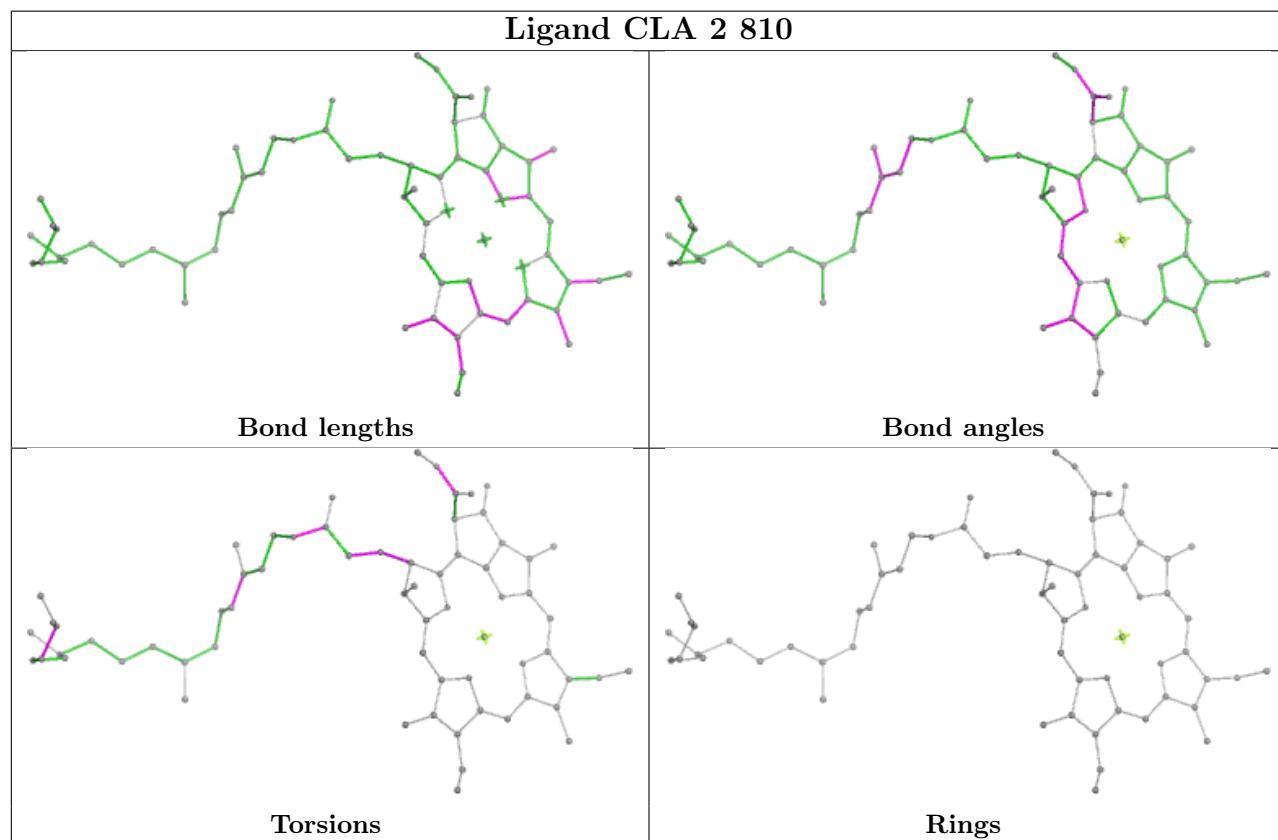
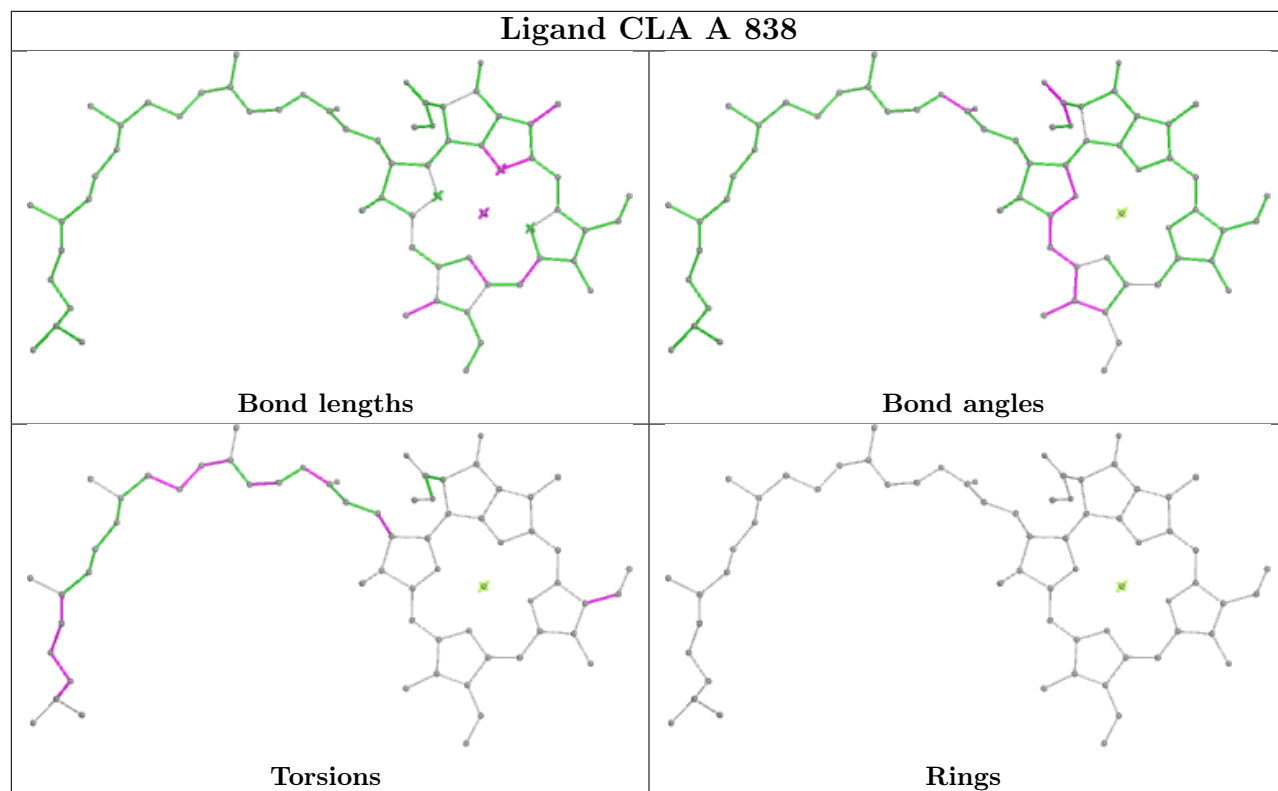


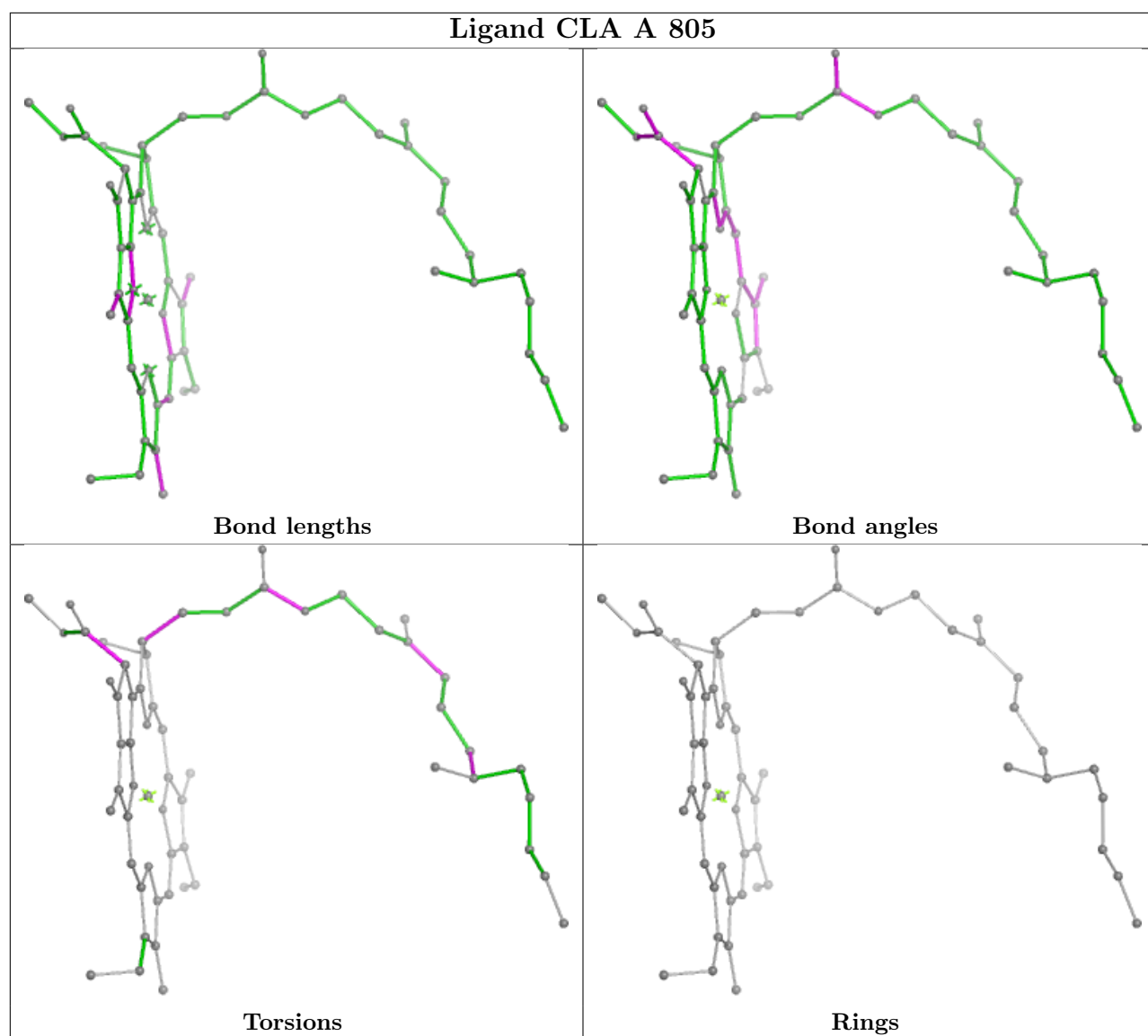
## Ligand CLA 1 1636

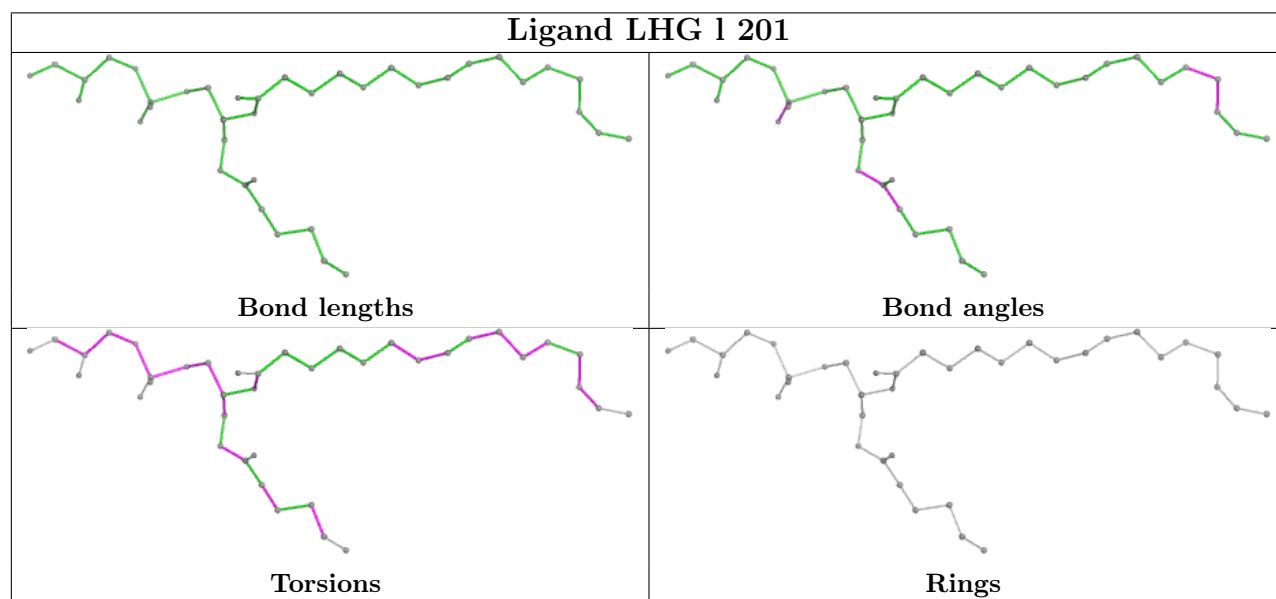
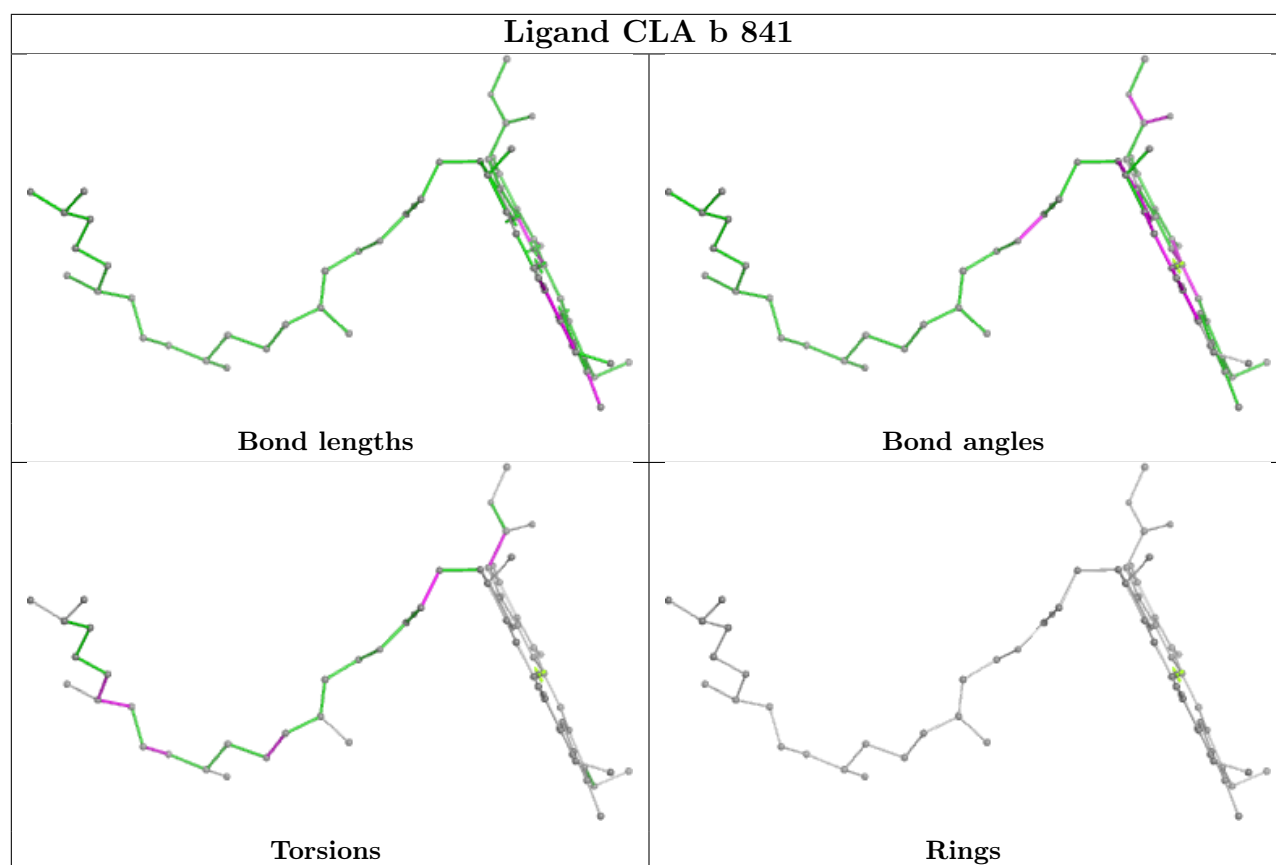


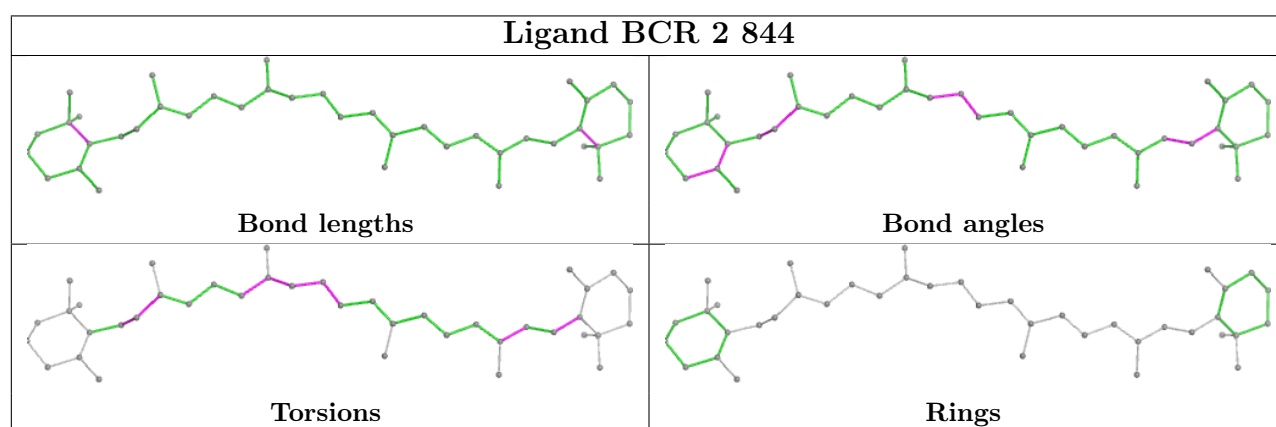
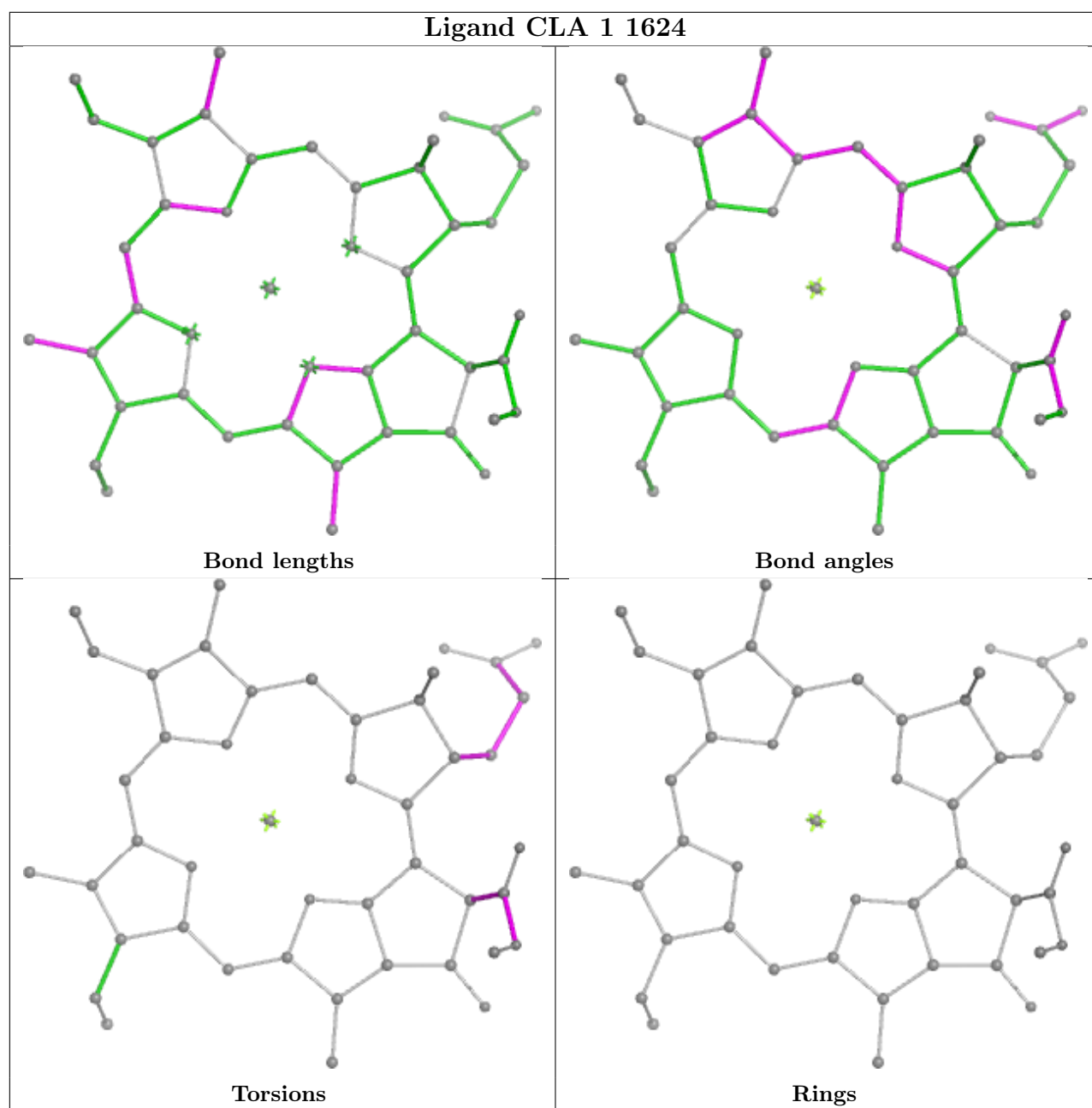


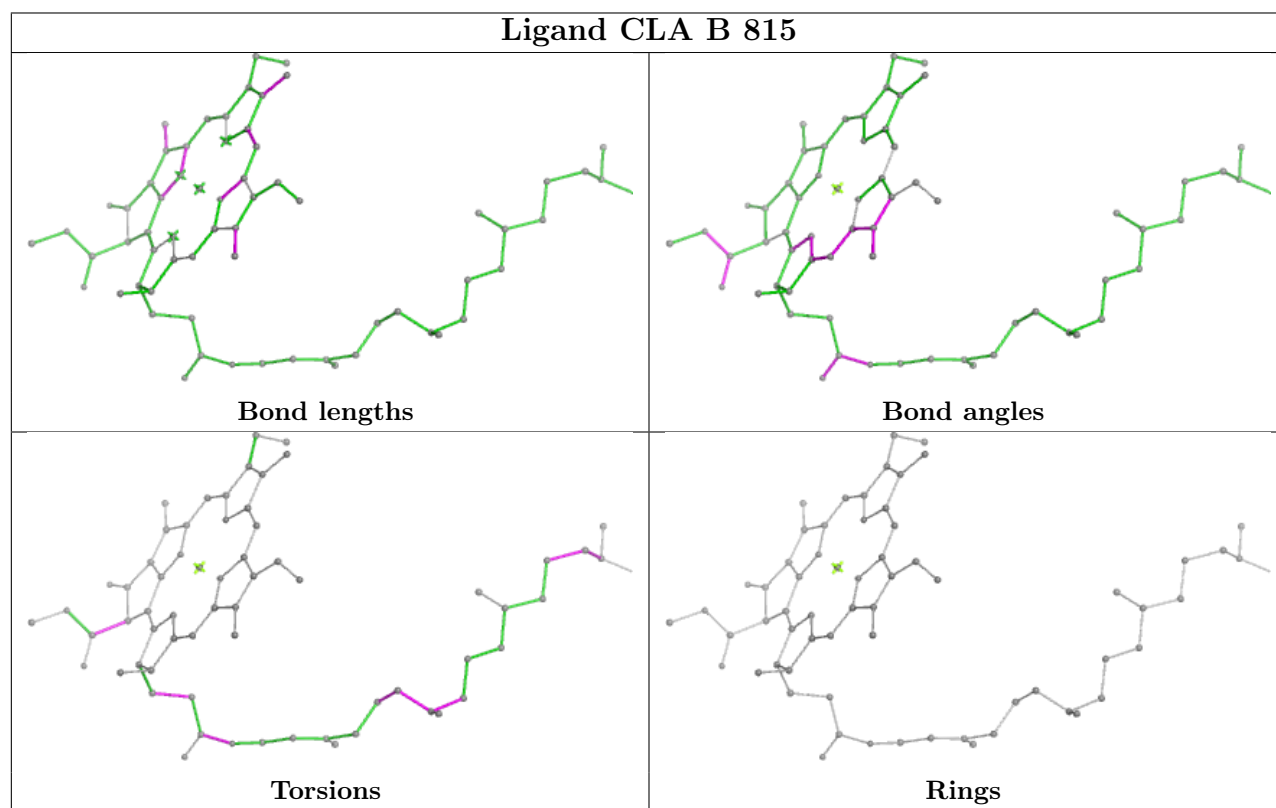
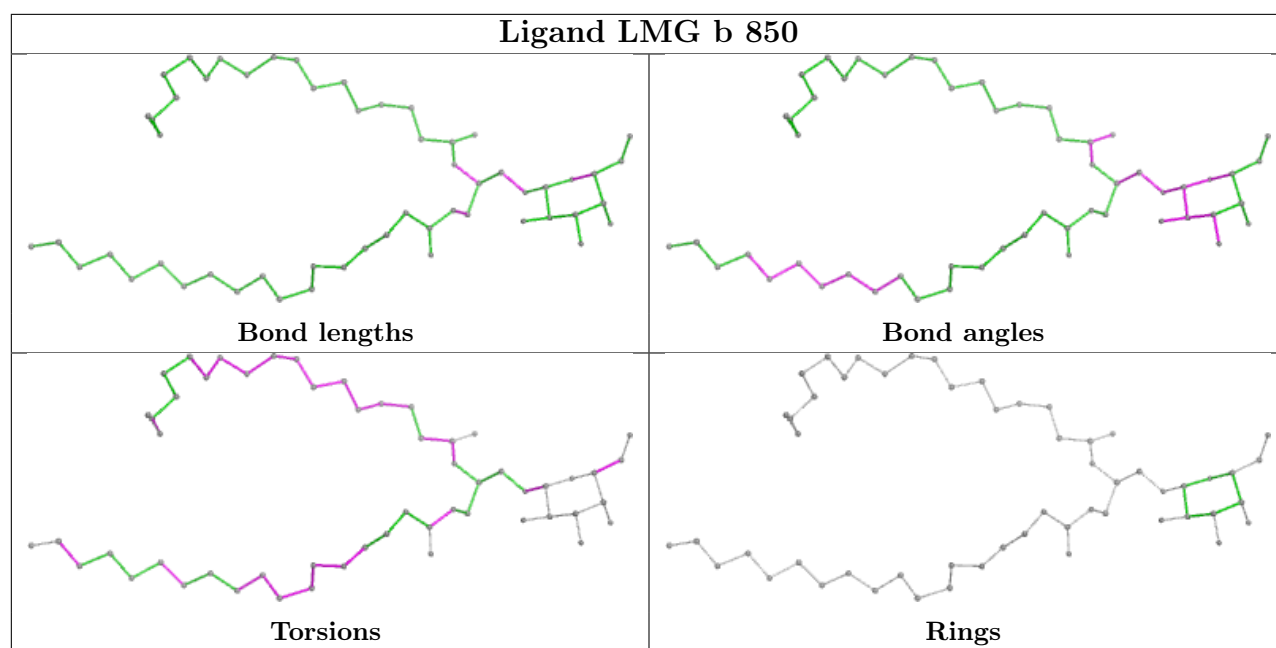


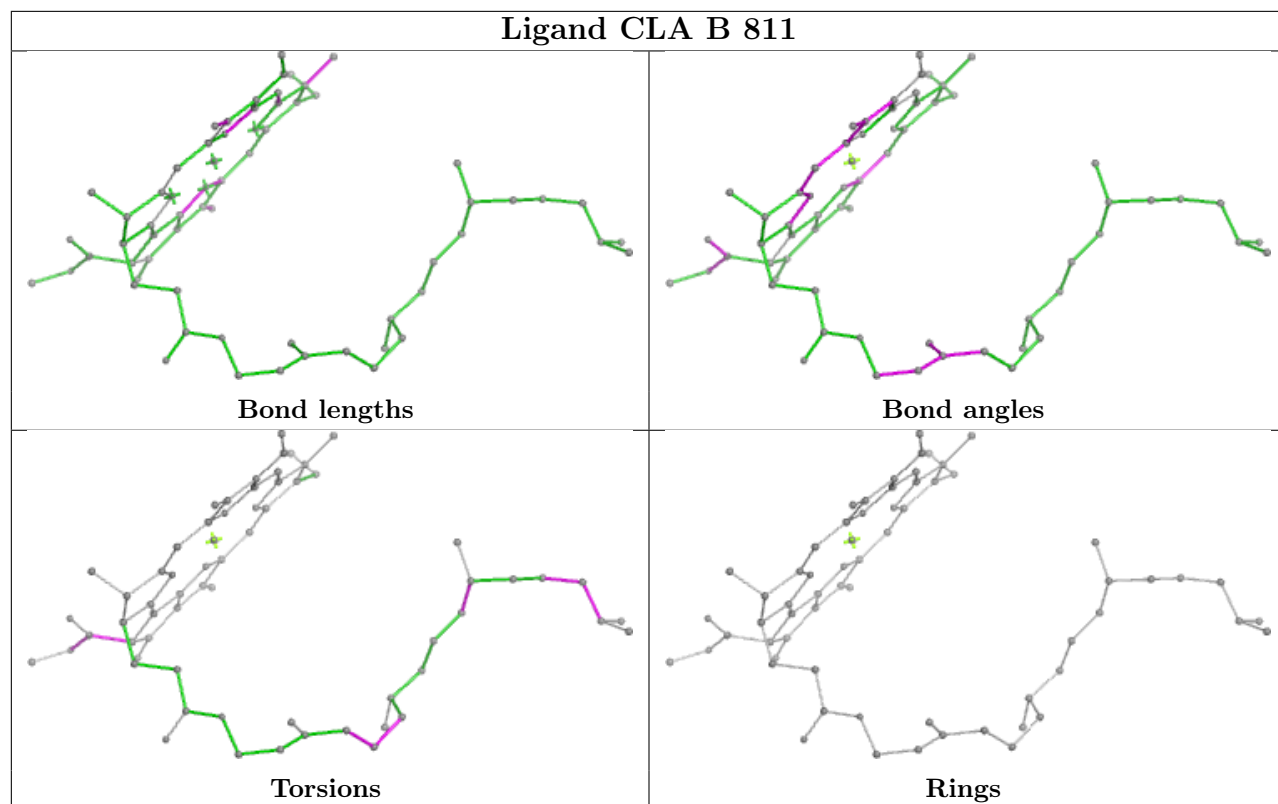




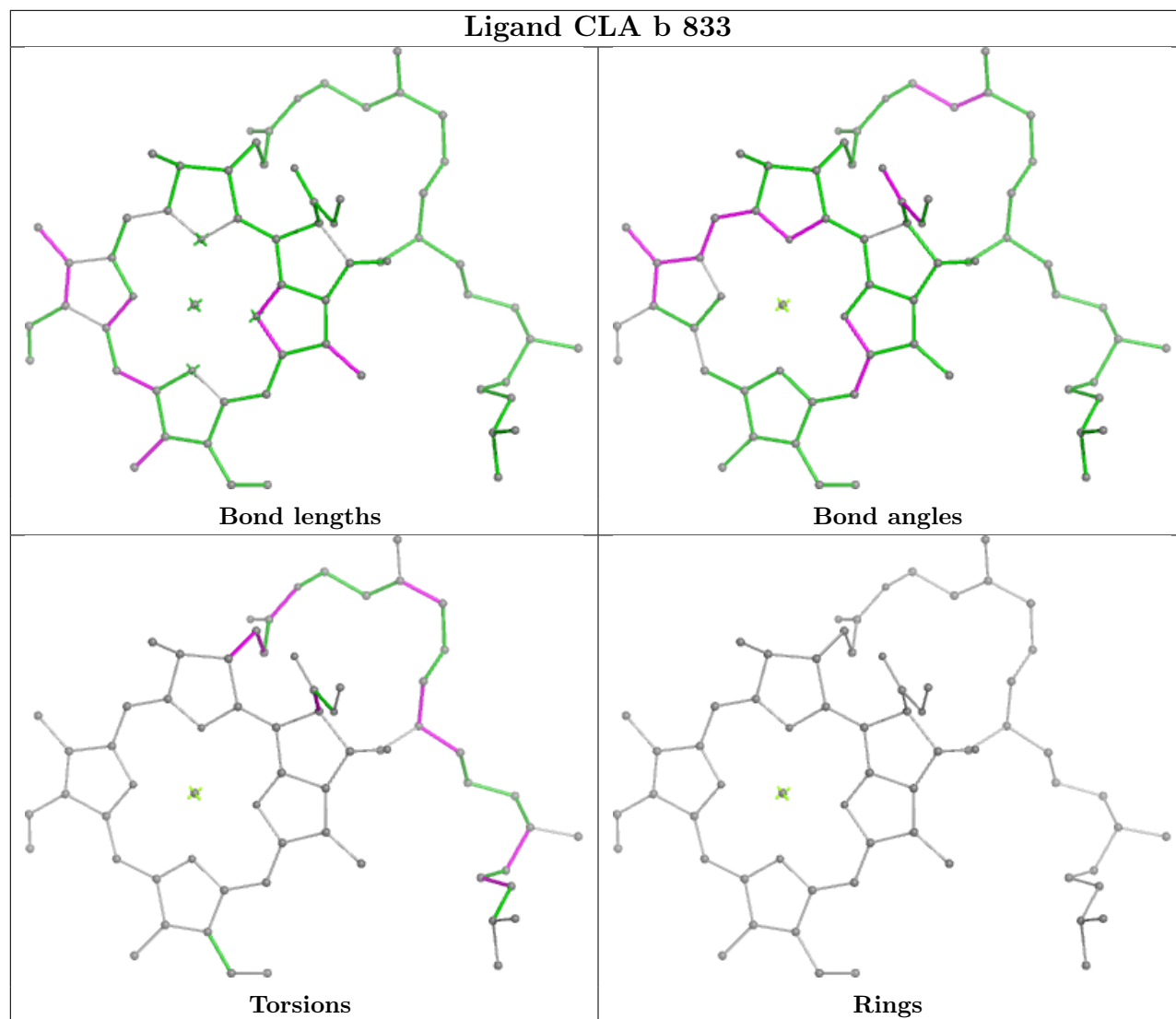






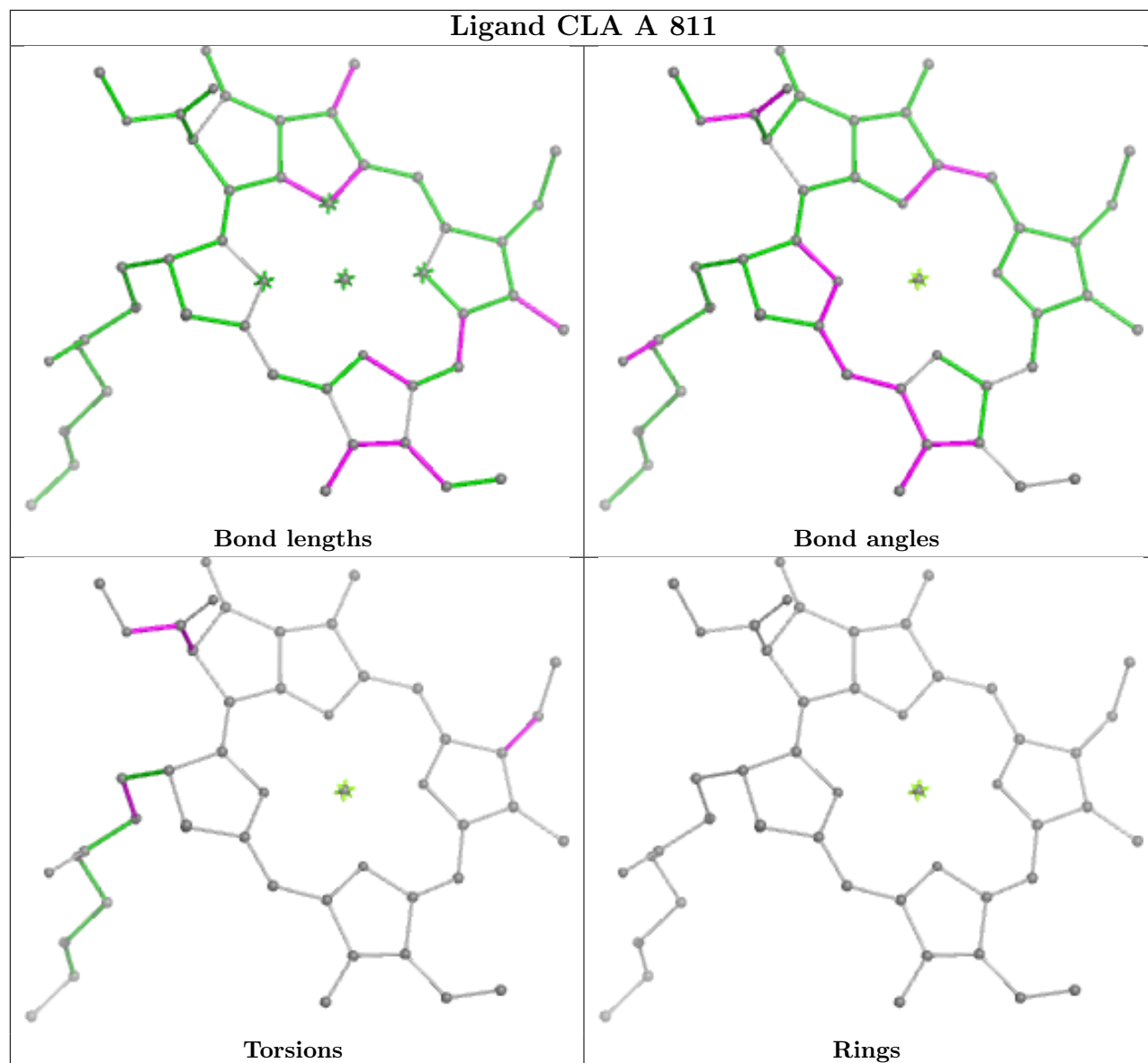


## Ligand CLA b 833

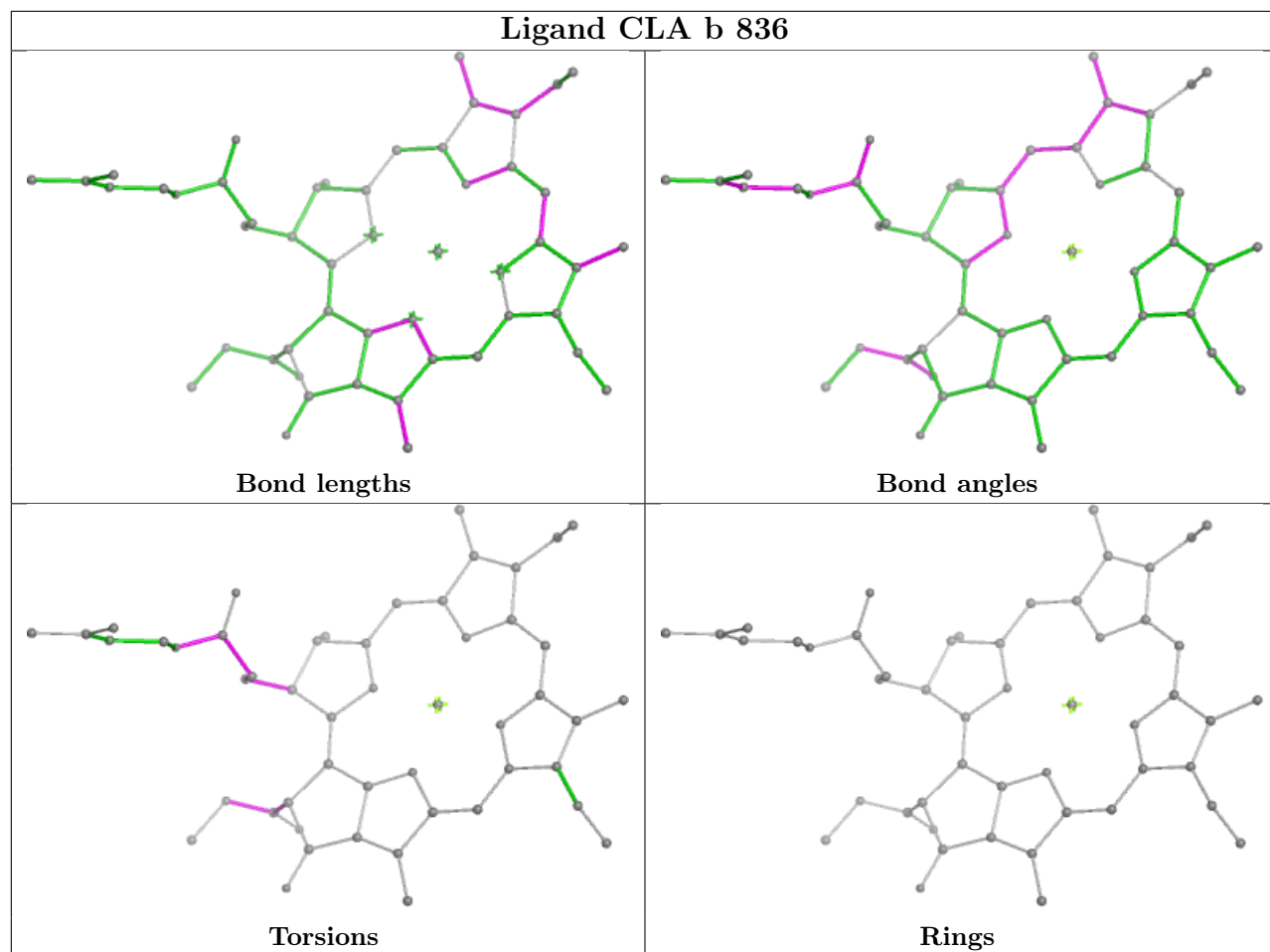


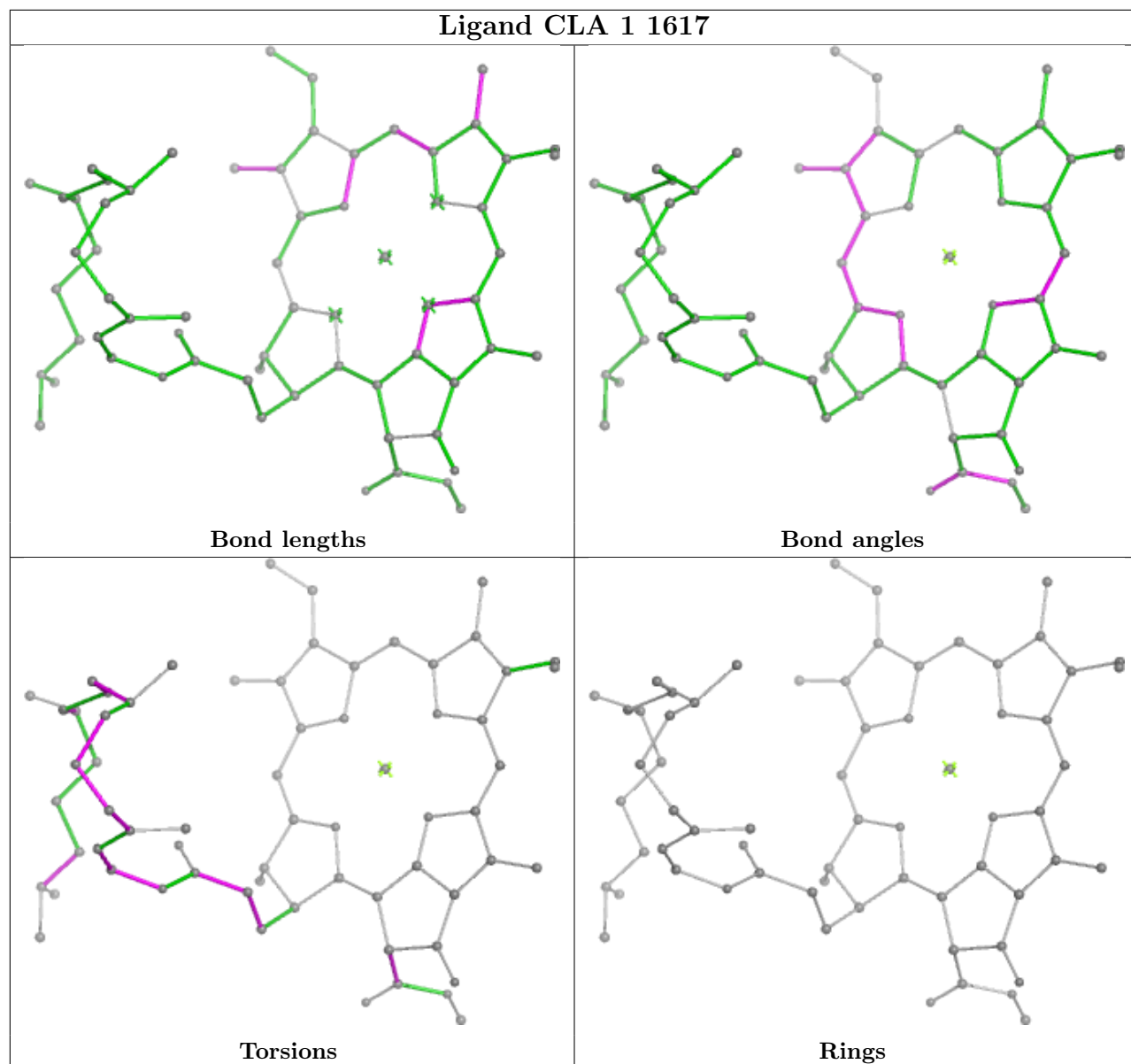


## Ligand CLA A 811

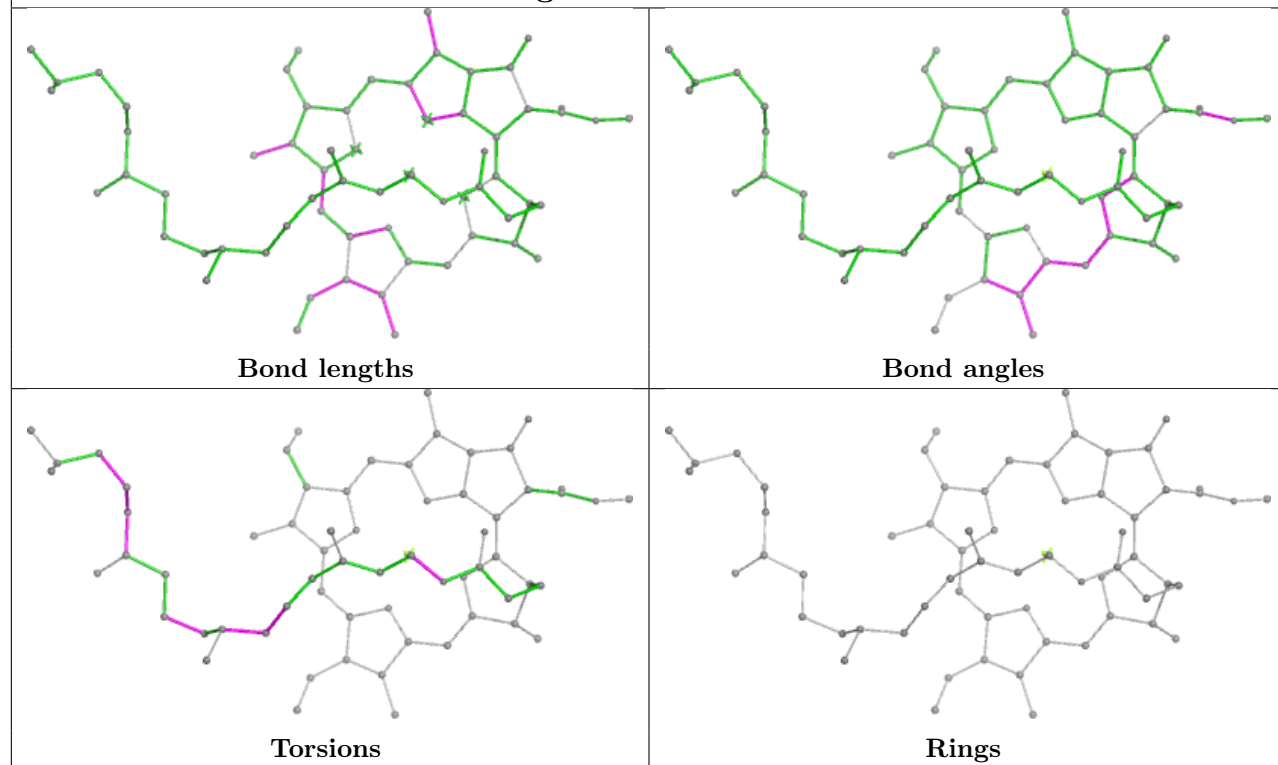


## Ligand CLA b 836

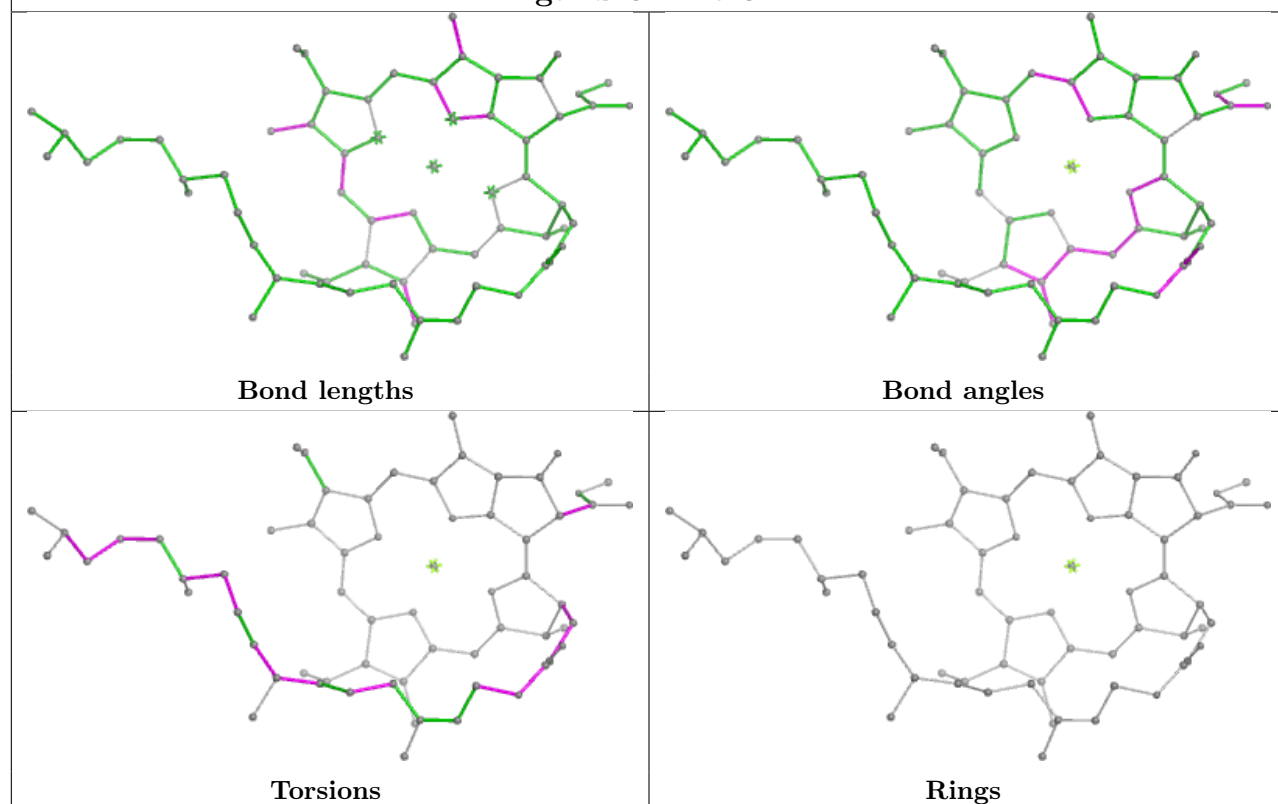




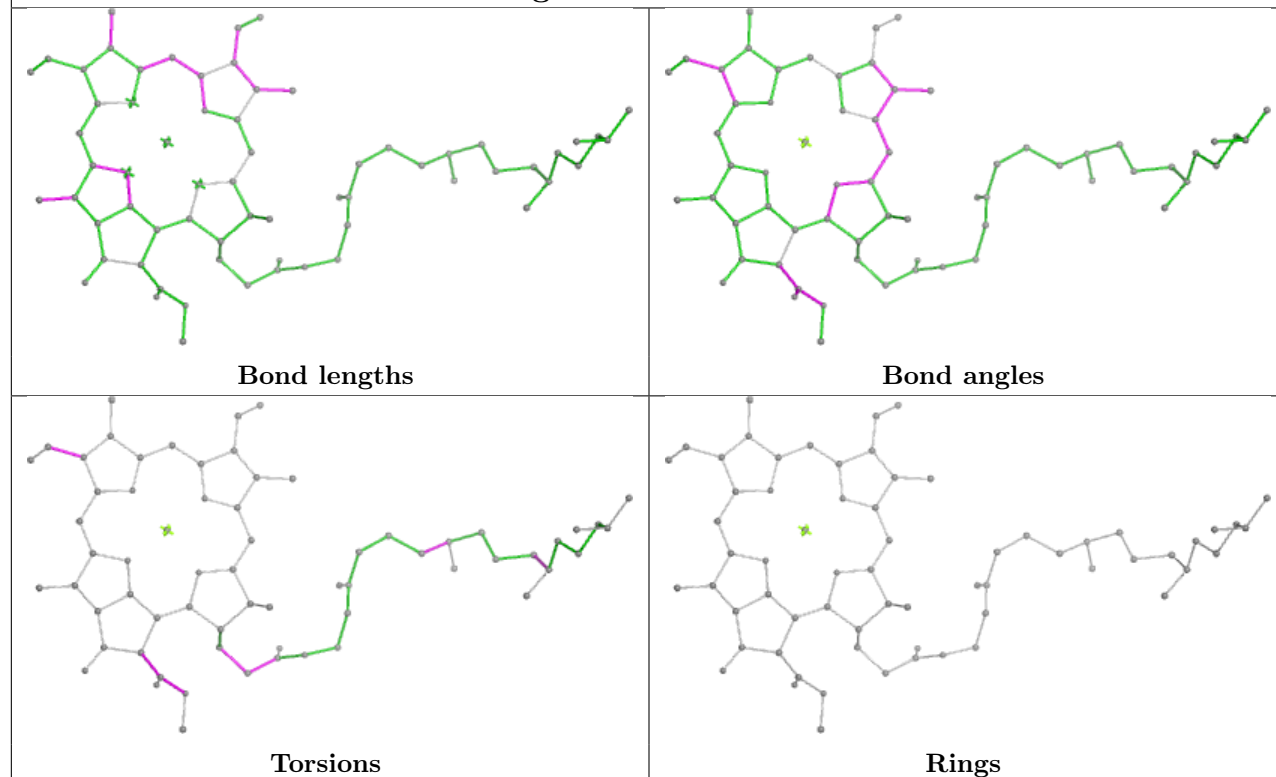
## Ligand CLA 2 839



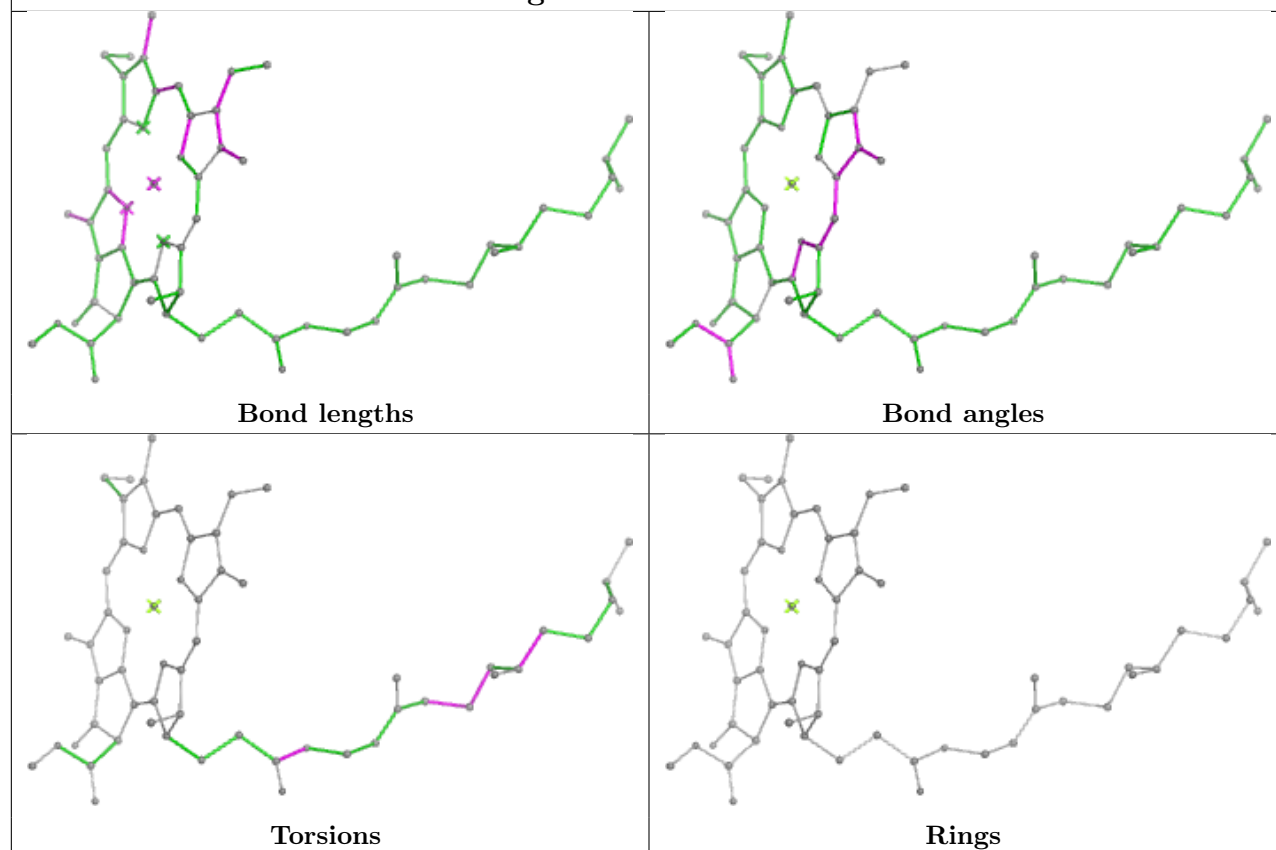
## Ligand CLA b 821

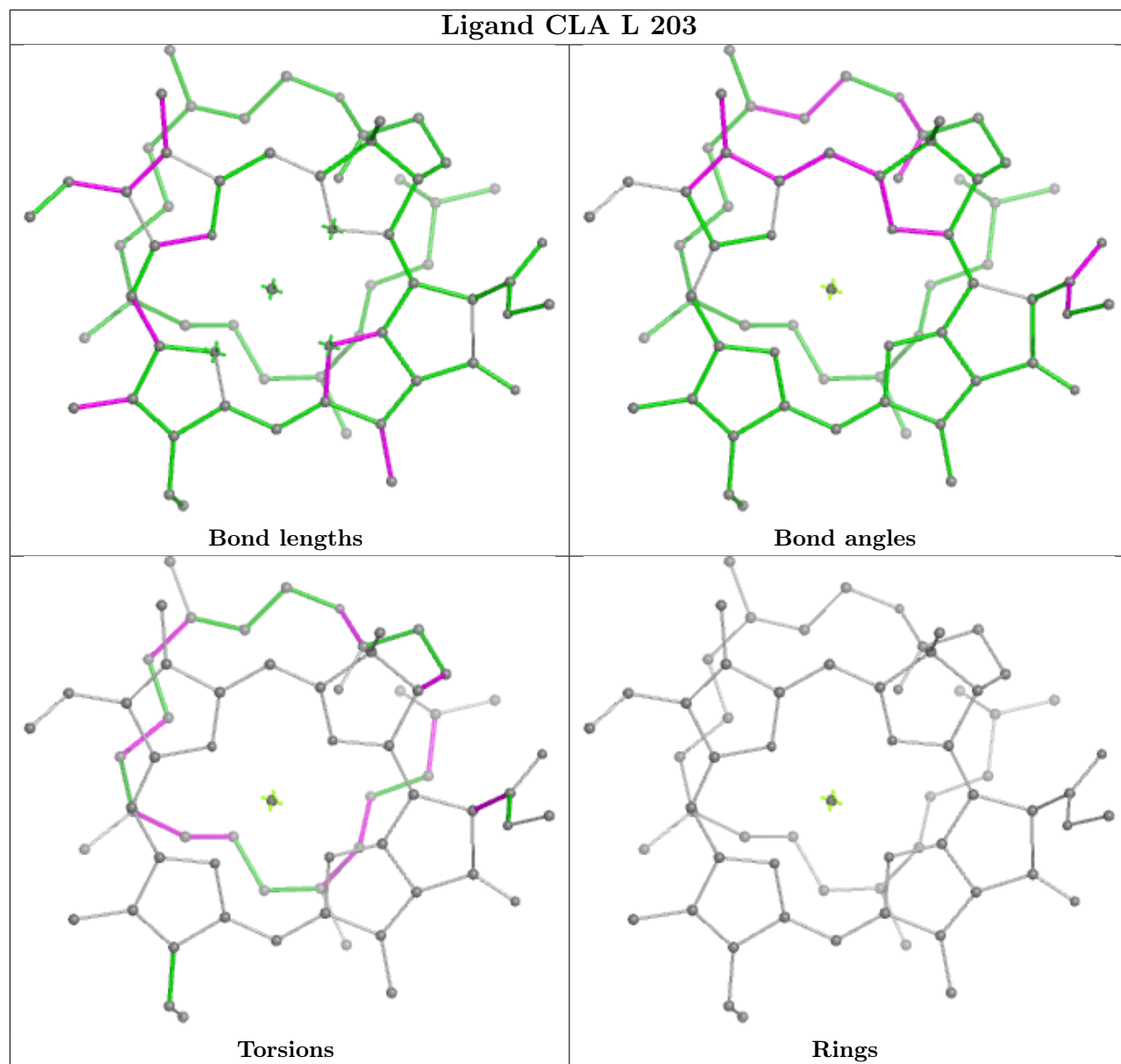


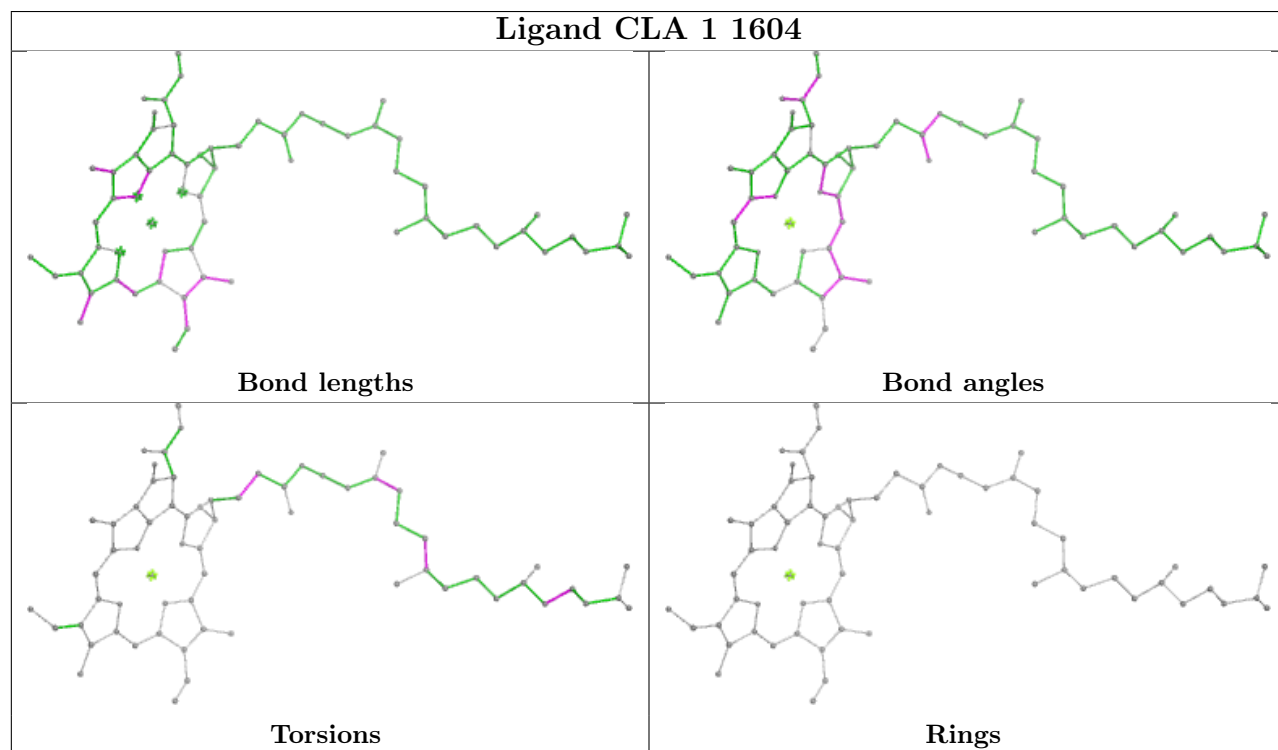
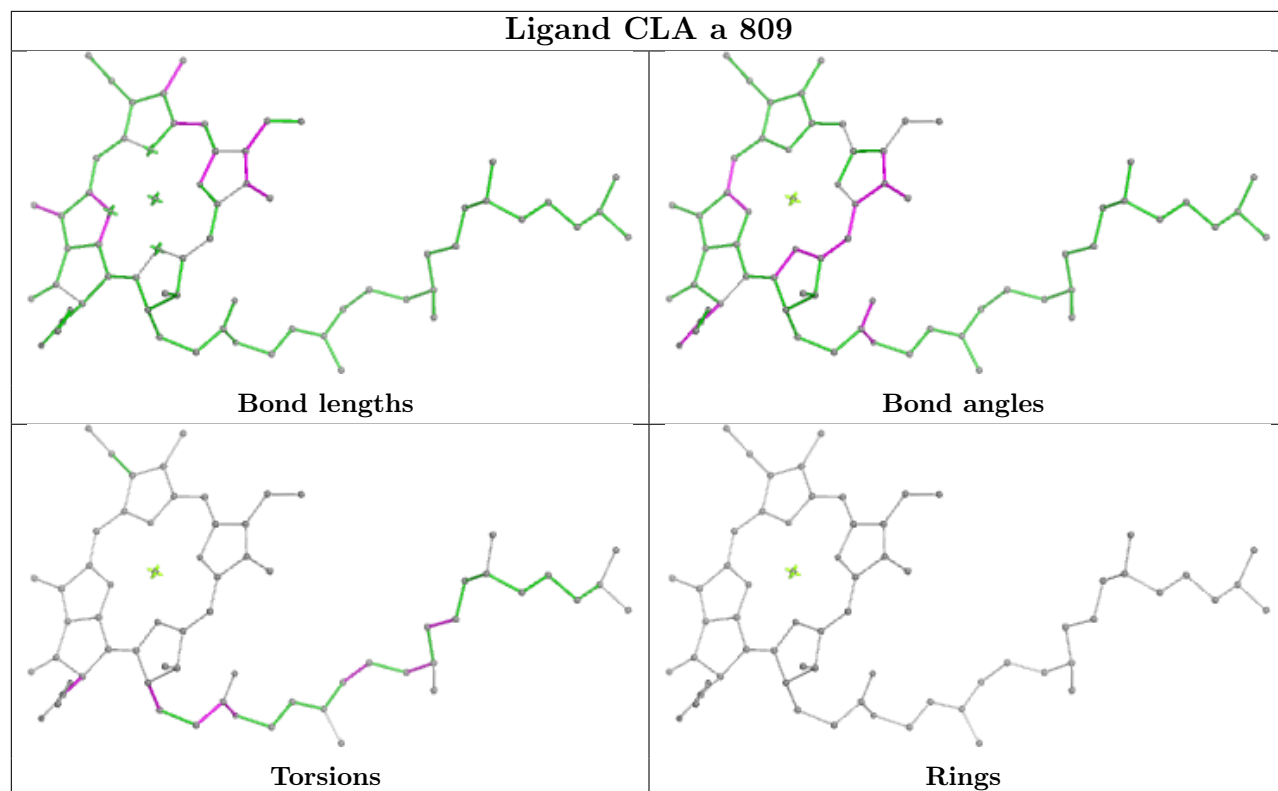
## Ligand CLA B 803



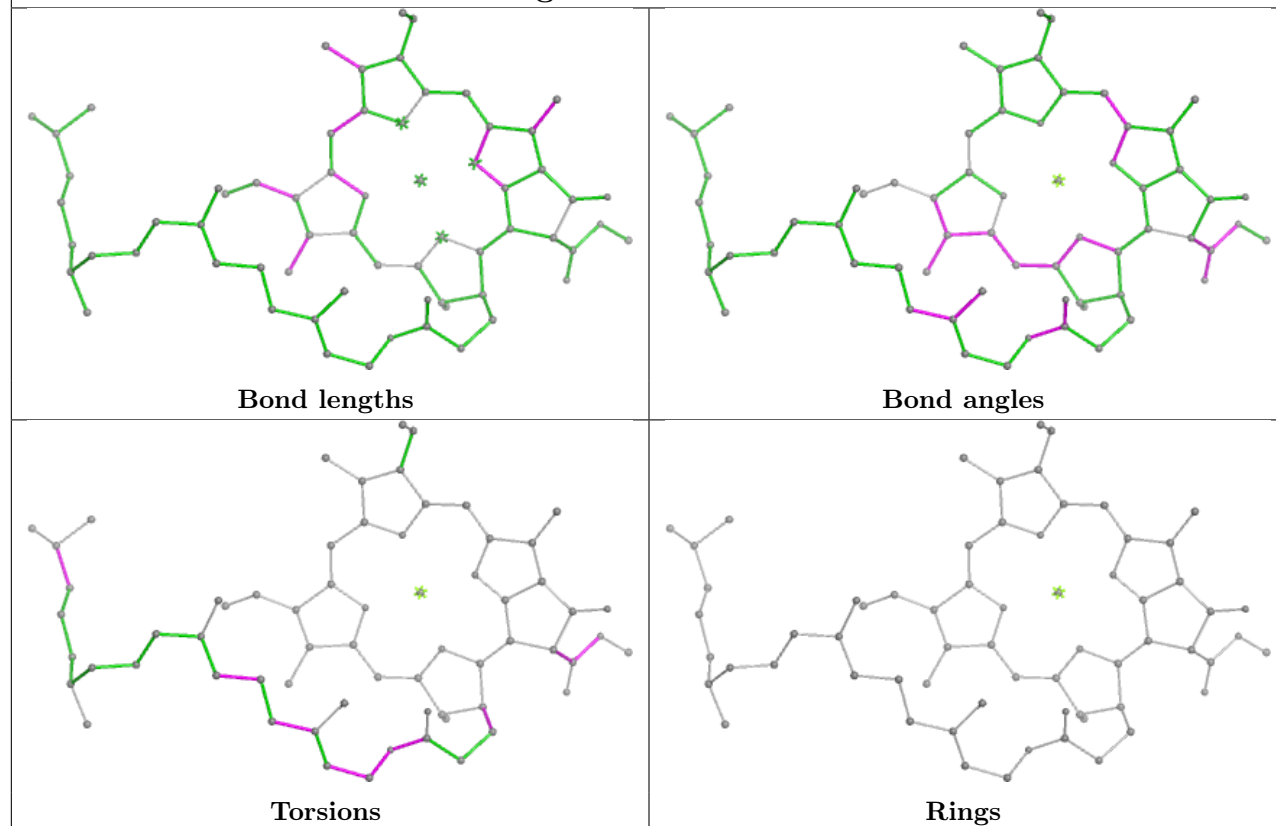
## Ligand CLA 1 1633



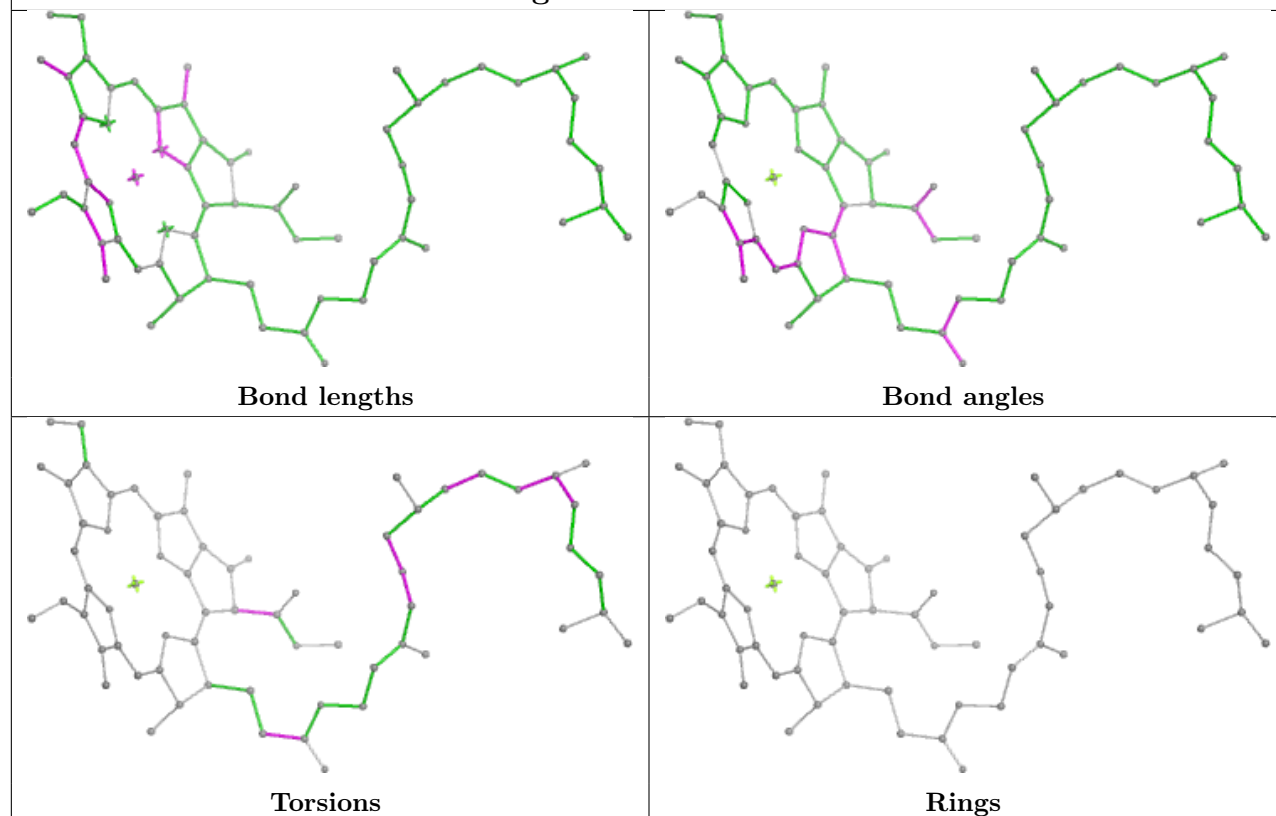




## Ligand CLA 2 819

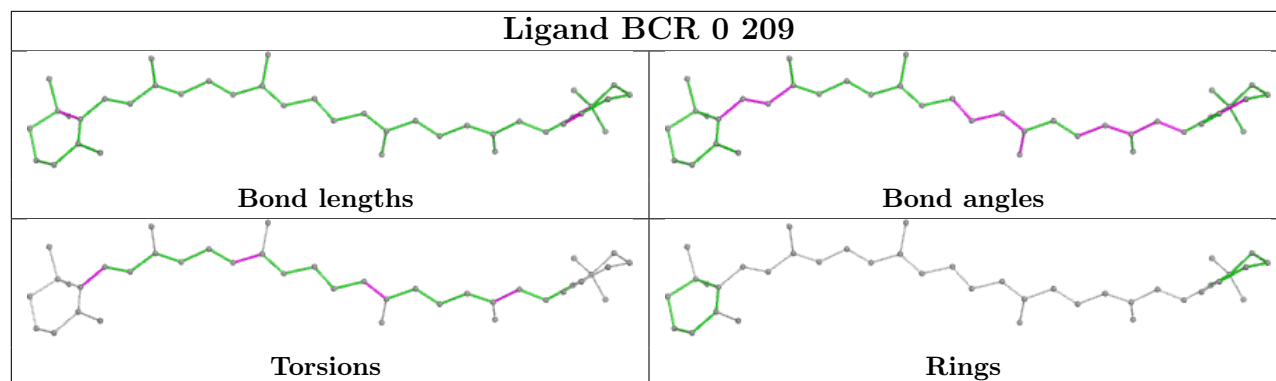


## Ligand CL0 1 1602

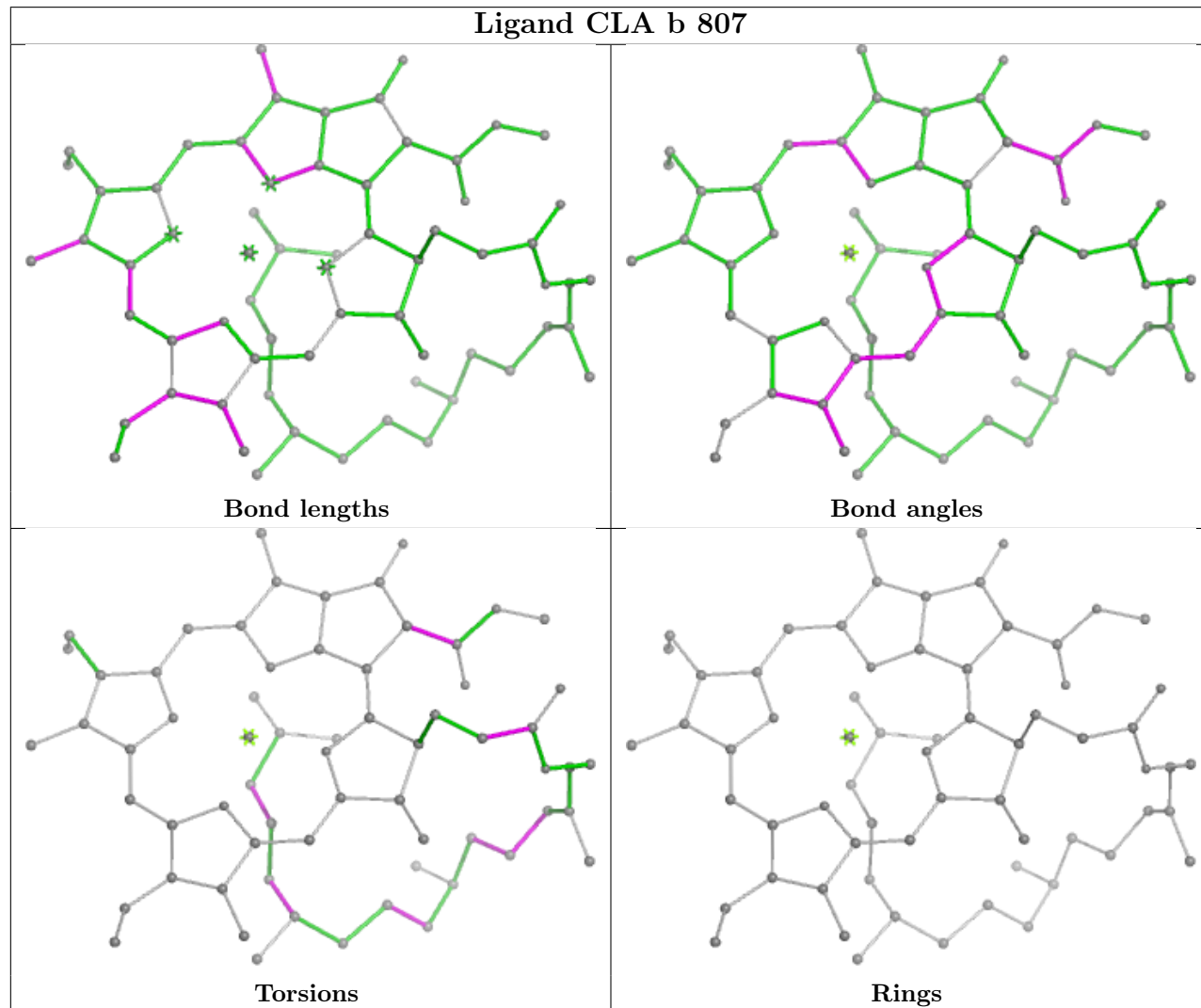




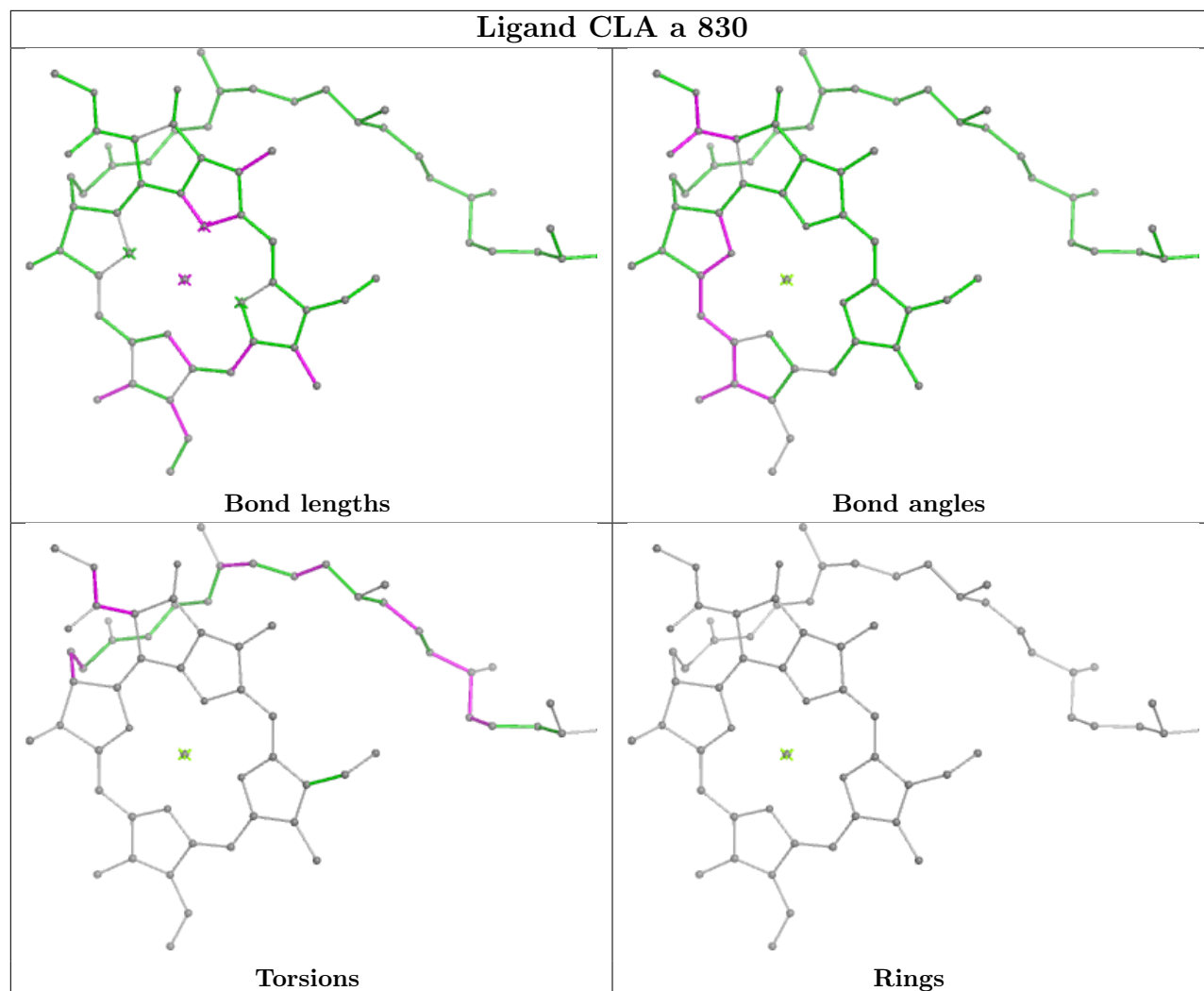
## Ligand BCR 0 209



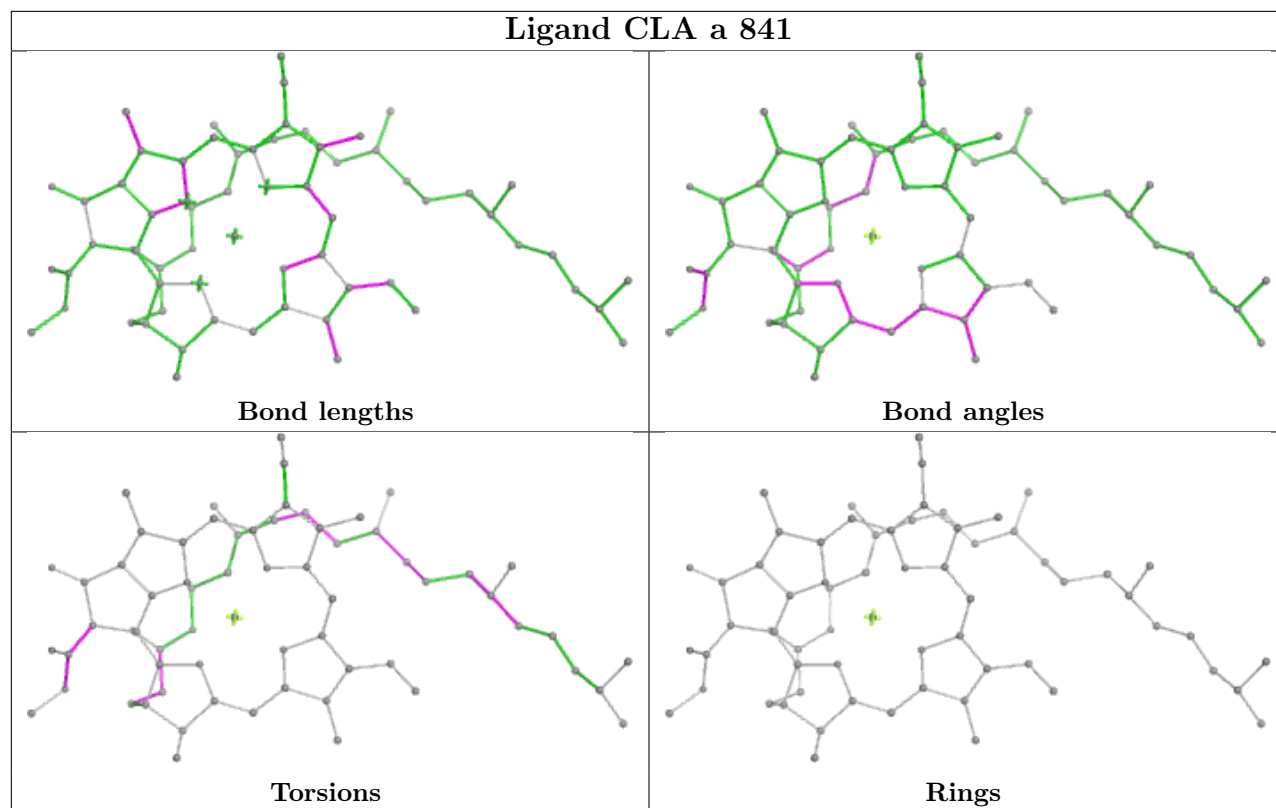
## Ligand CLA b 807



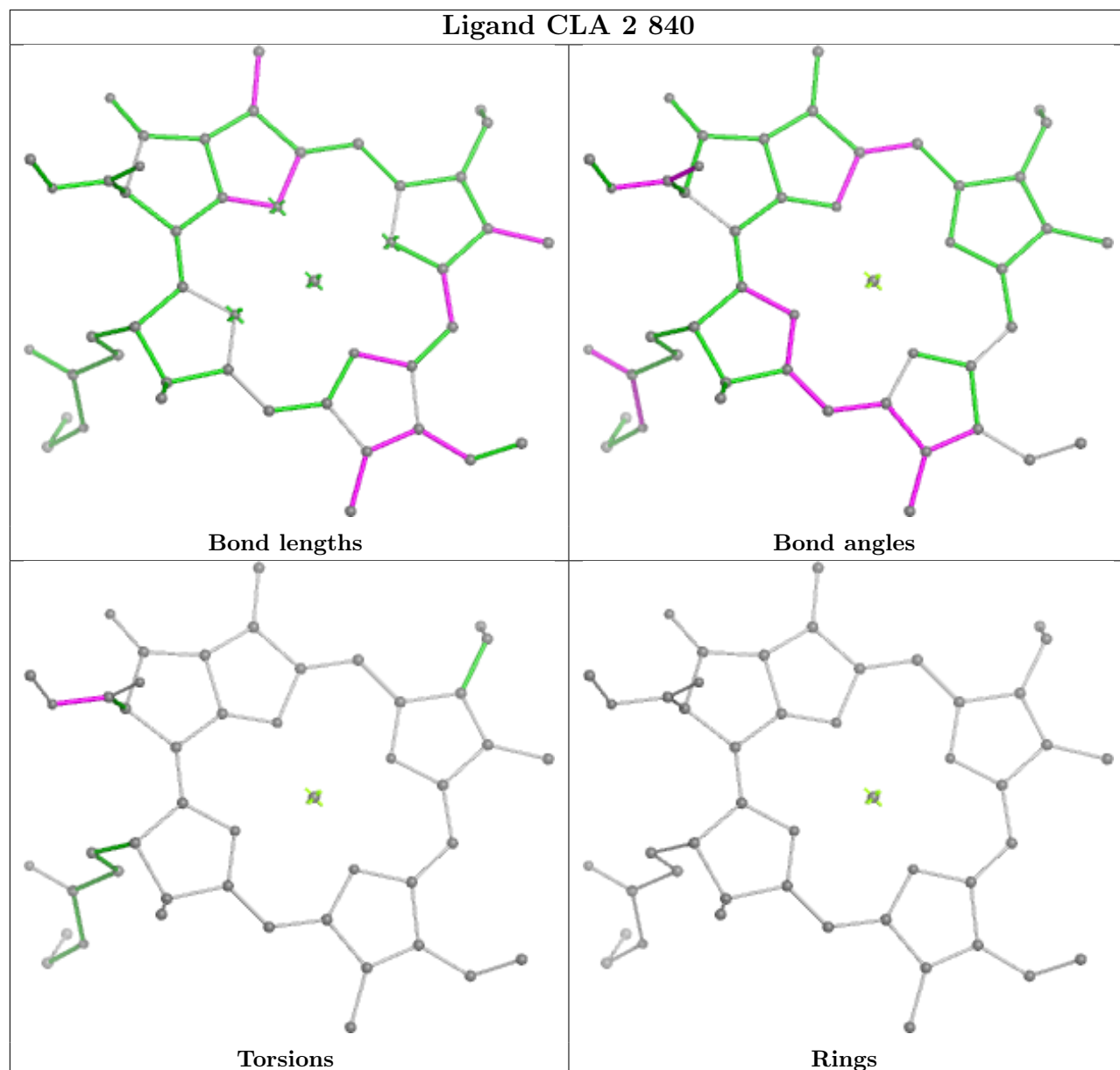
## Ligand CLA a 830



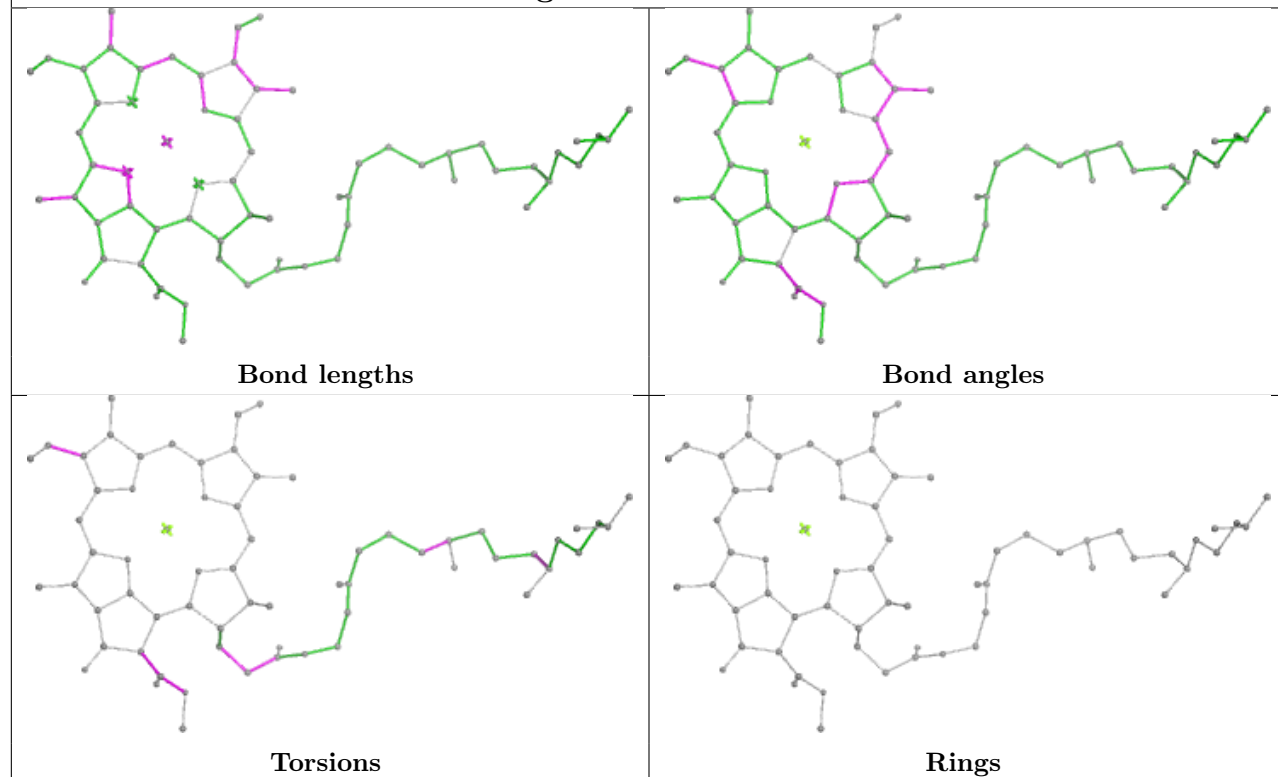
## Ligand CLA a 841



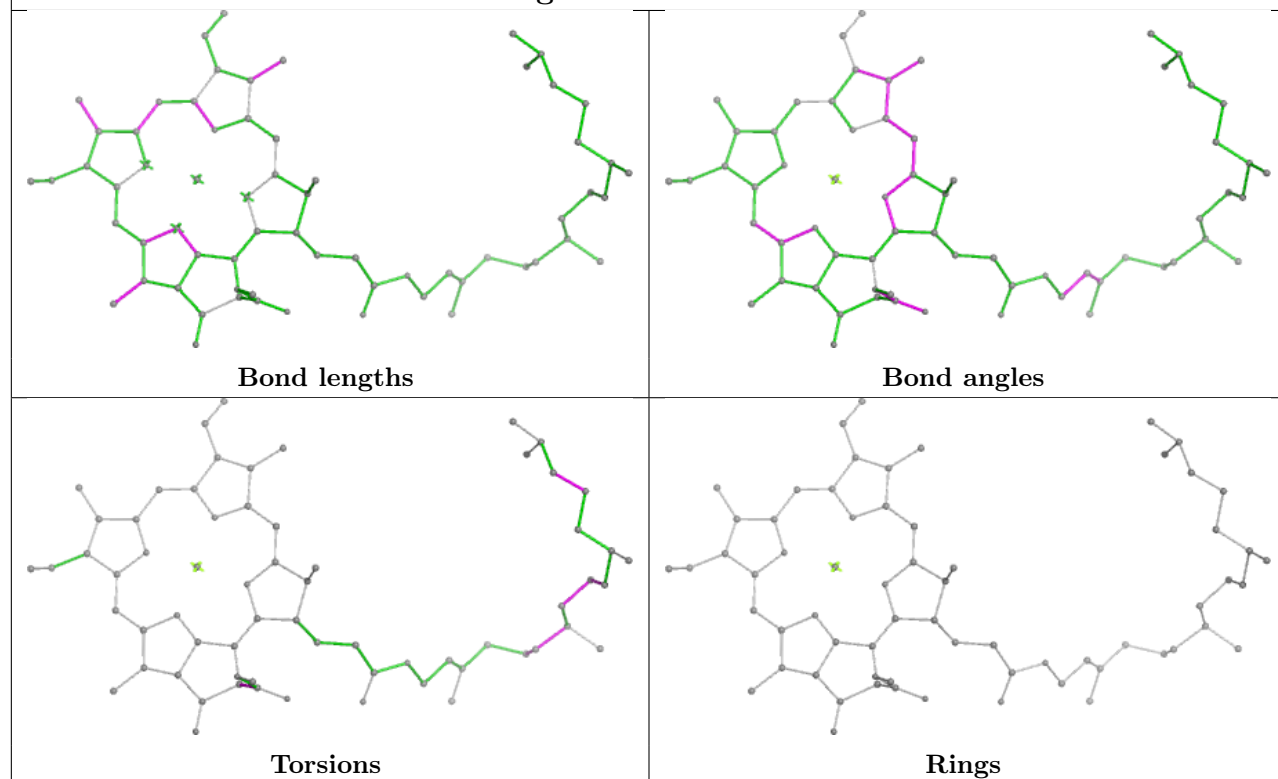
## Ligand CLA 2 840

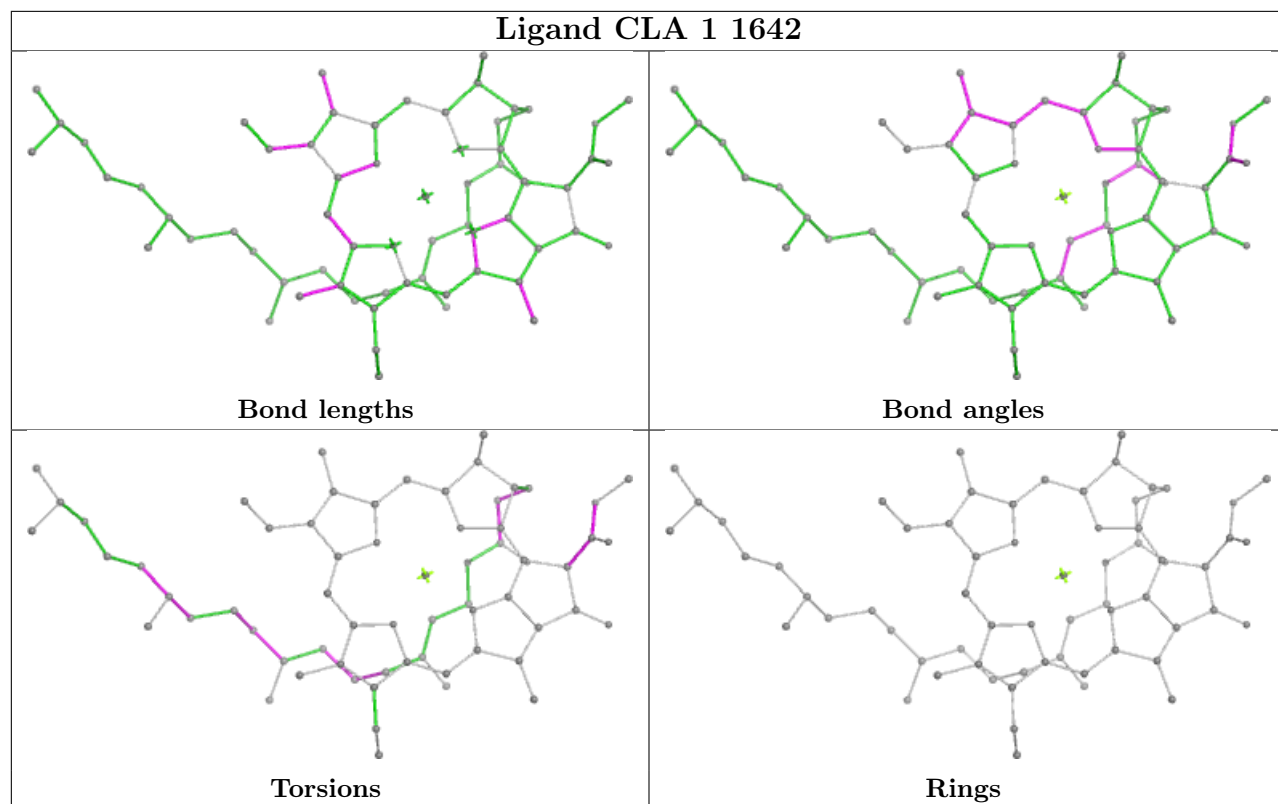


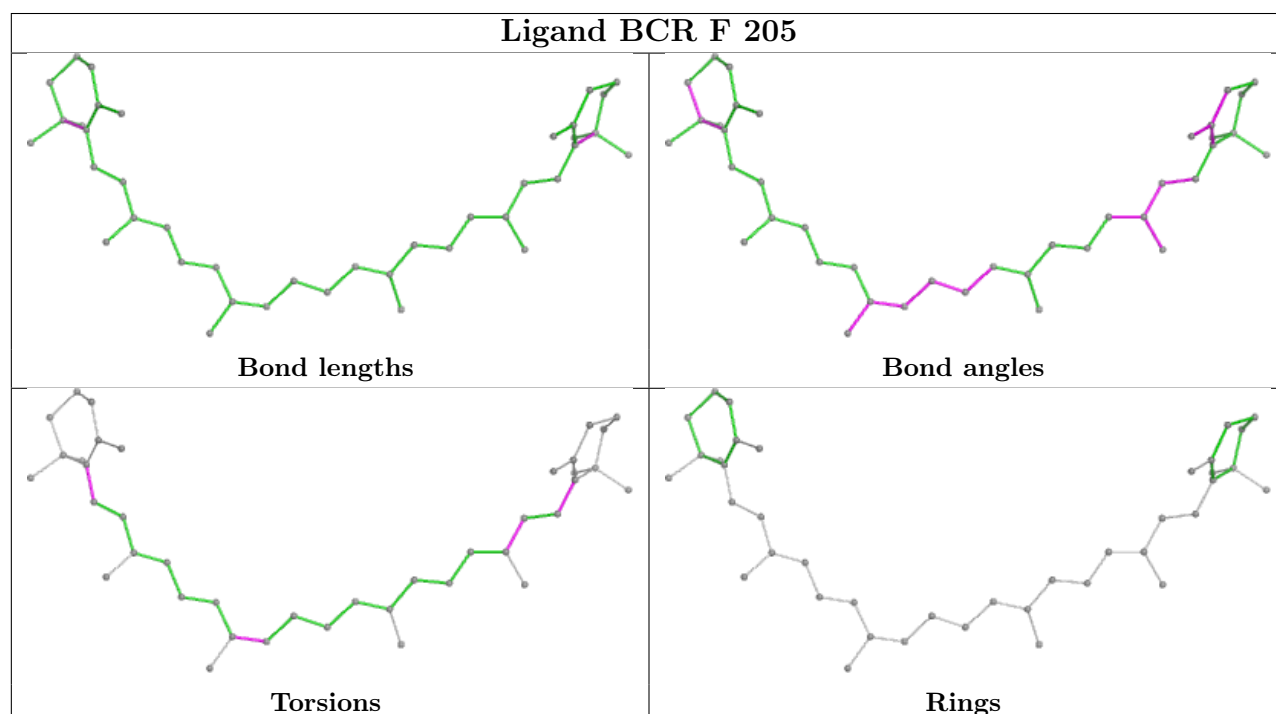
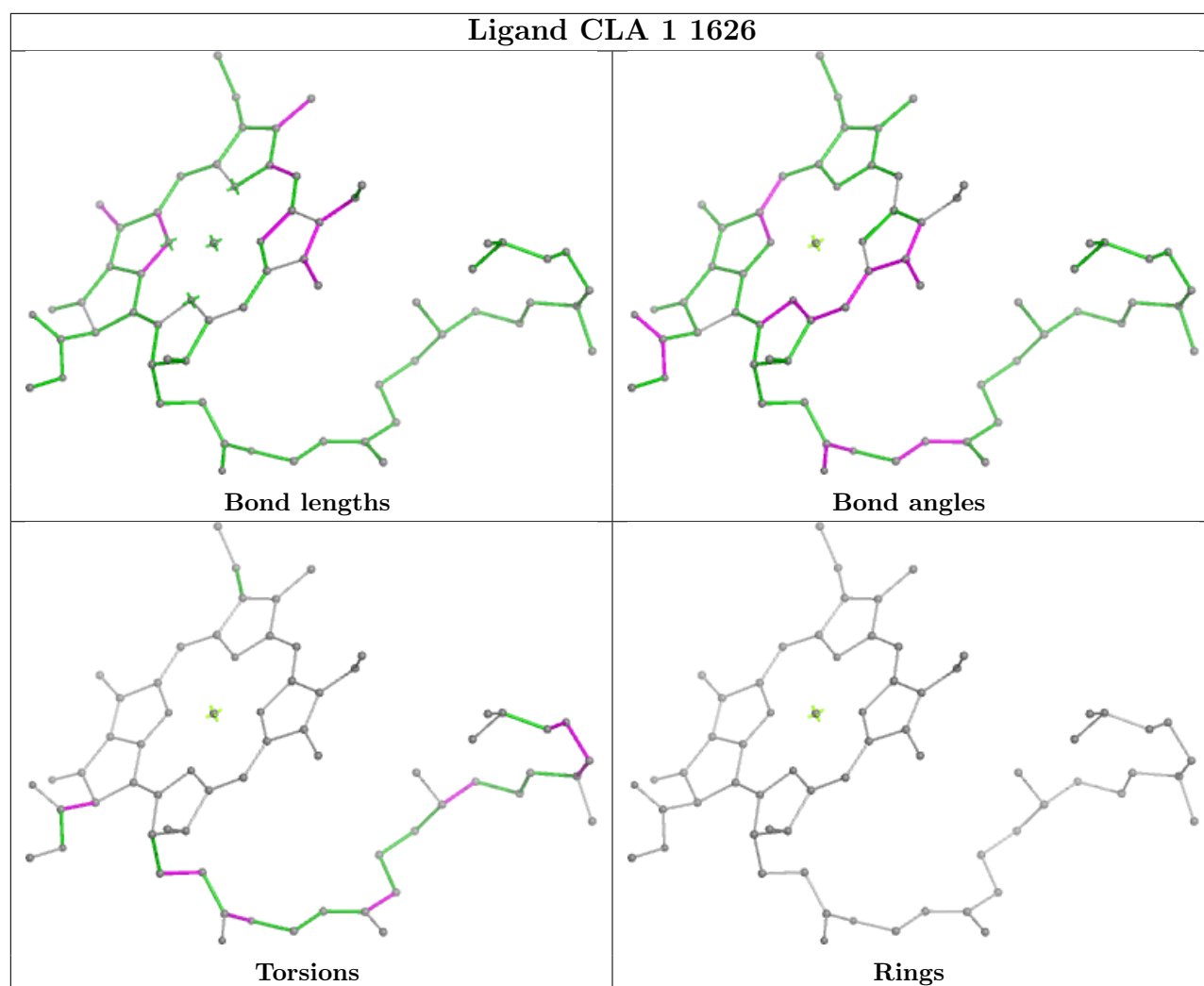
## Ligand CLA 2 804

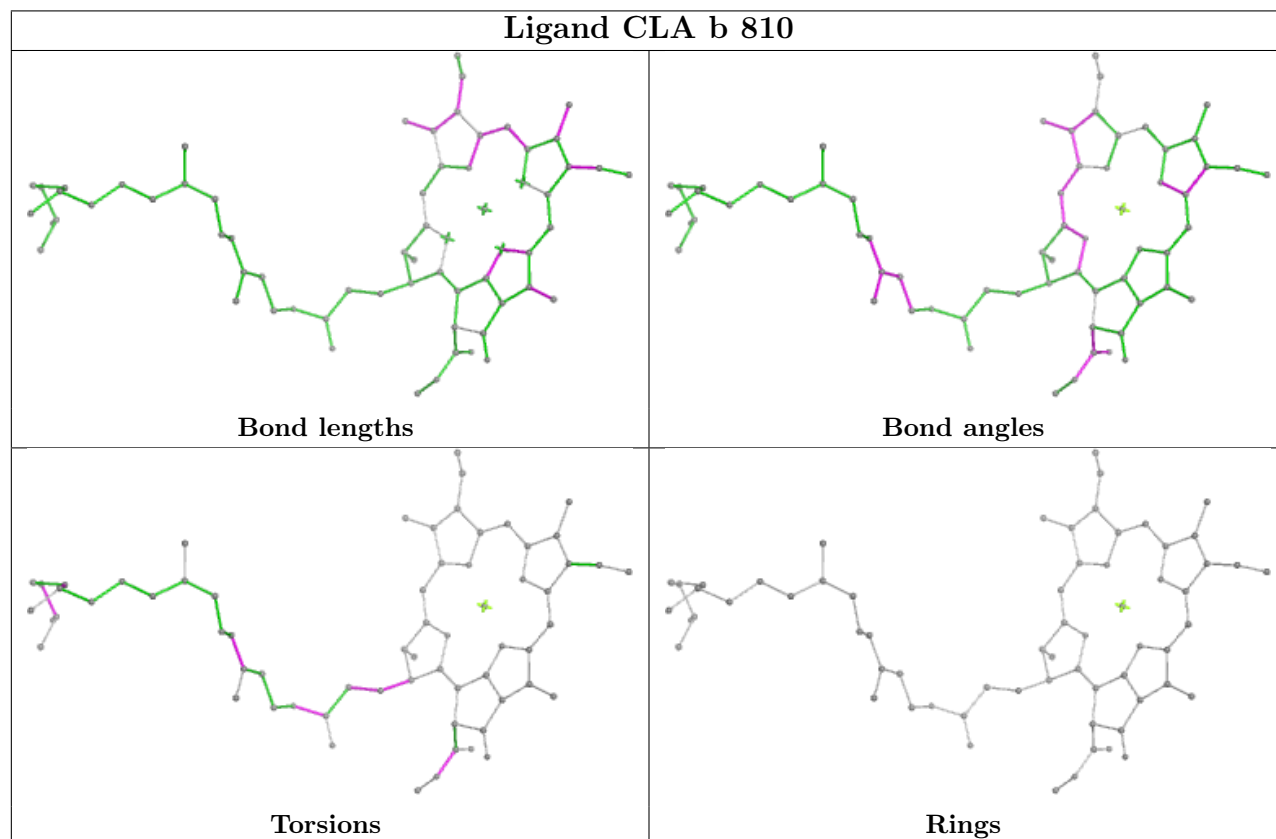
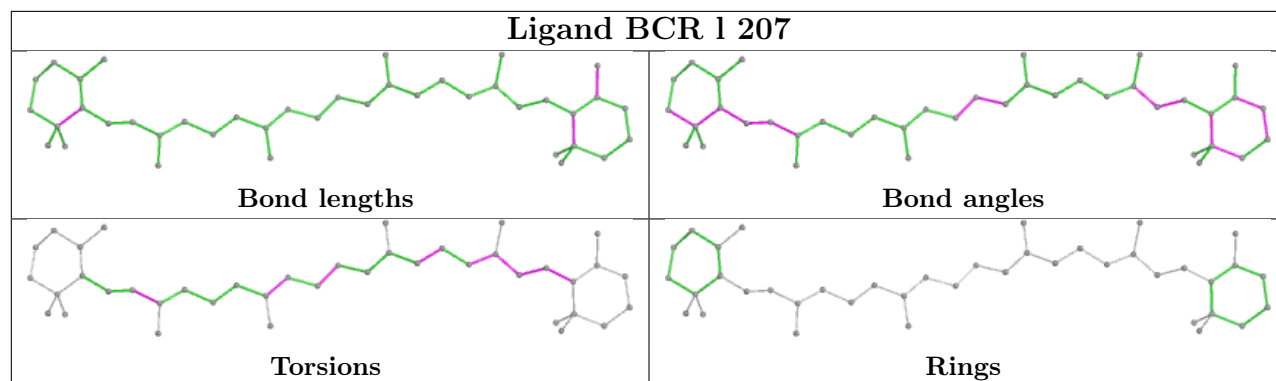


## Ligand CLA a 828

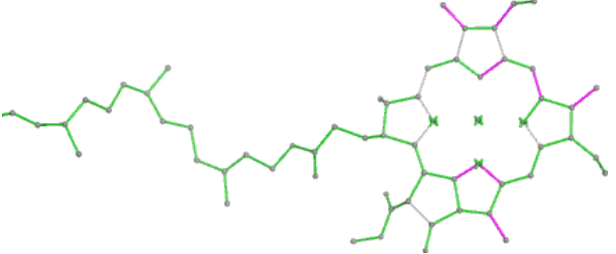
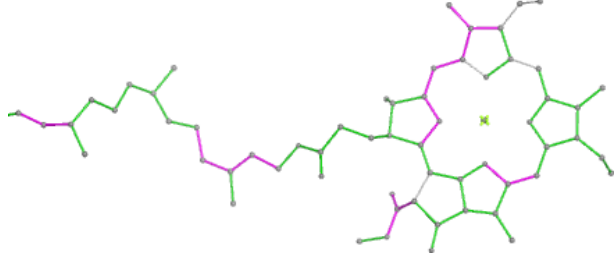
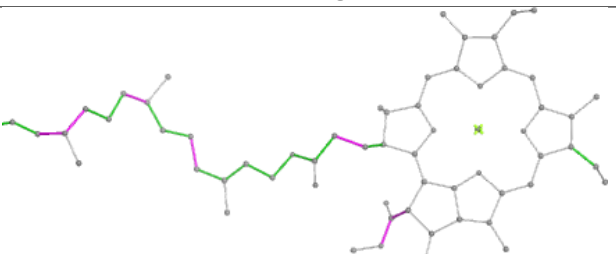
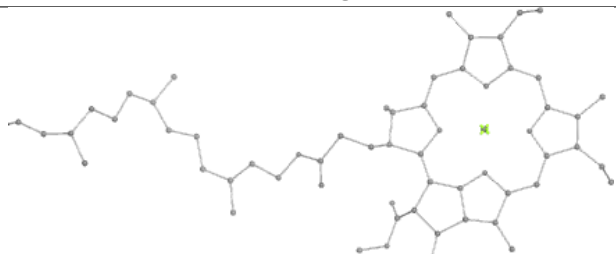
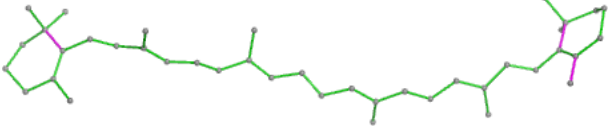
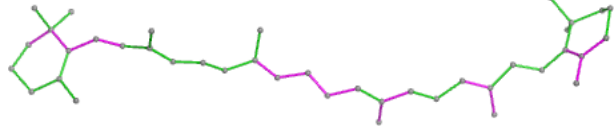
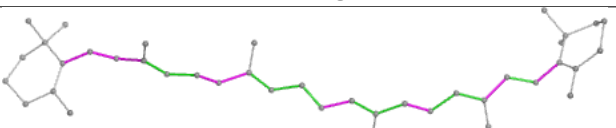
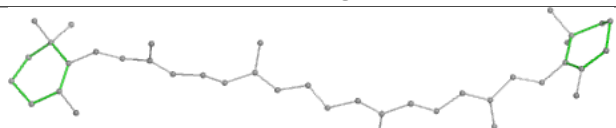
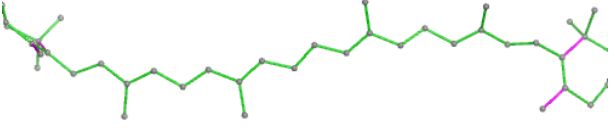
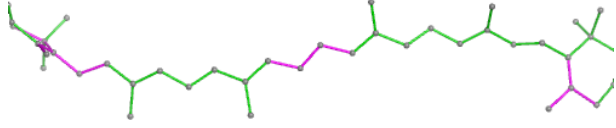
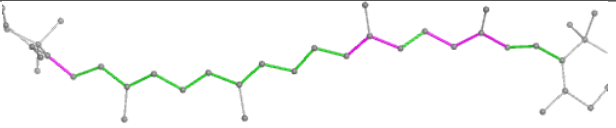
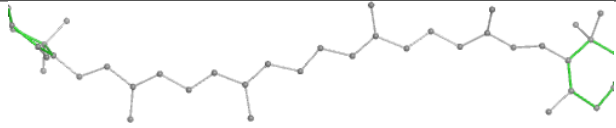


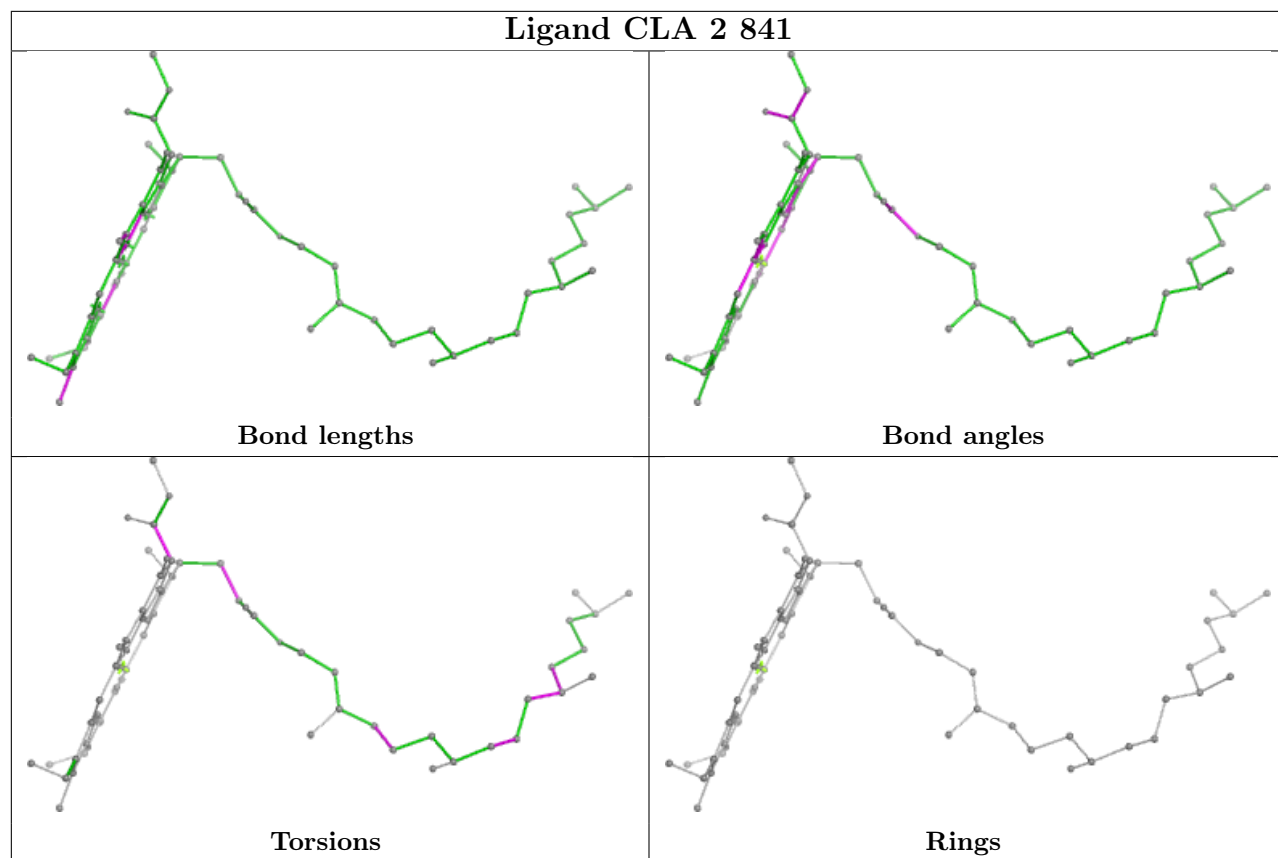


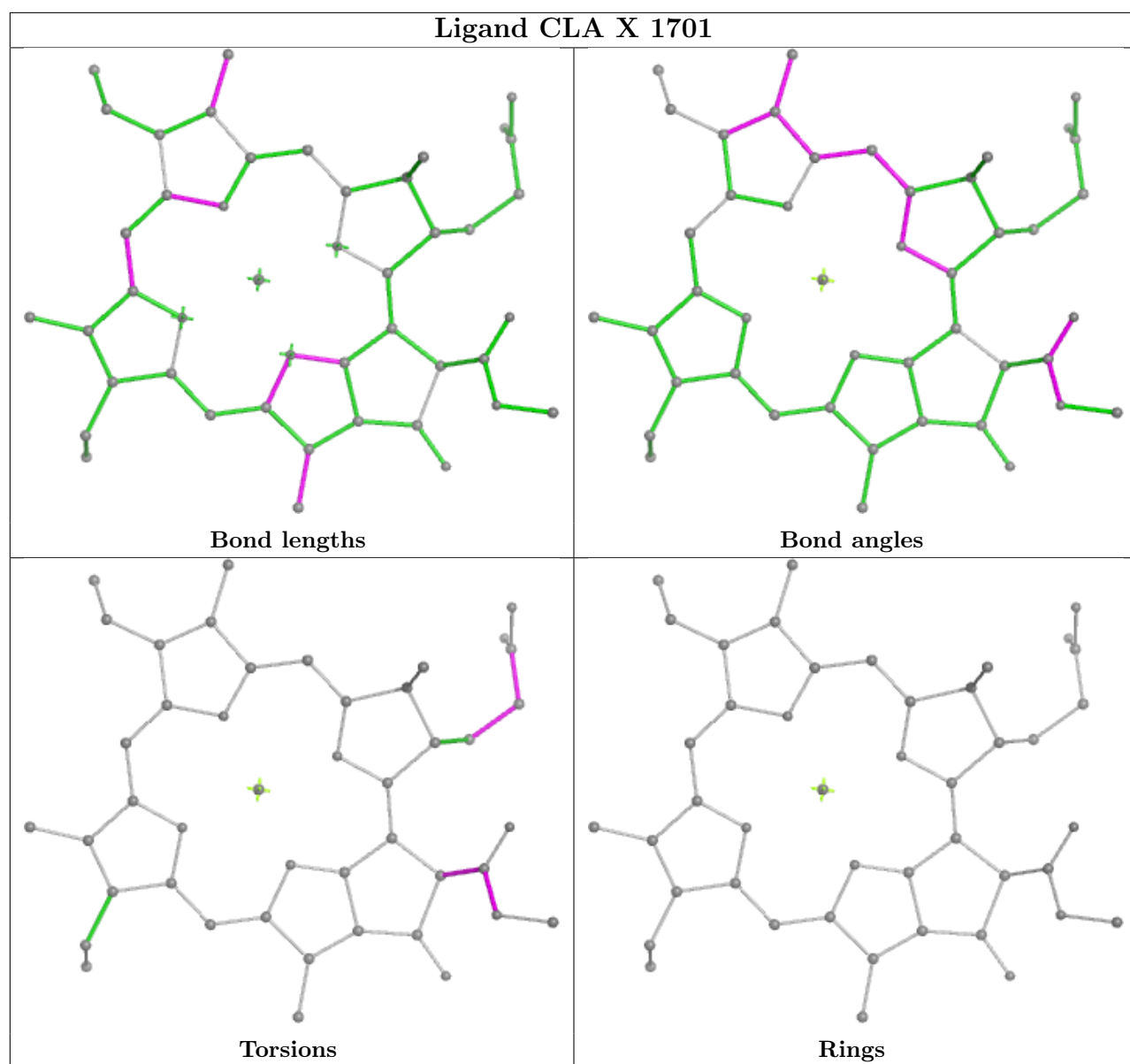




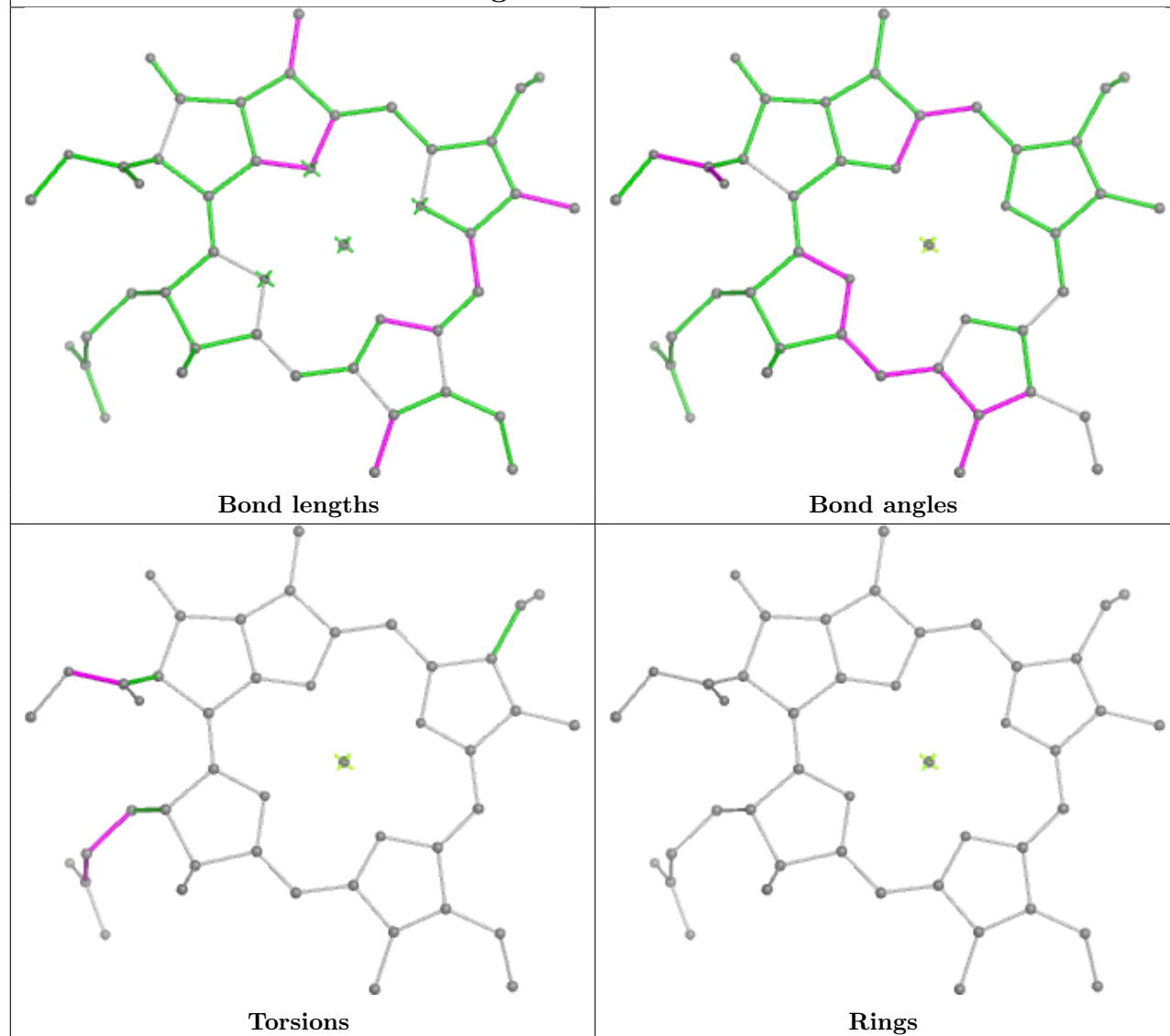


| Ligand CLA 1 1635   |   |
|---|---|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand BCR 2 848  |   |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>     |  <p>Rings</p>       |
| Ligand BCR 1 1651   |   |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

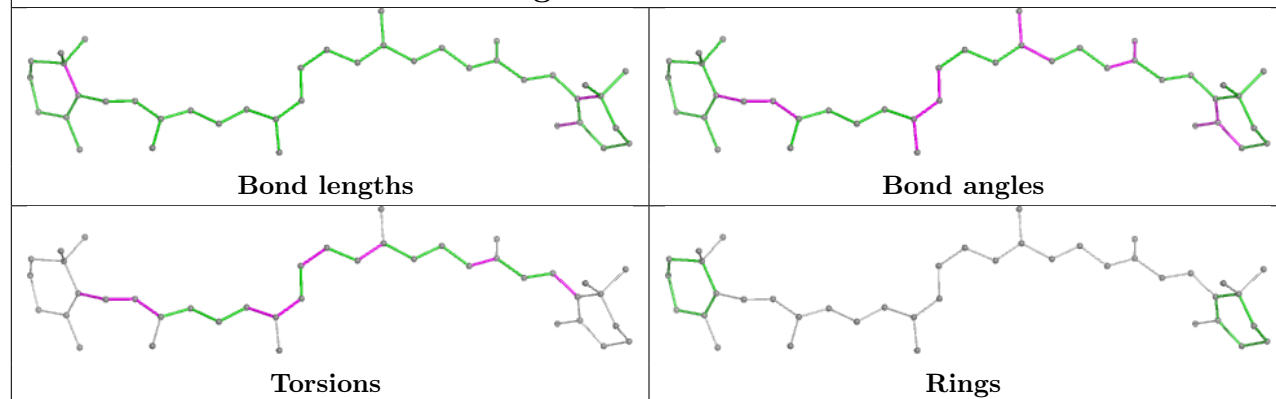


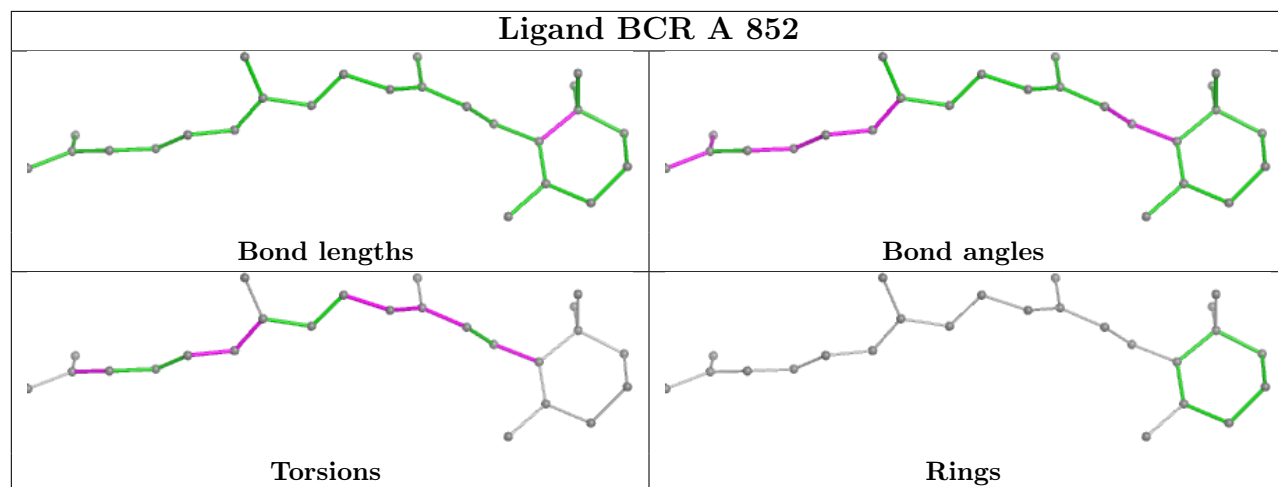
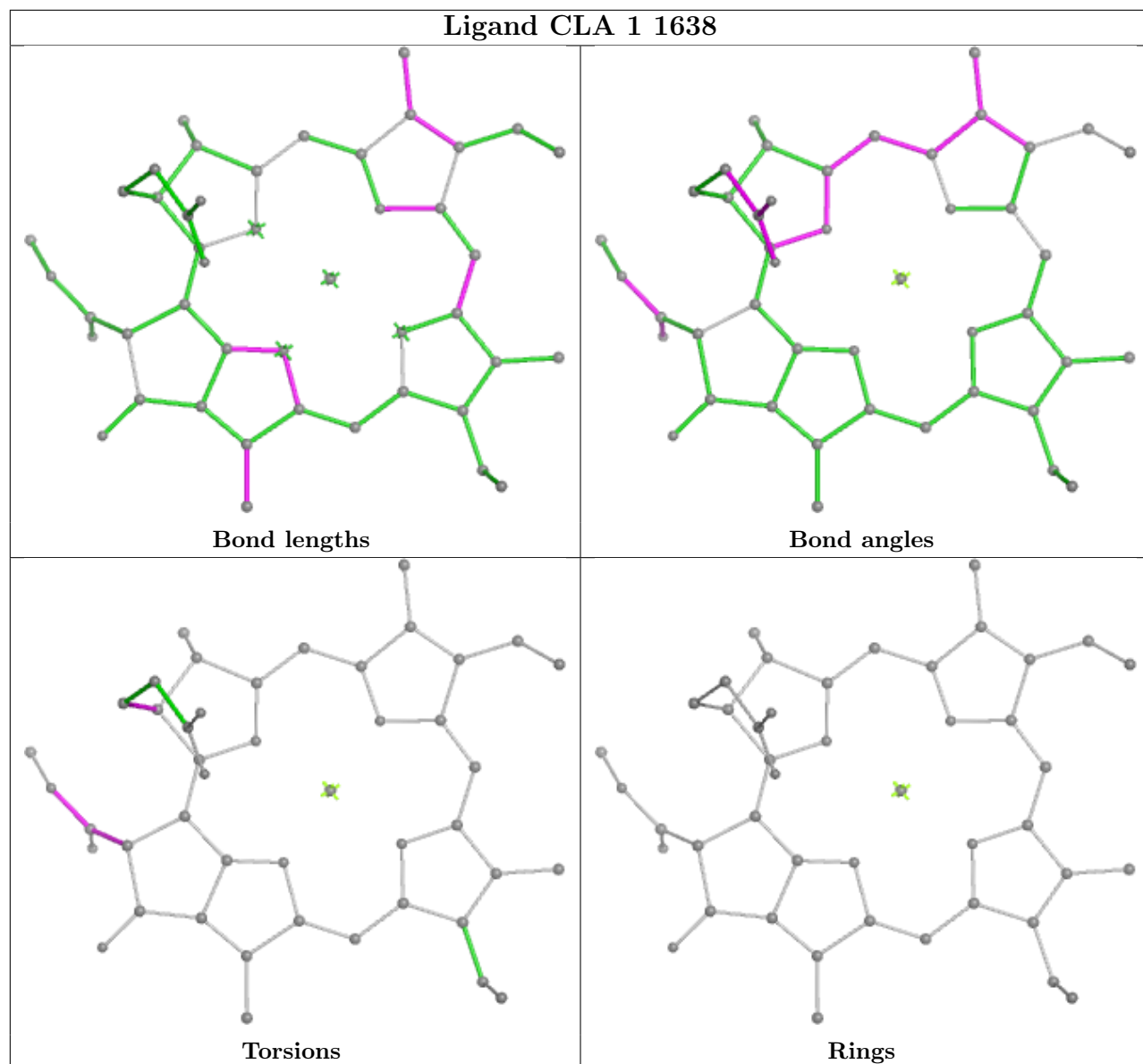


## Ligand CLA b 824

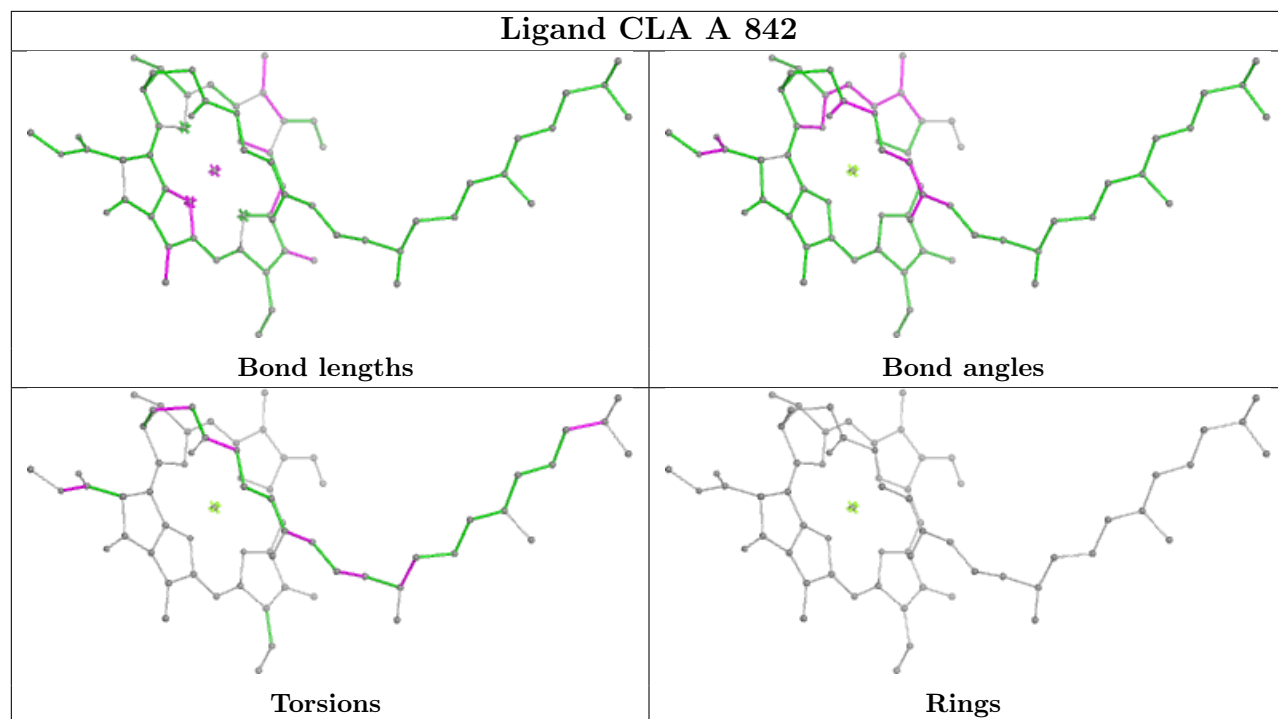


## Ligand BCR b 847

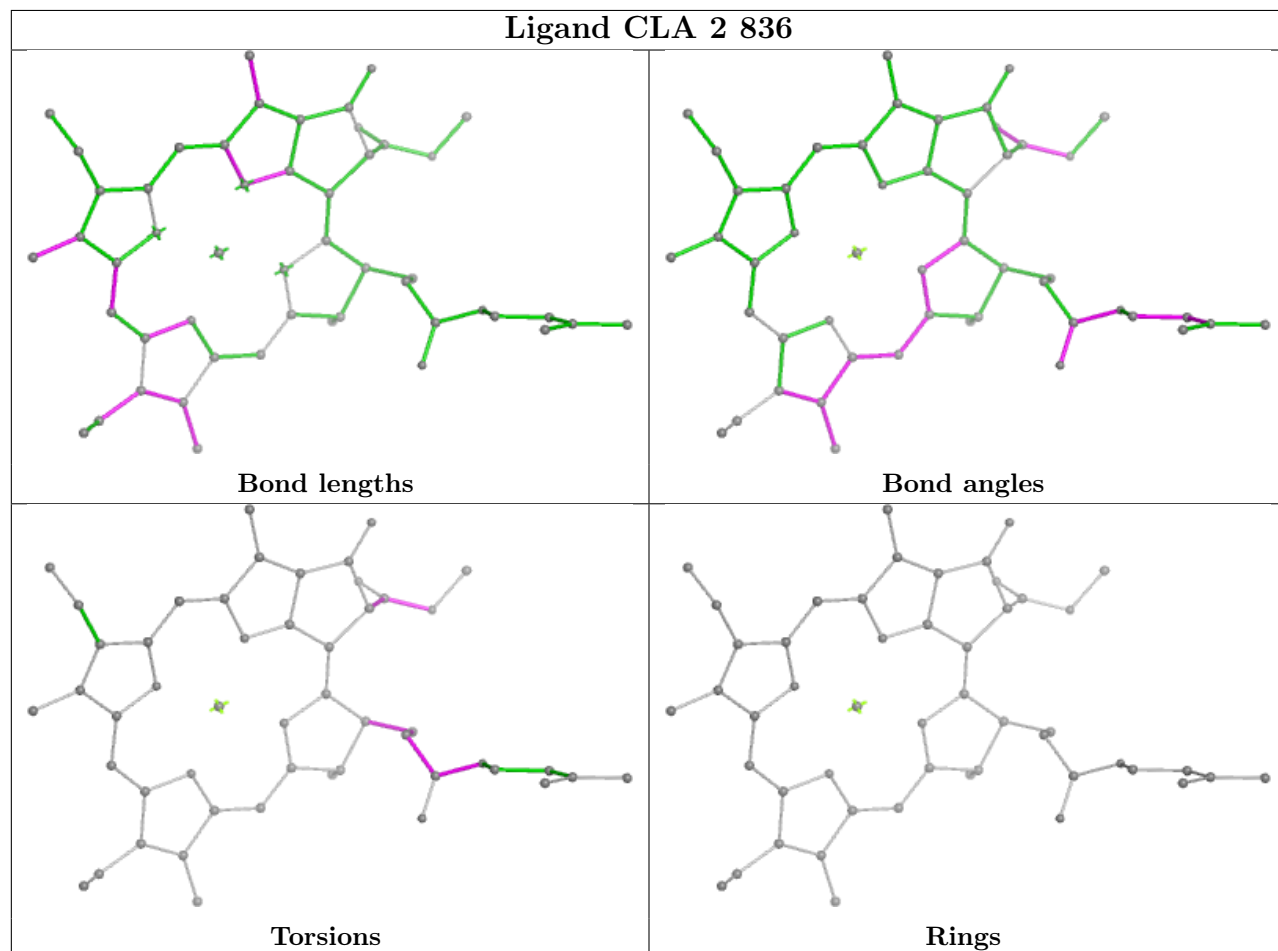


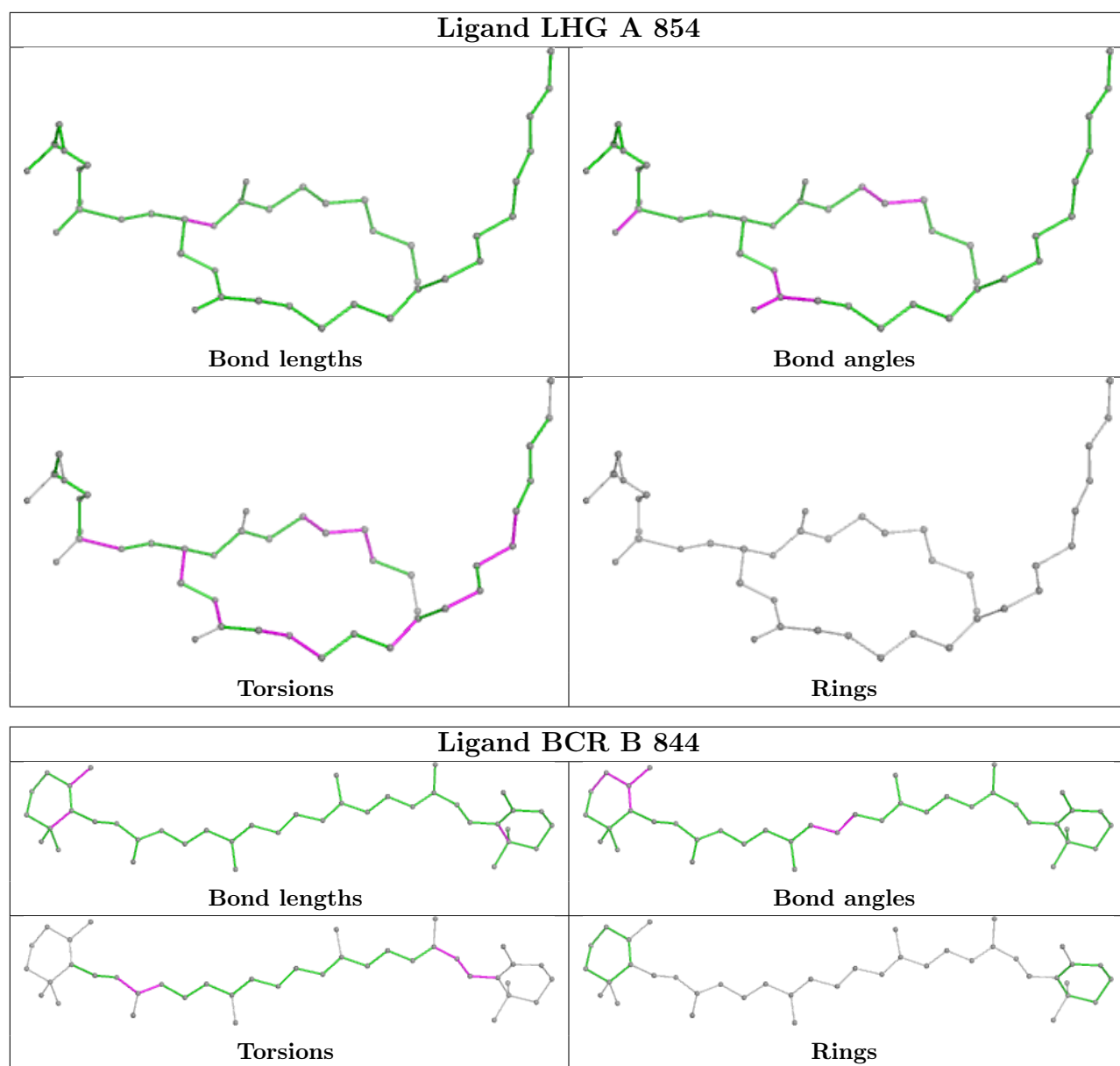


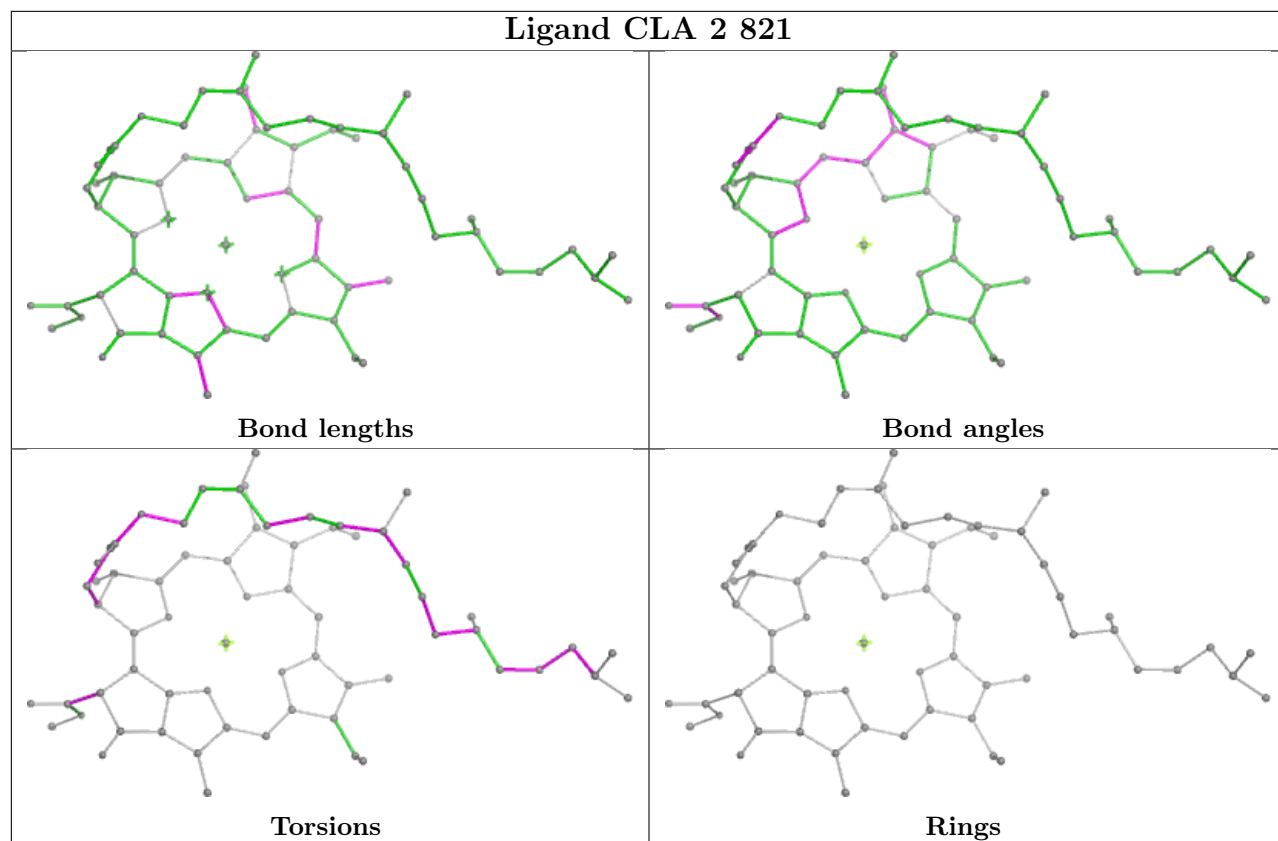
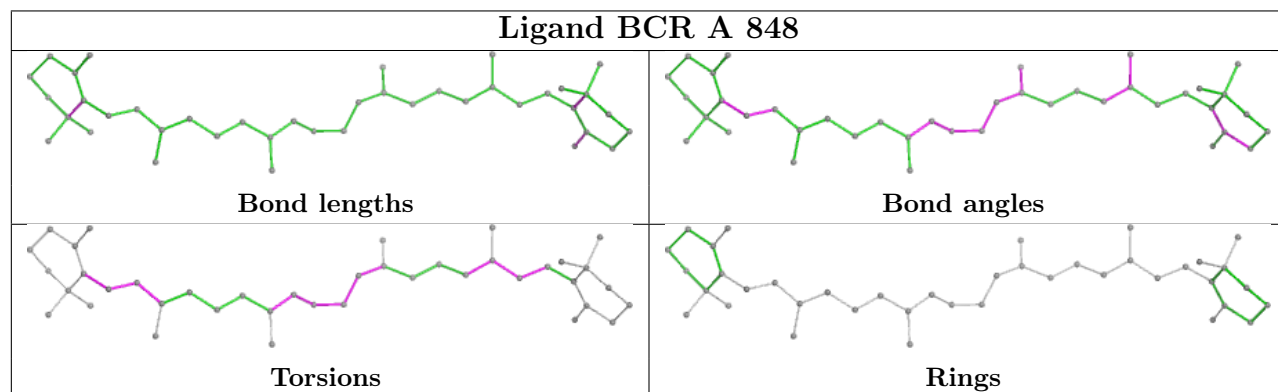
## Ligand CLA A 842



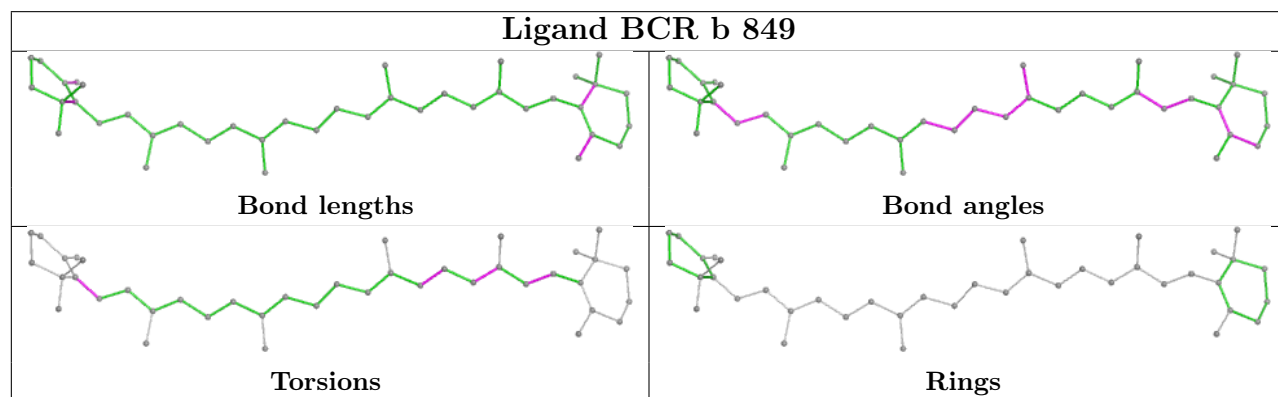
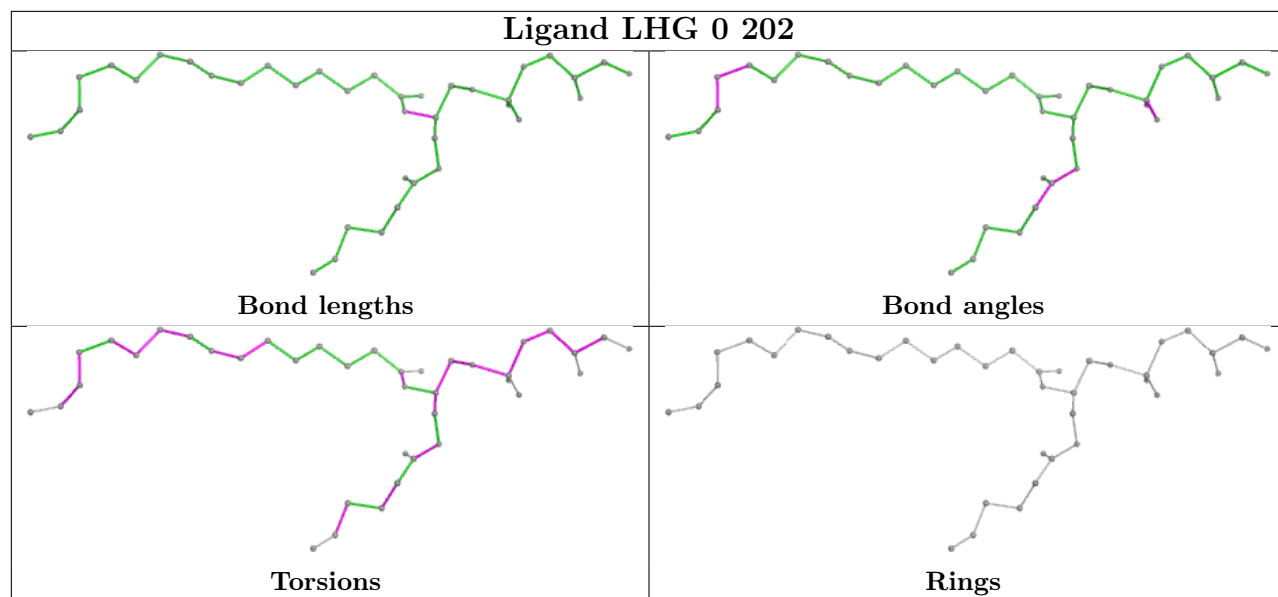
## Ligand CLA 2 836

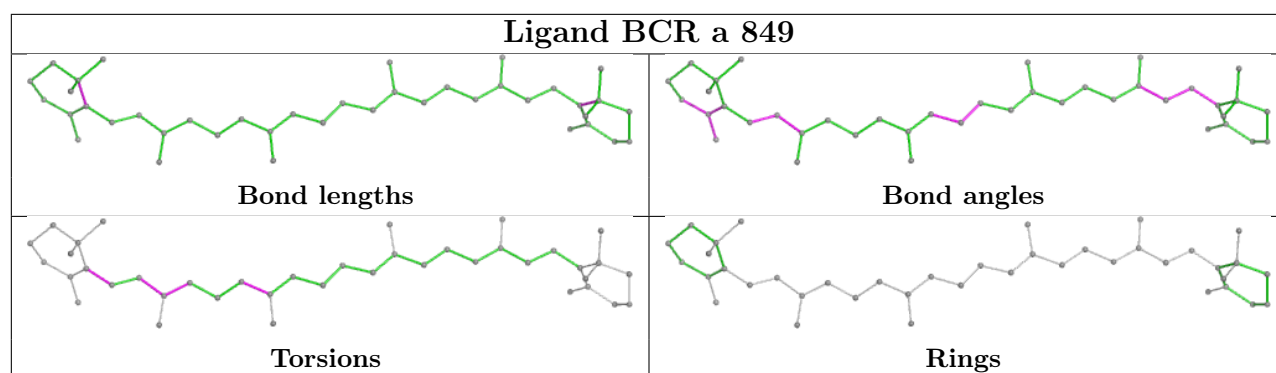
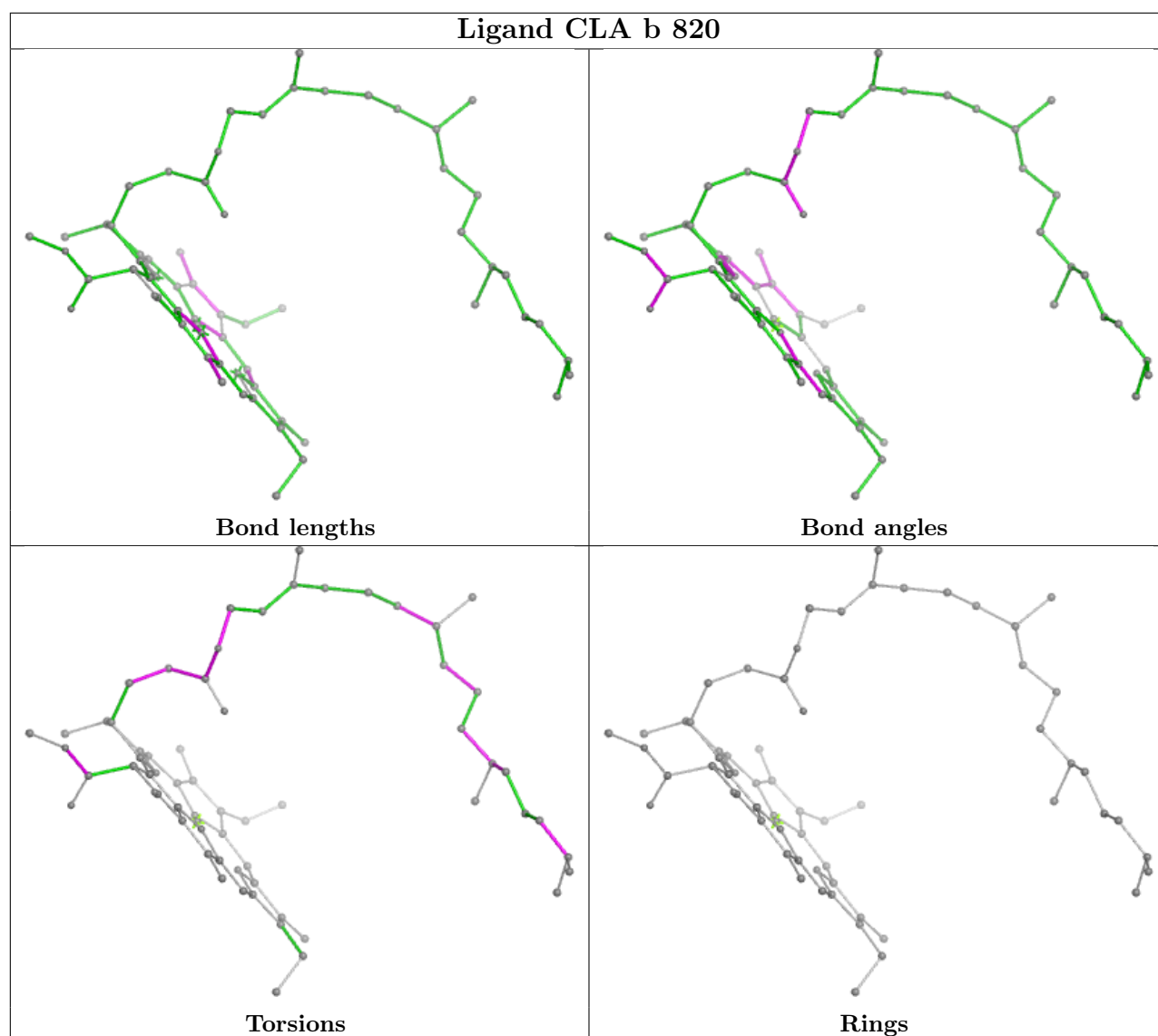




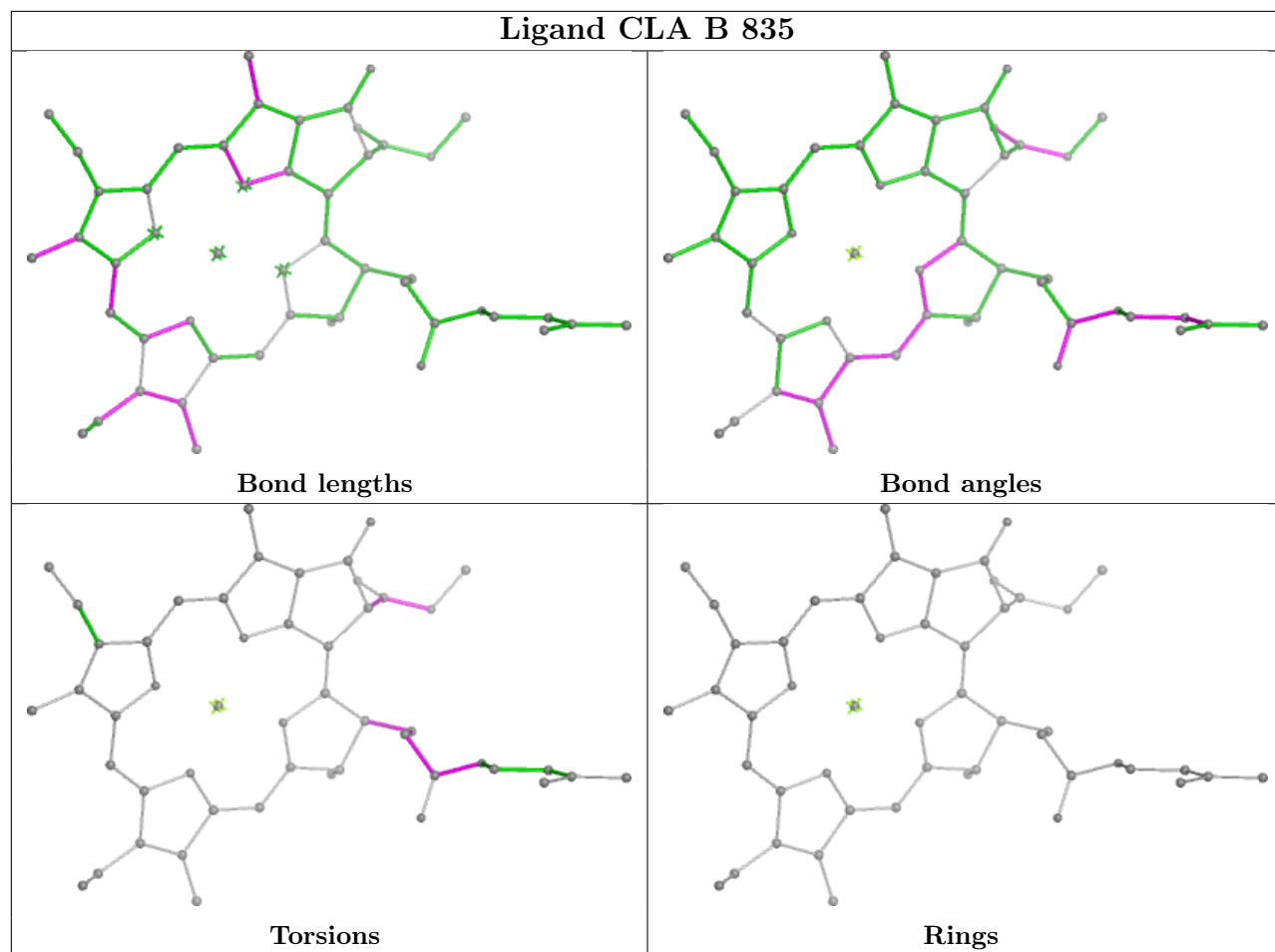
**Ligand CLA 2 821****Ligand BCR A 848**



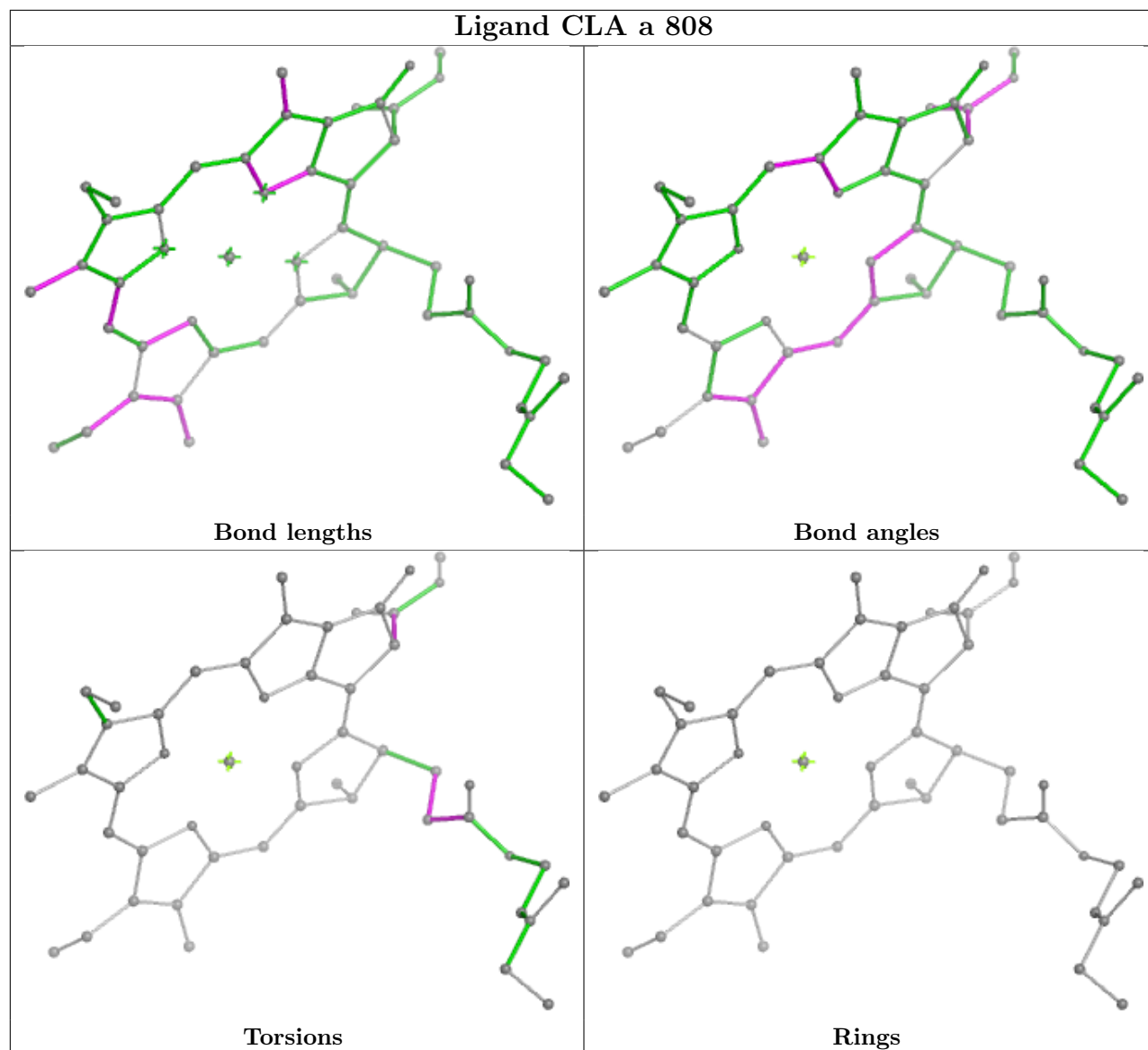


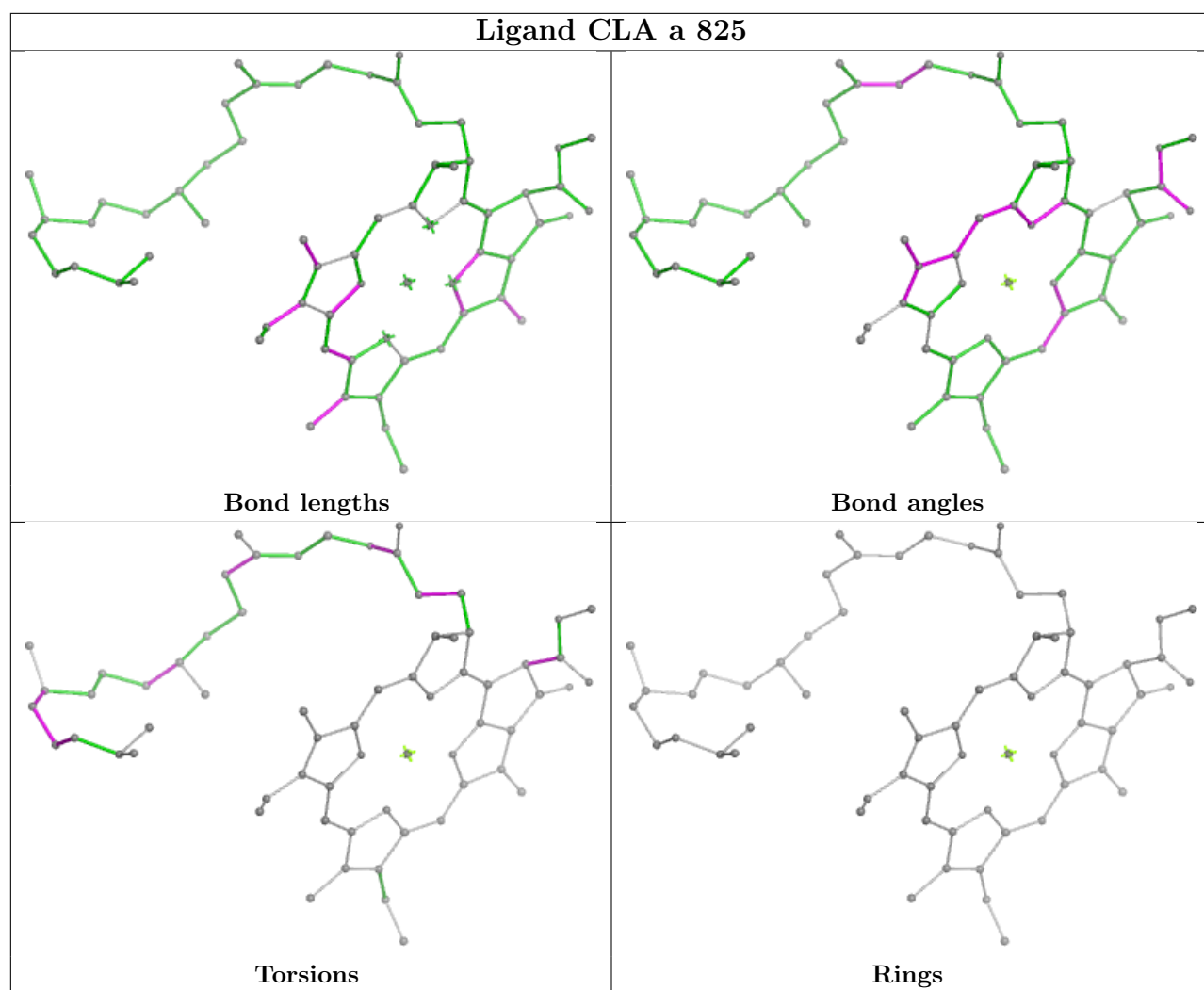


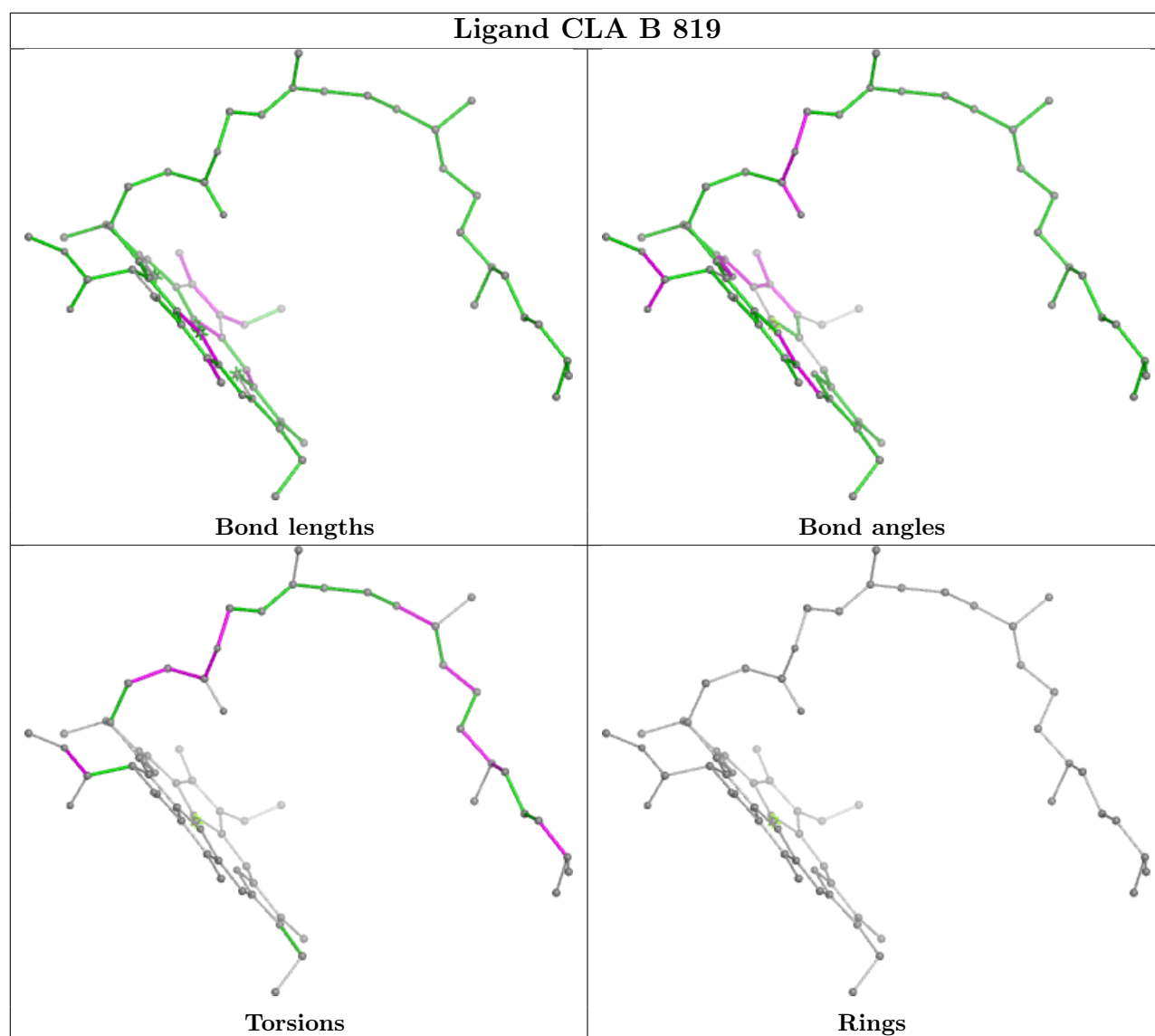
## Ligand CLA B 835

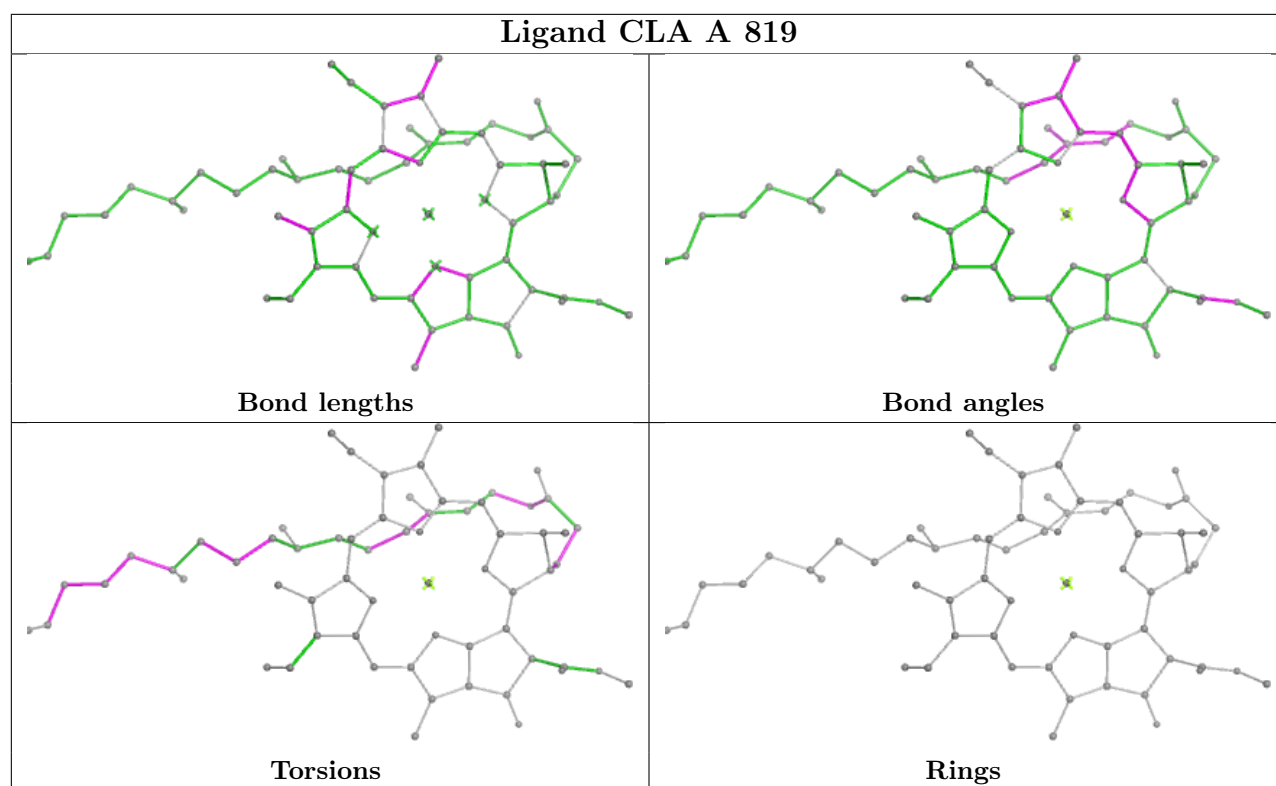


## Ligand CLA a 808

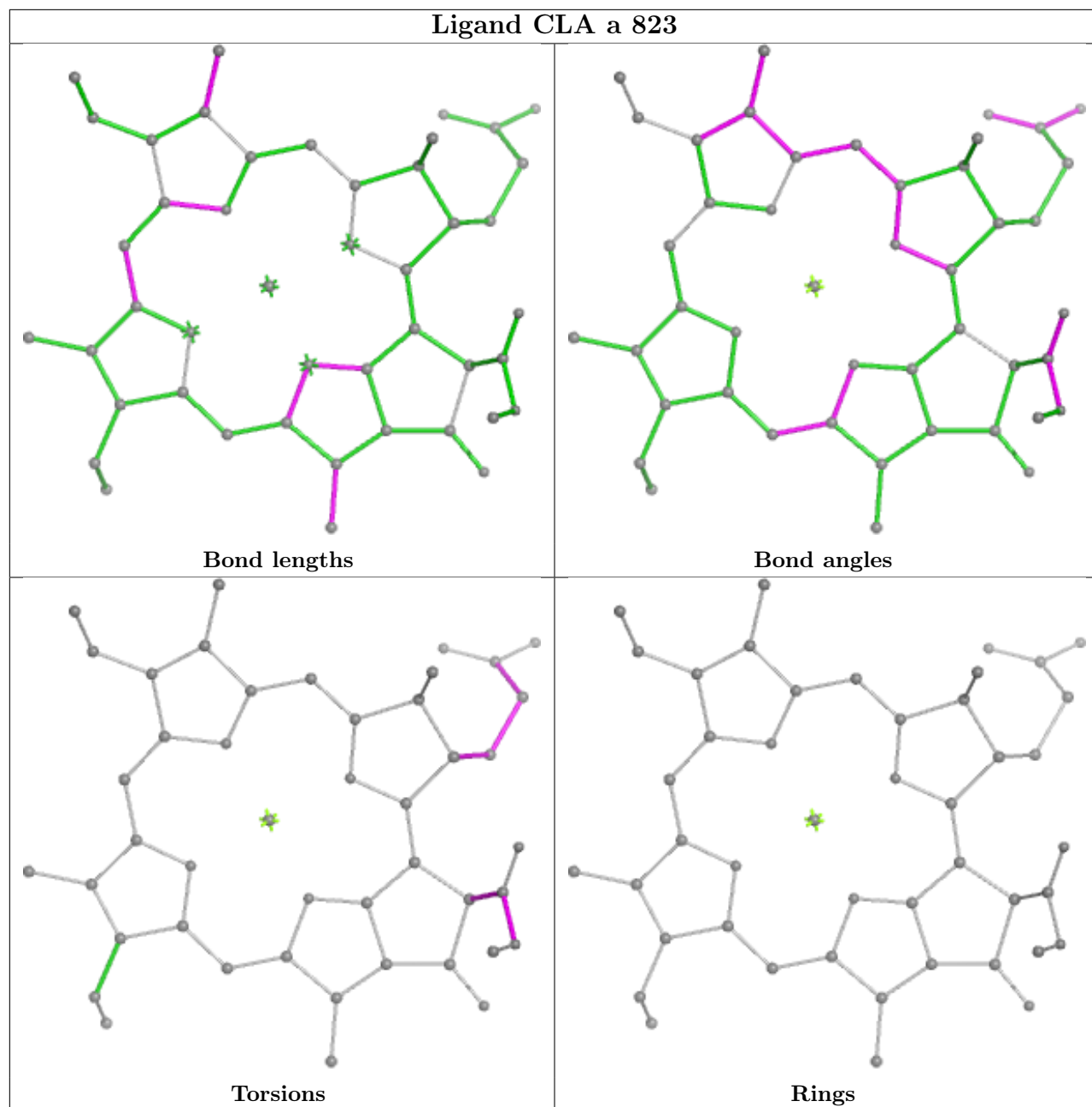




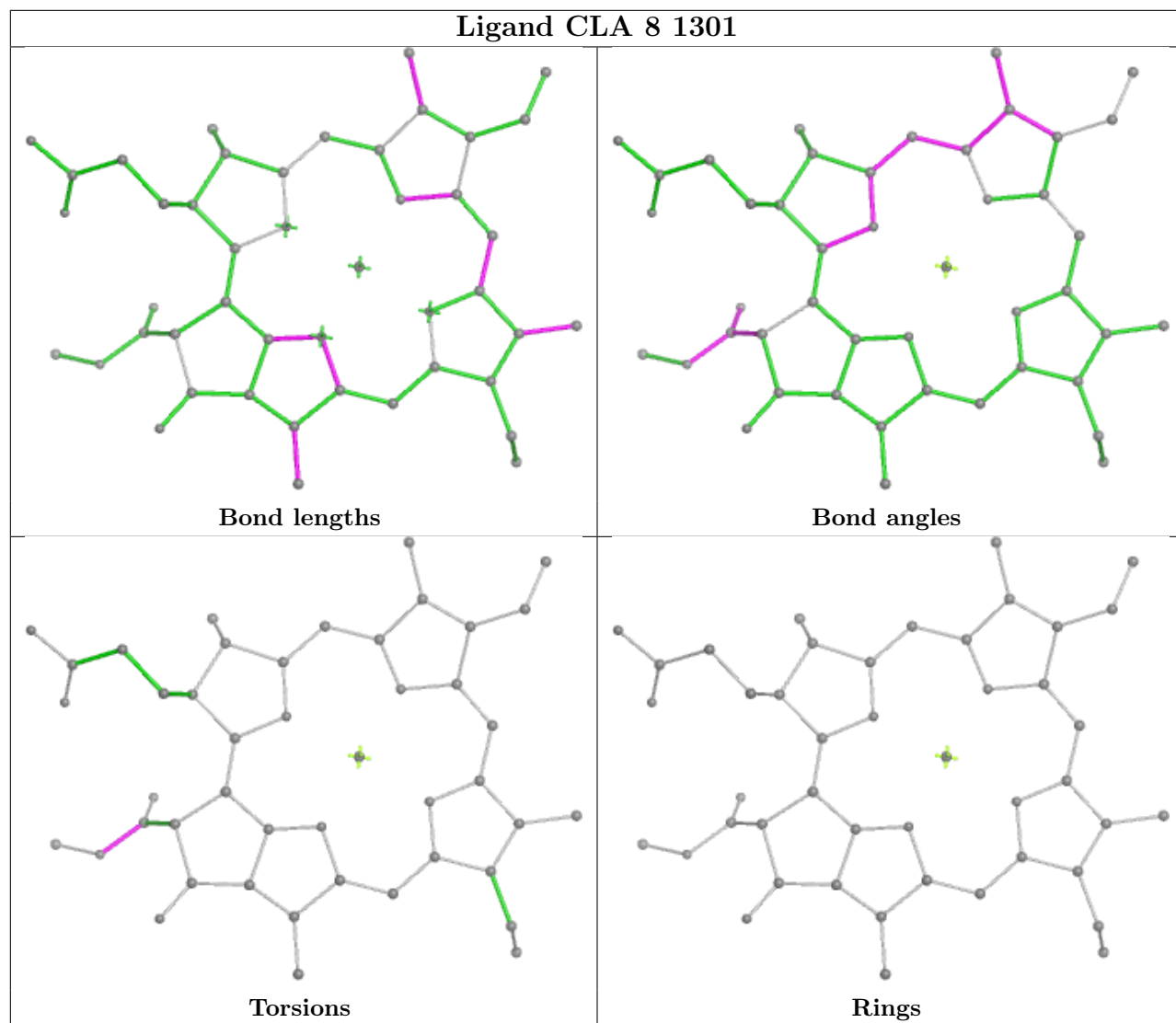




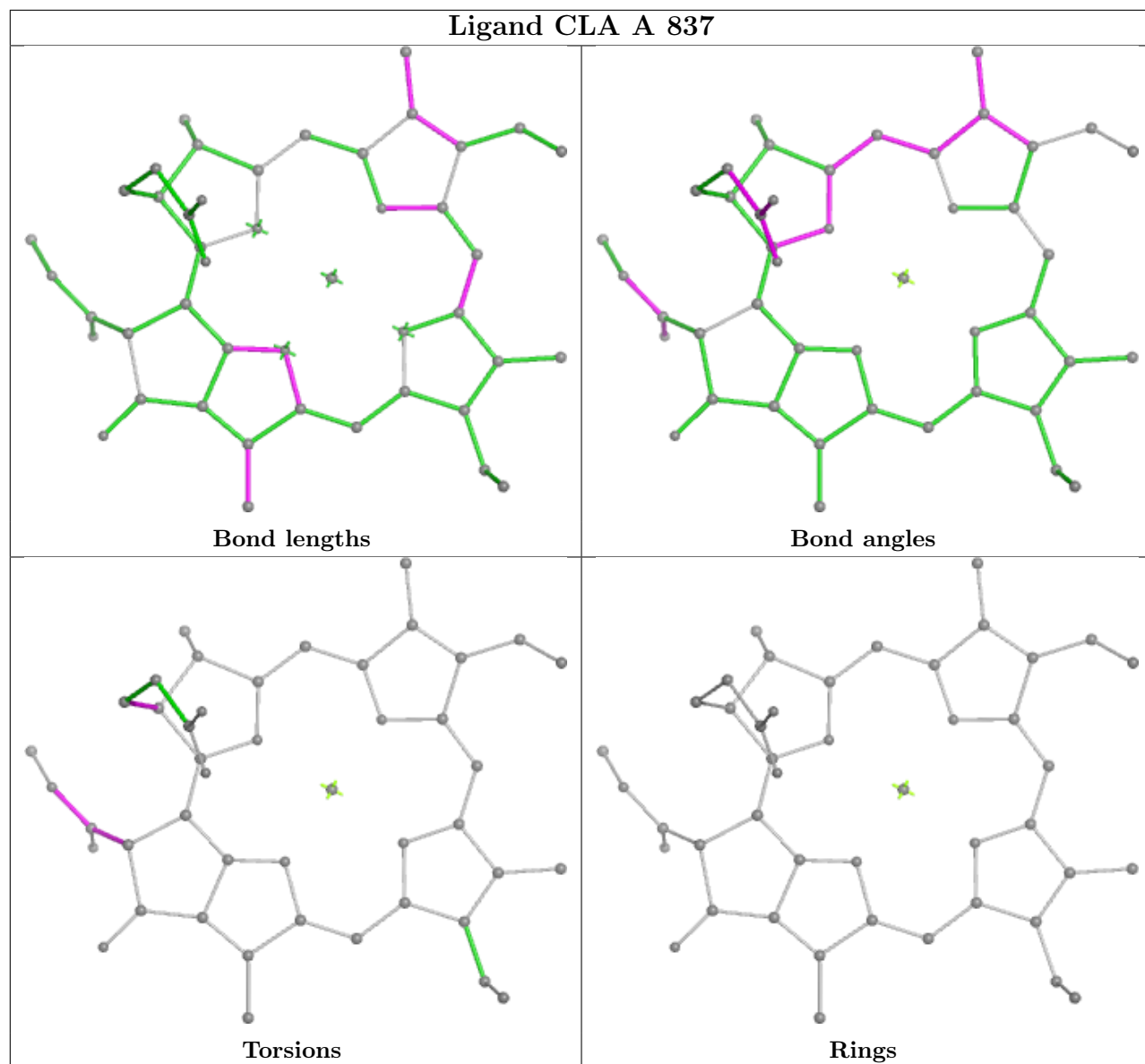
## Ligand CLA a 823



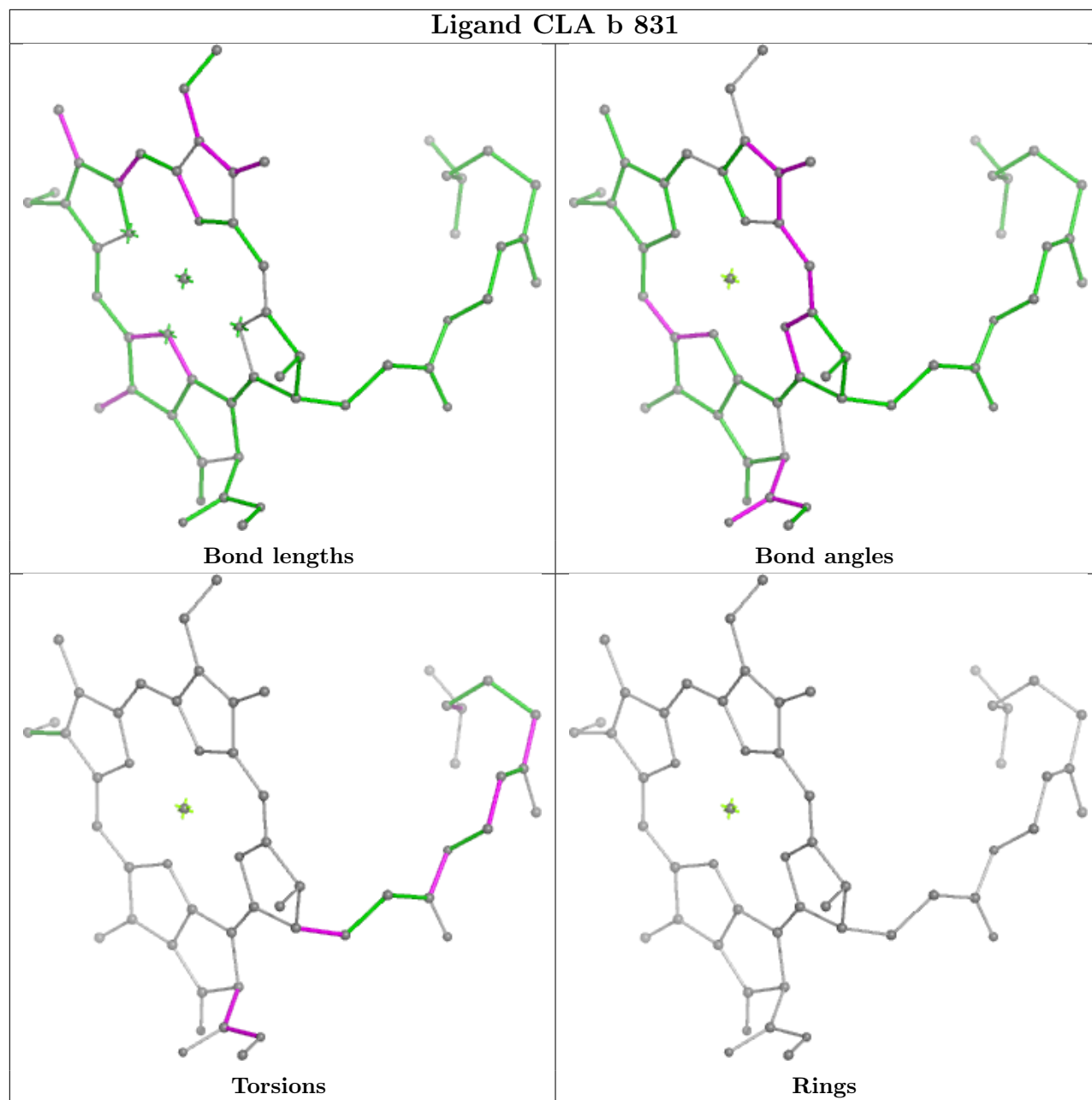


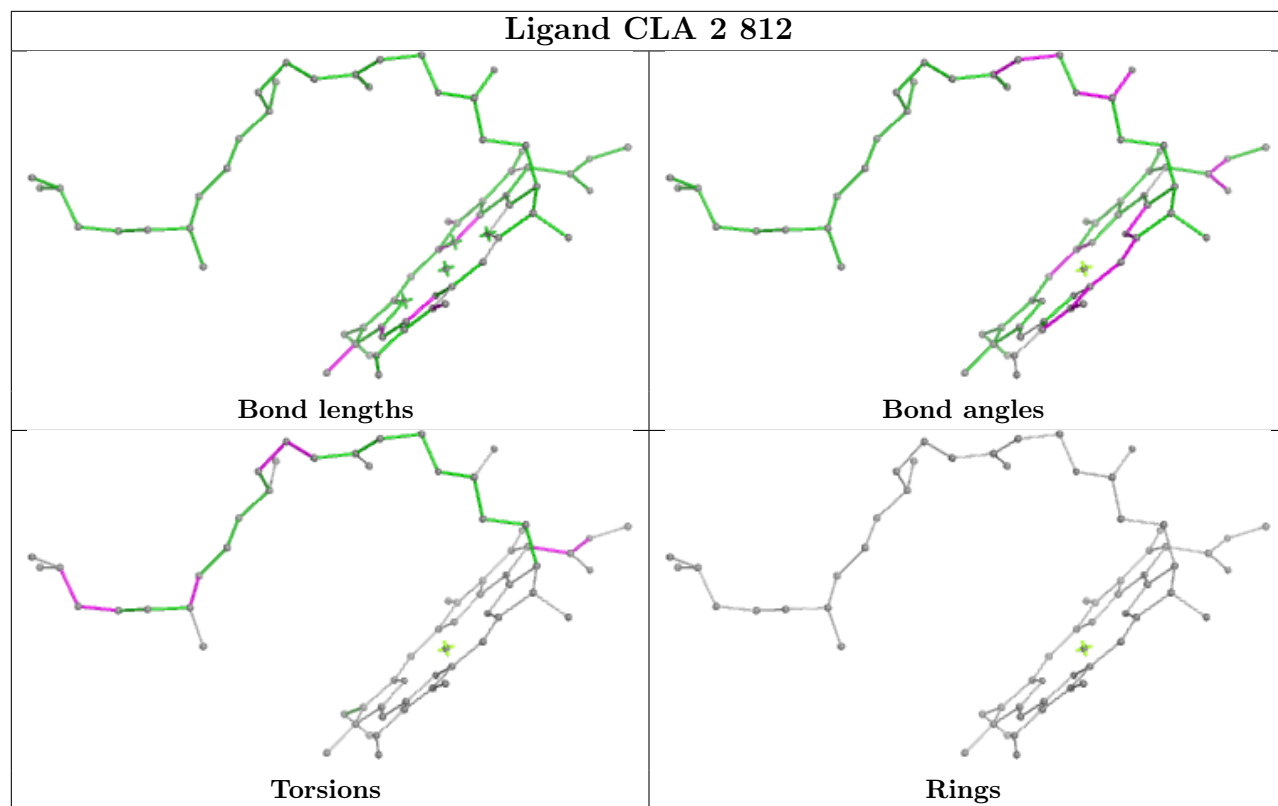


## Ligand CLA A 837

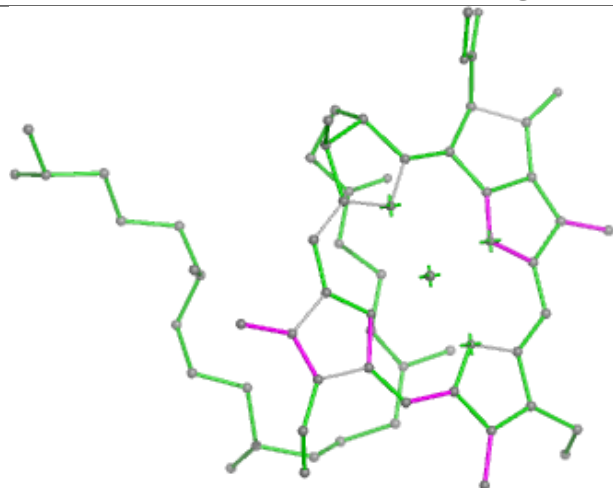


## Ligand CLA b 831

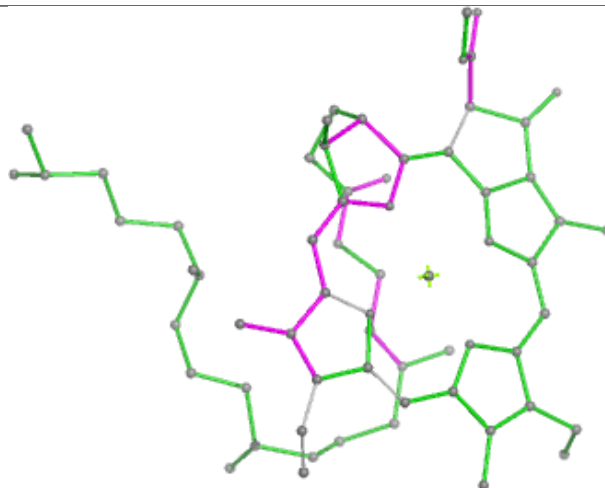




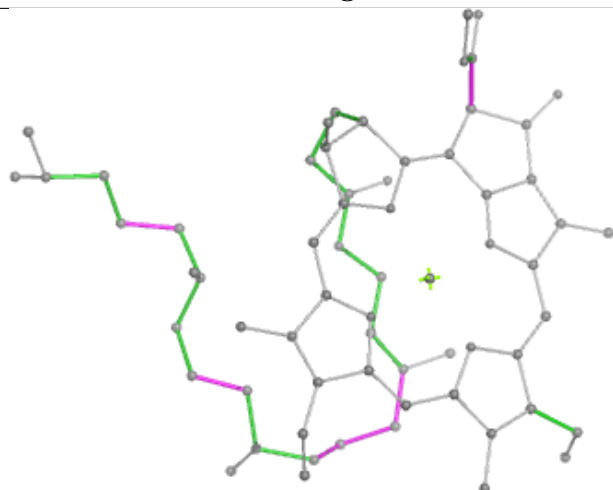
## Ligand CLA B 808



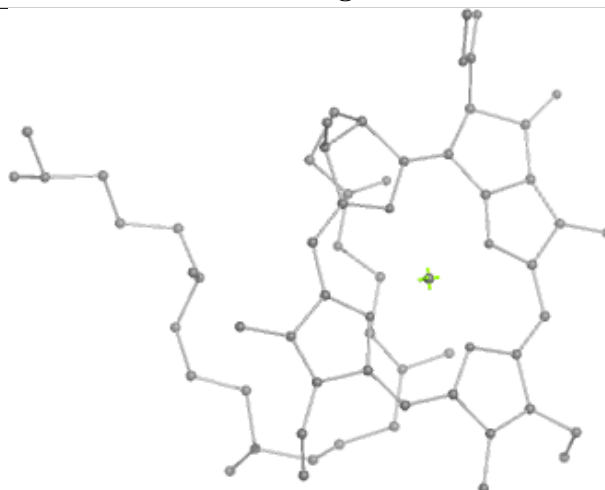
Bond lengths



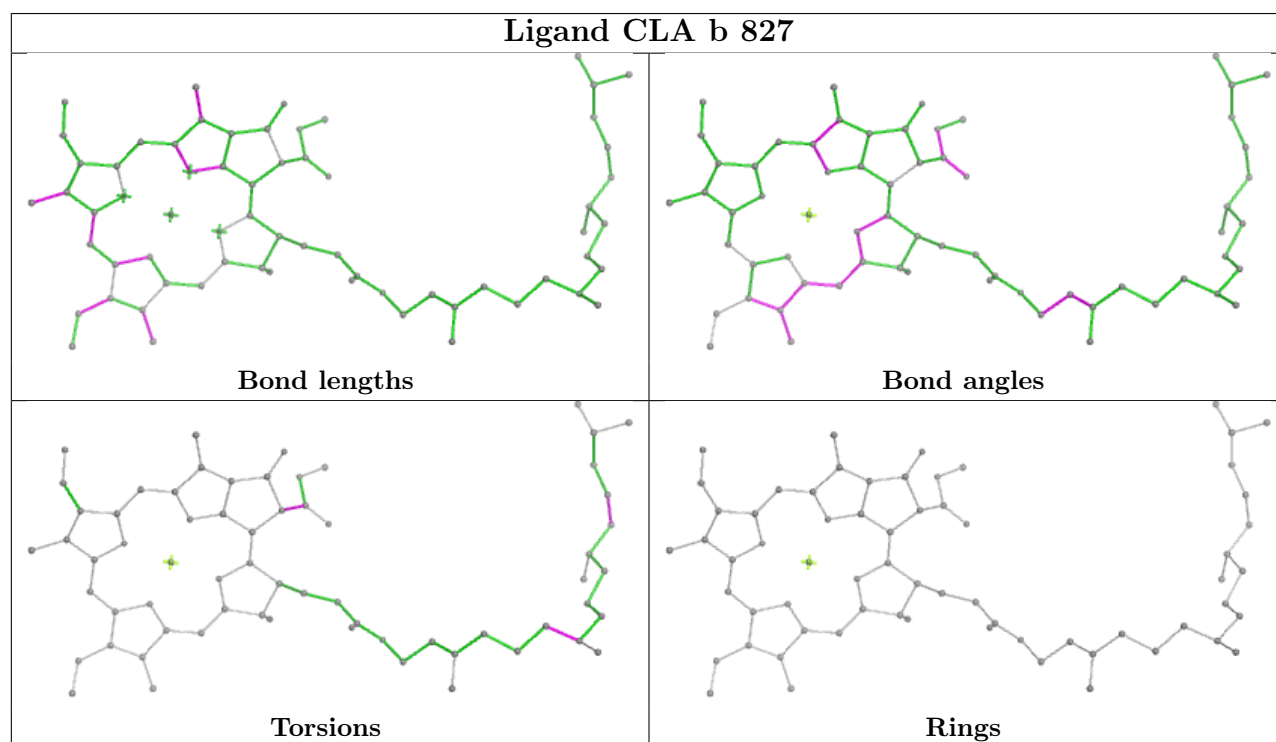
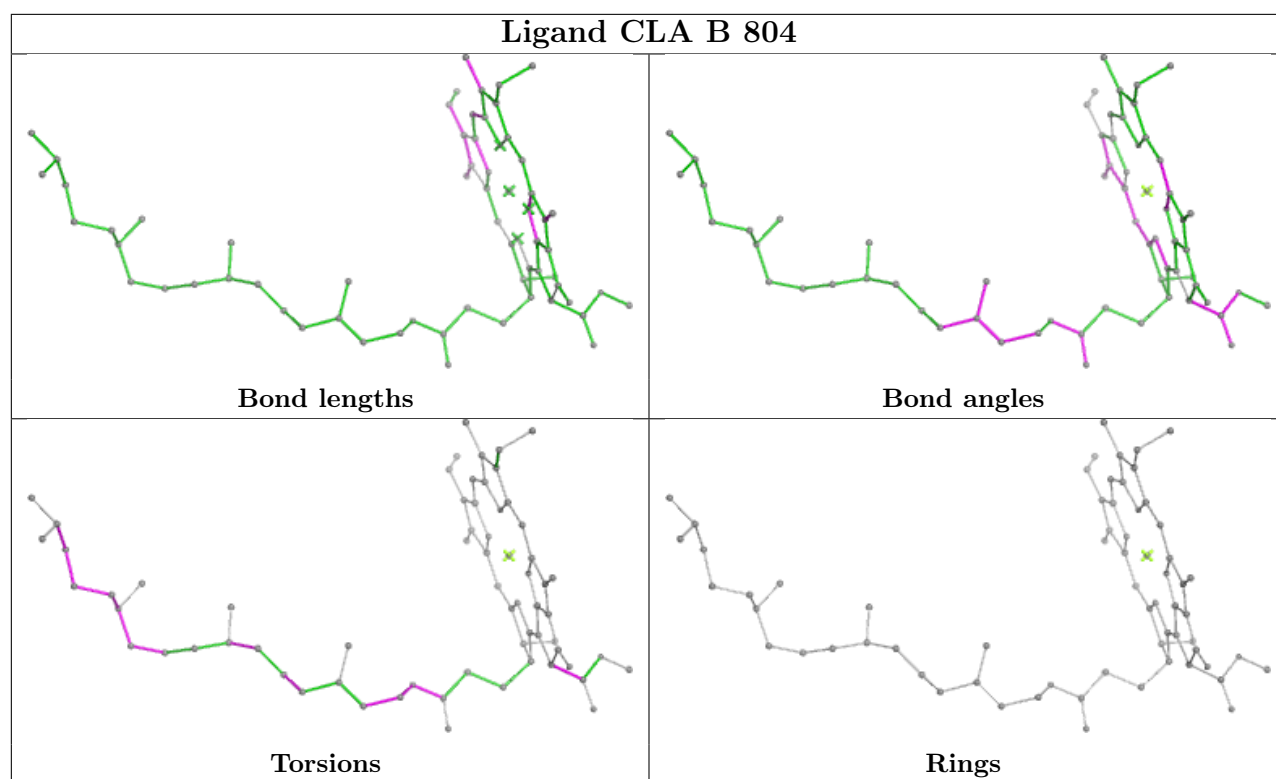
Bond angles

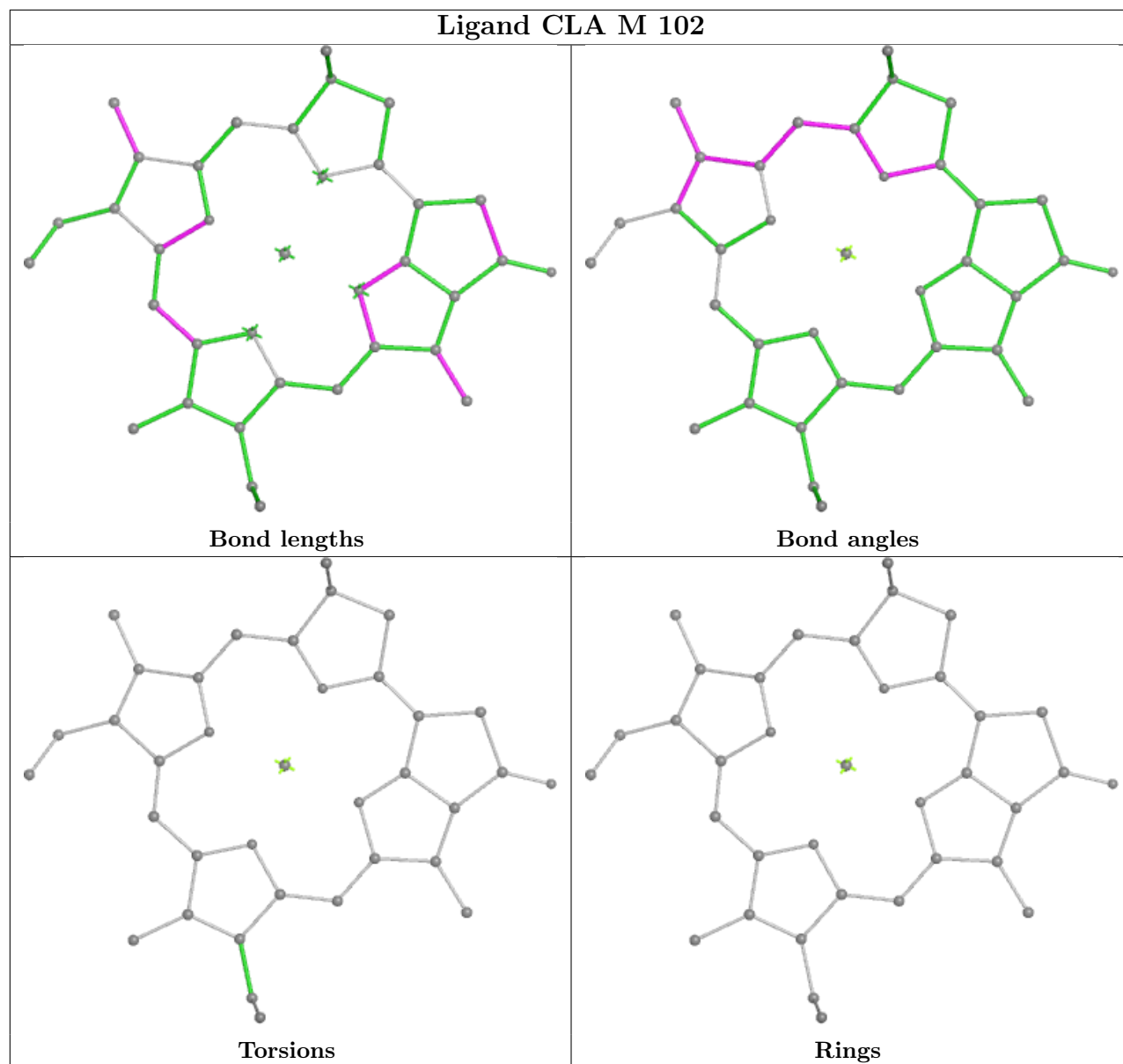


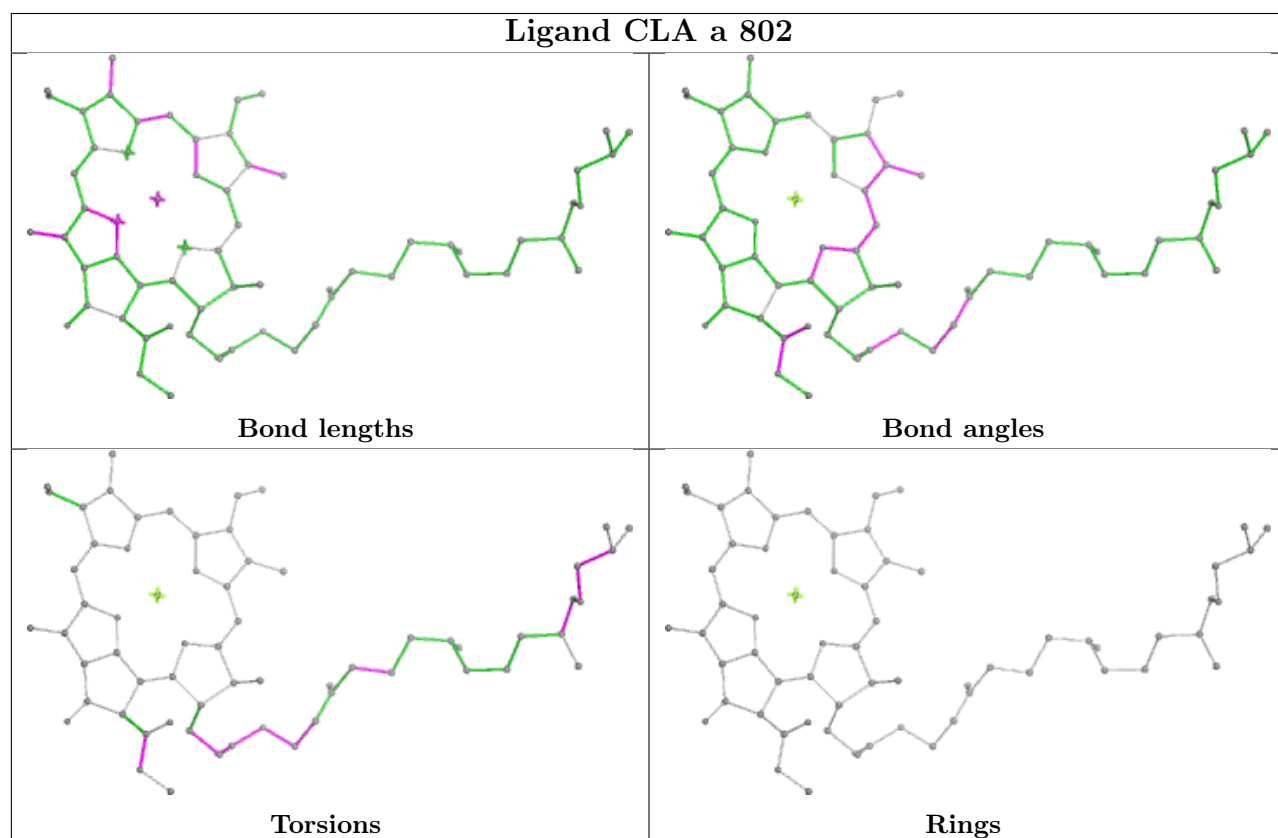
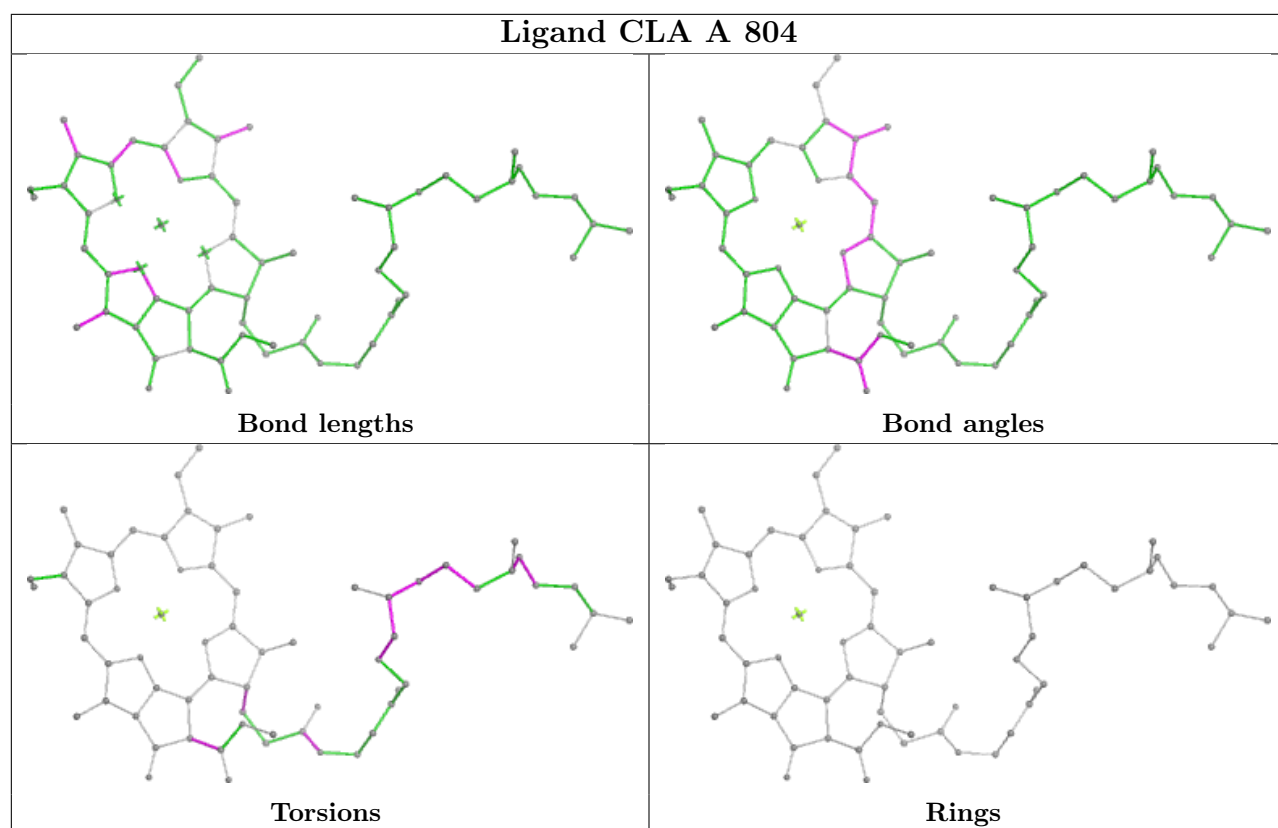
Torsions



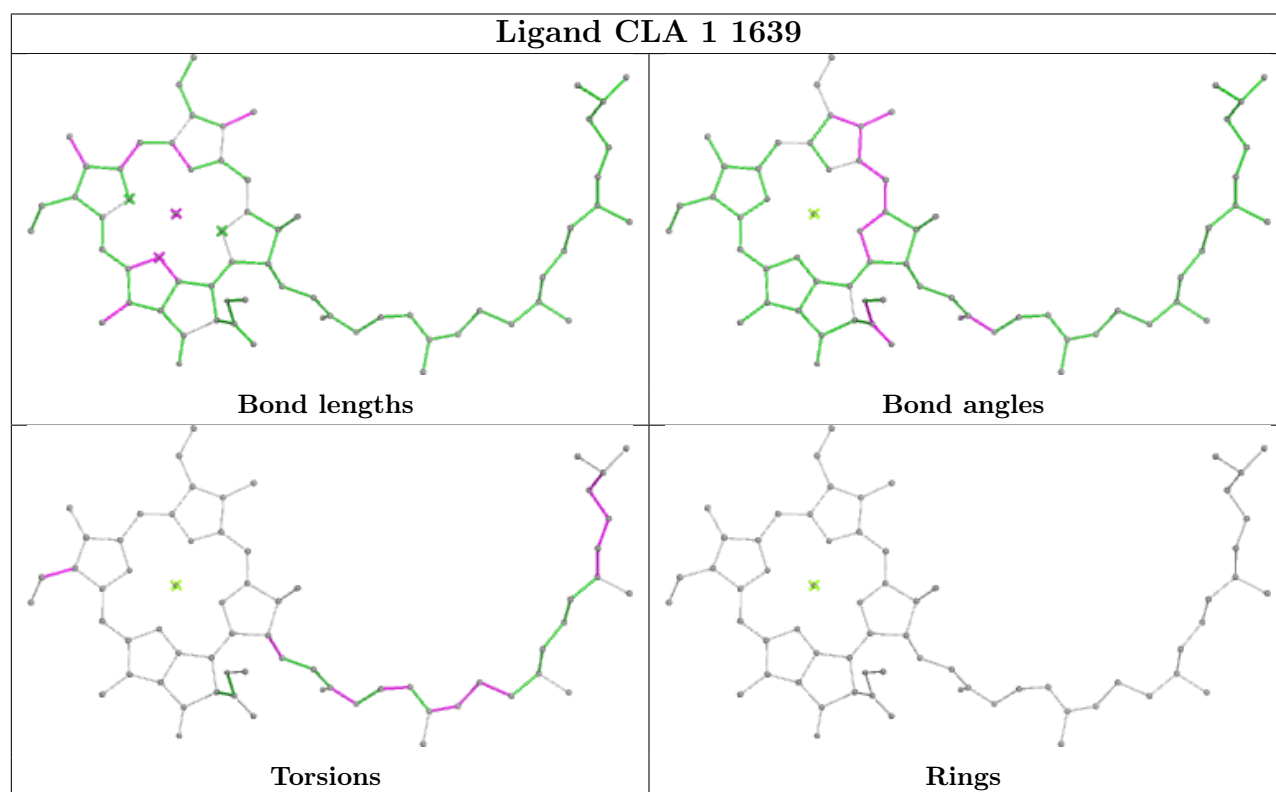
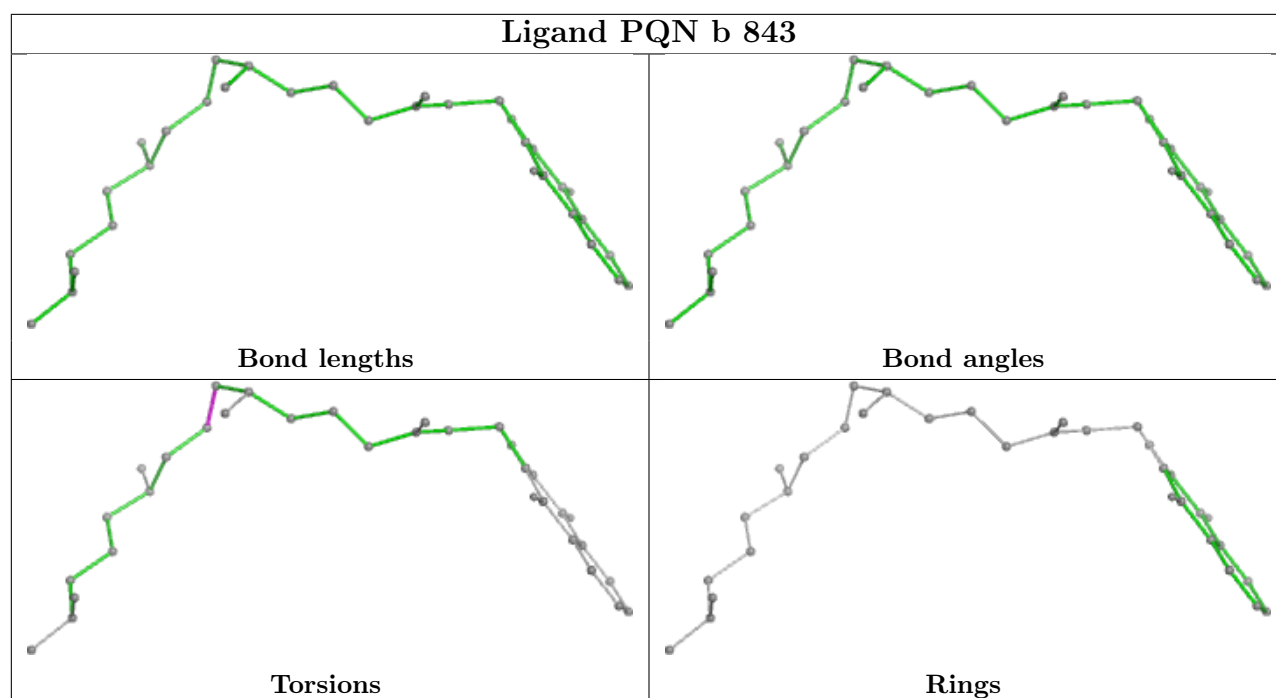
Rings



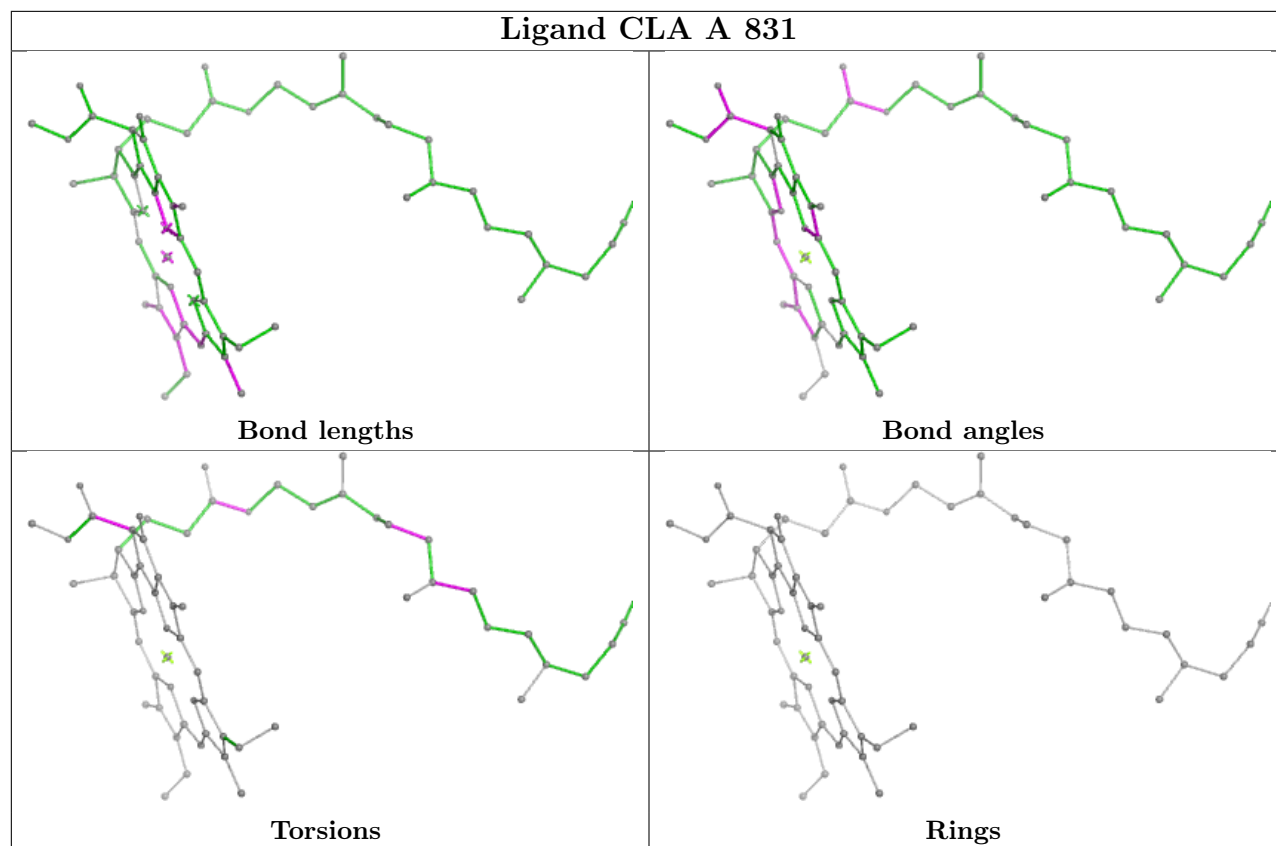




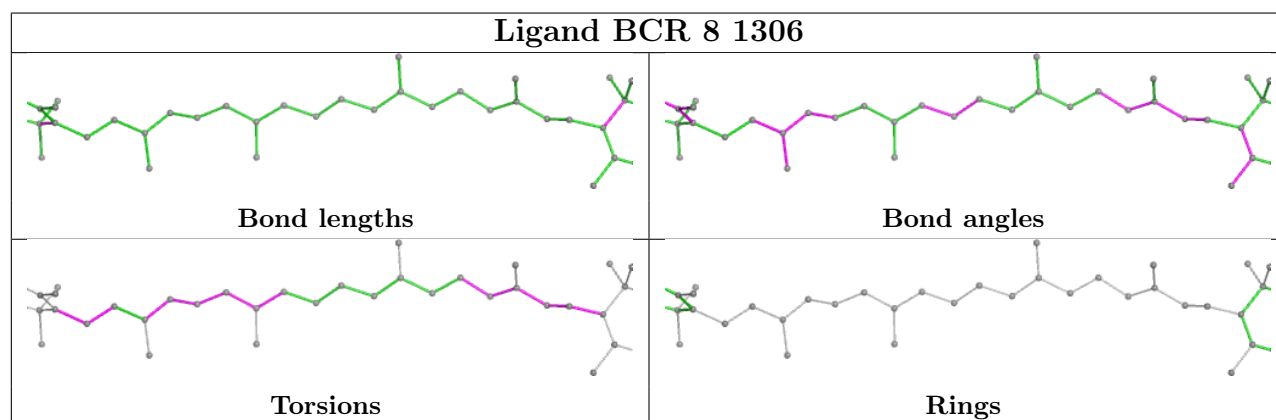




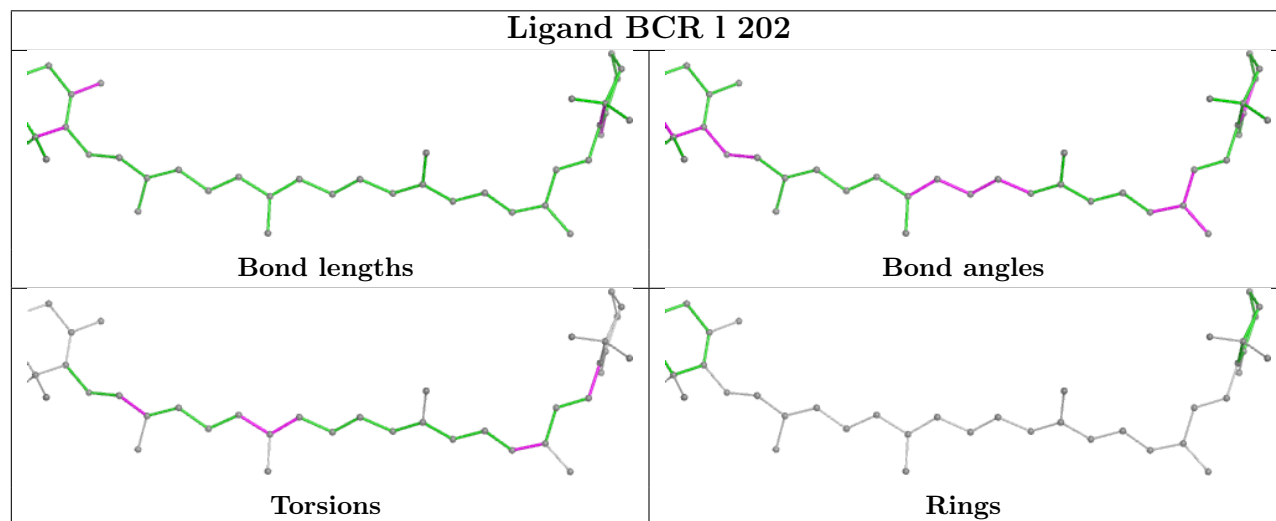
## Ligand CLA A 831

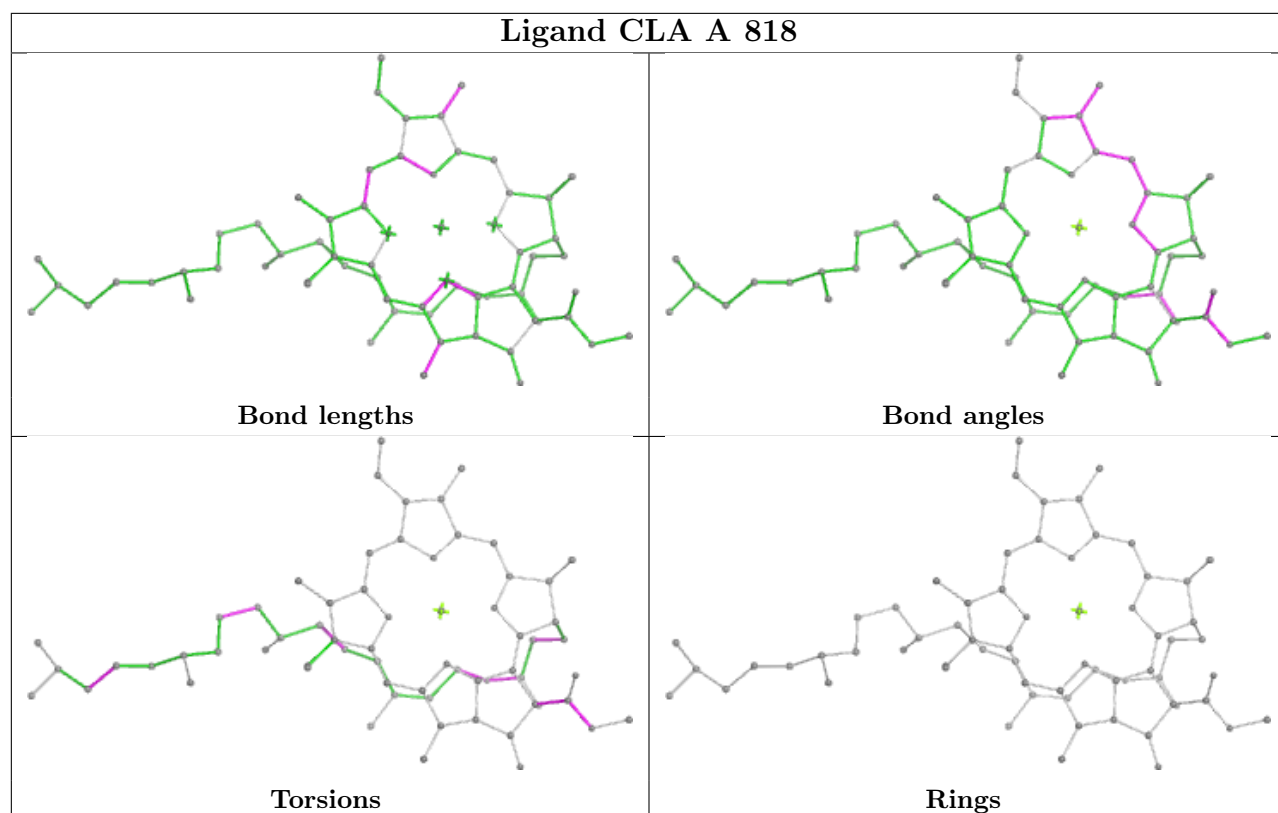
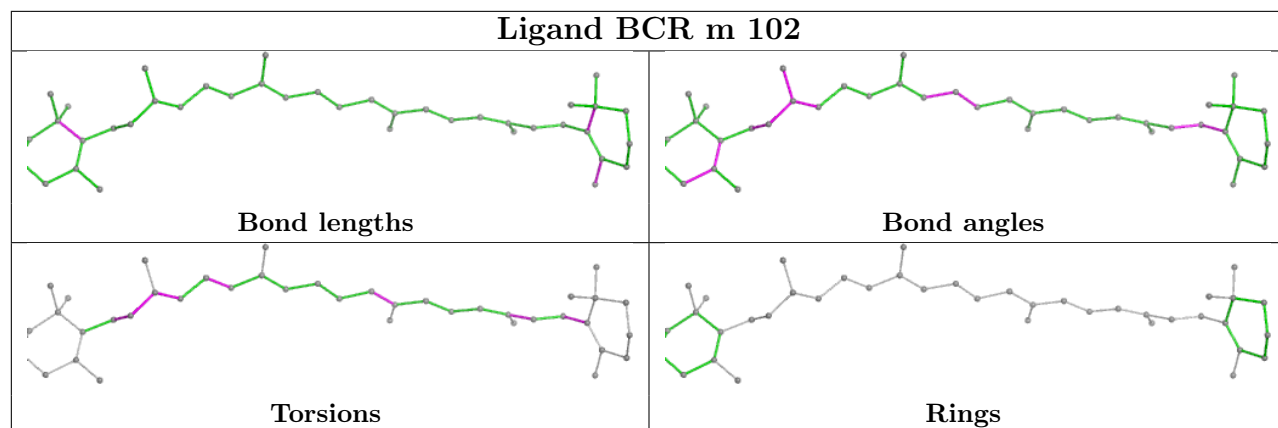


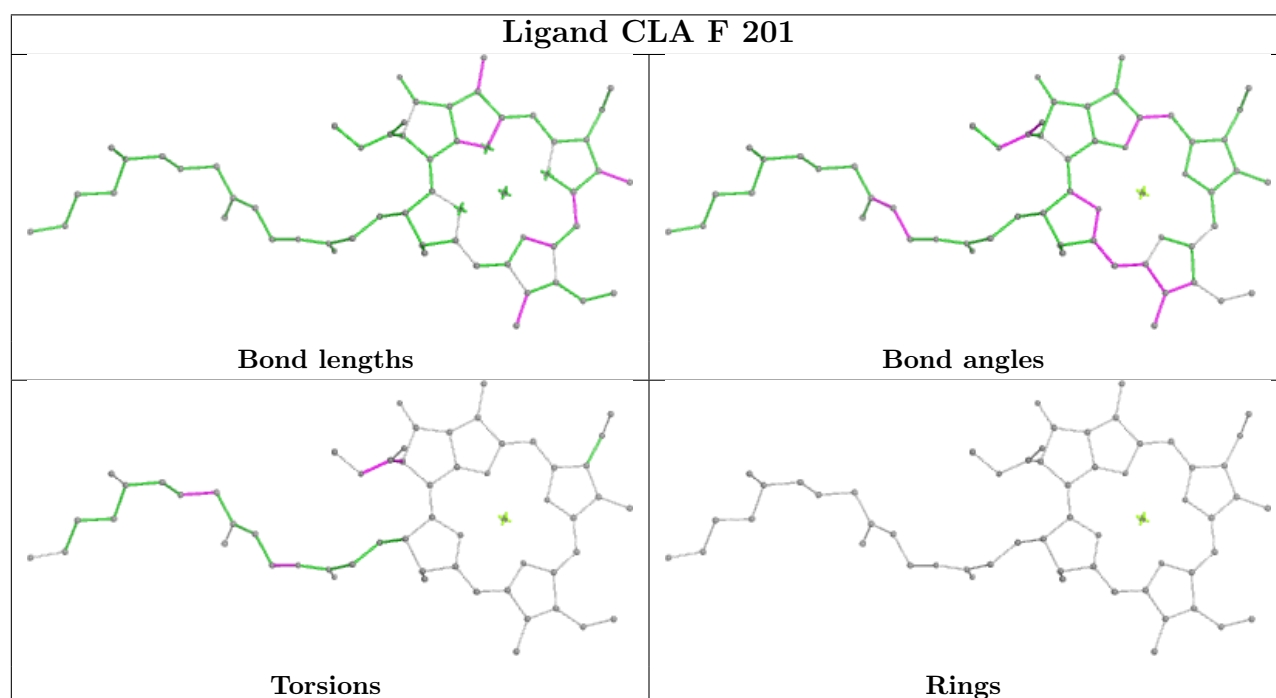
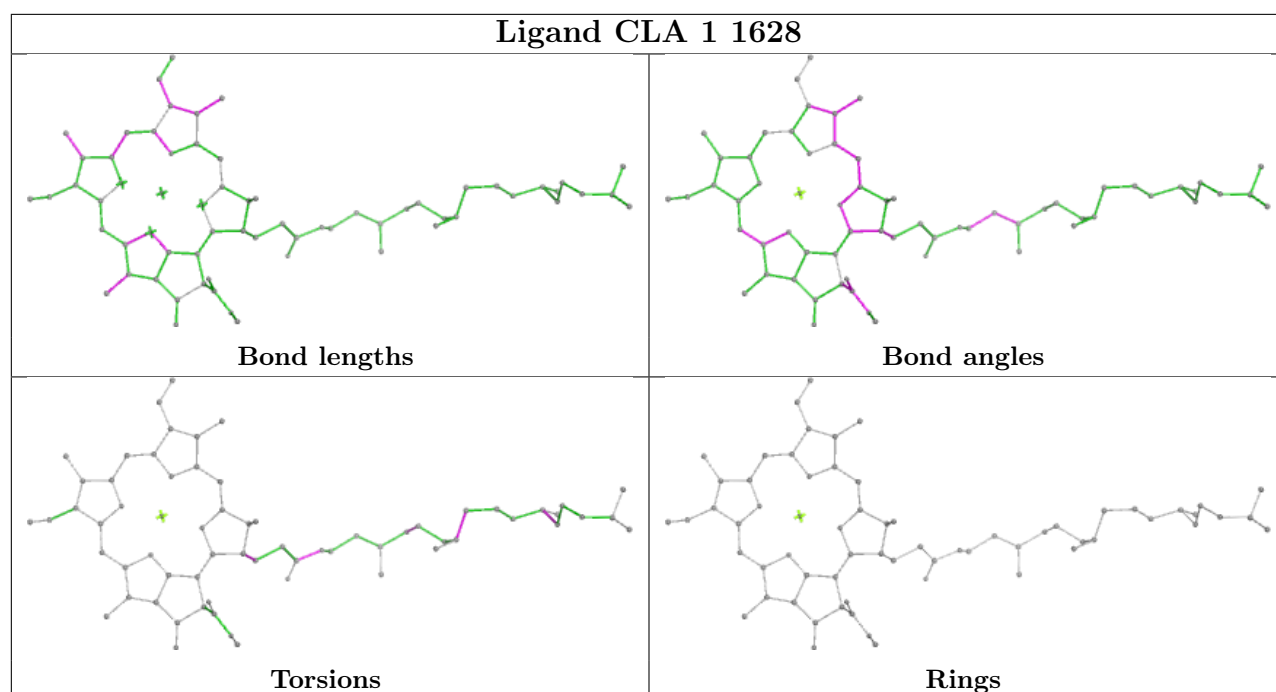
## Ligand BCR 8 1306

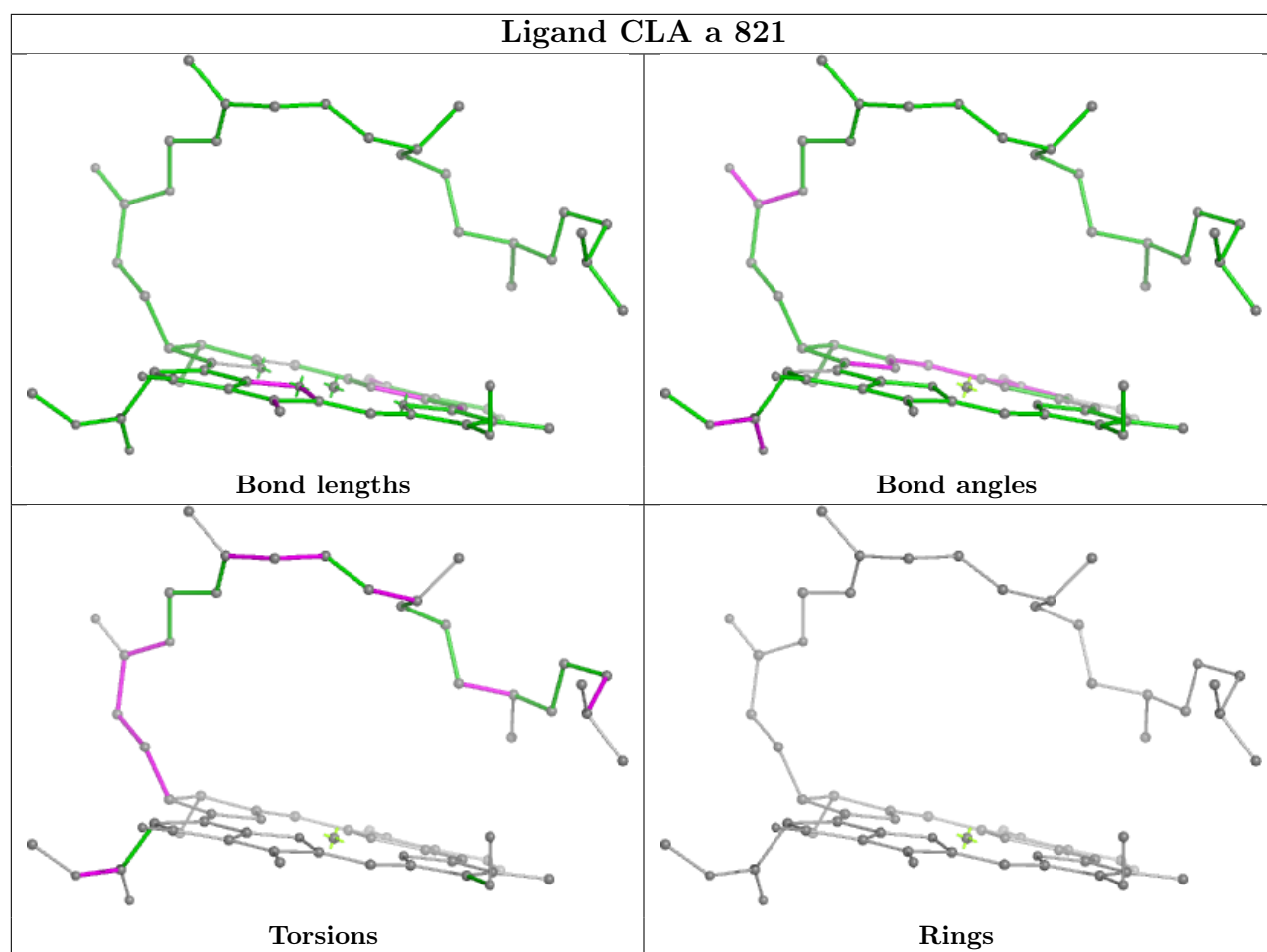


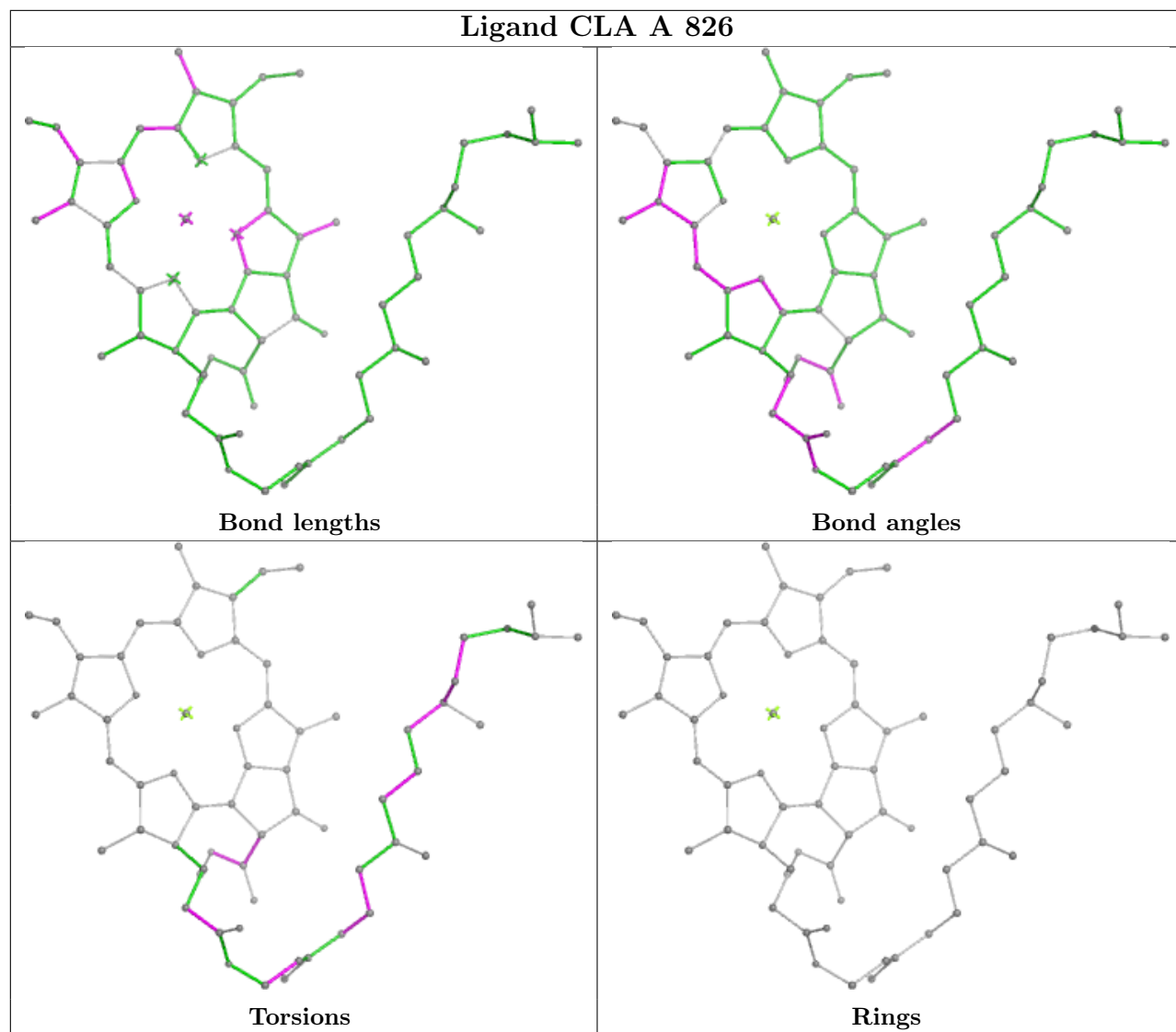
## Ligand BCR 1 202

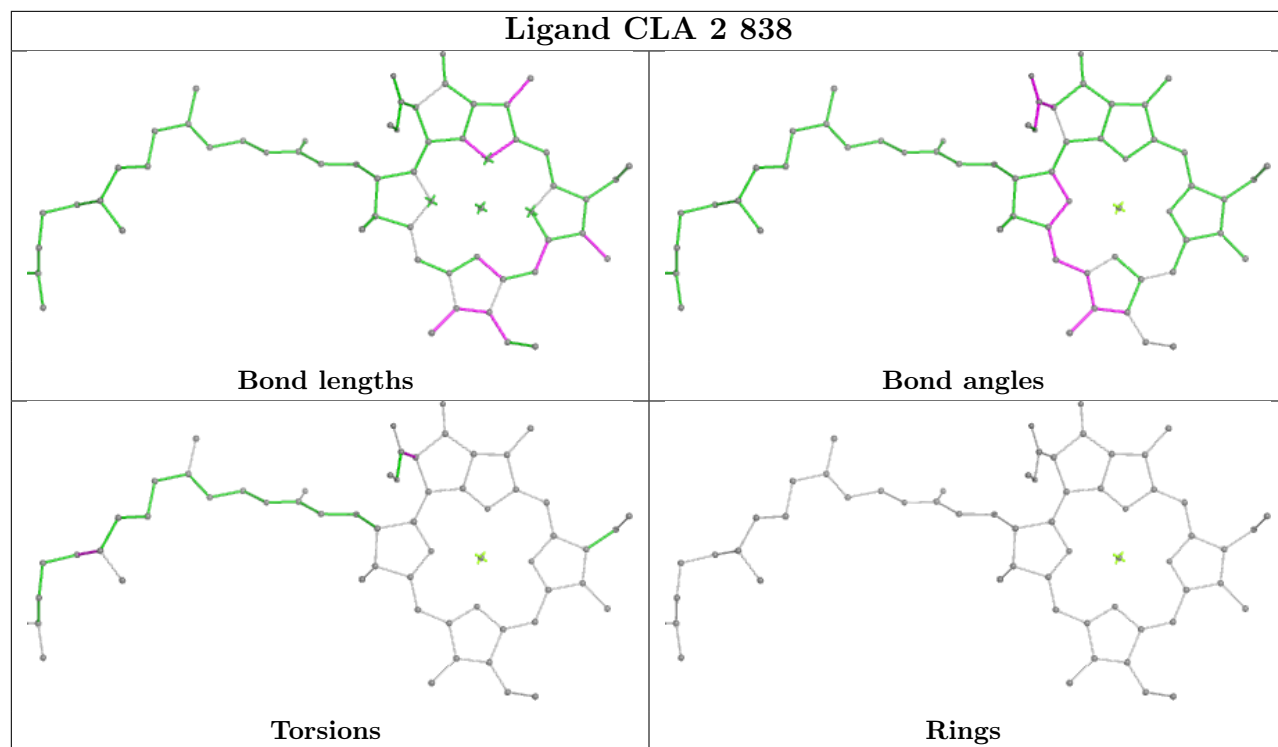




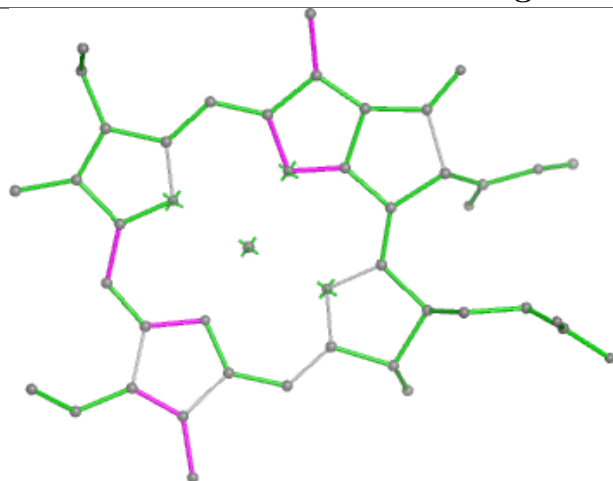




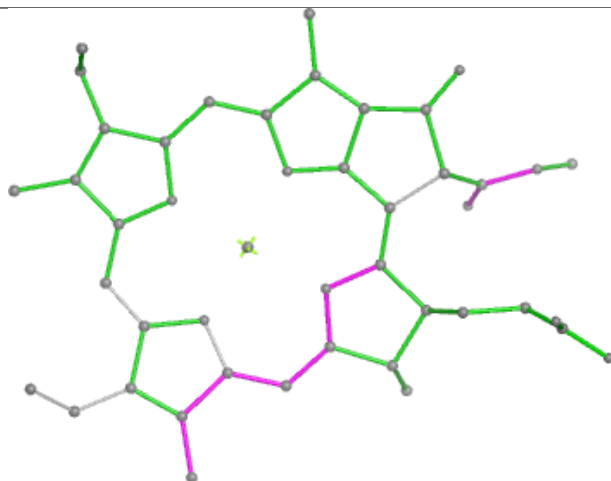




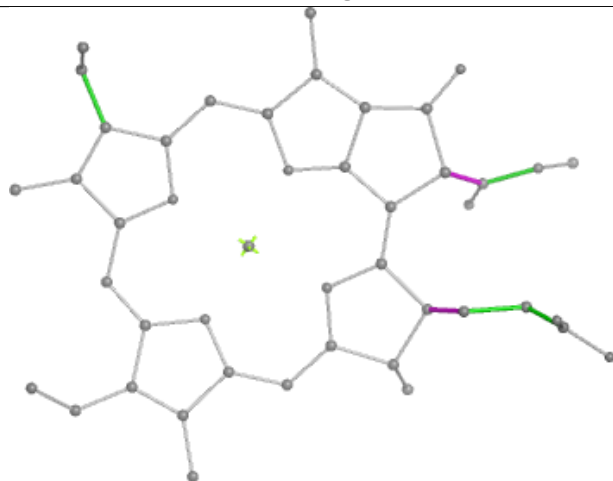
## Ligand CLA B 836



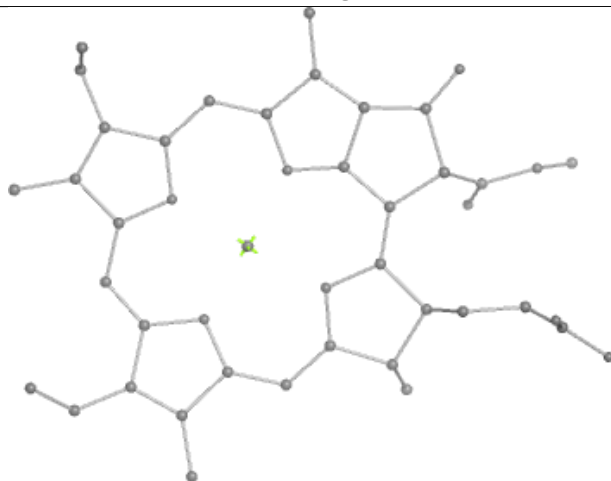
Bond lengths



Bond angles

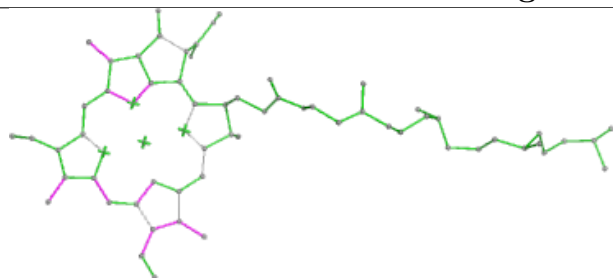


Torsions

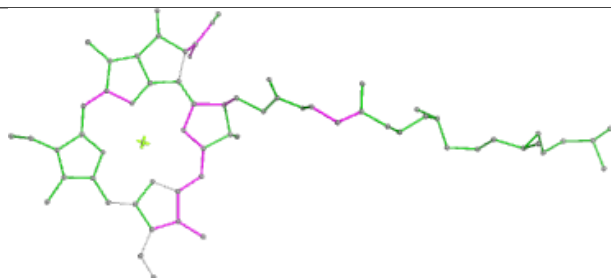


Rings

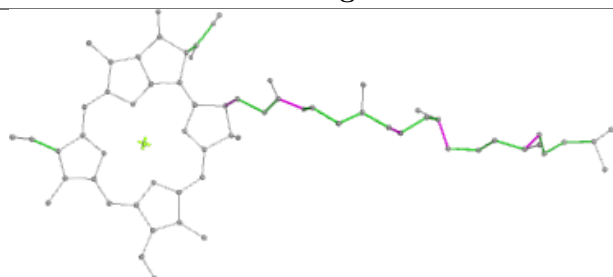
## Ligand CLA a 827



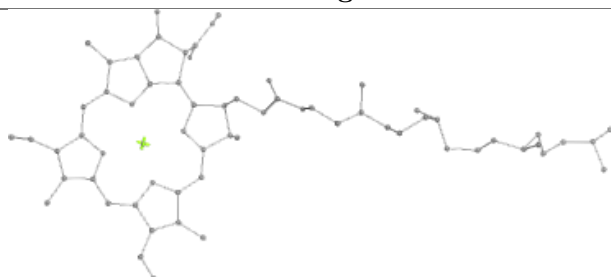
Bond lengths



Bond angles

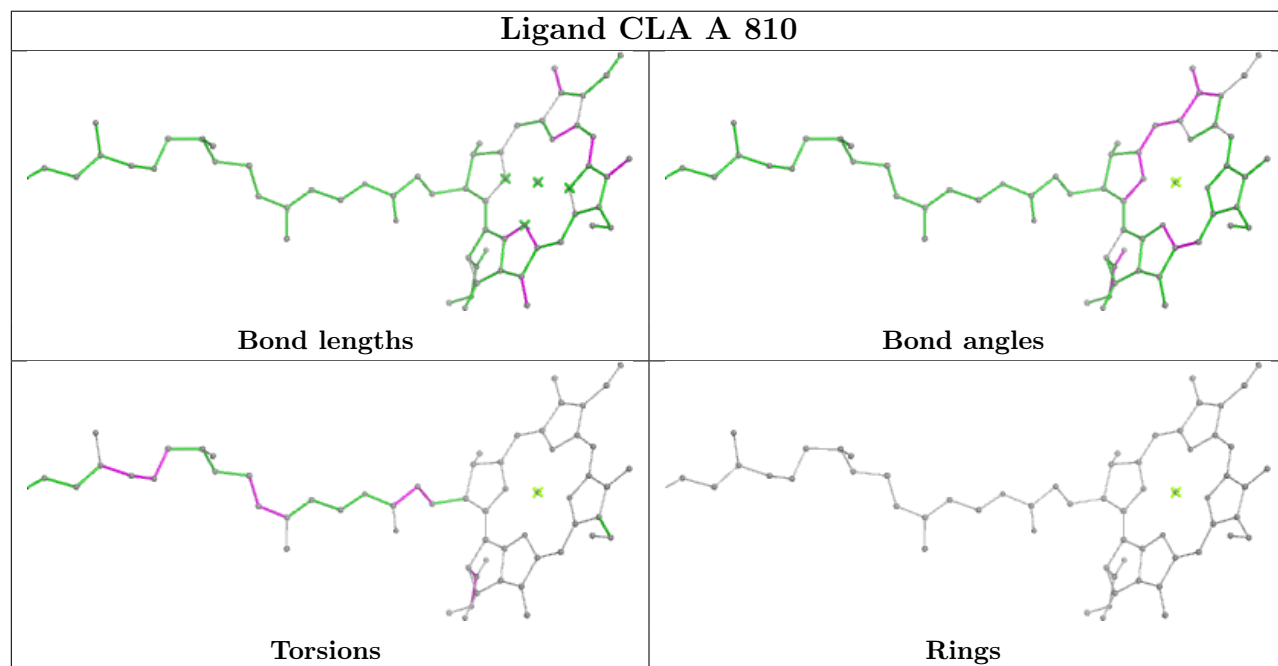
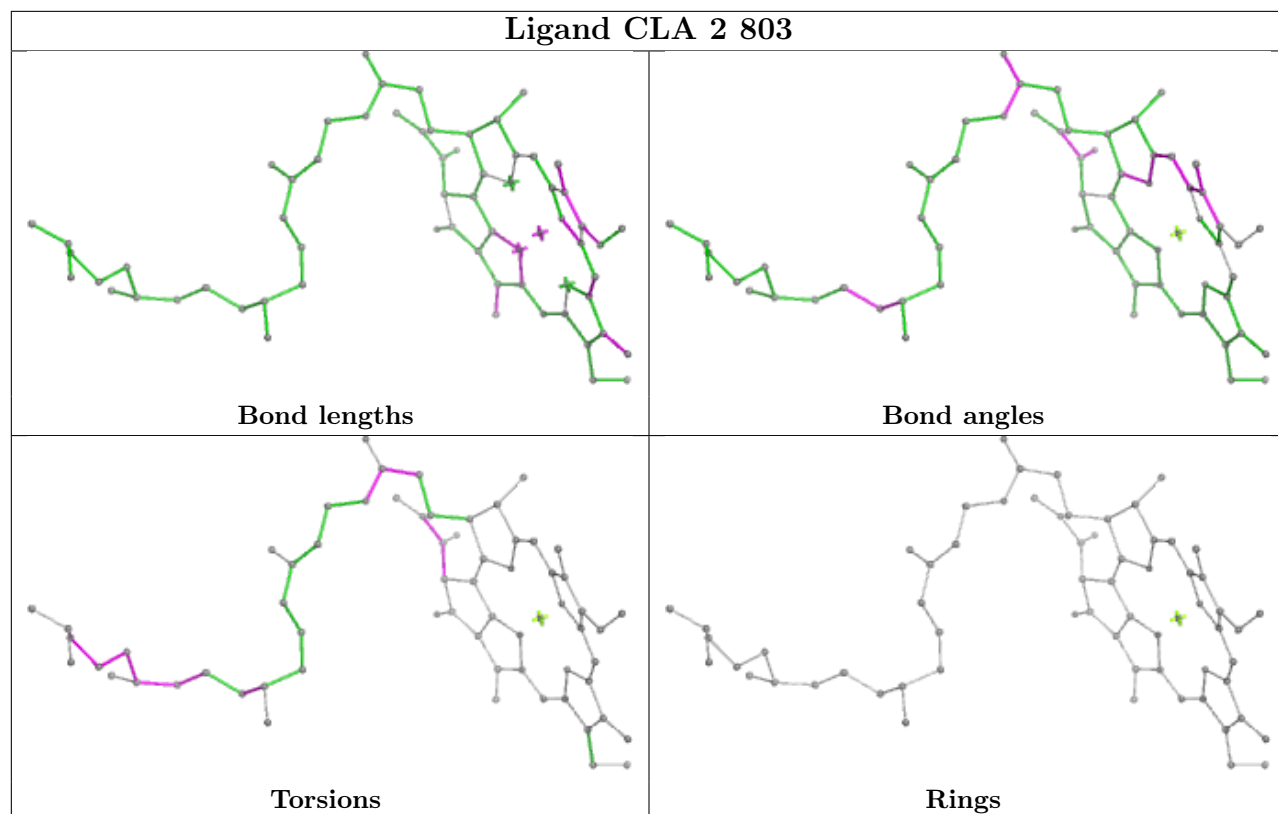


Torsions

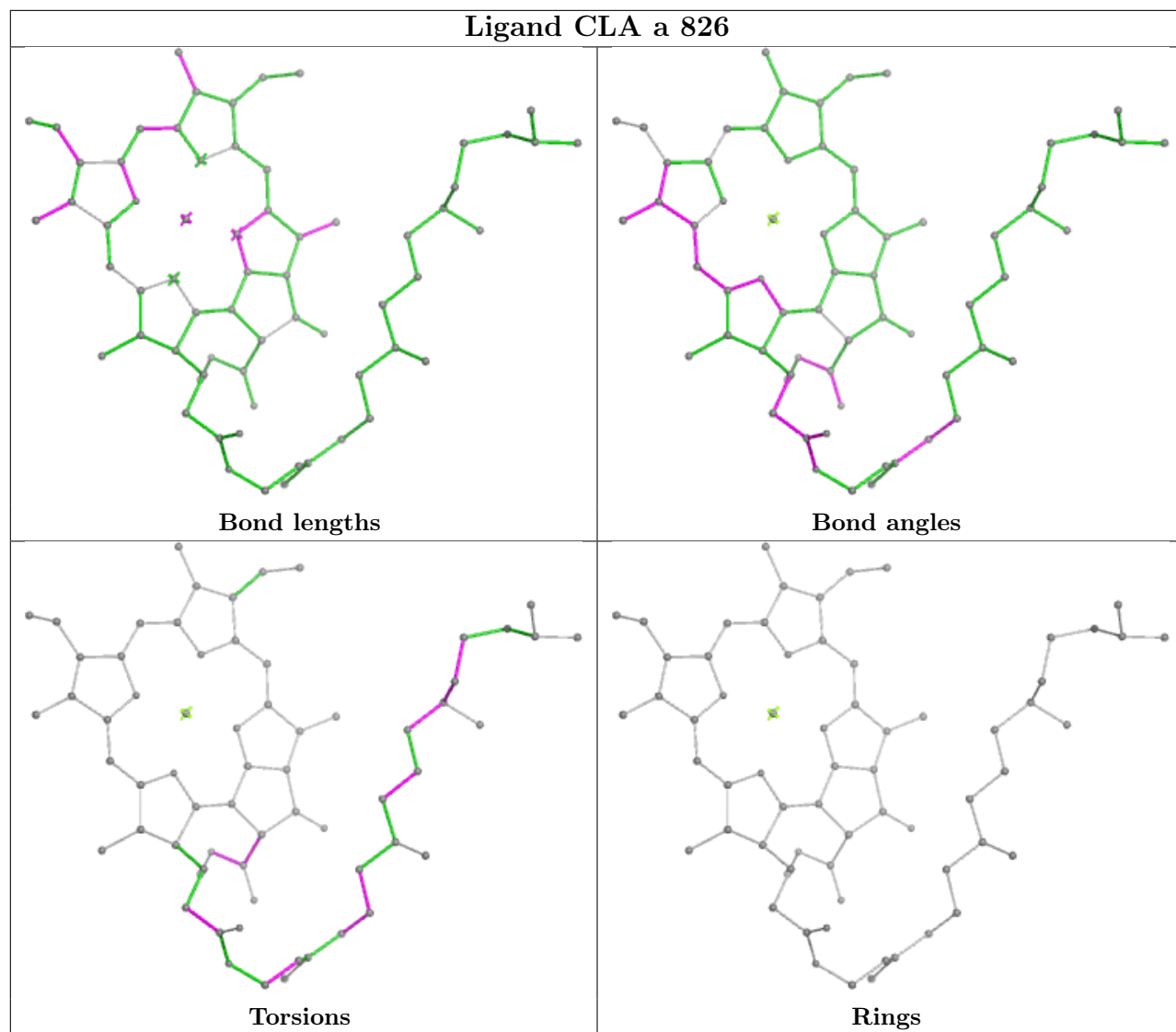


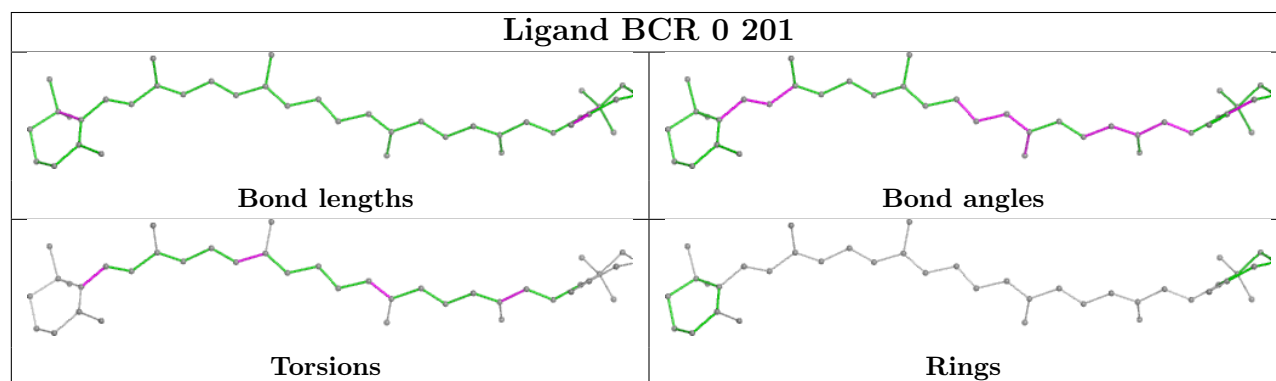
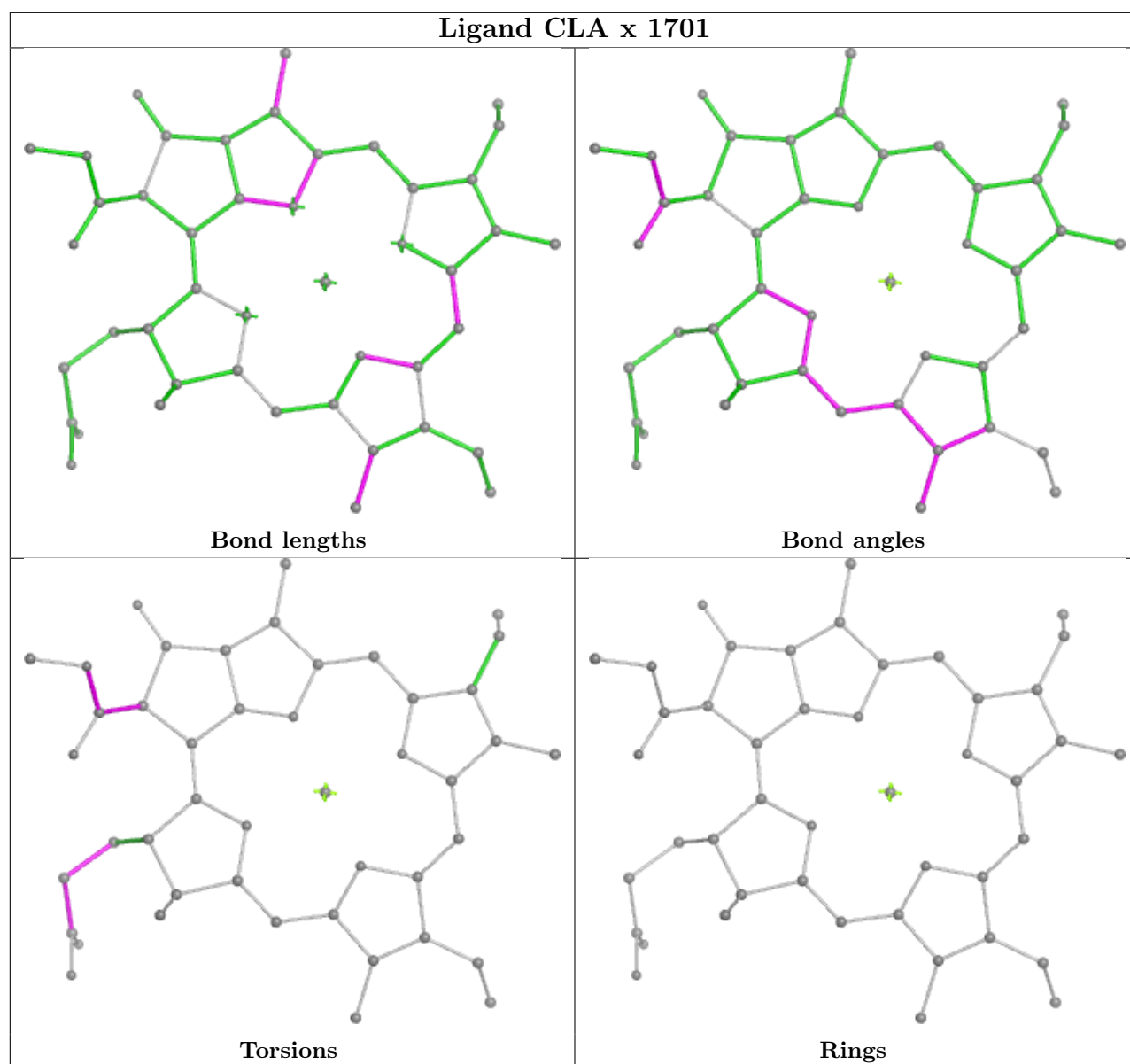
Rings



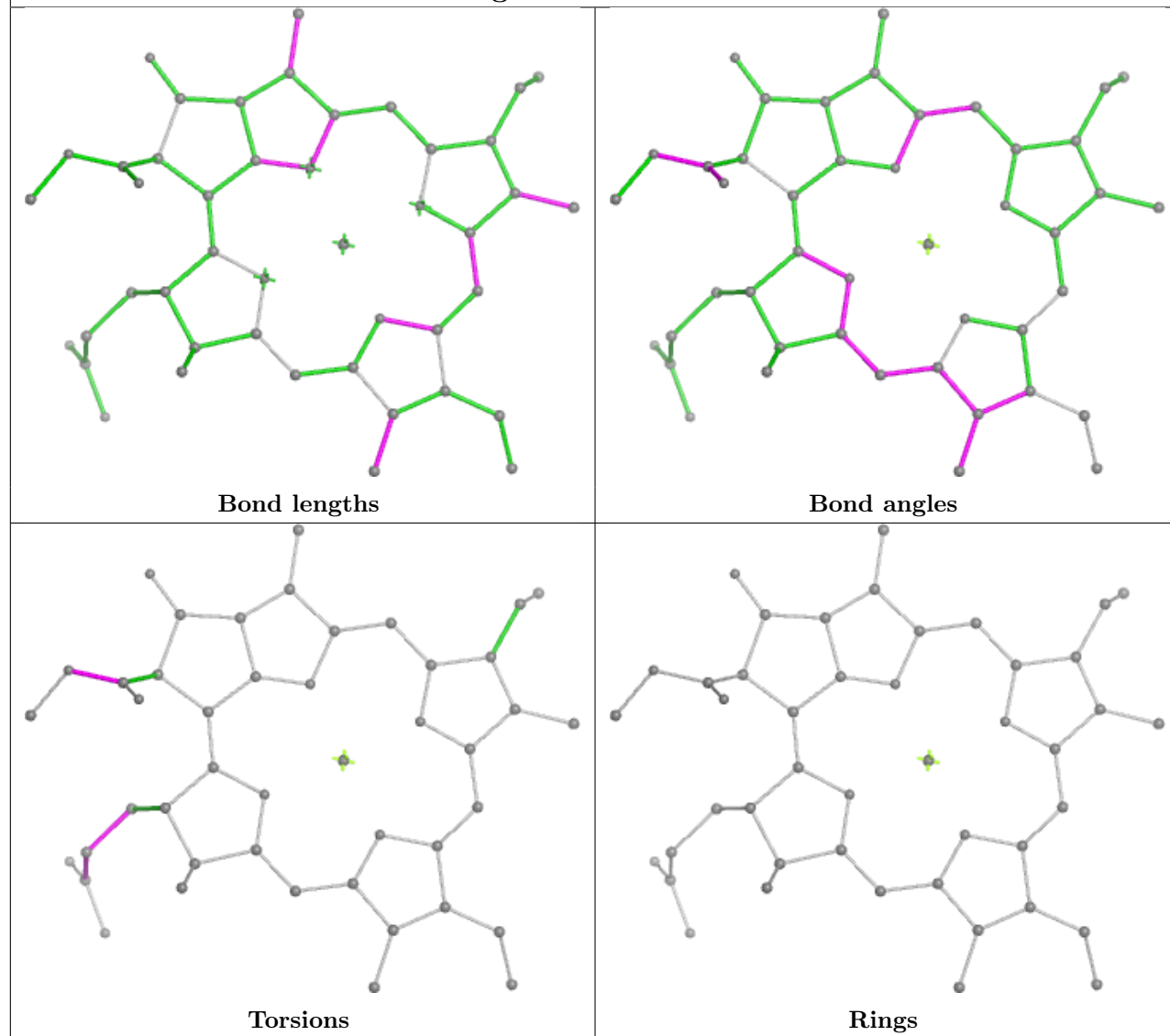


## Ligand CLA a 826

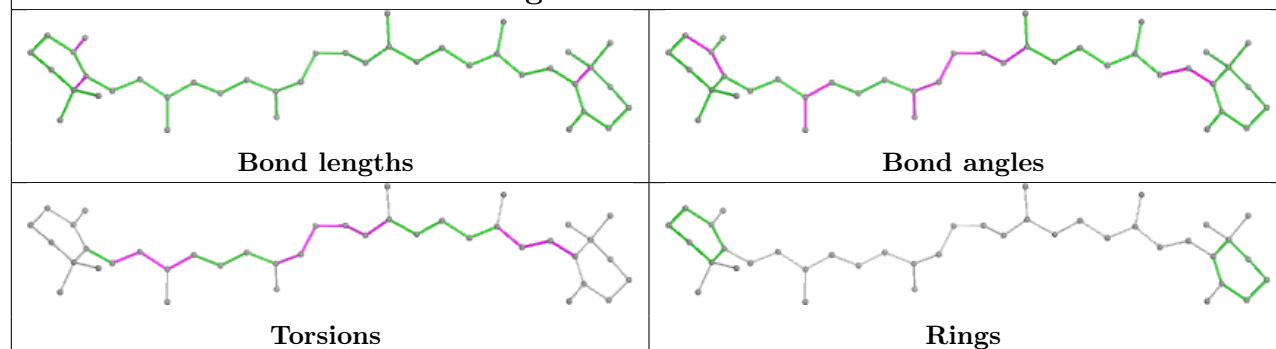


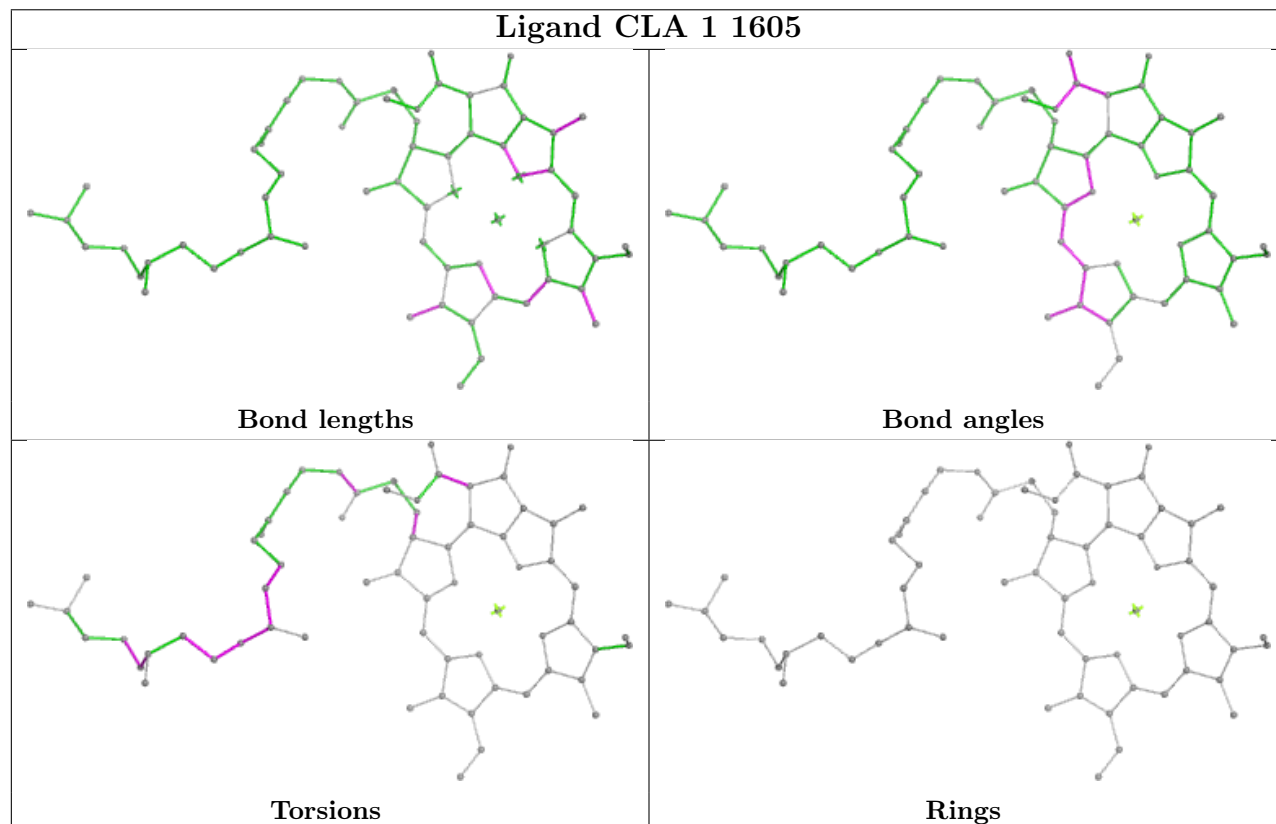
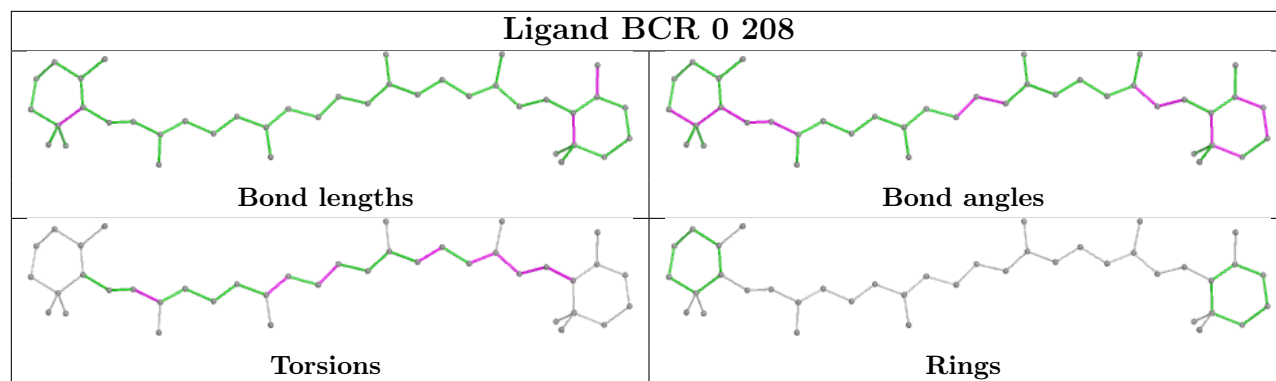


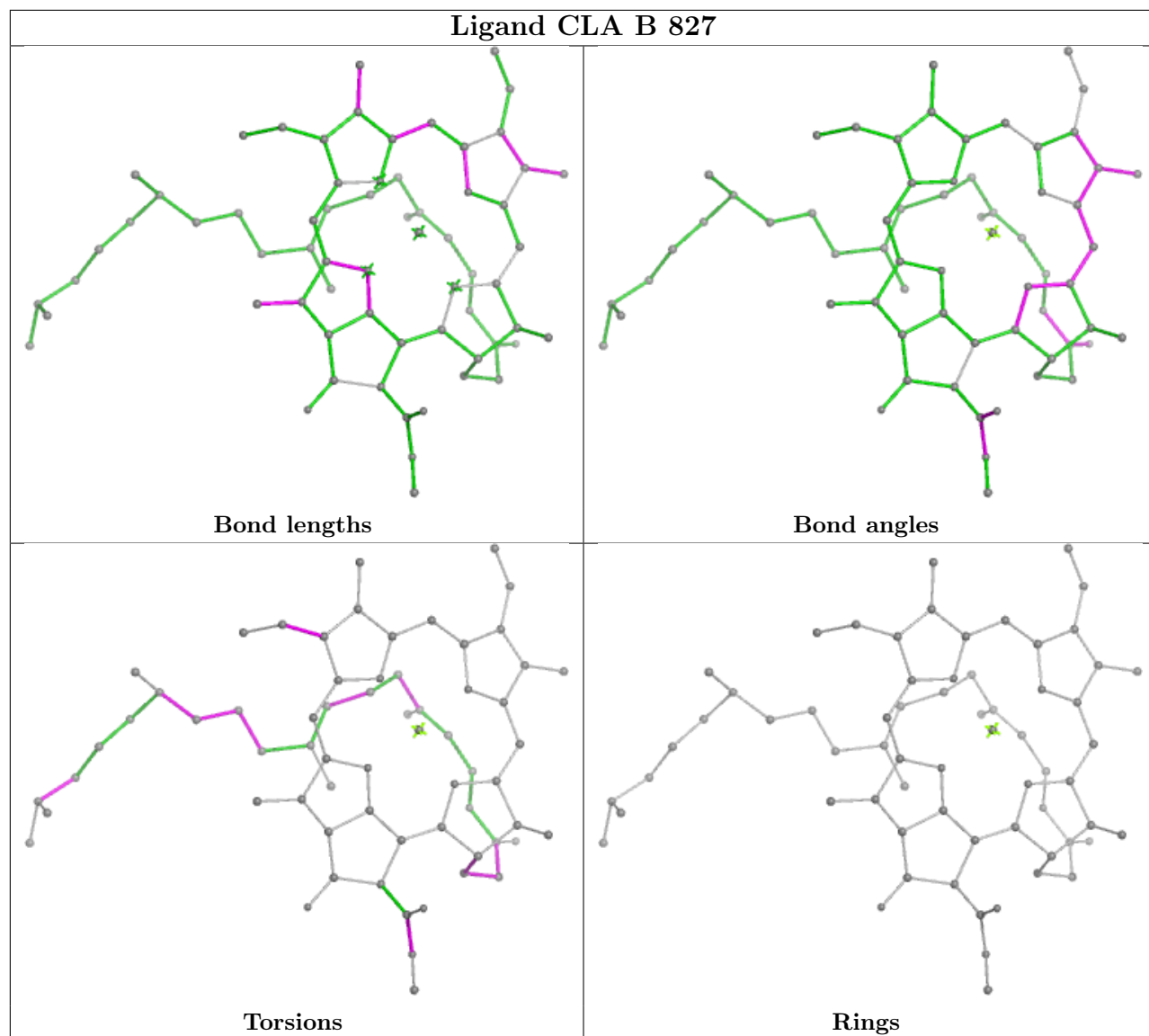
## Ligand CLA 2 824

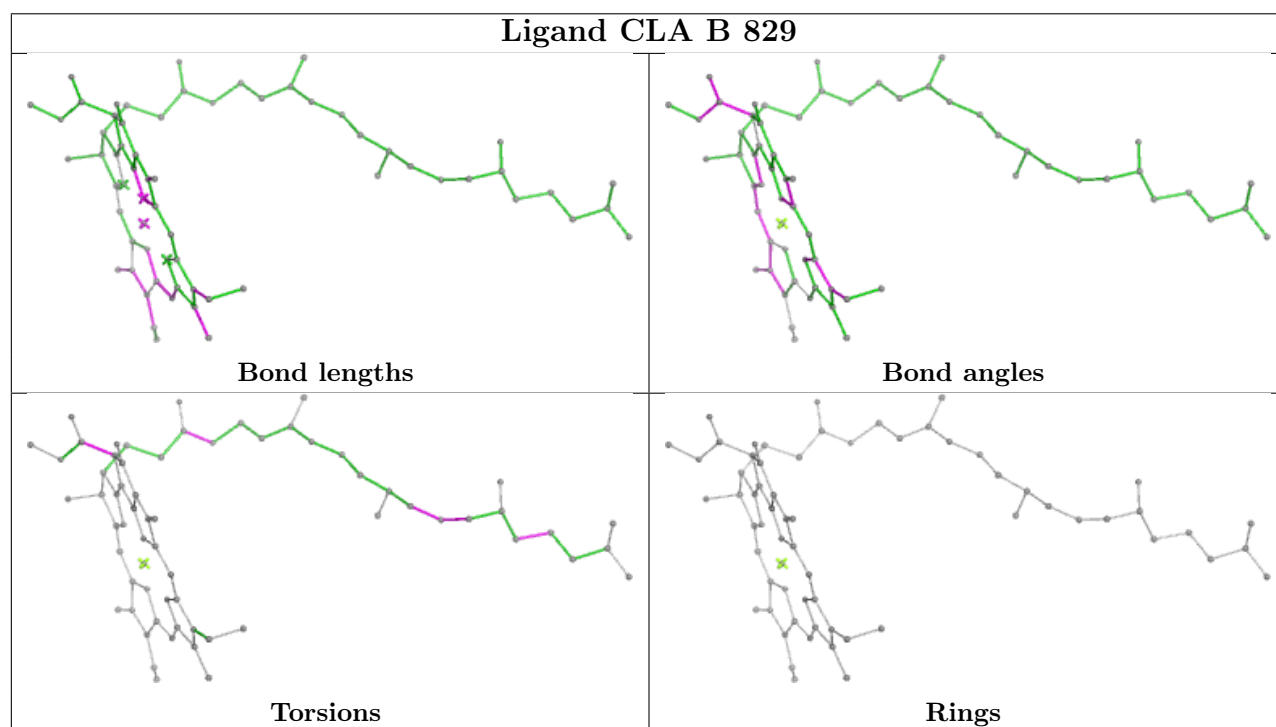
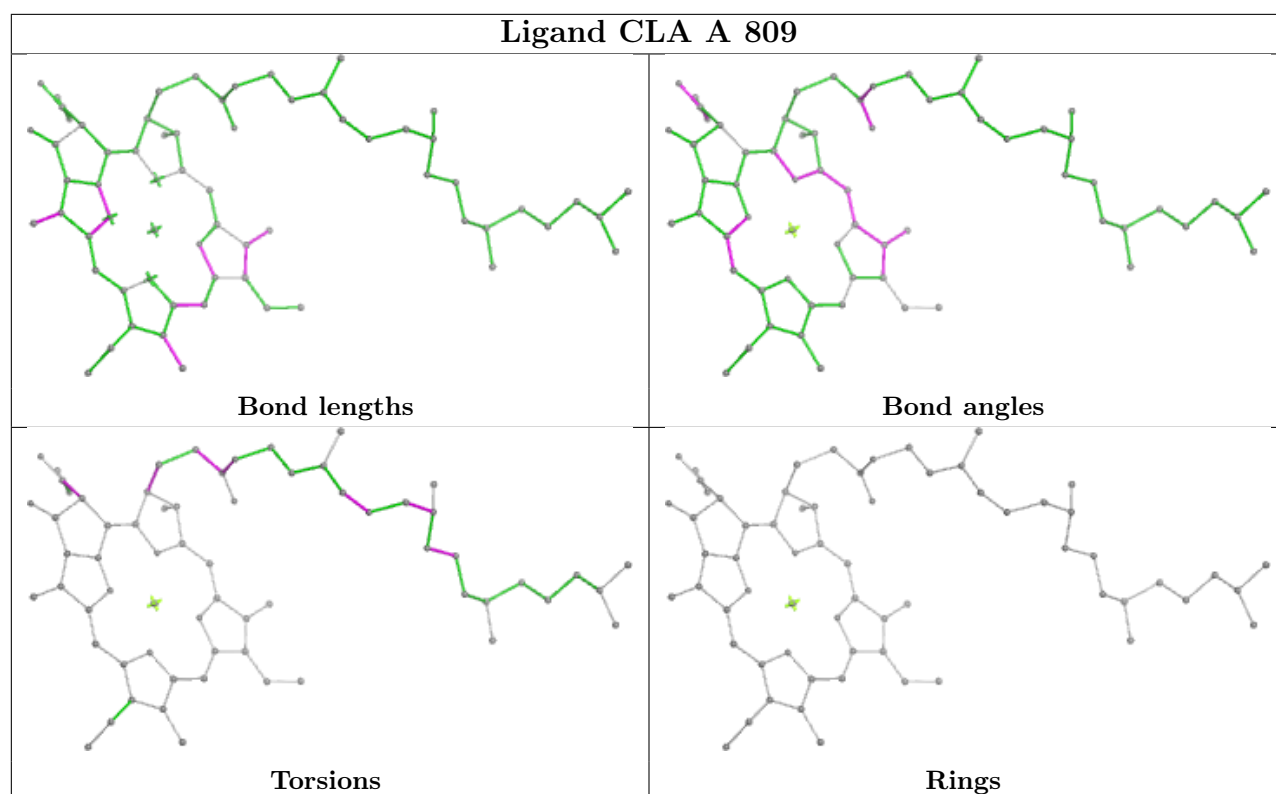


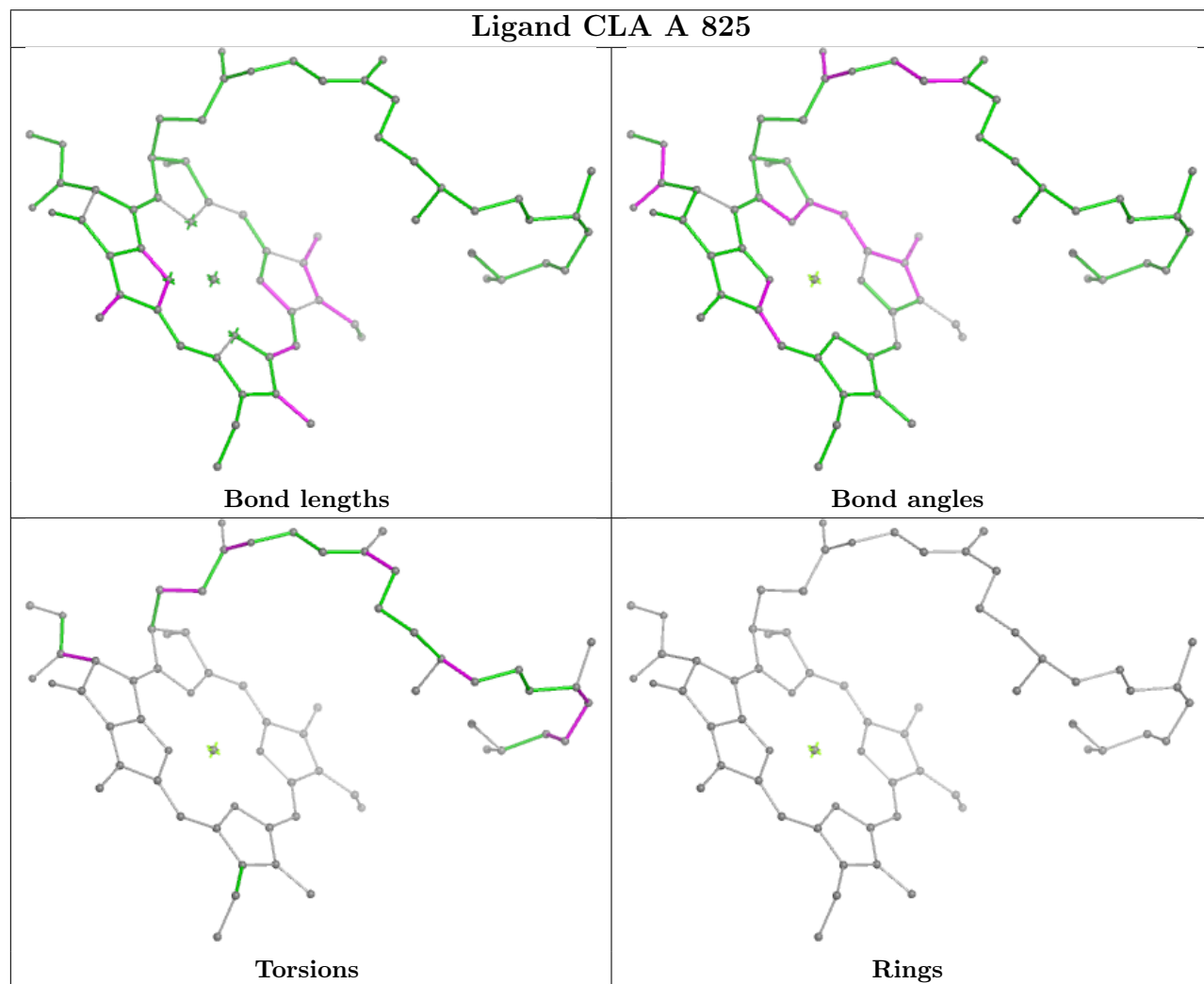
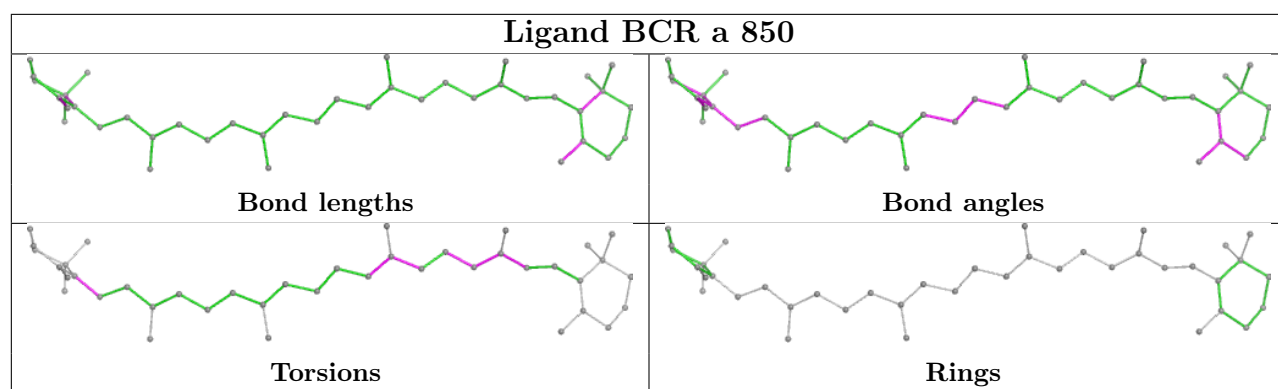
## Ligand BCR 1 1649





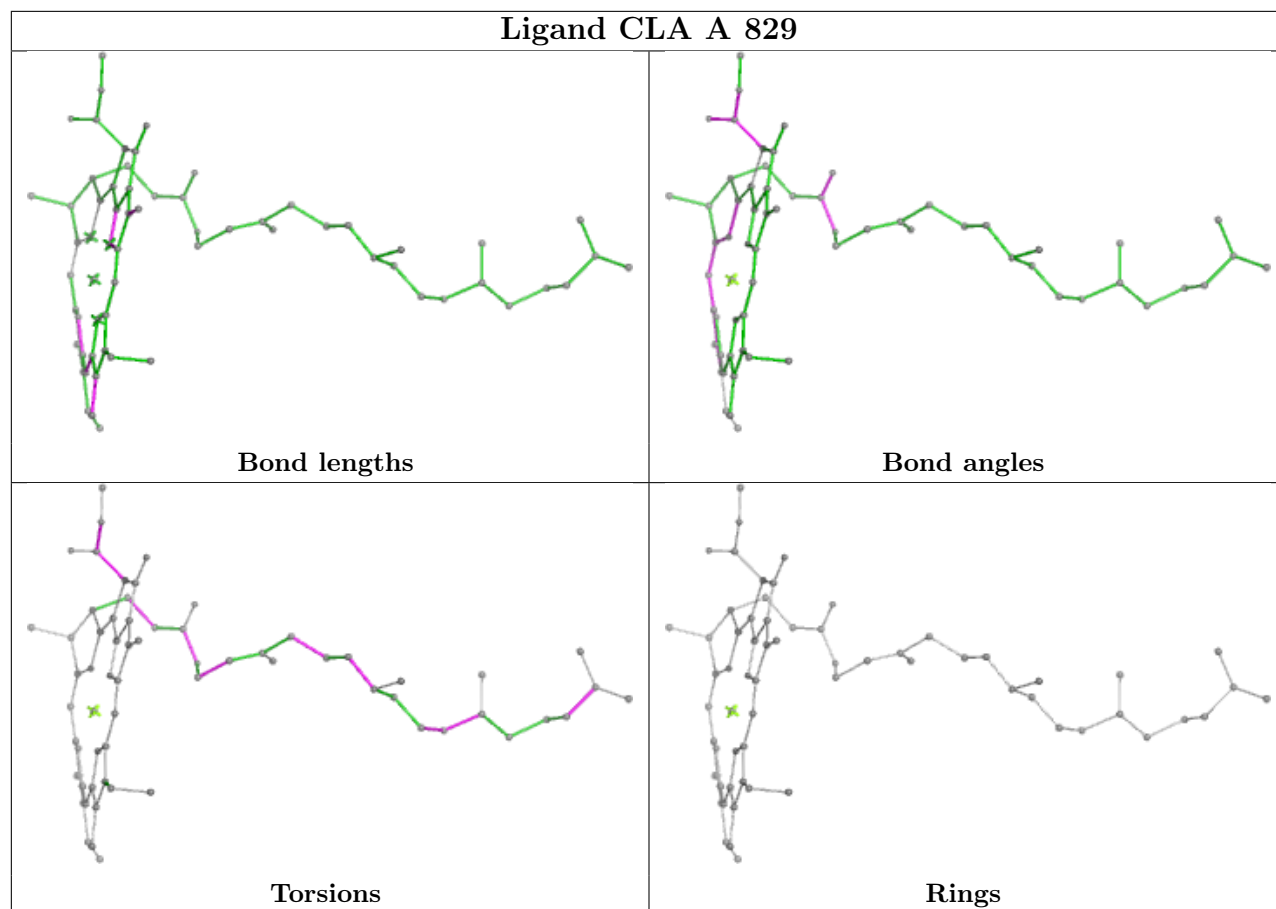




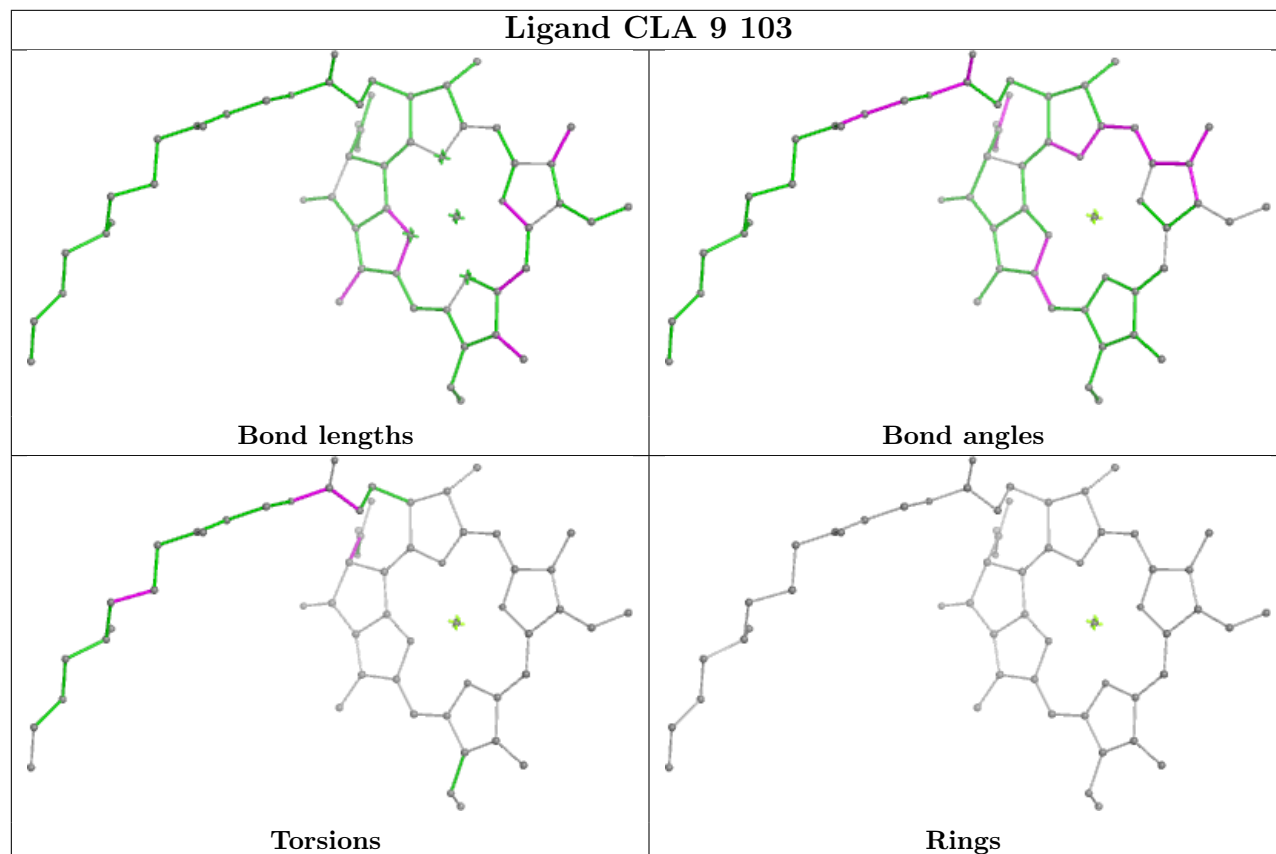


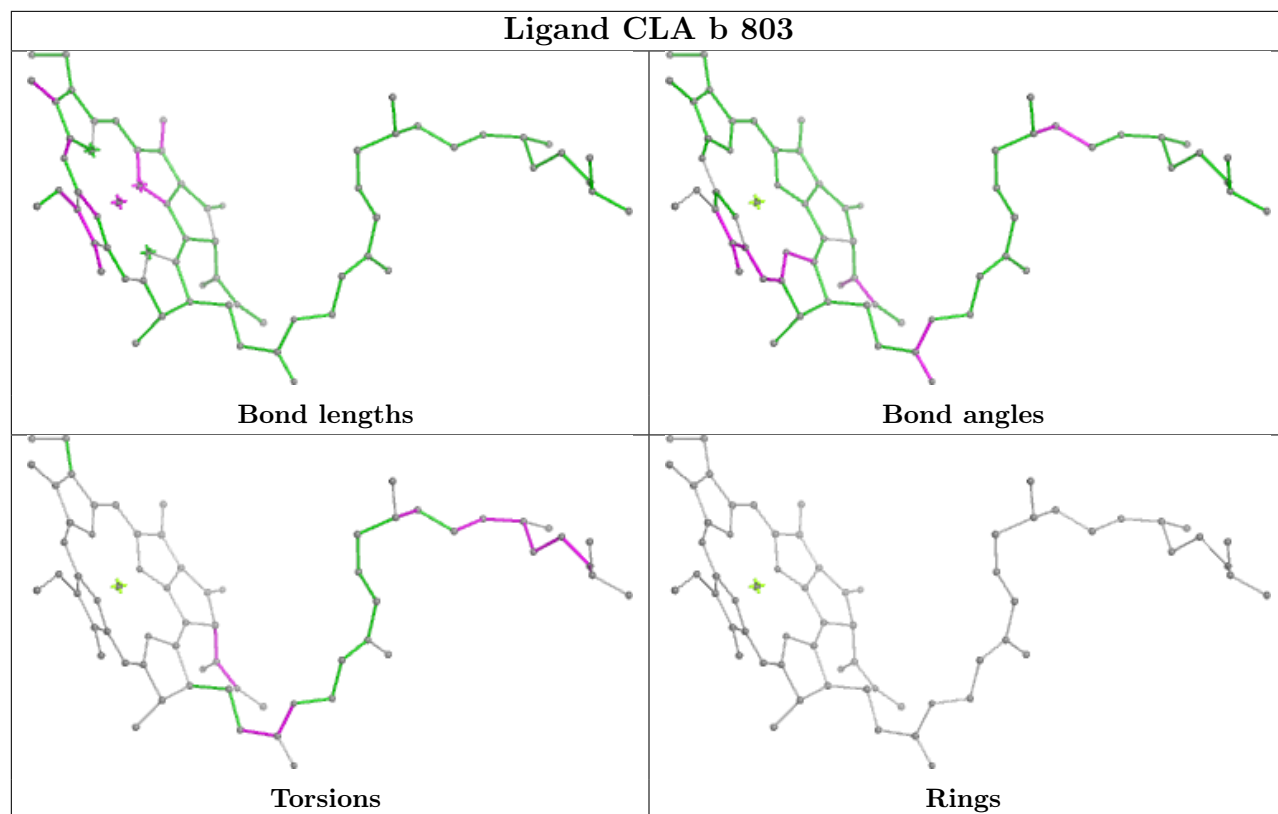


## Ligand CLA A 829

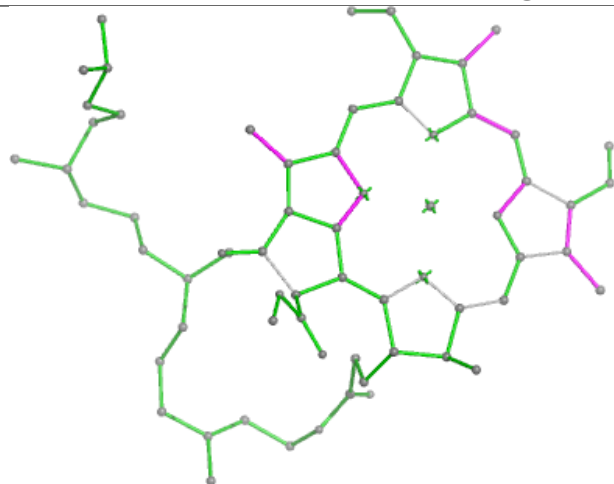


## Ligand CLA 9 103

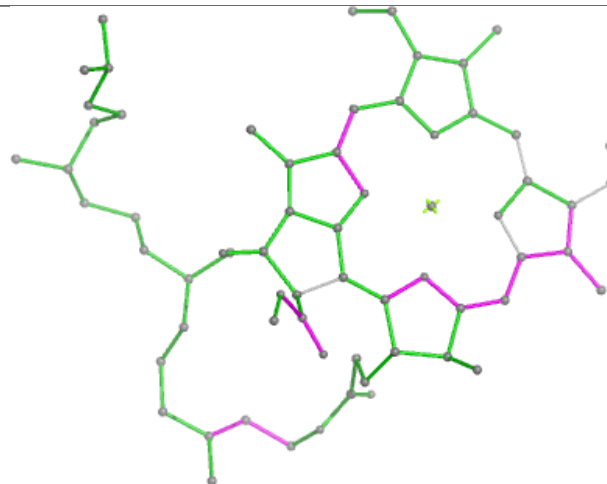




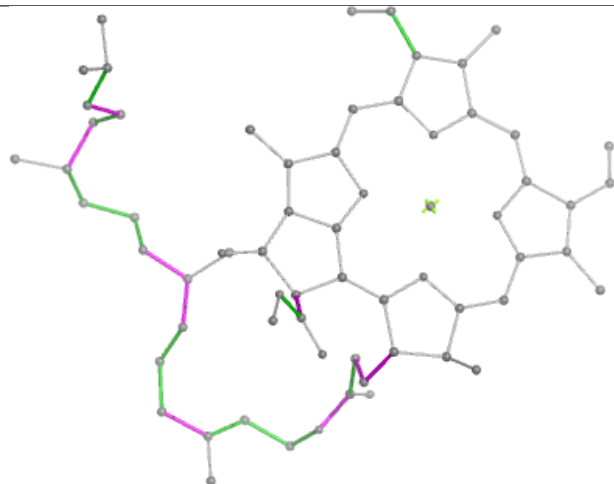
## Ligand CLA 2 833



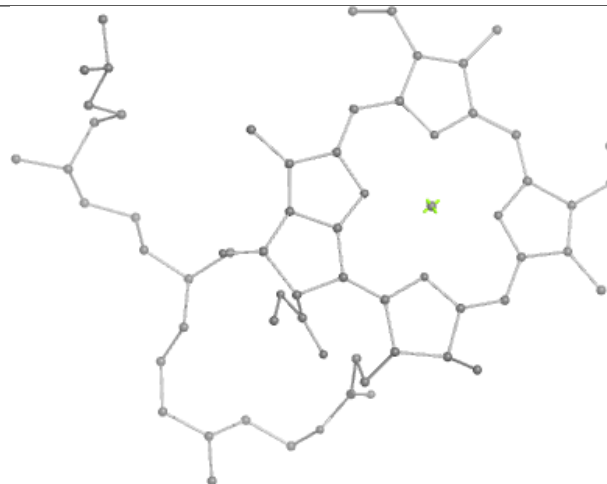
Bond lengths



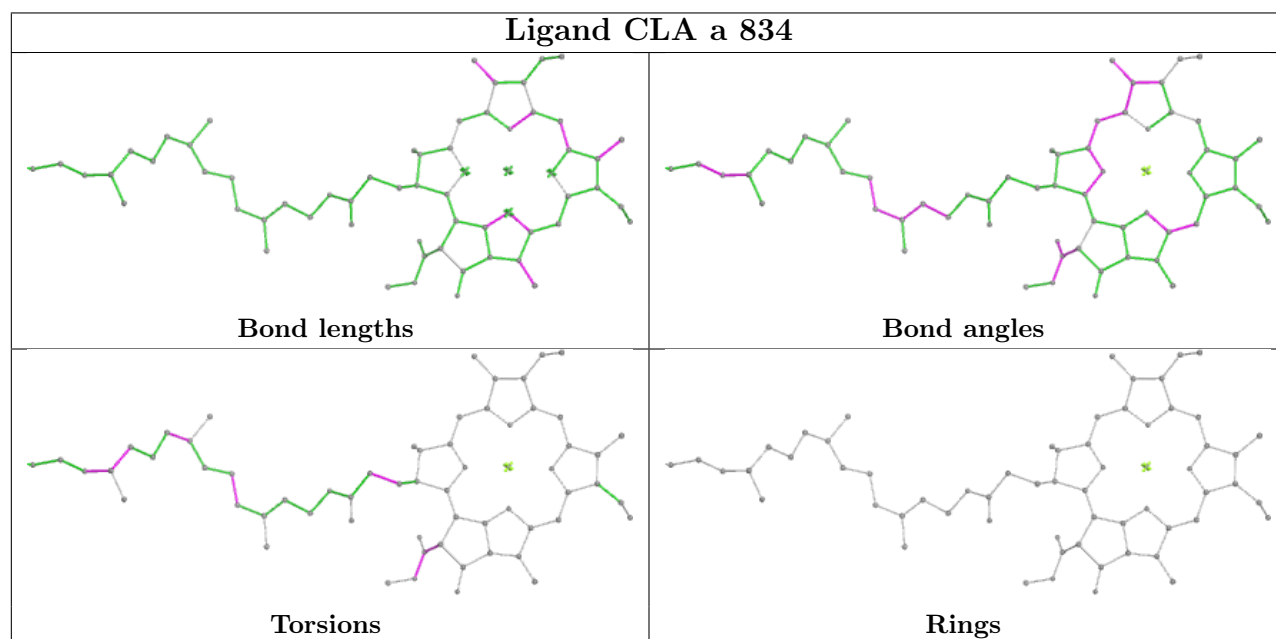
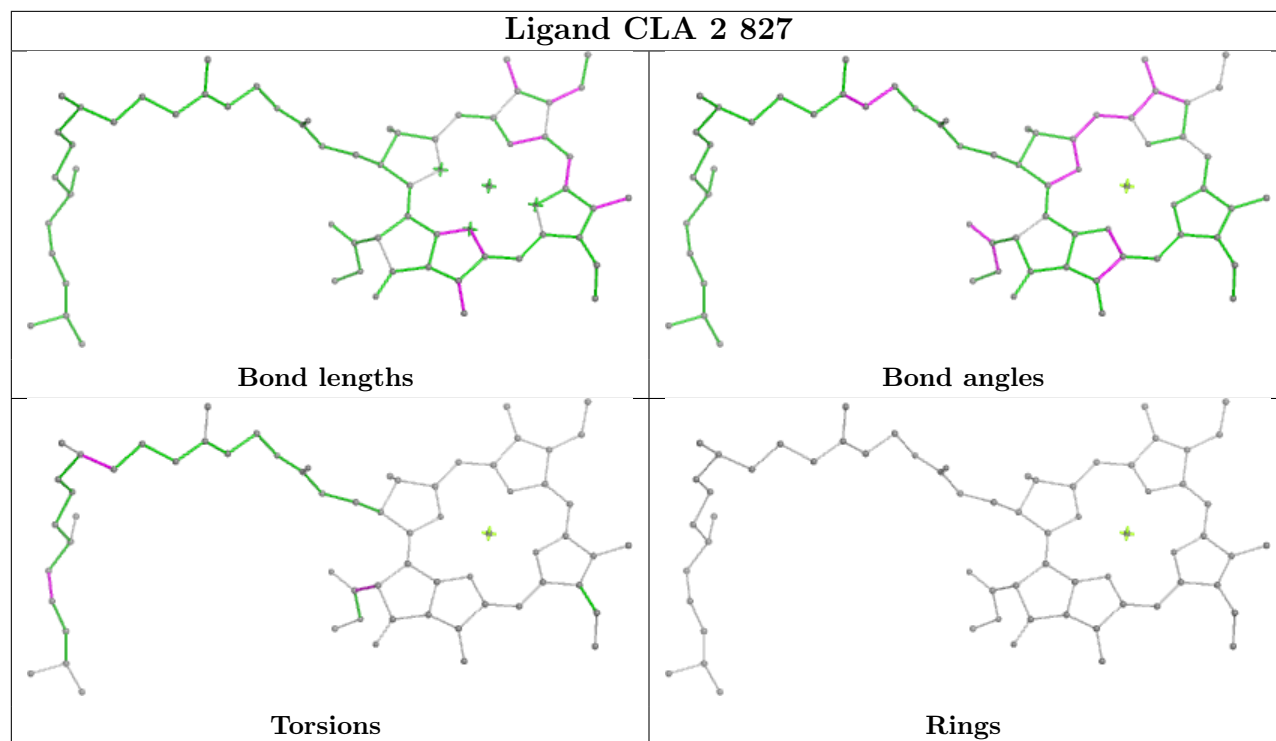
Bond angles

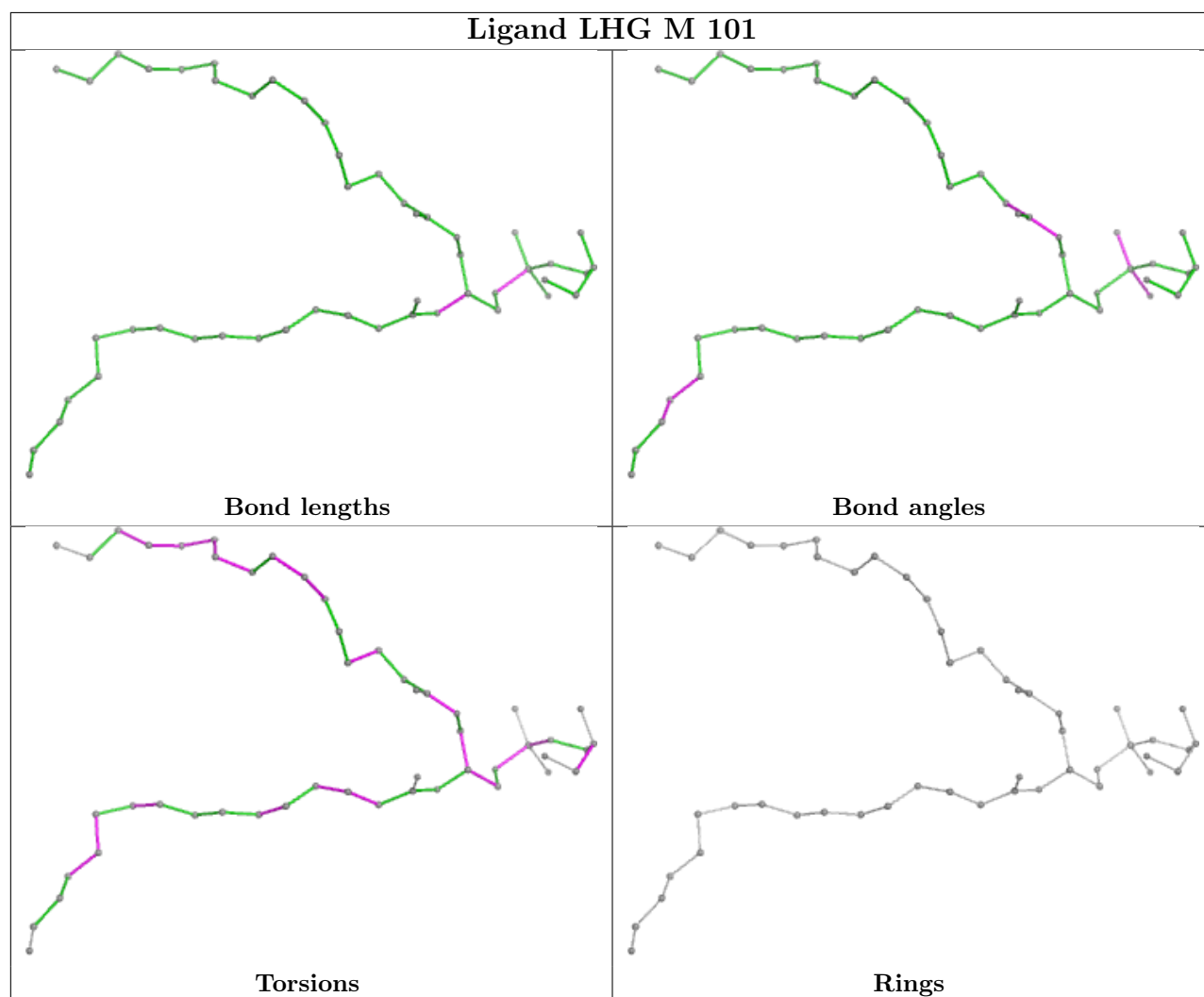
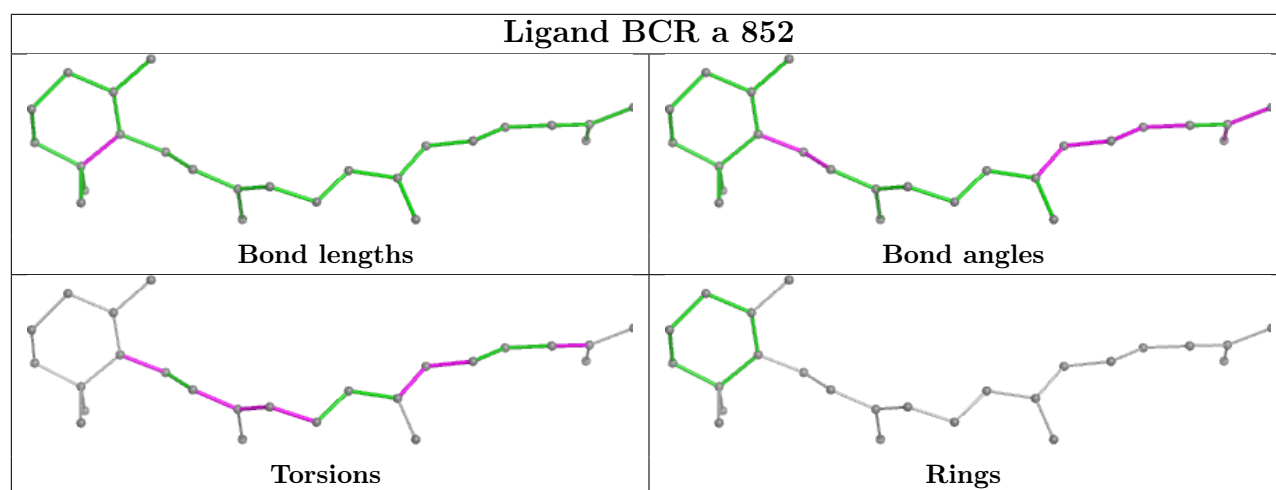


Torsions

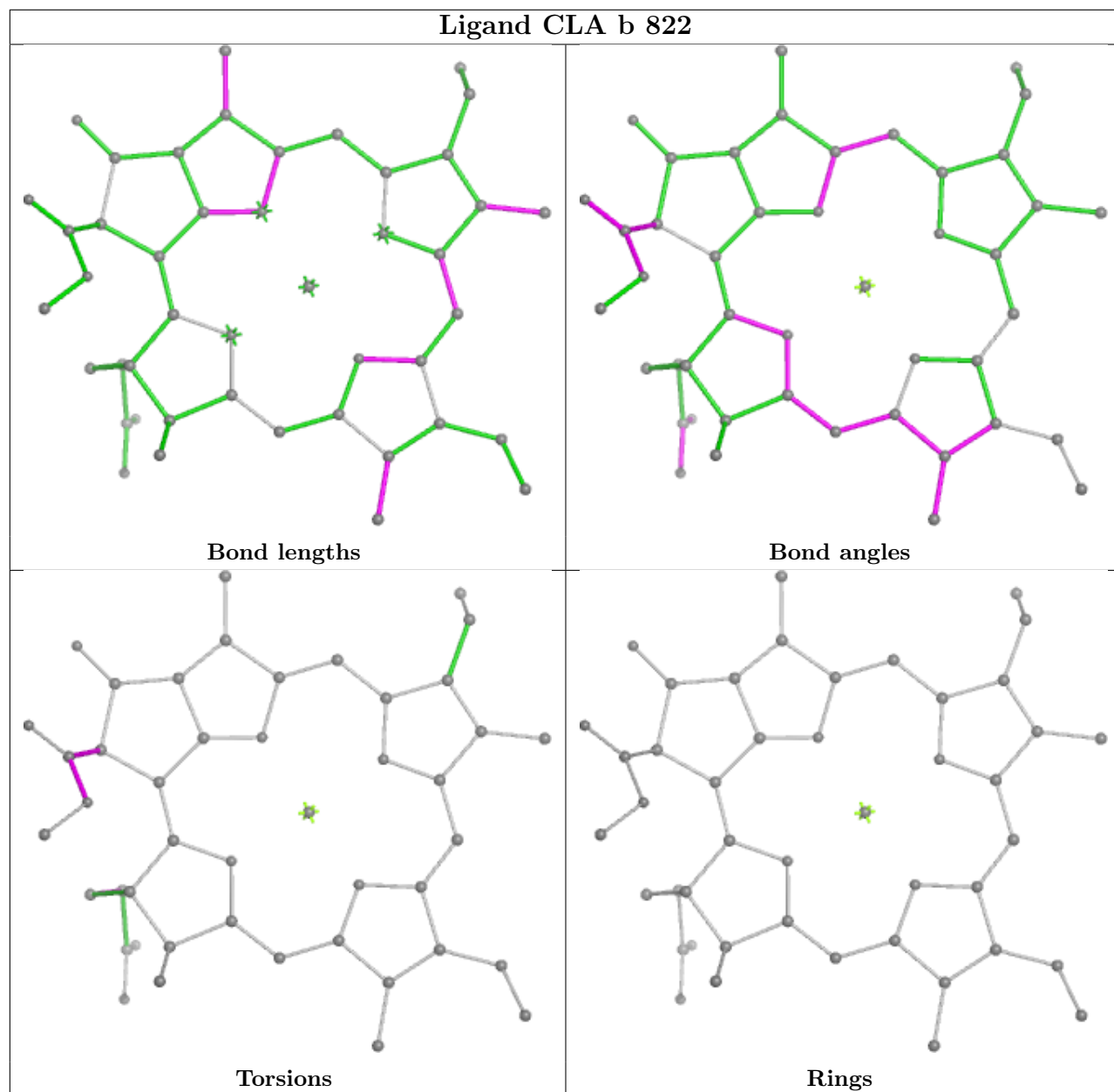


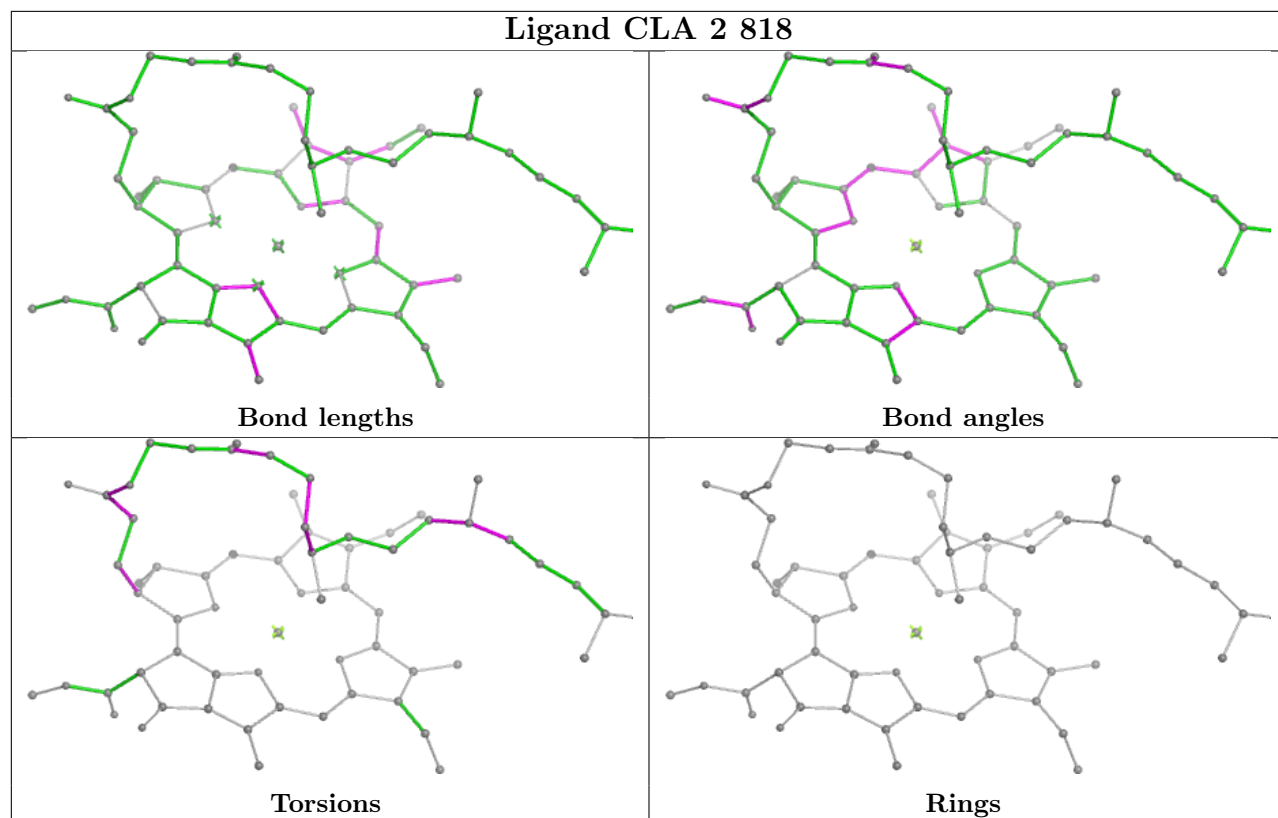
Rings



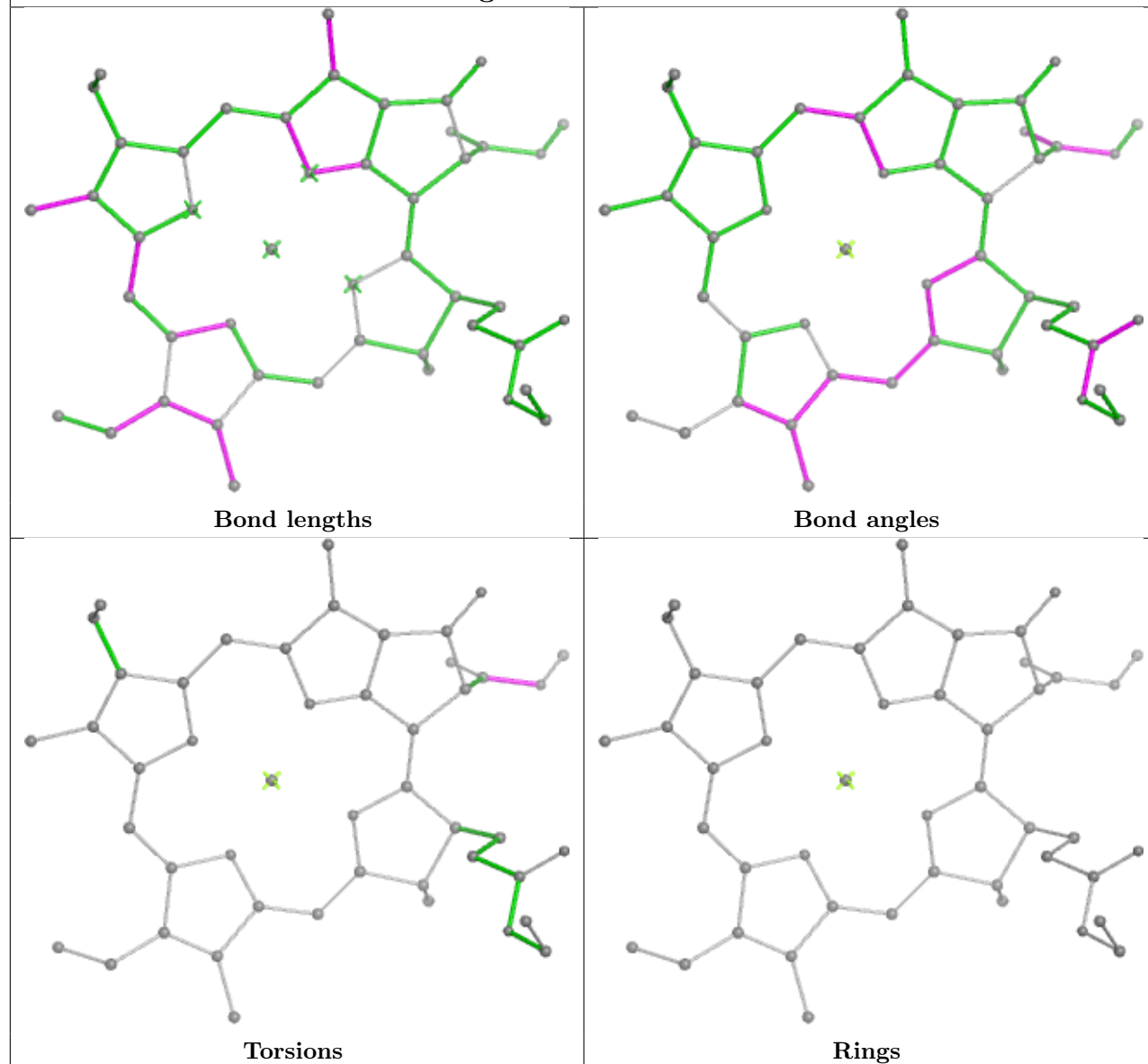


## Ligand CLA b 822

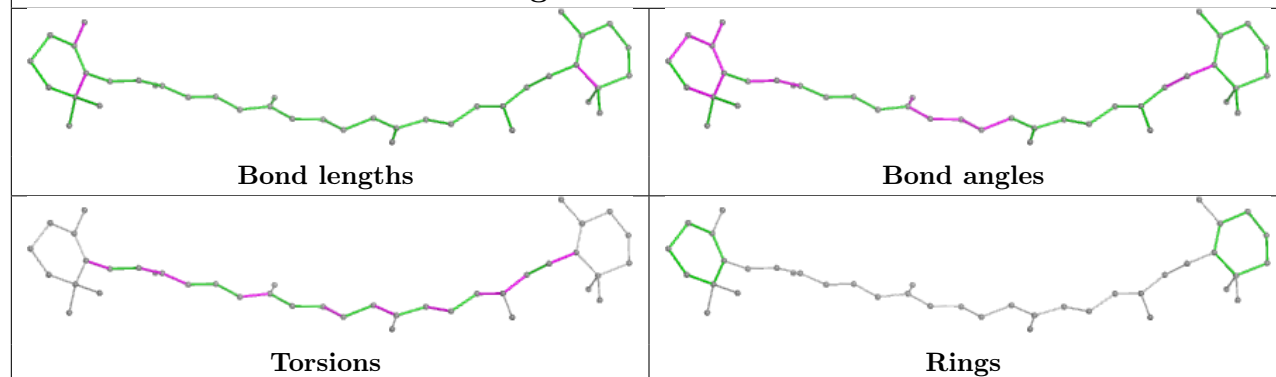




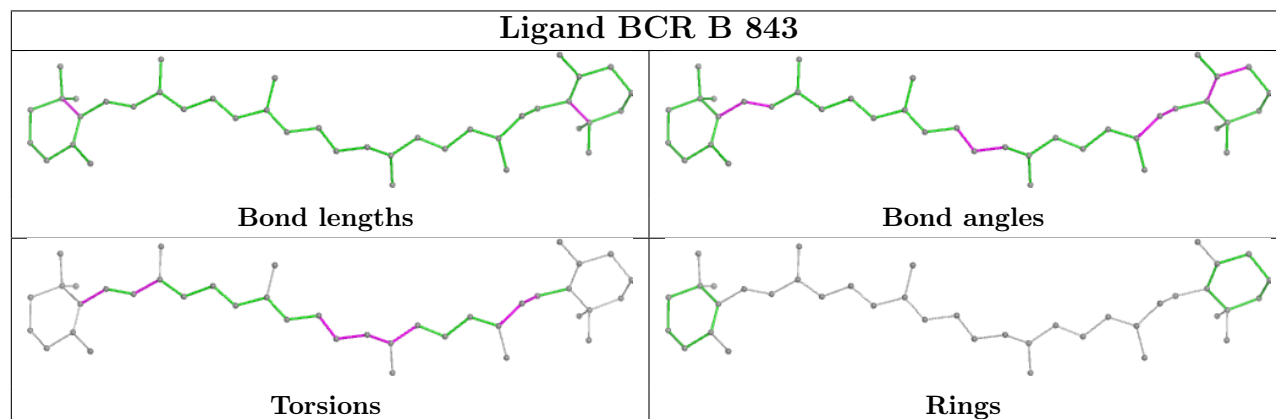
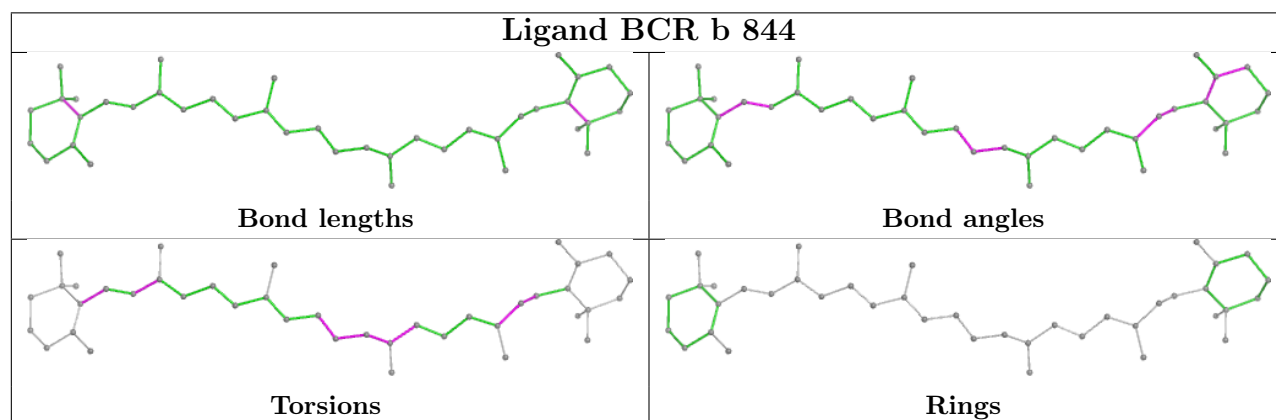
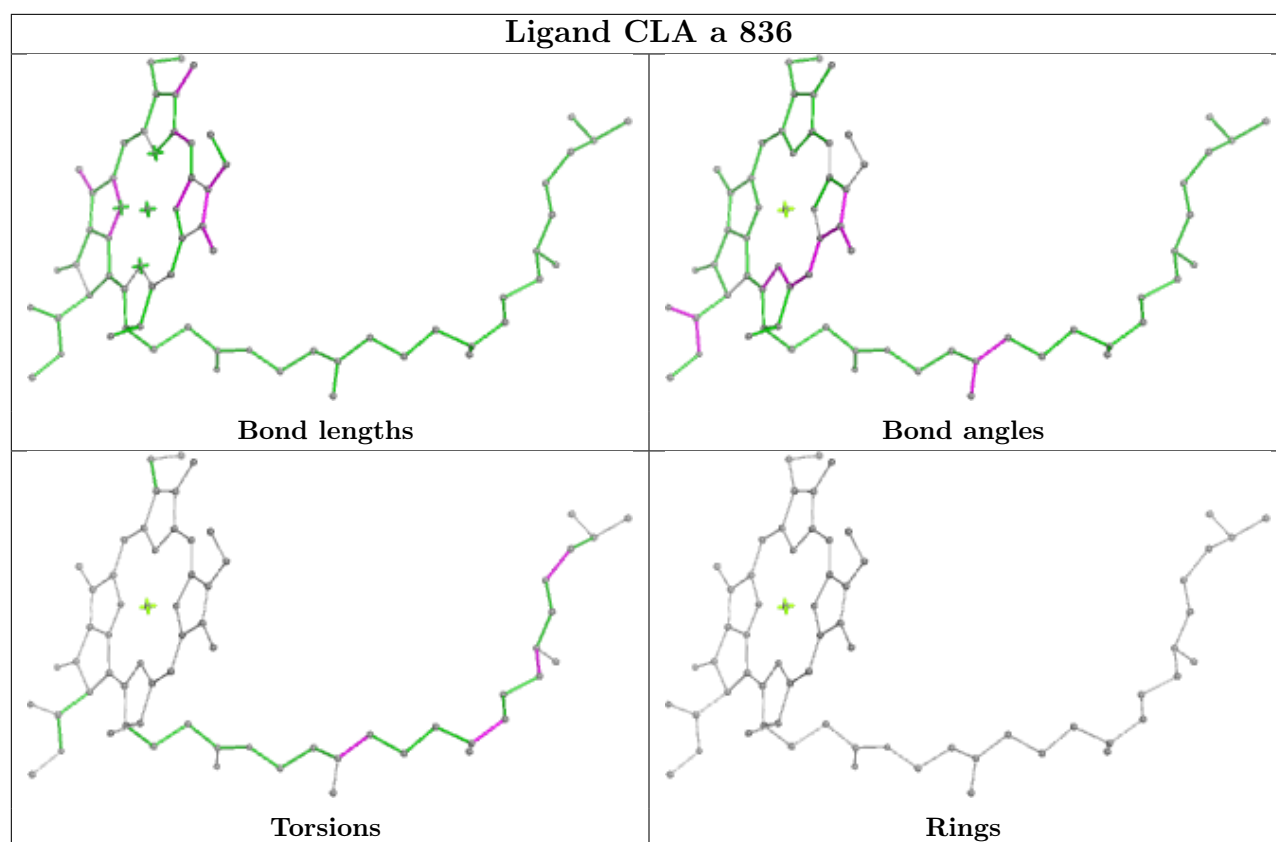
## Ligand CLA B 839



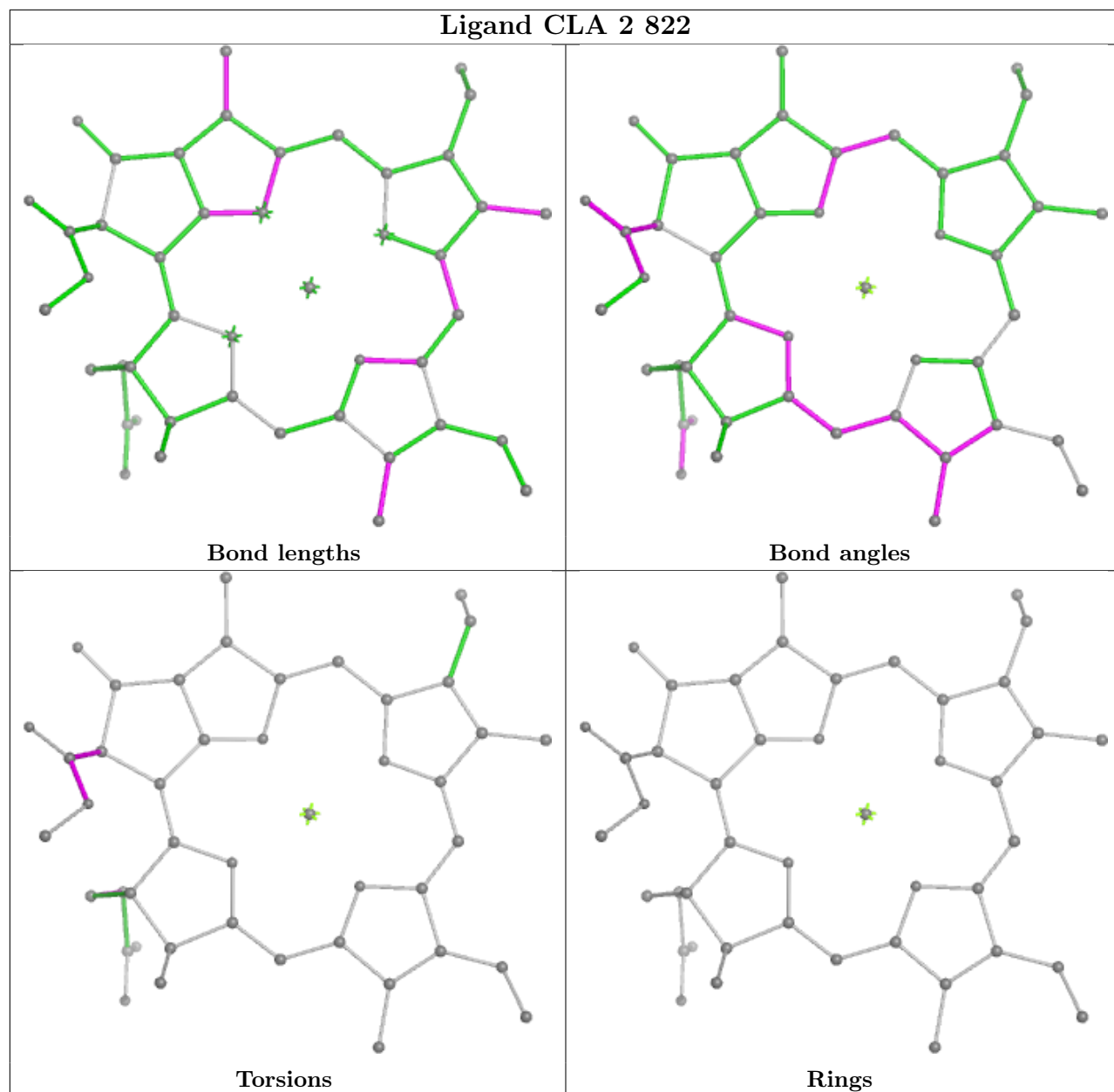
## Ligand BCR A 856



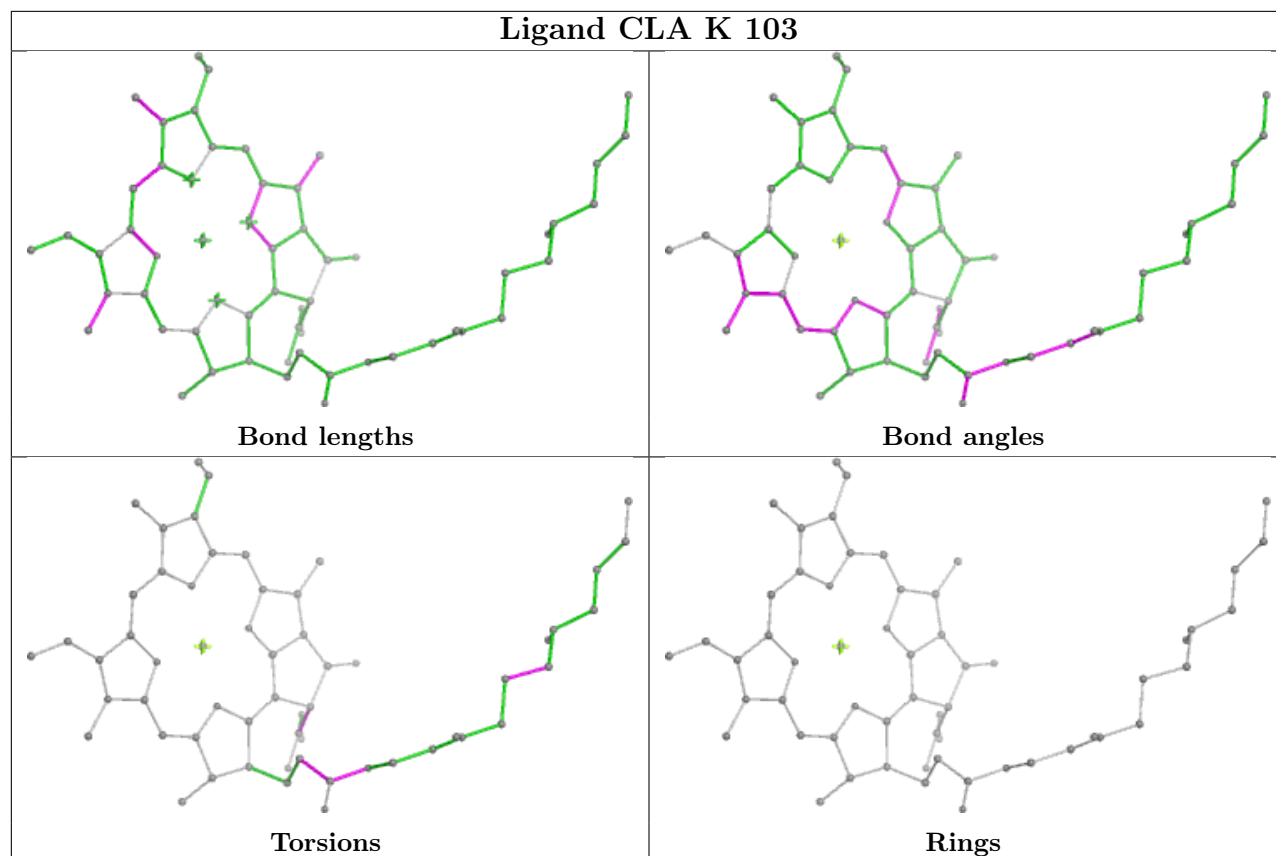




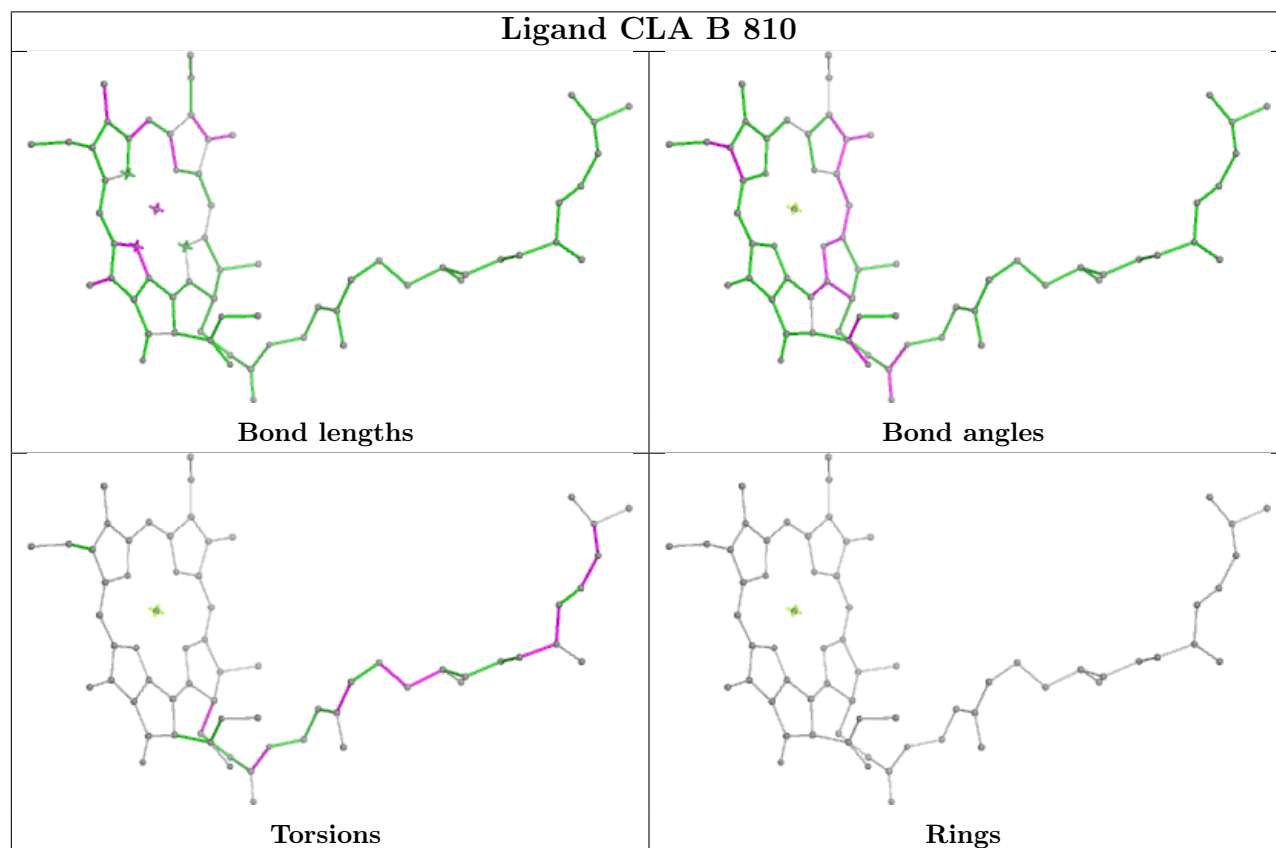
## Ligand CLA 2 822

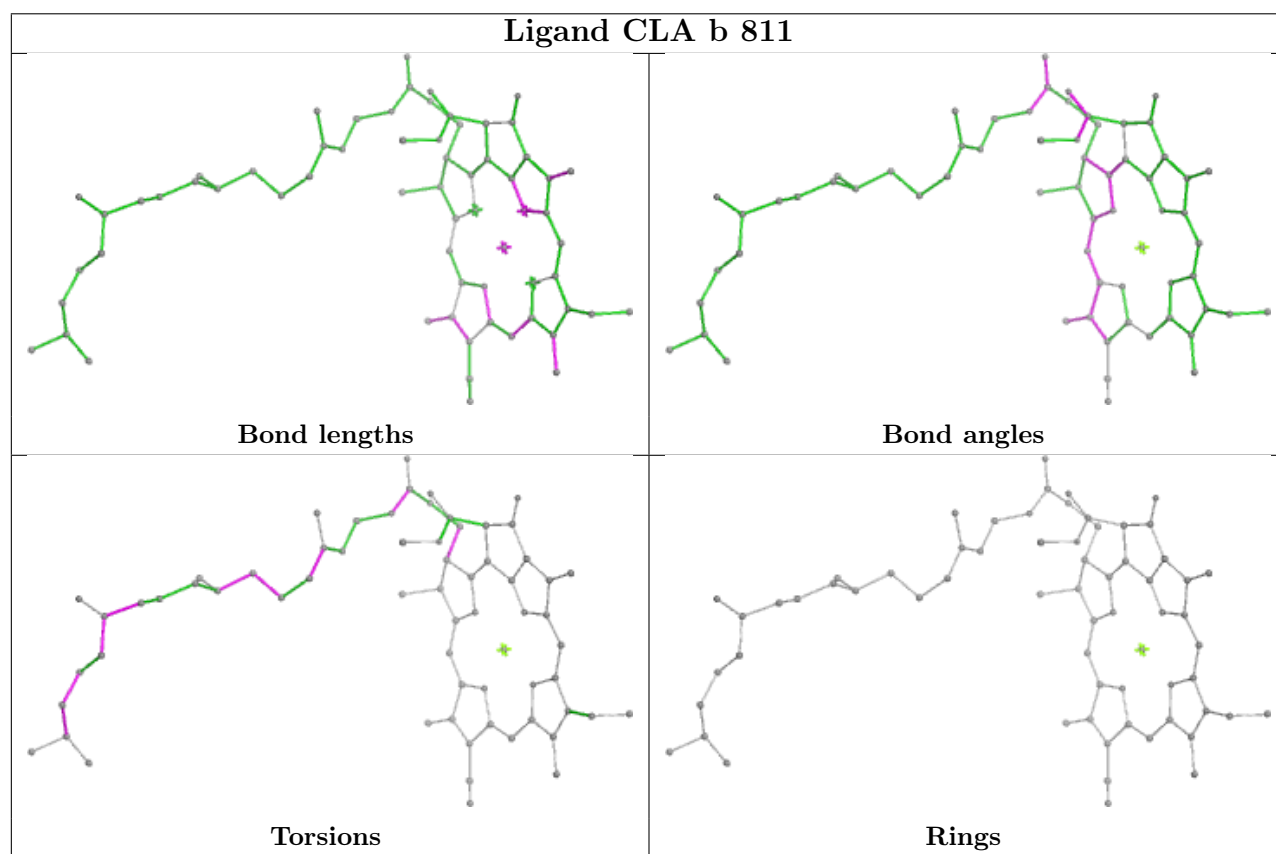
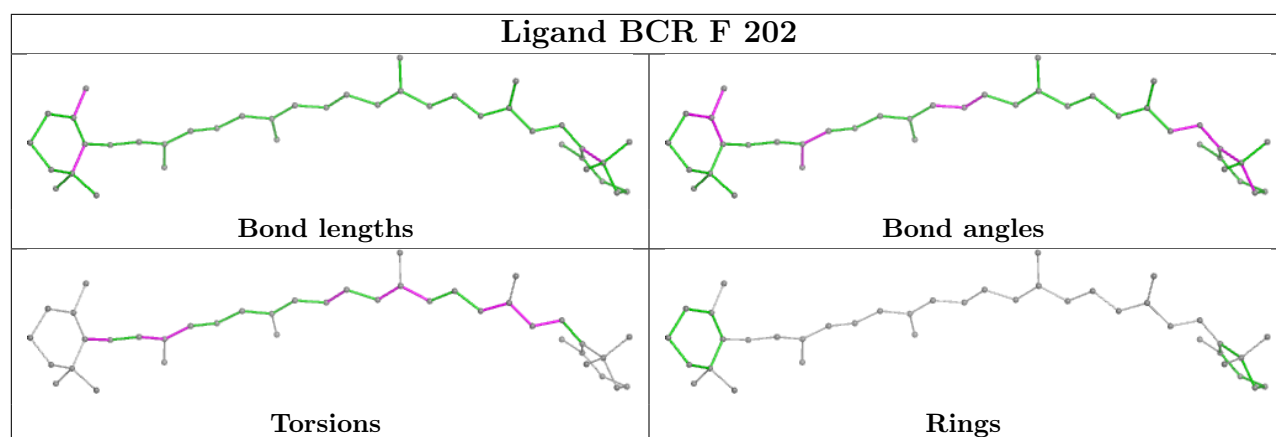


## Ligand CLA K 103

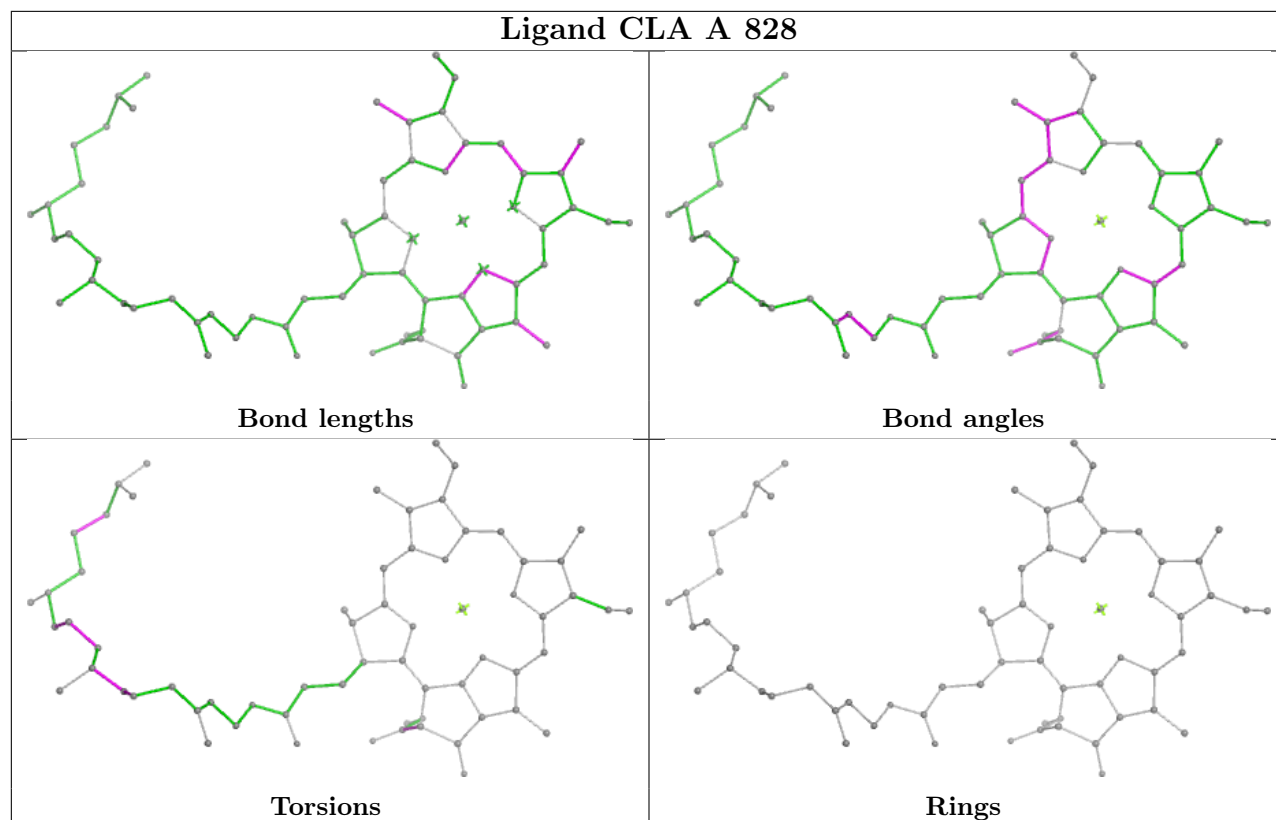


## Ligand CLA B 810

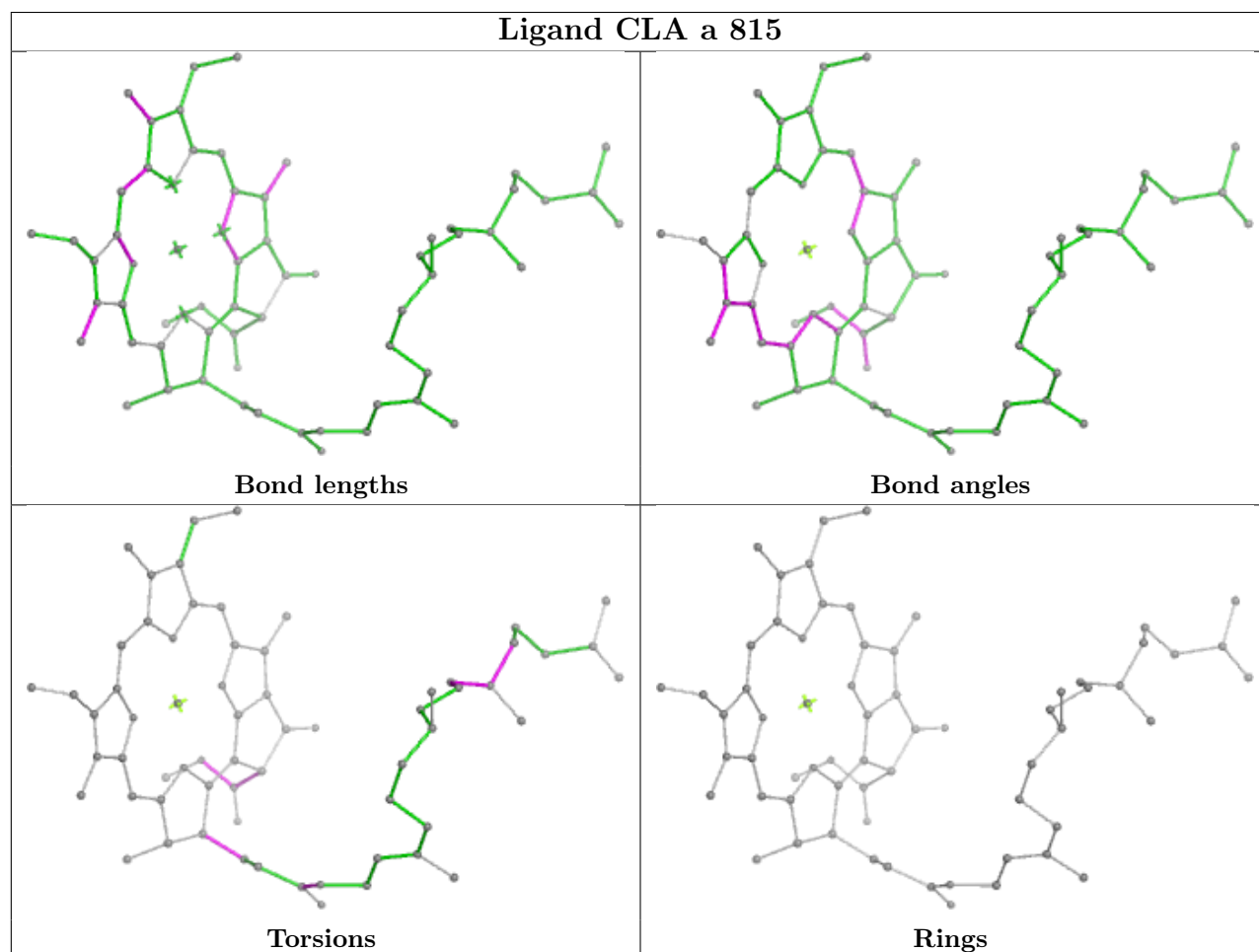




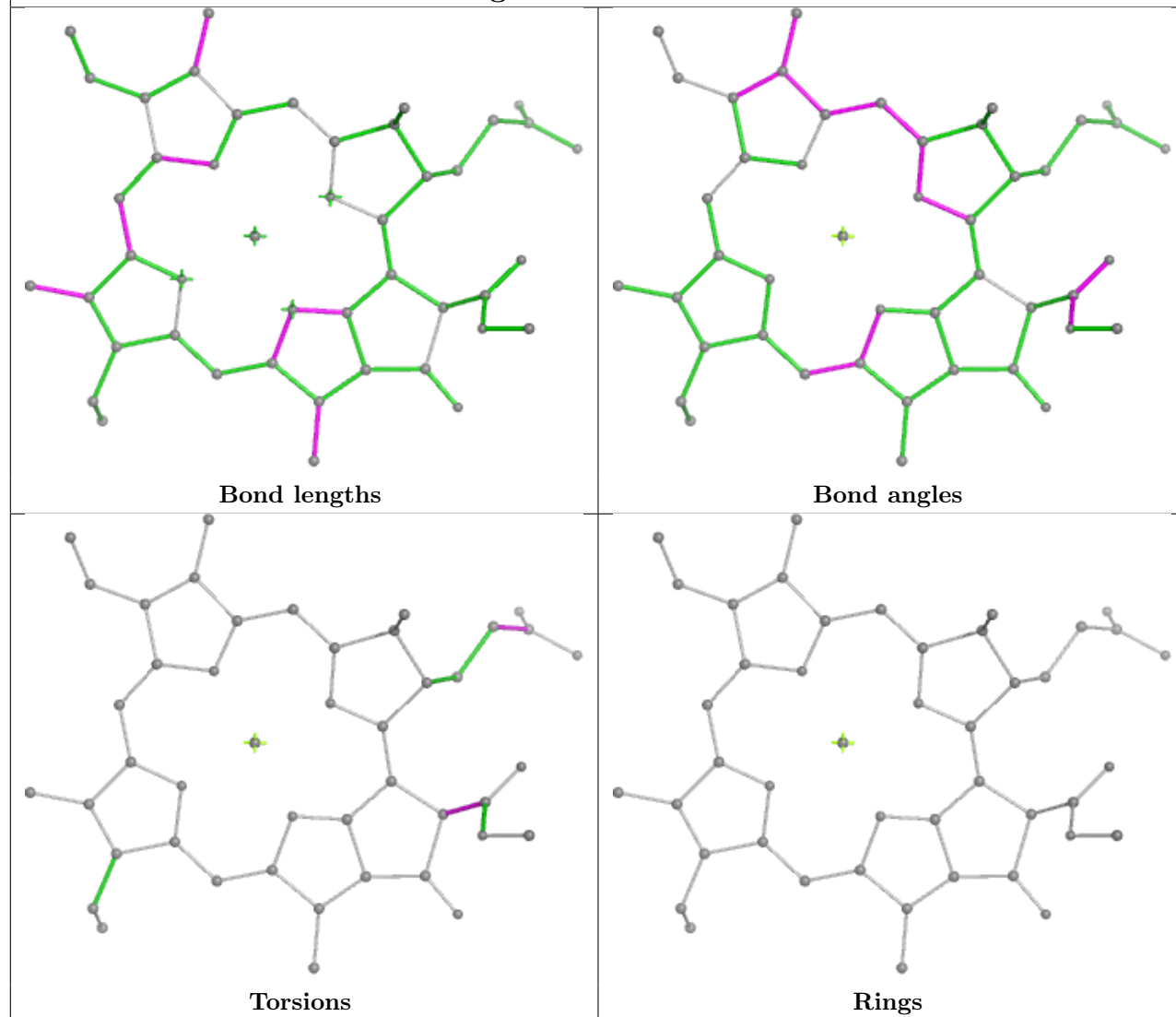
## Ligand CLA A 828

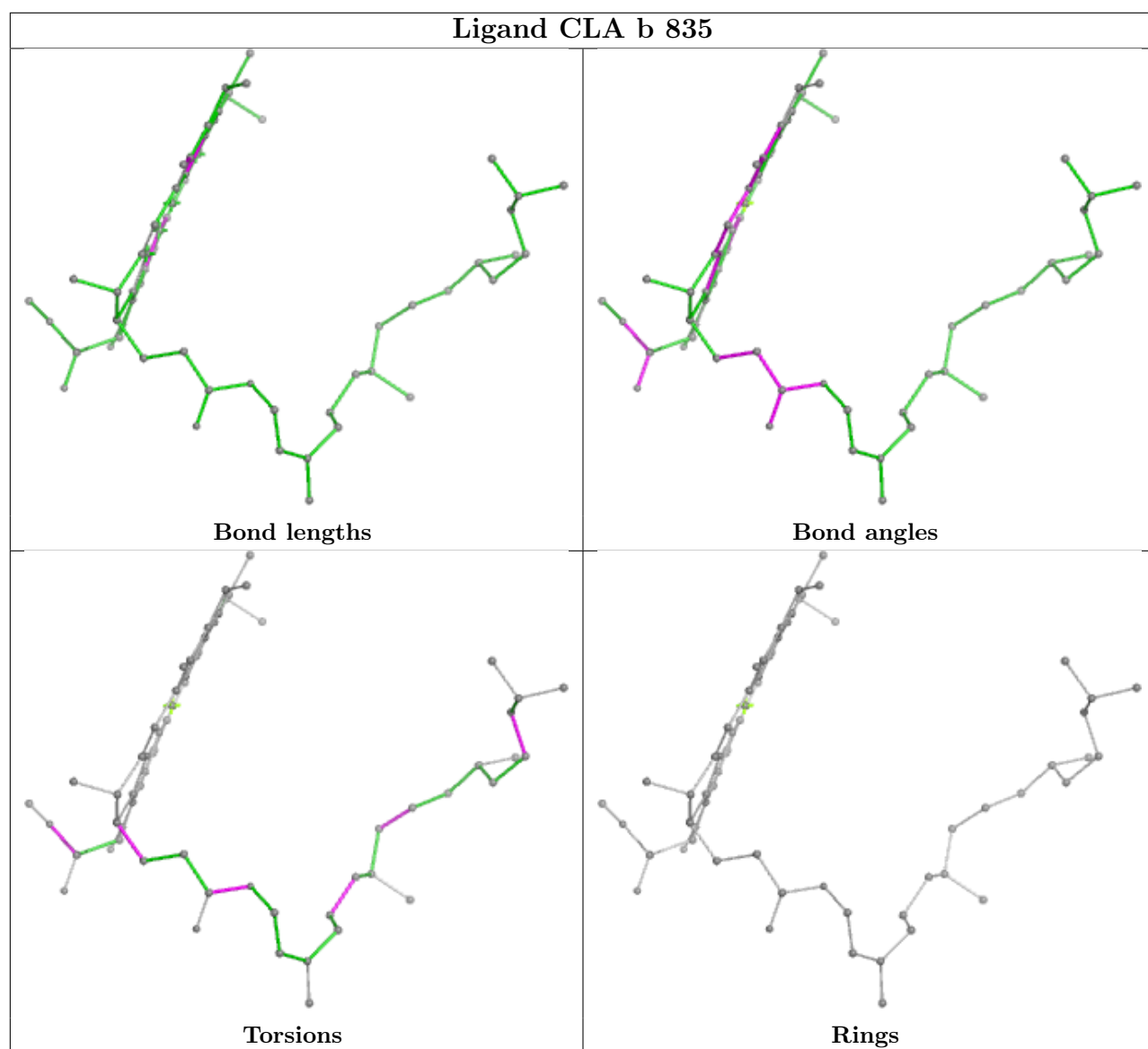


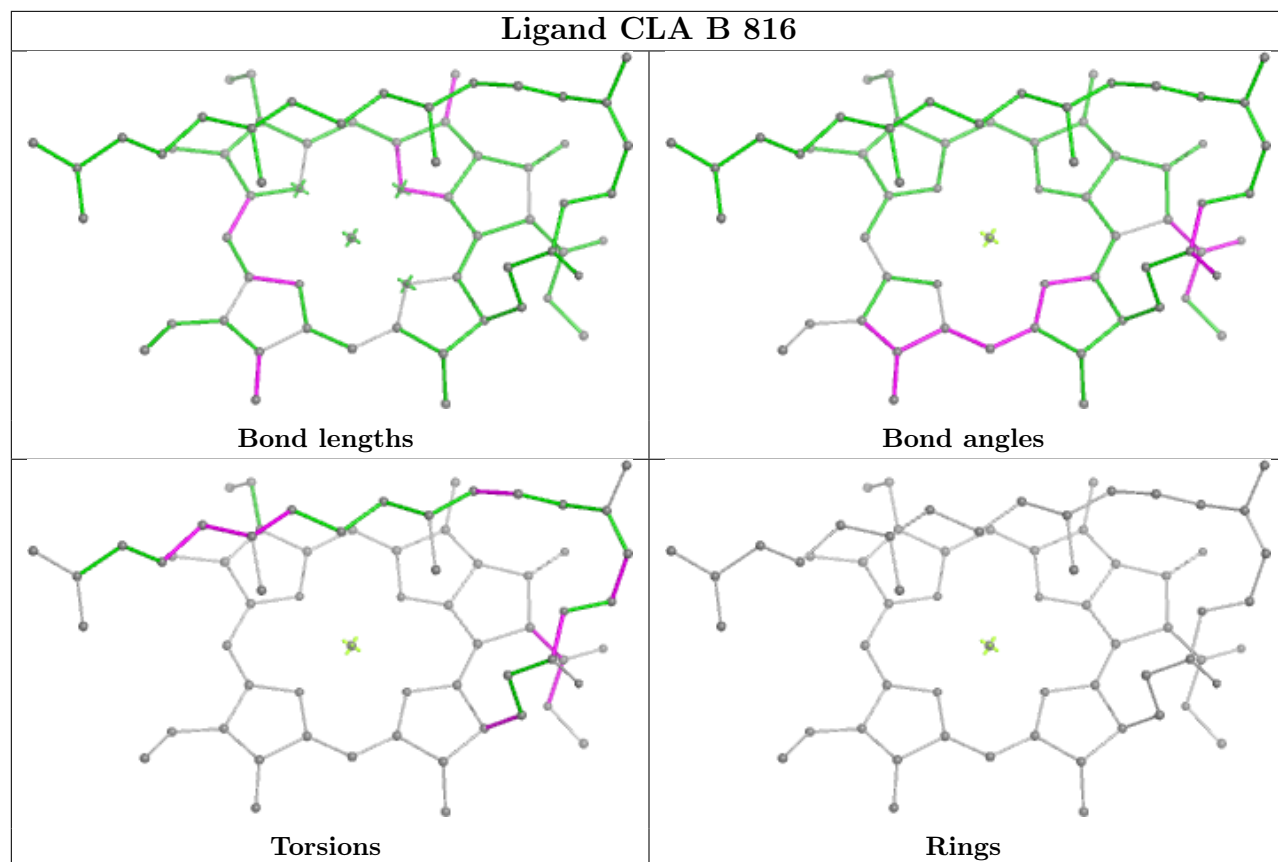
## Ligand CLA a 815



## Ligand CLA A 844

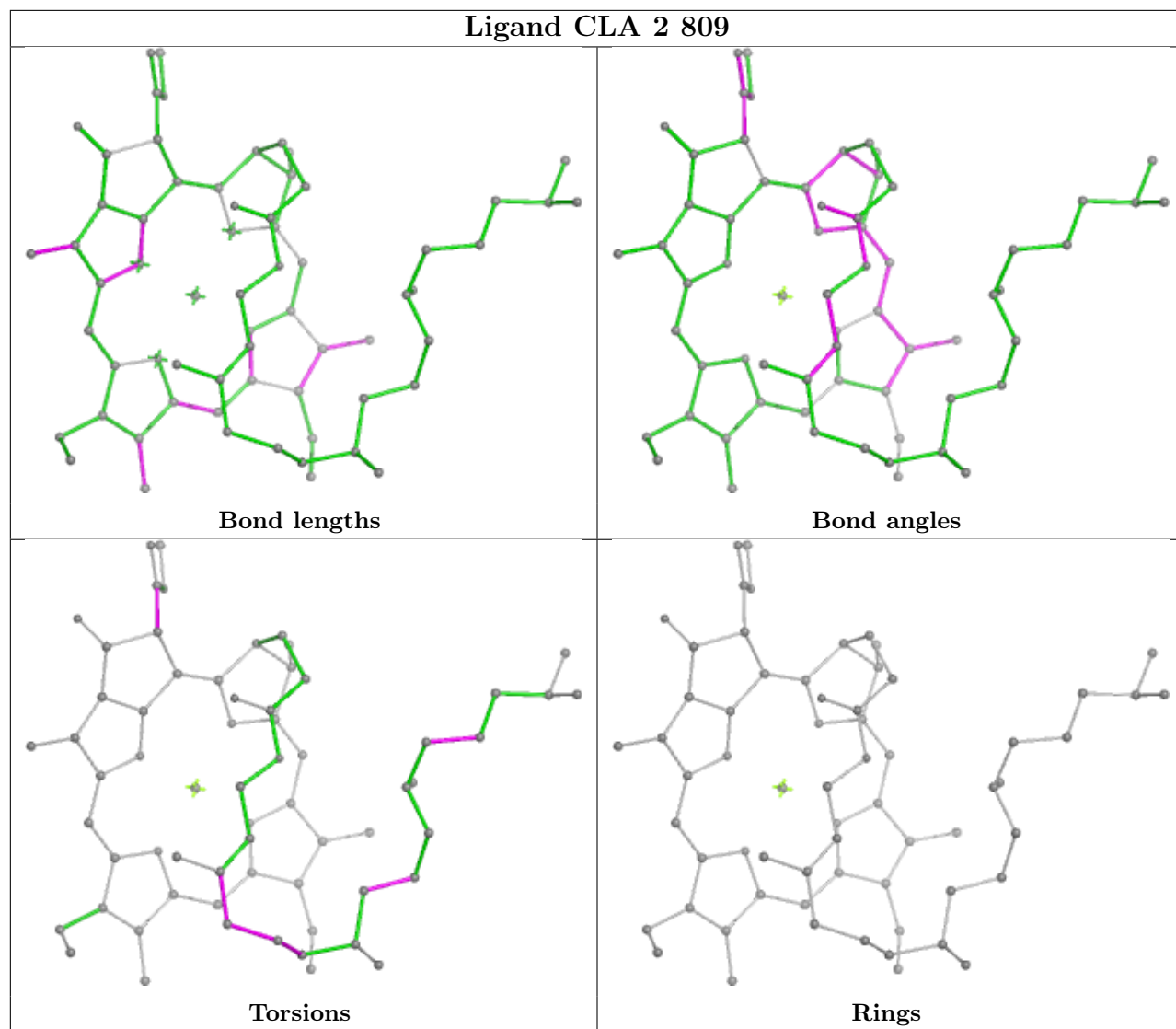


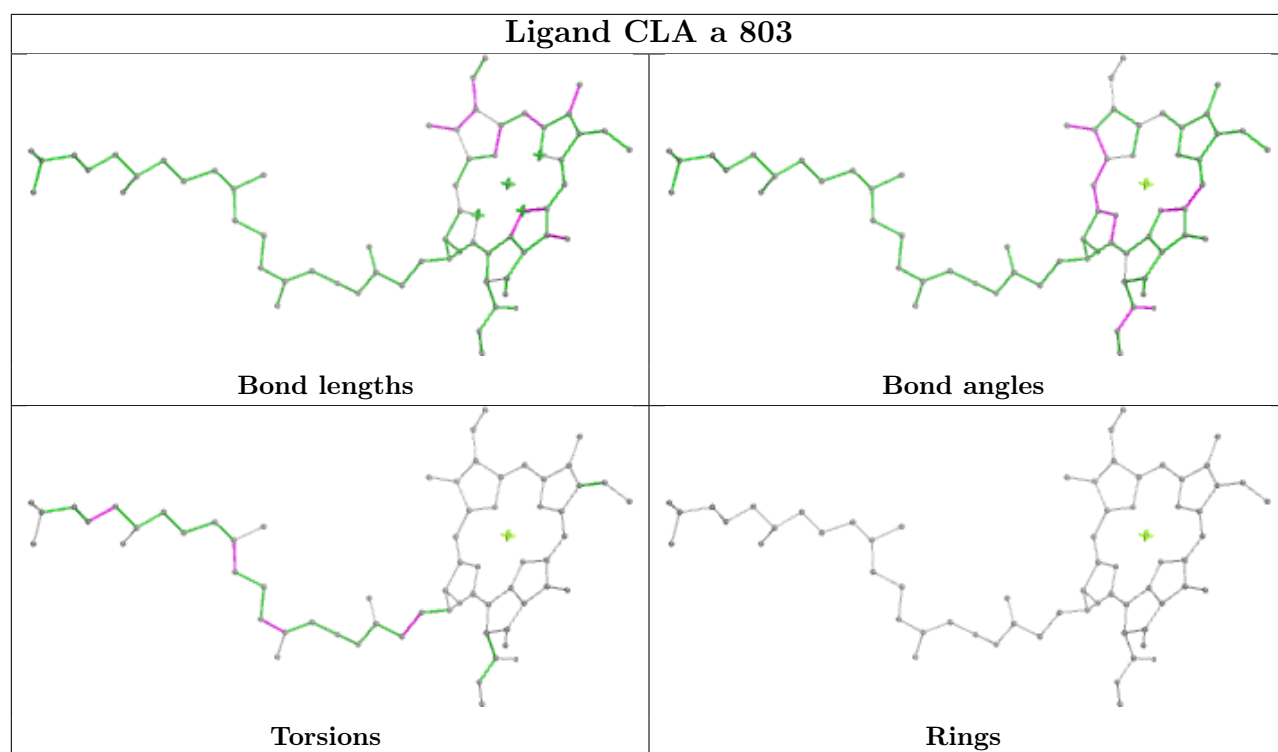




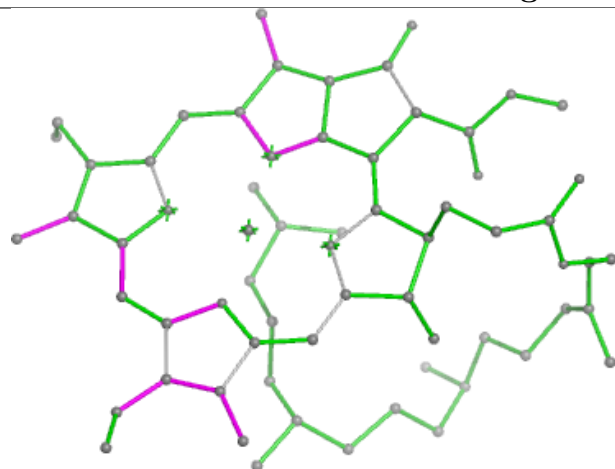


## Ligand CLA 2 809

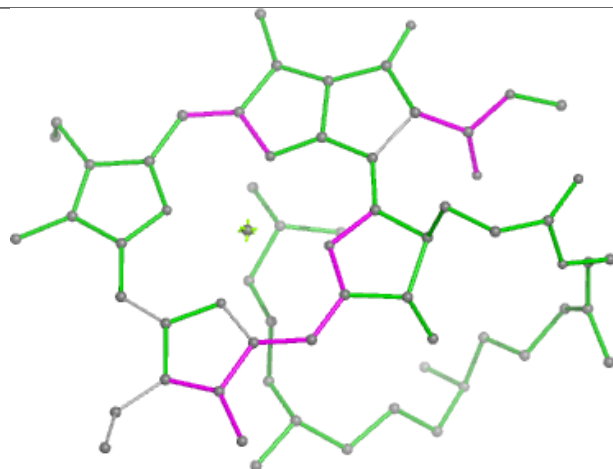




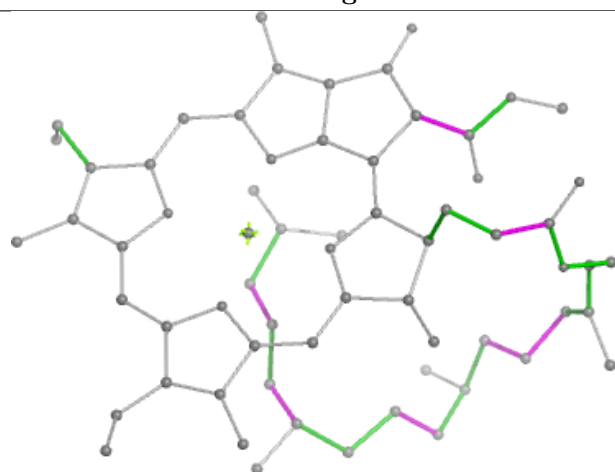
## Ligand CLA 2 807



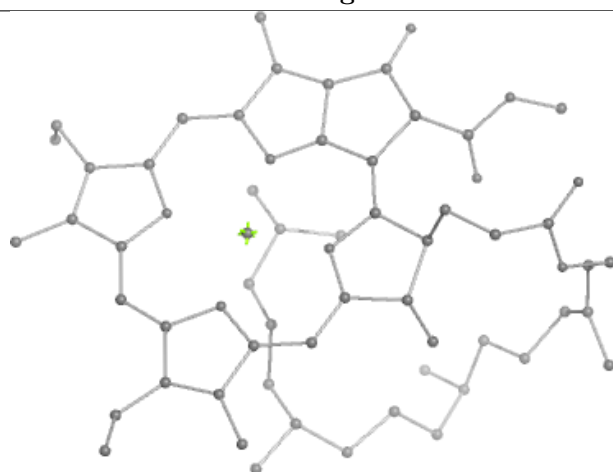
Bond lengths



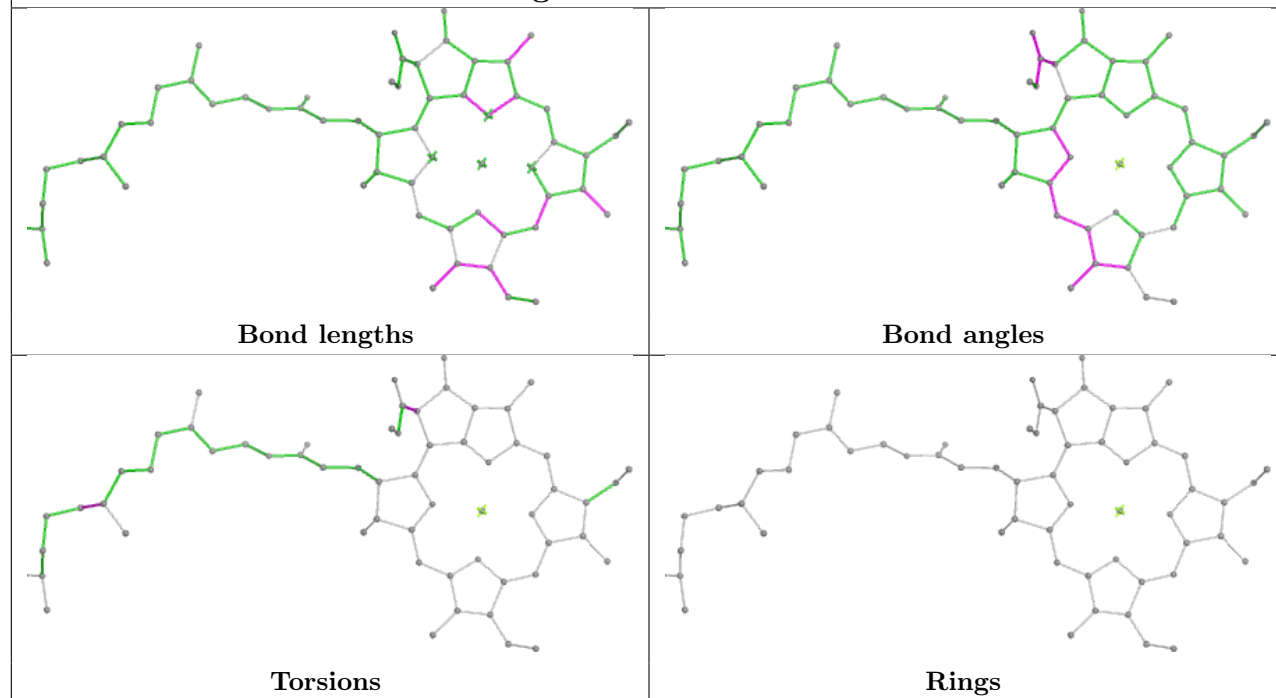
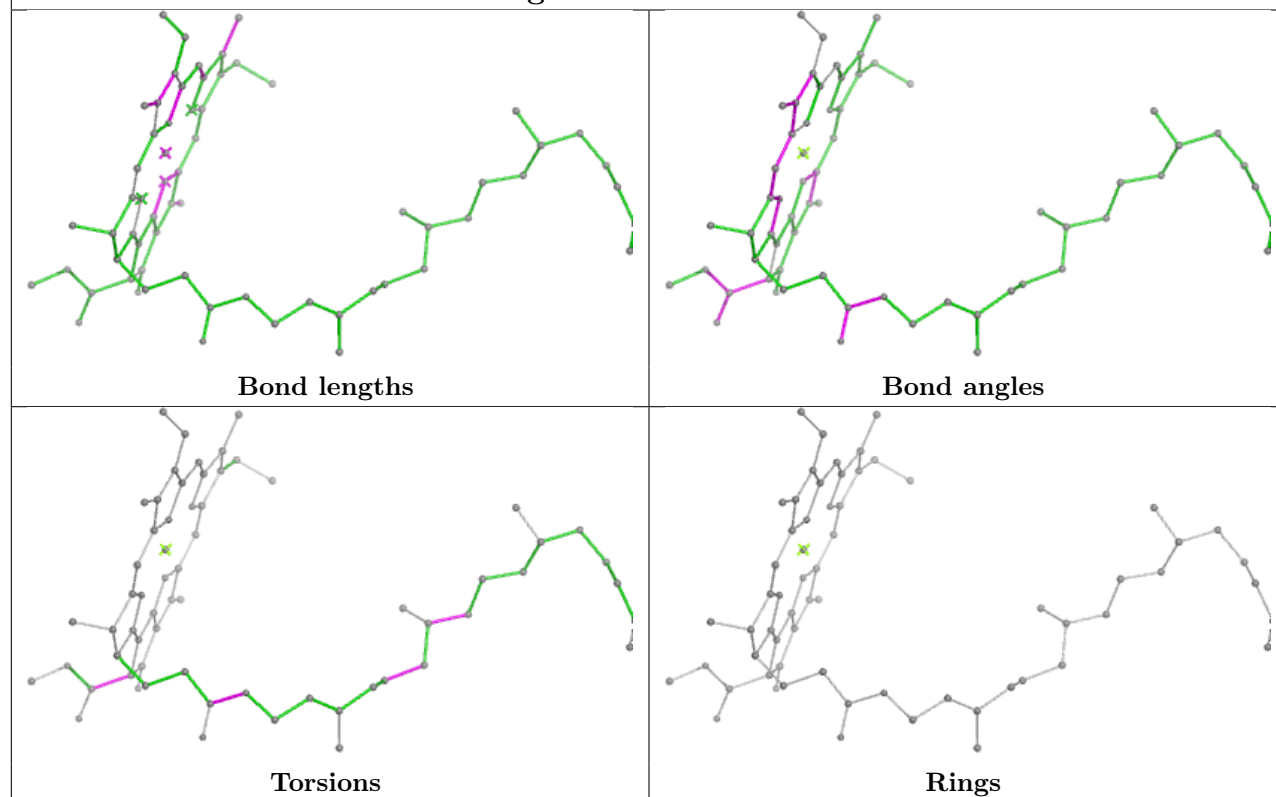
Bond angles

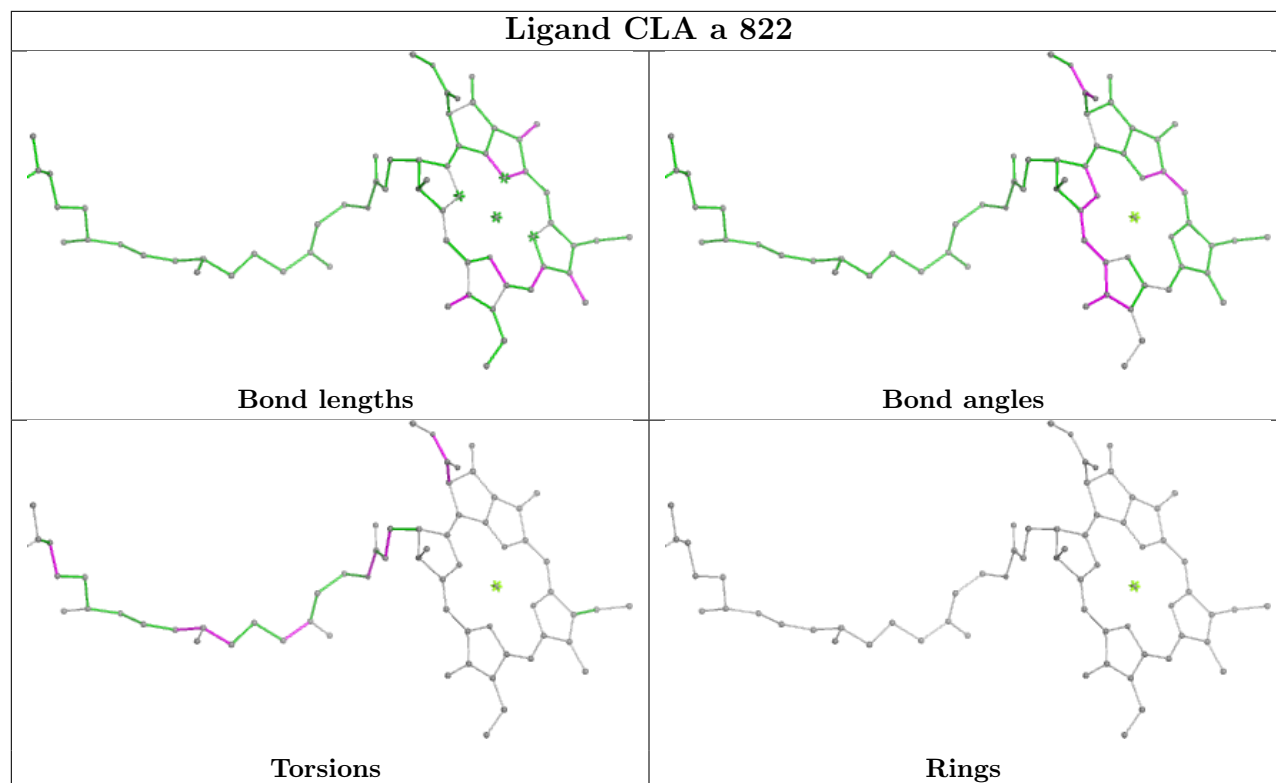


Torsions

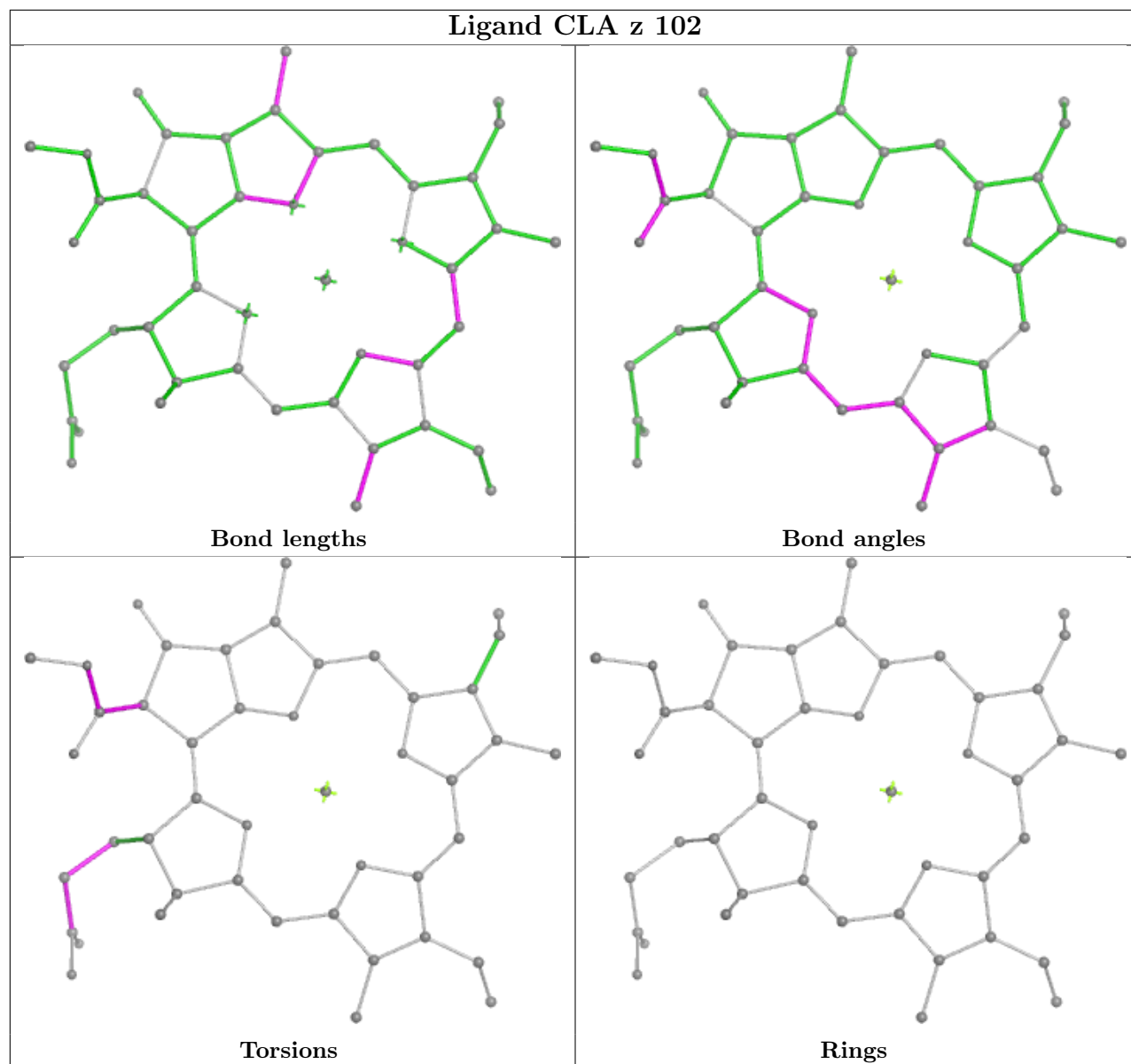


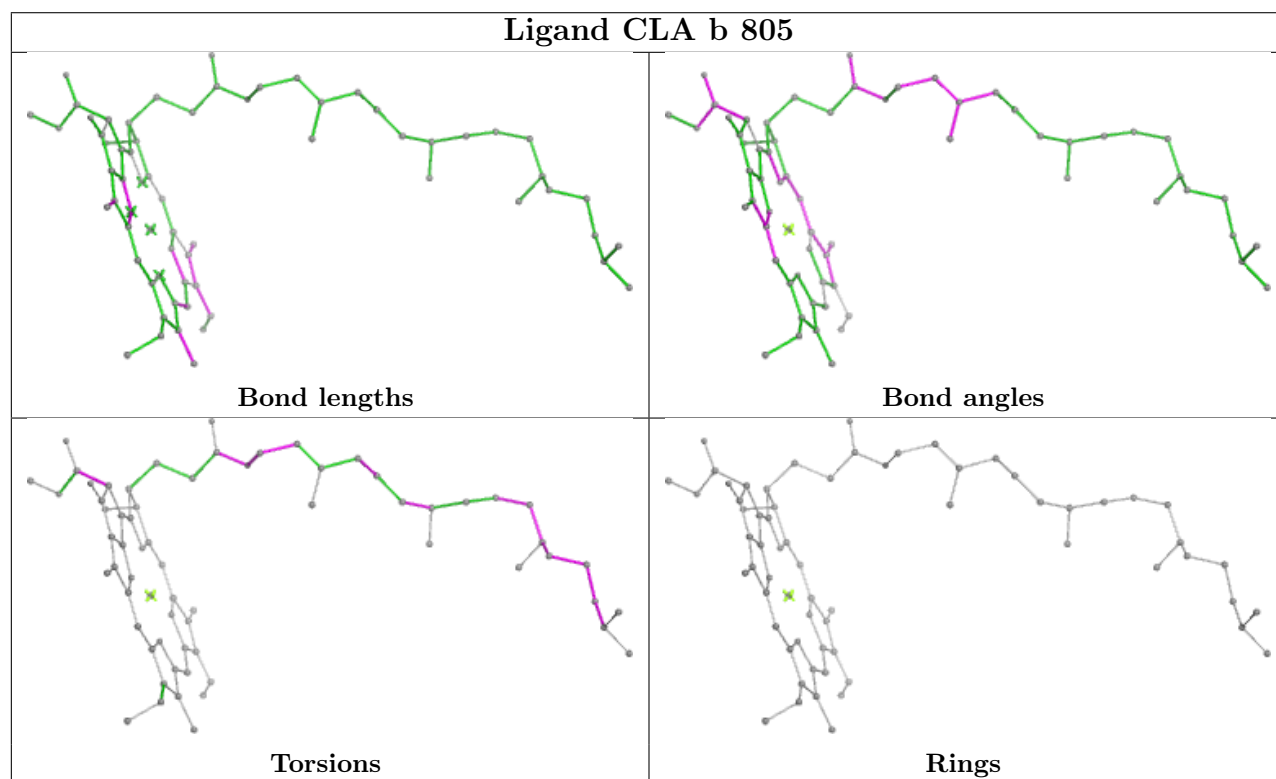
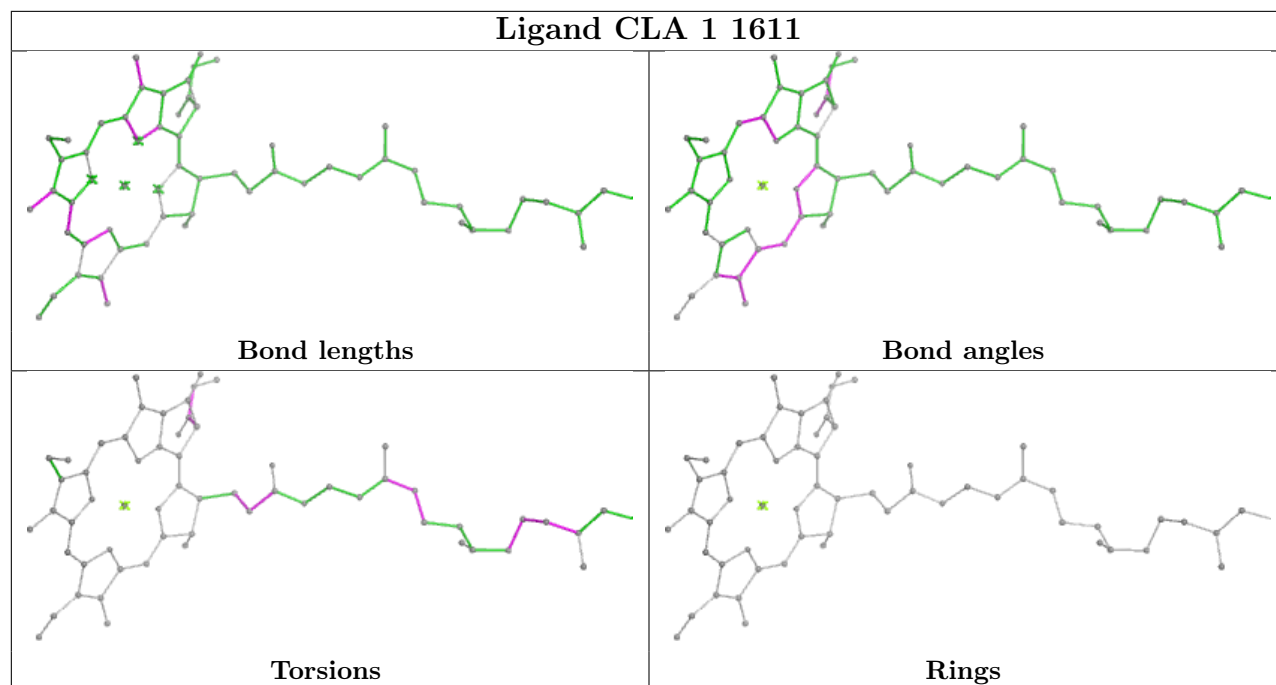
Rings

**Ligand CLA B 837****Ligand CLA 1 1632**

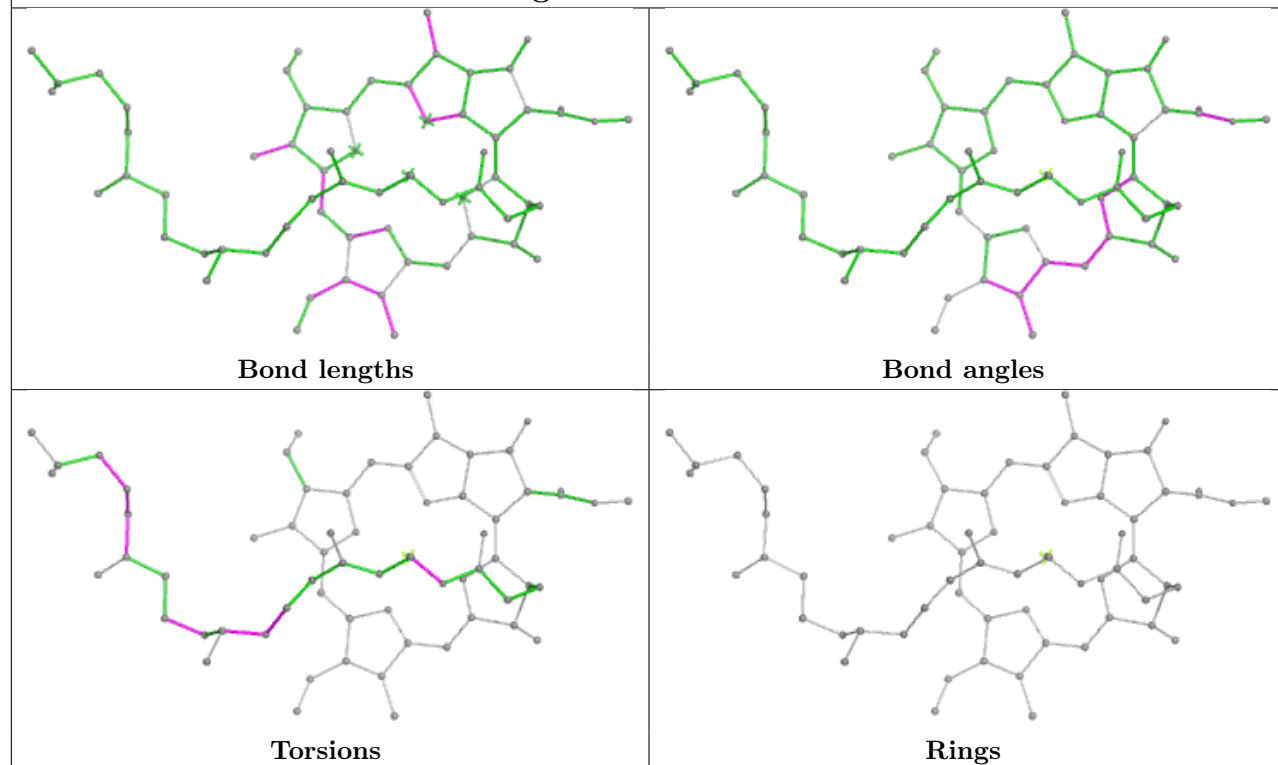


## Ligand CLA z 102

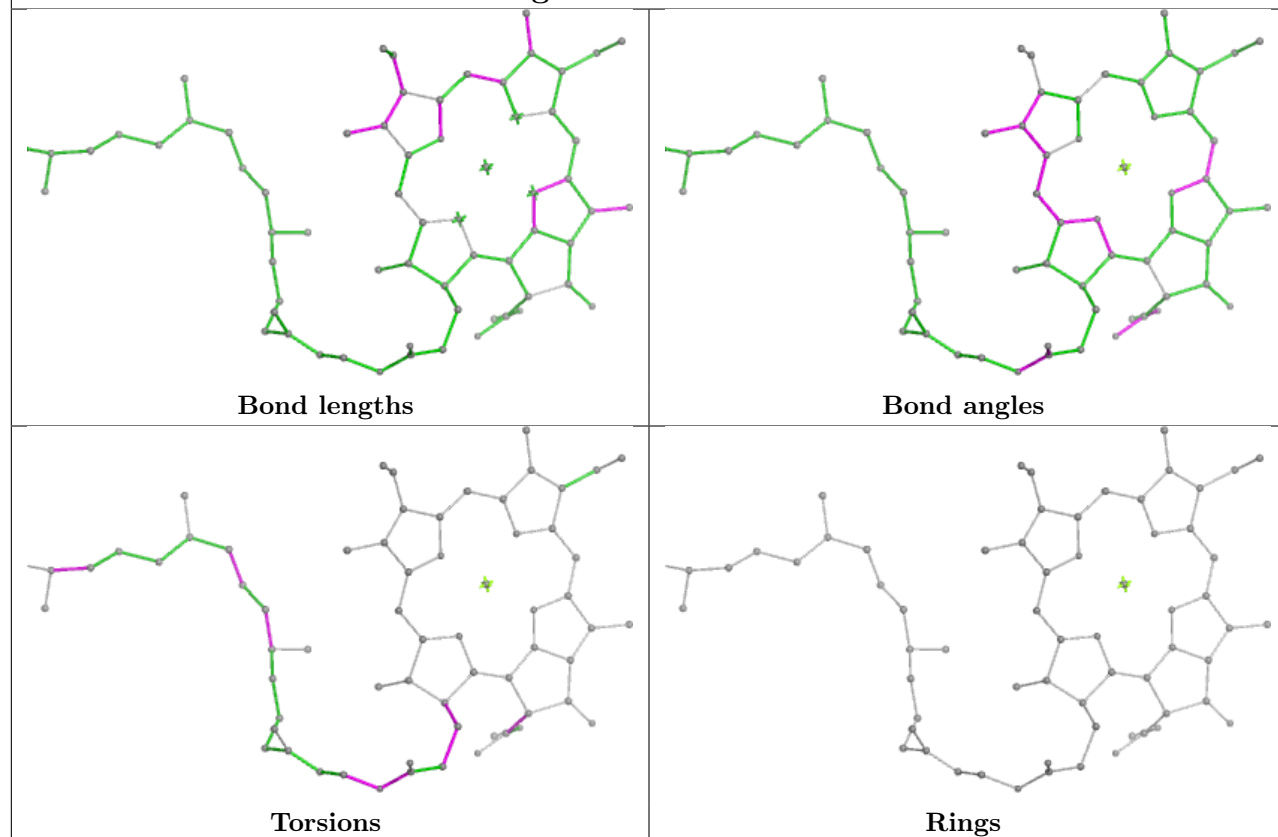




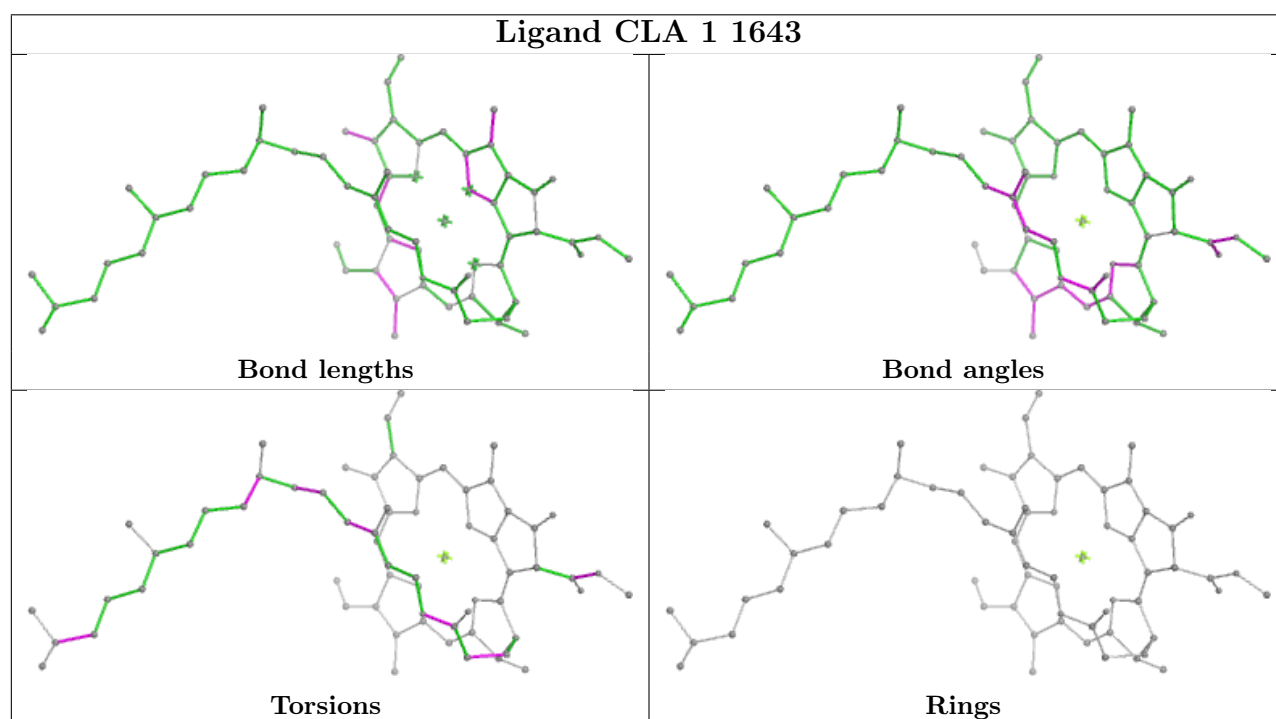
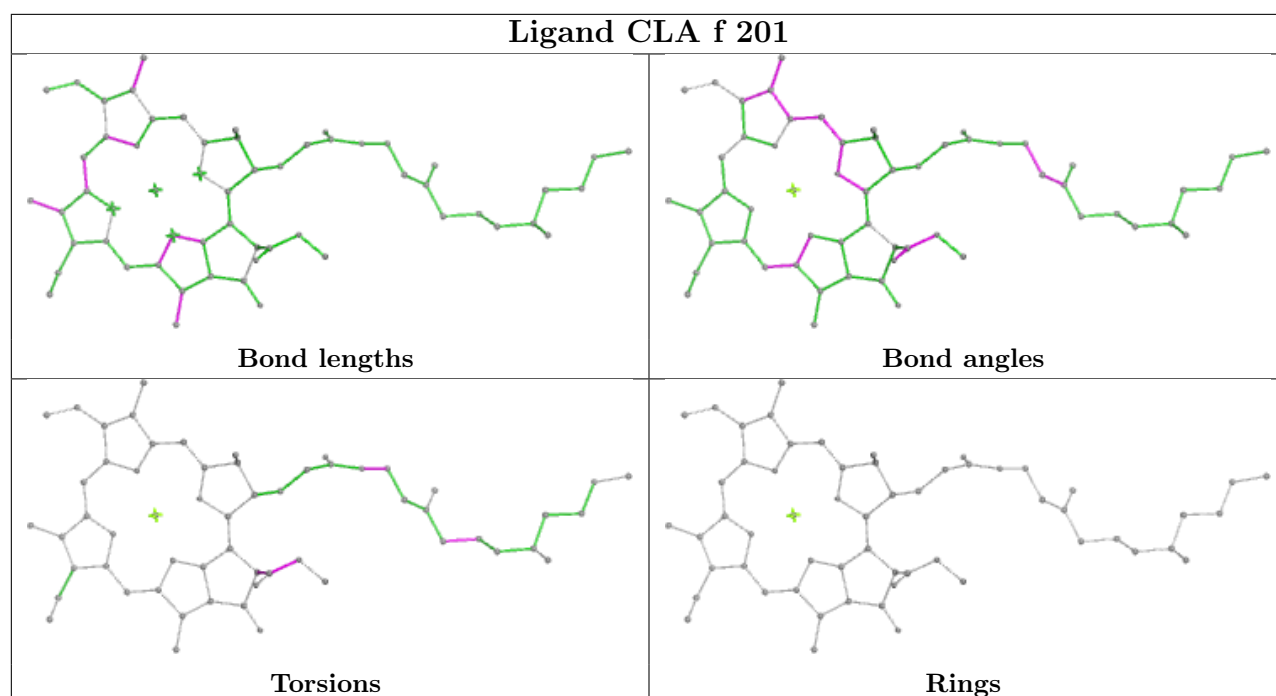
## Ligand CLA B 838

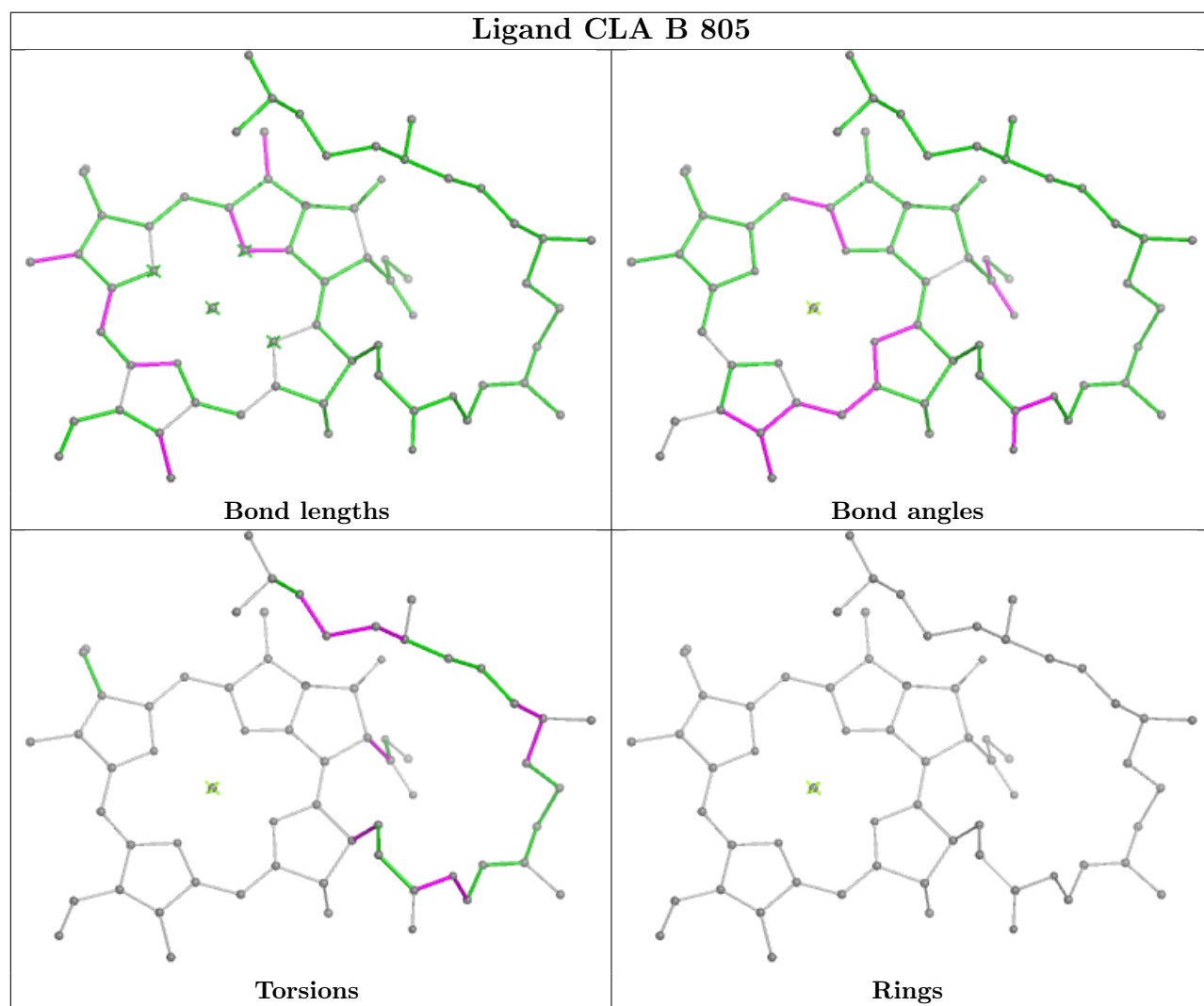
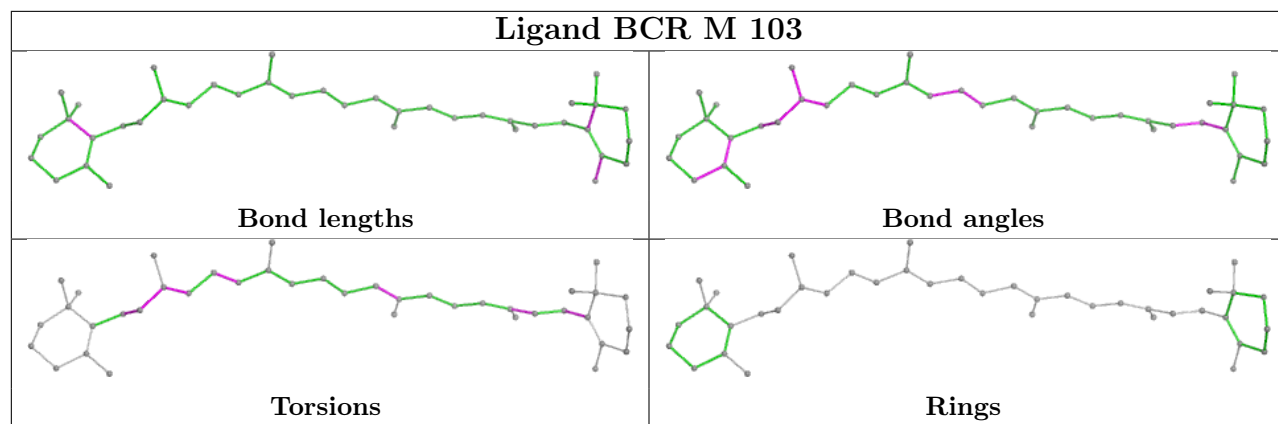


## Ligand CLA A 814

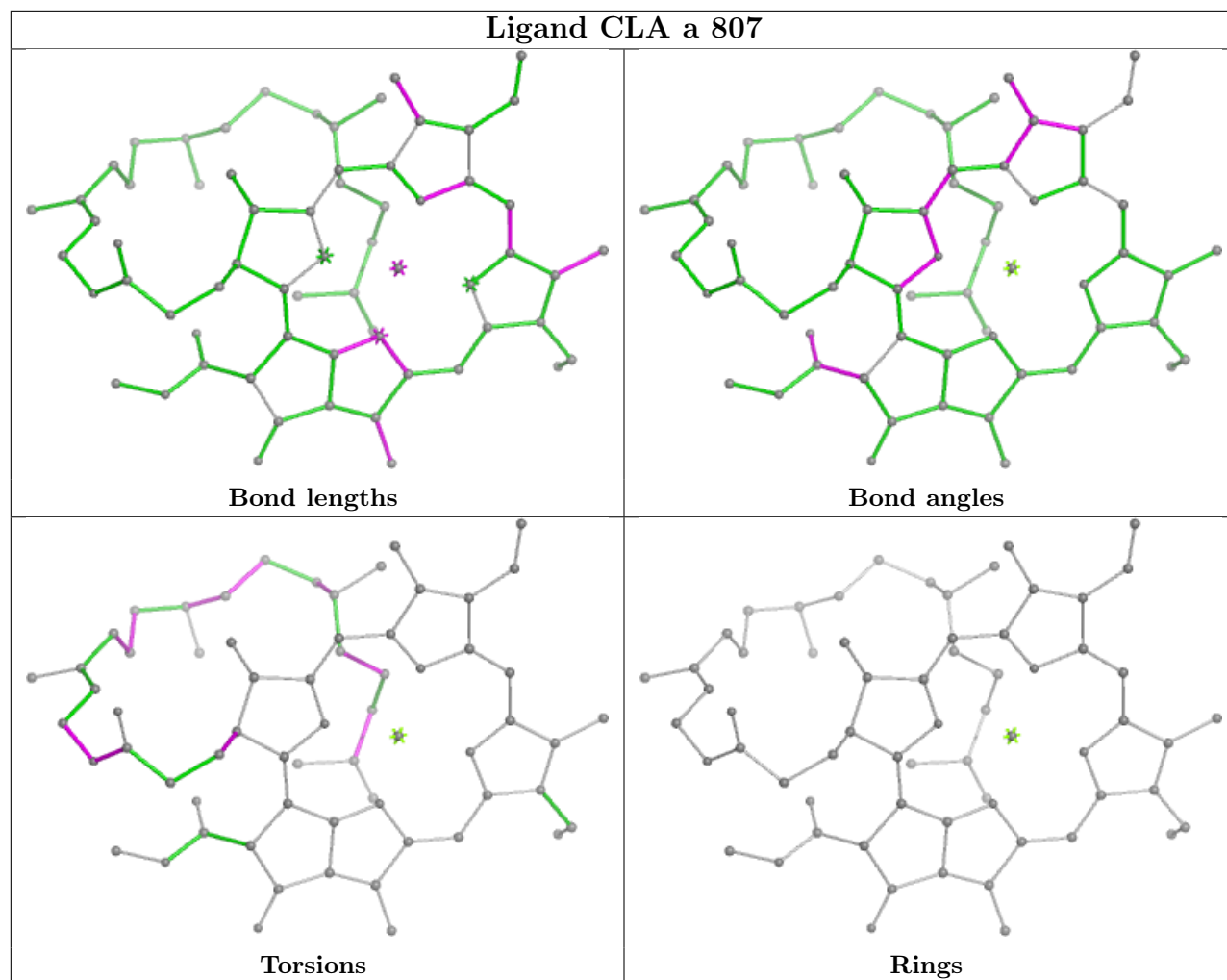




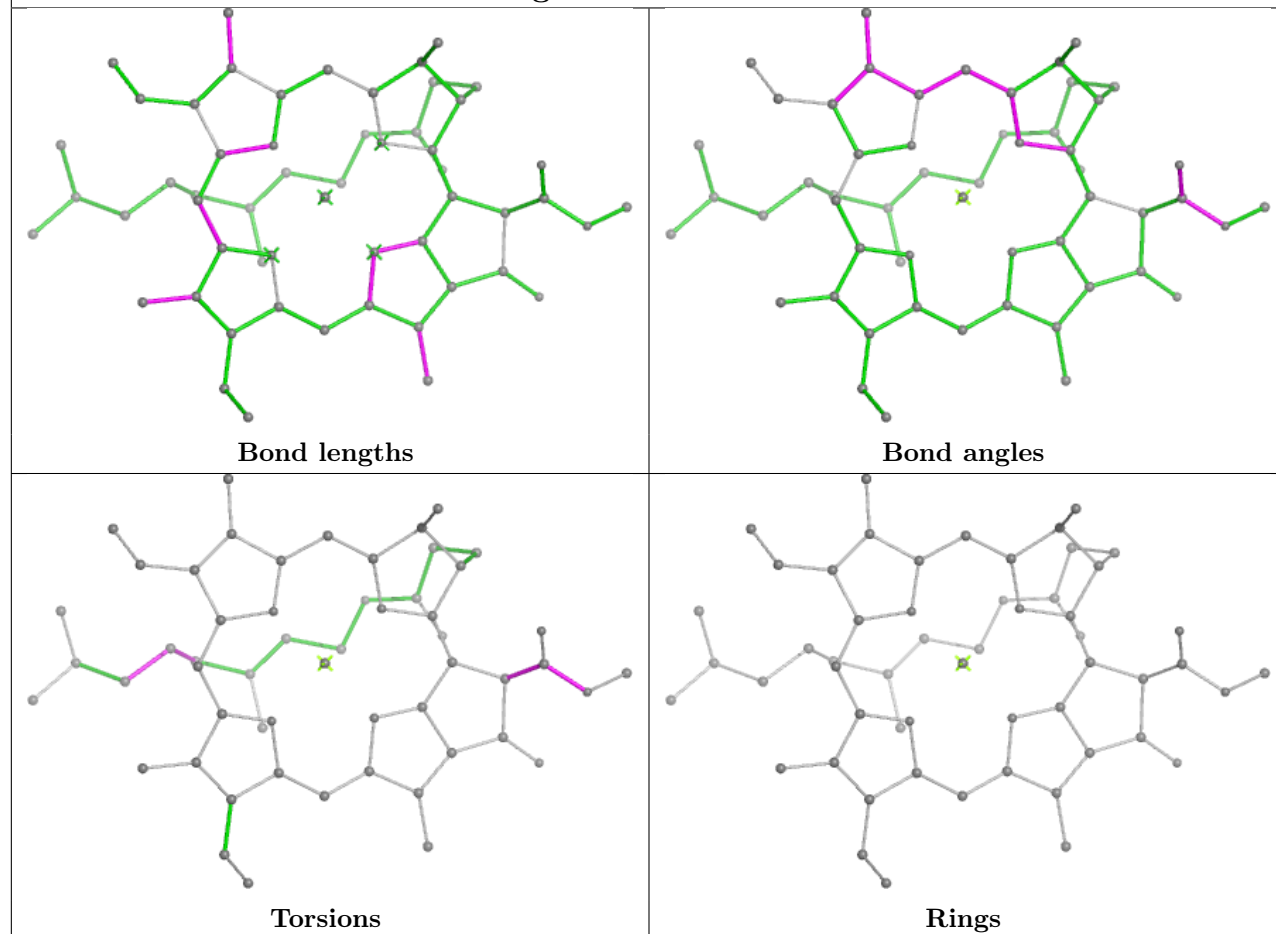




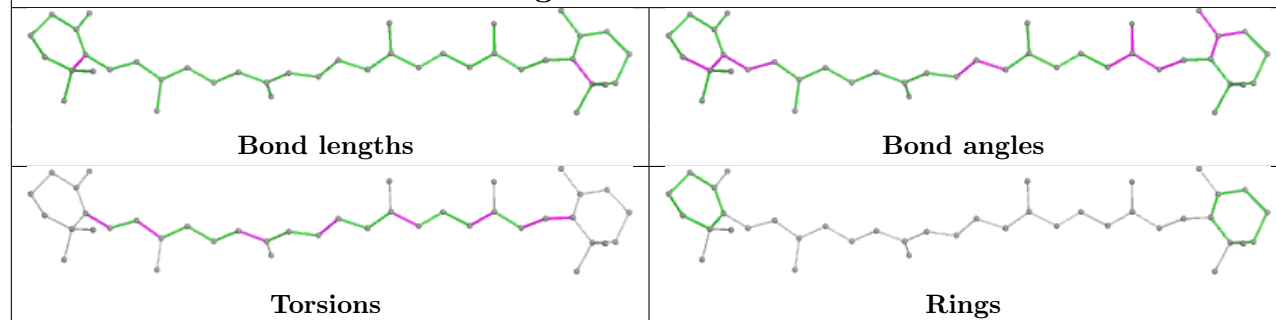
## Ligand CLA a 807

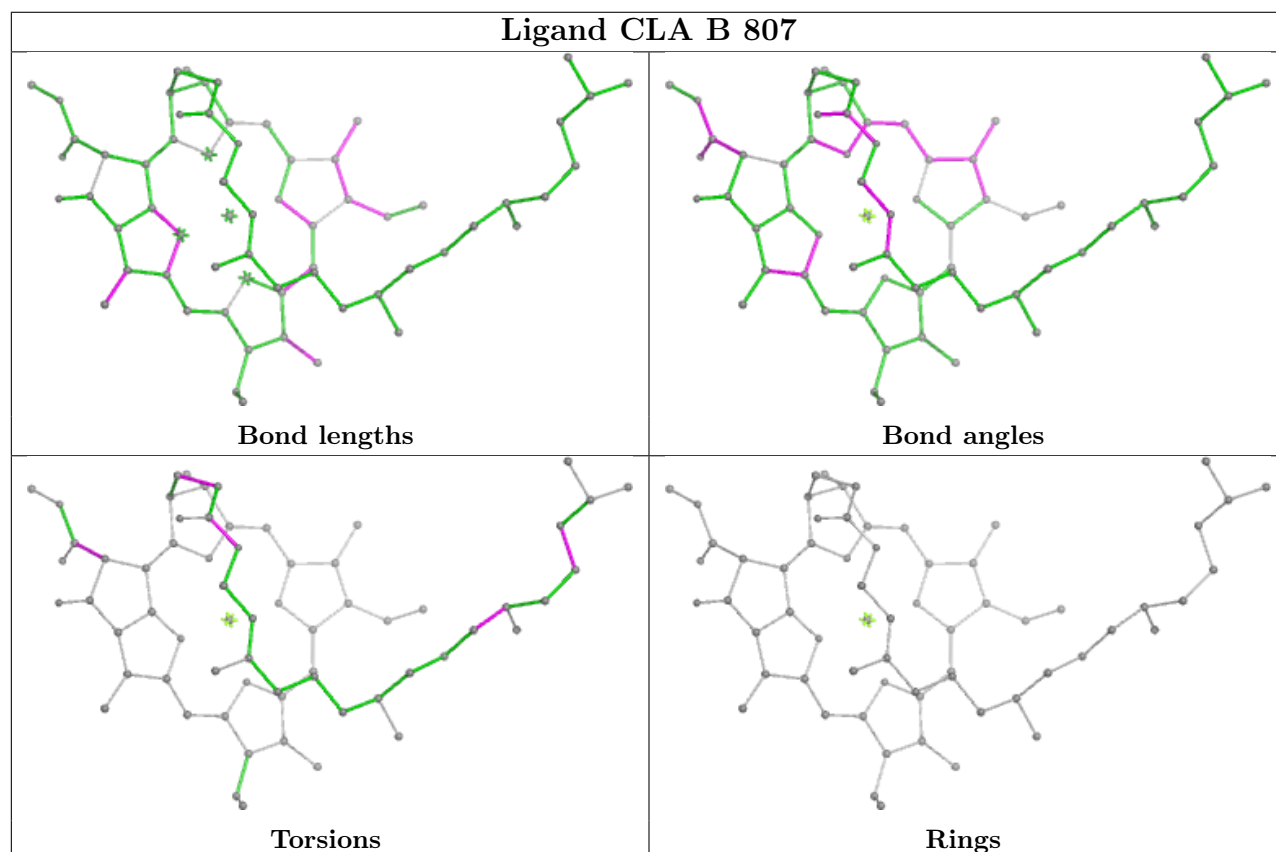
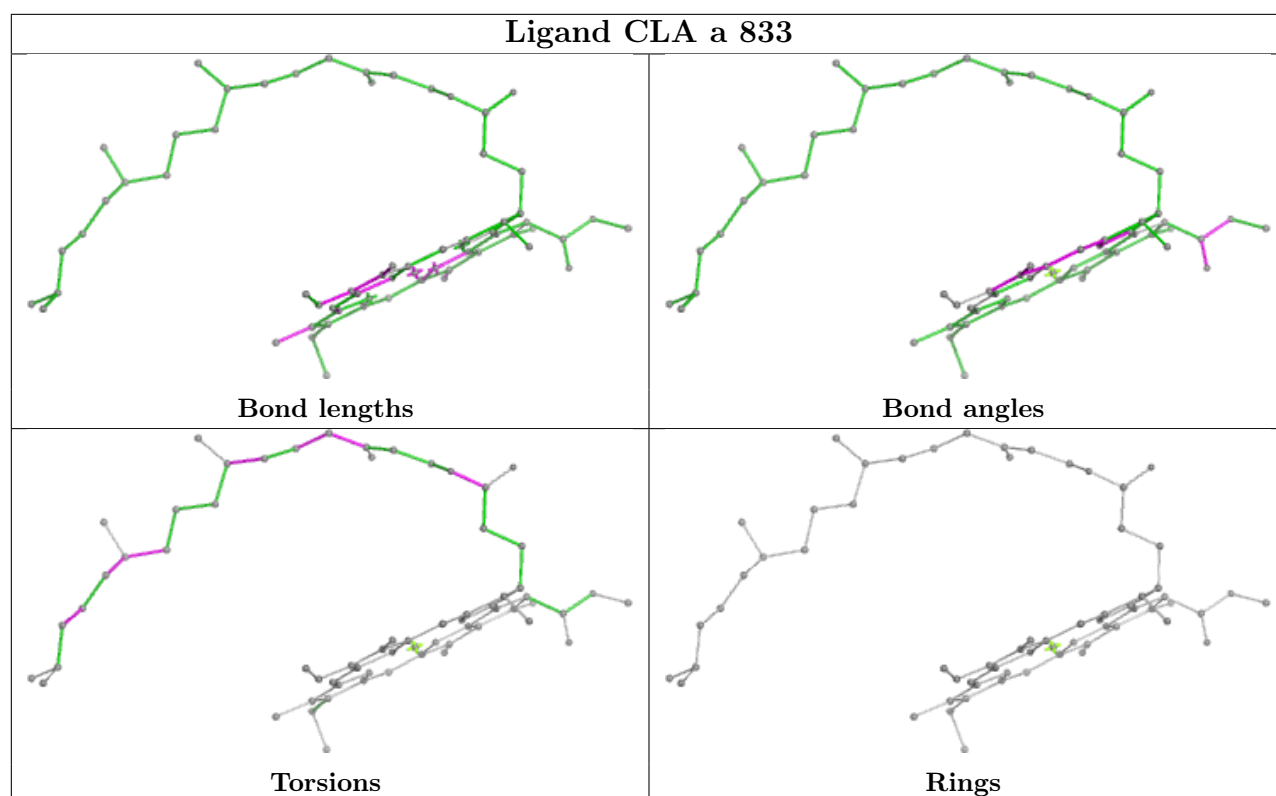


## Ligand CLA B 822

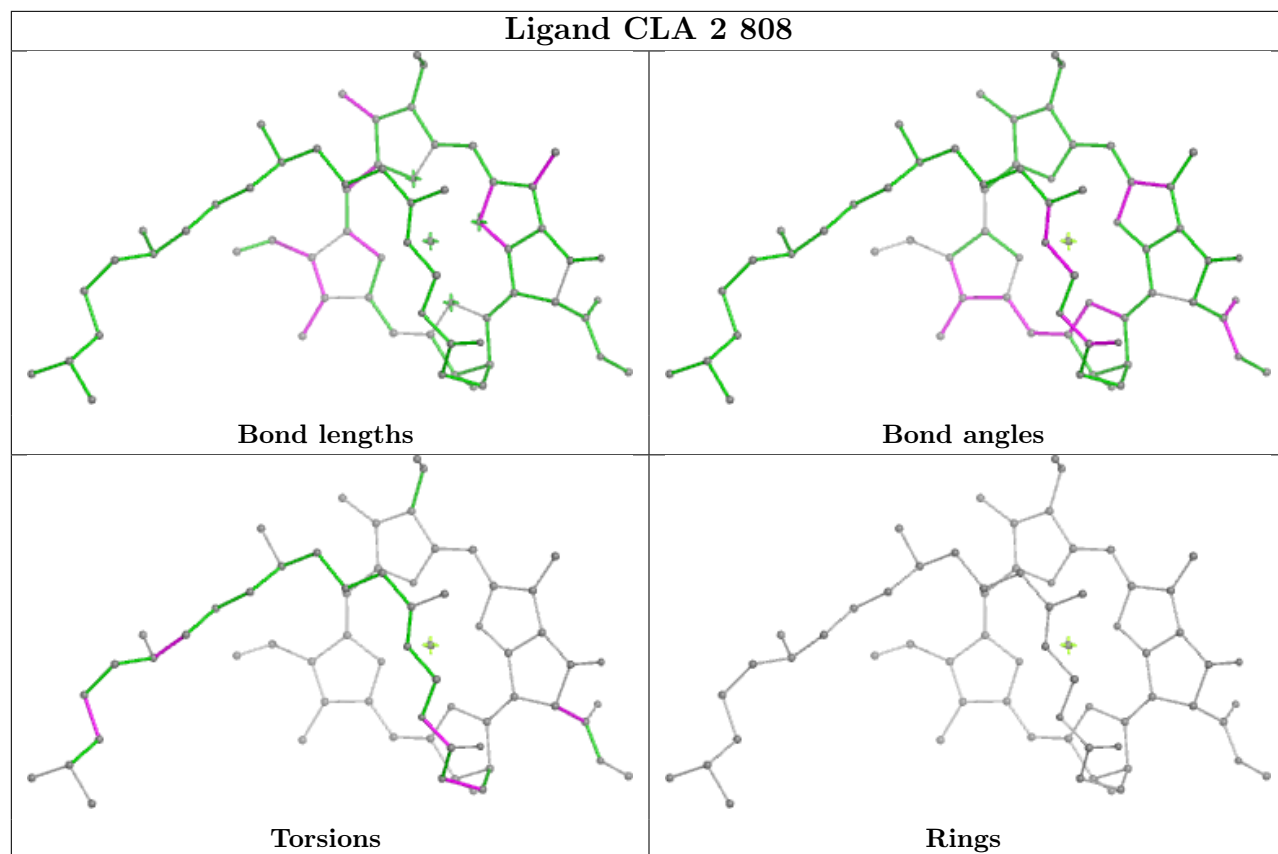


## Ligand BCR a 847

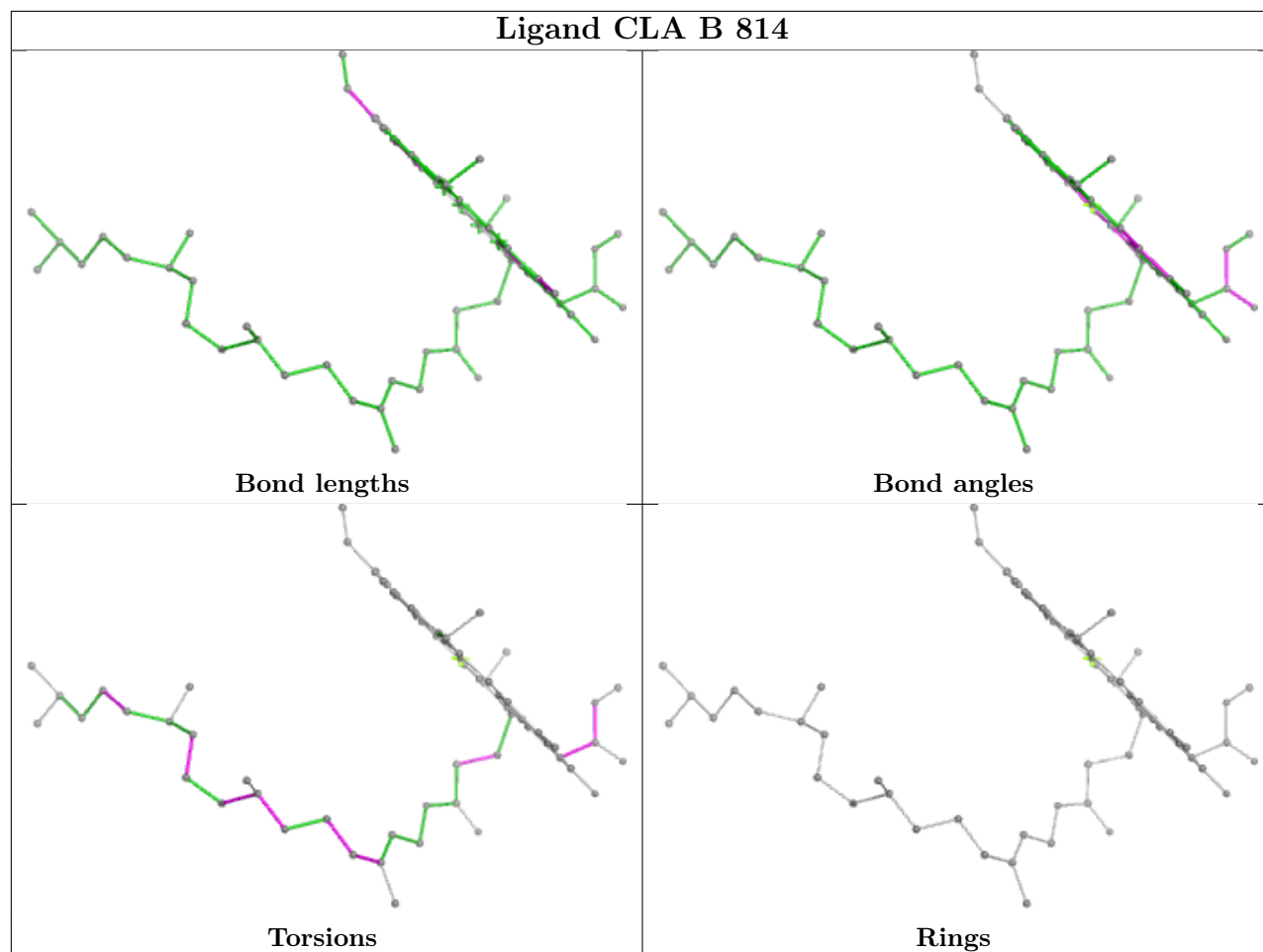




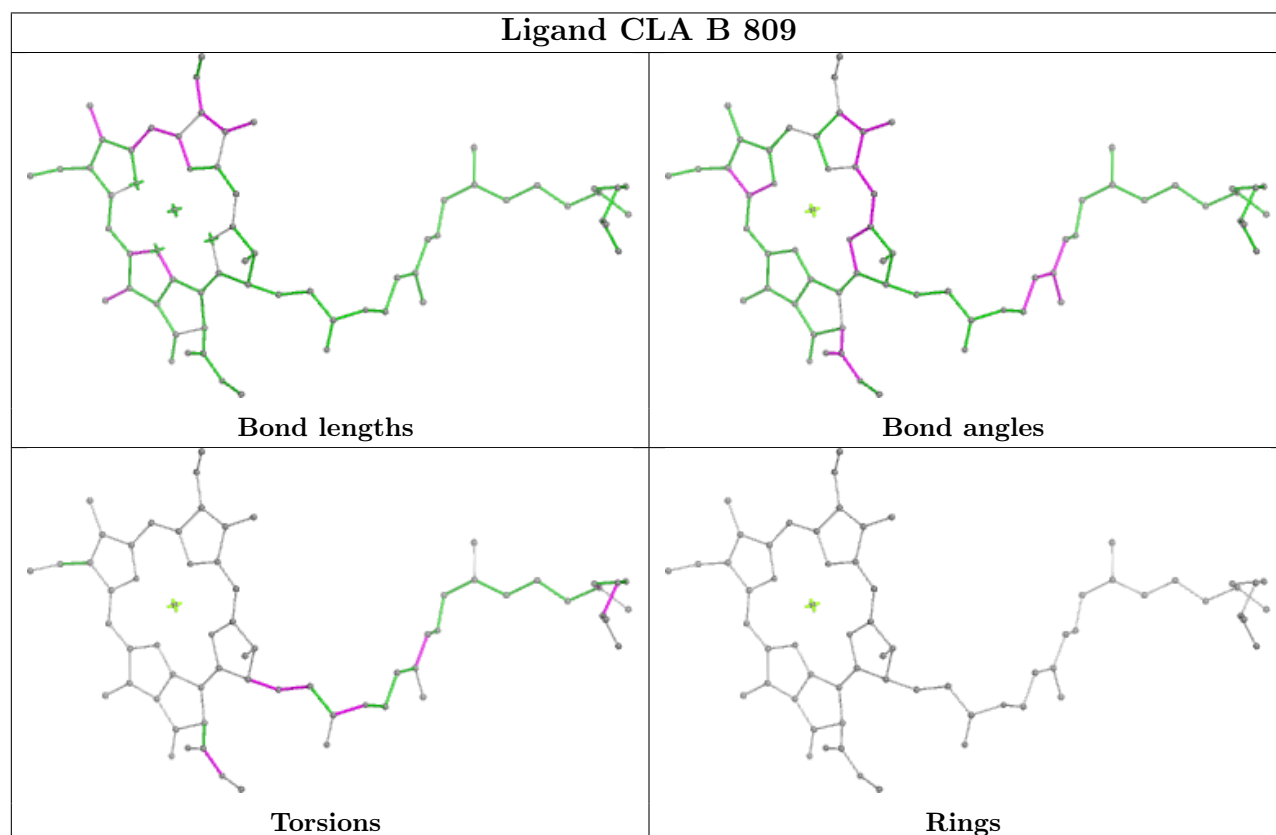
## Ligand CLA 2 808

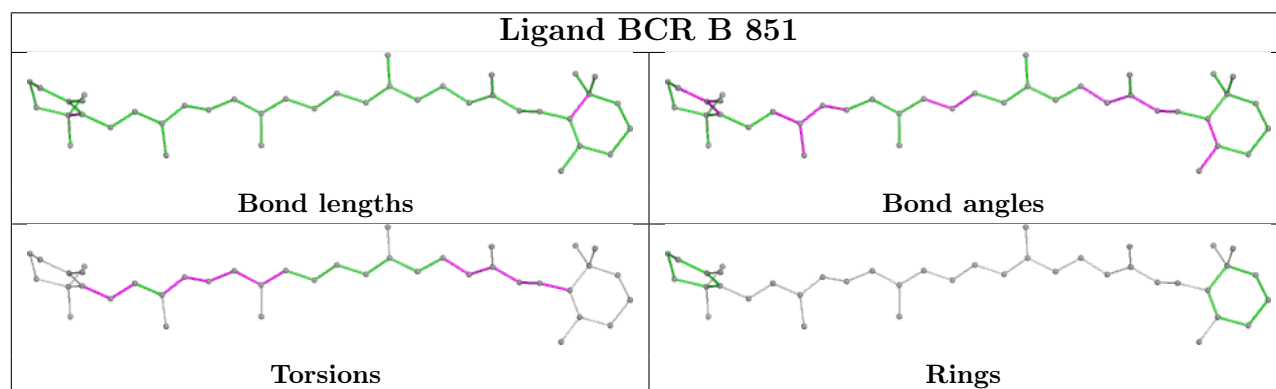
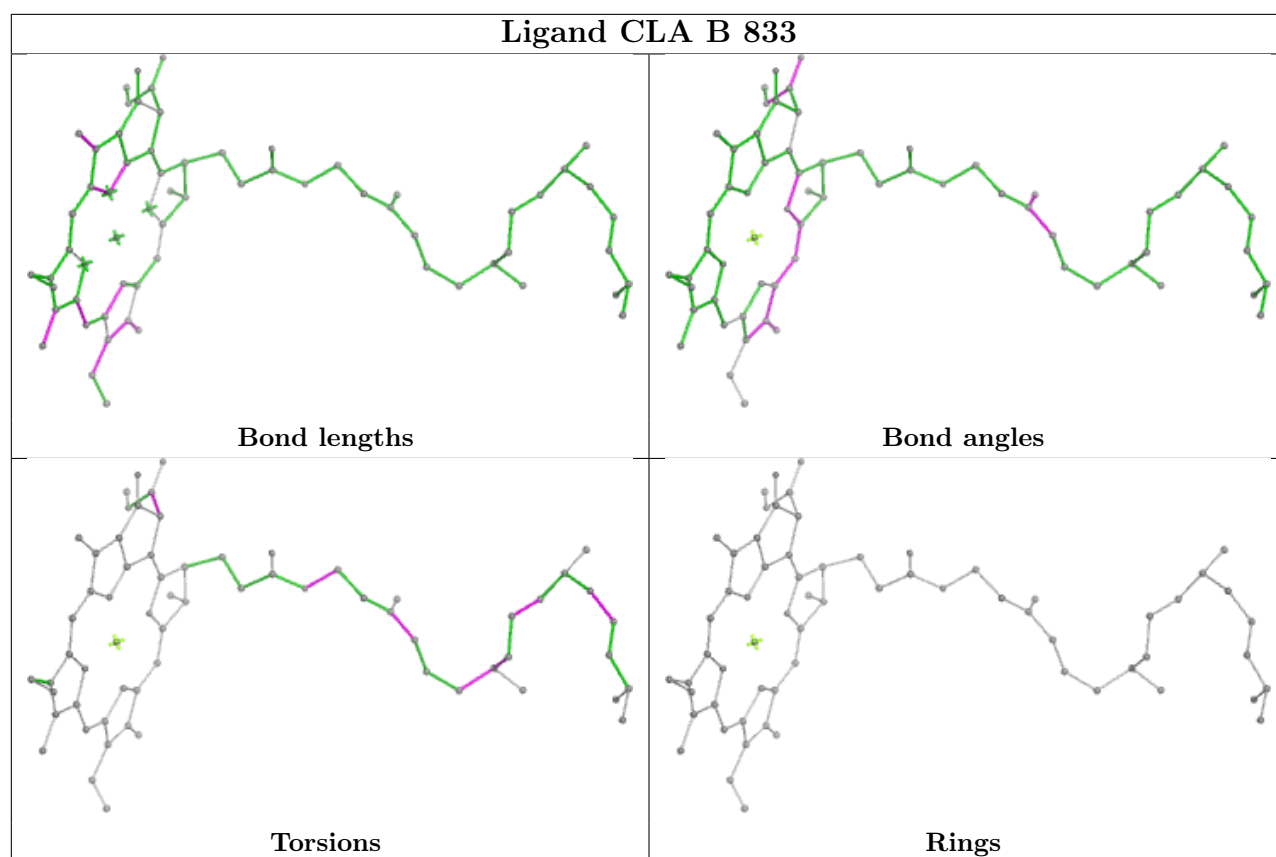


## Ligand CLA B 814

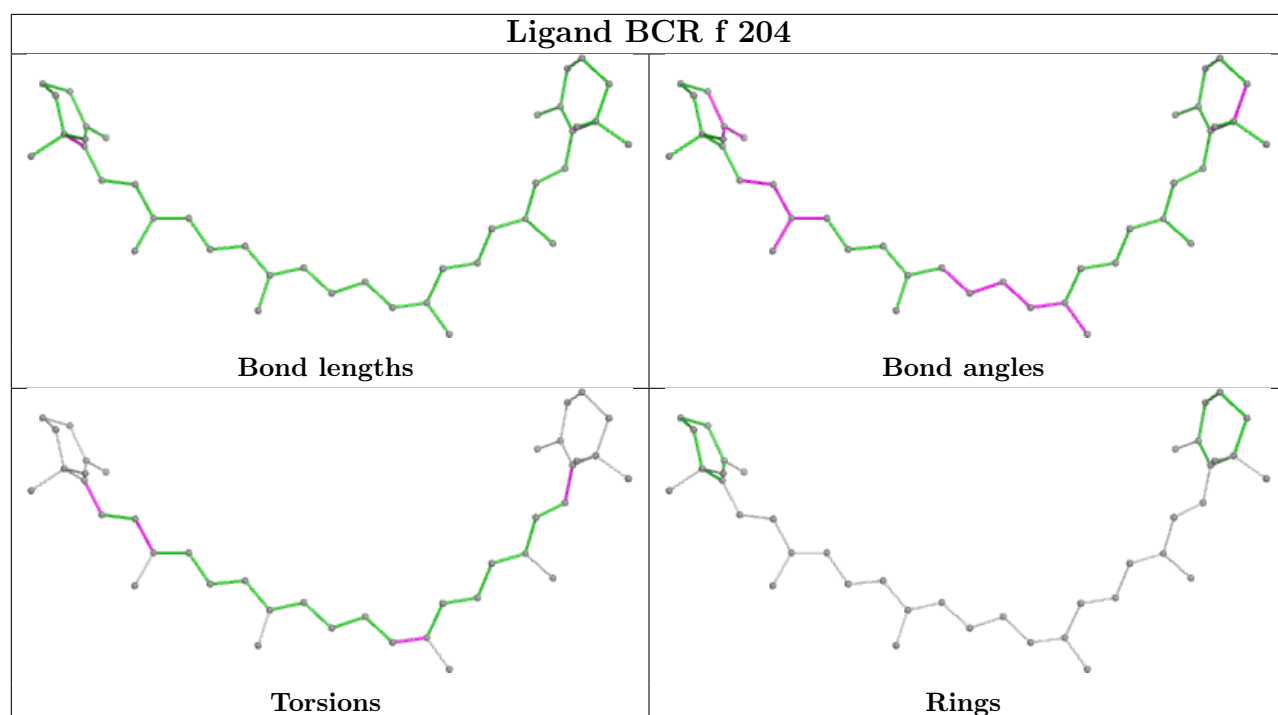


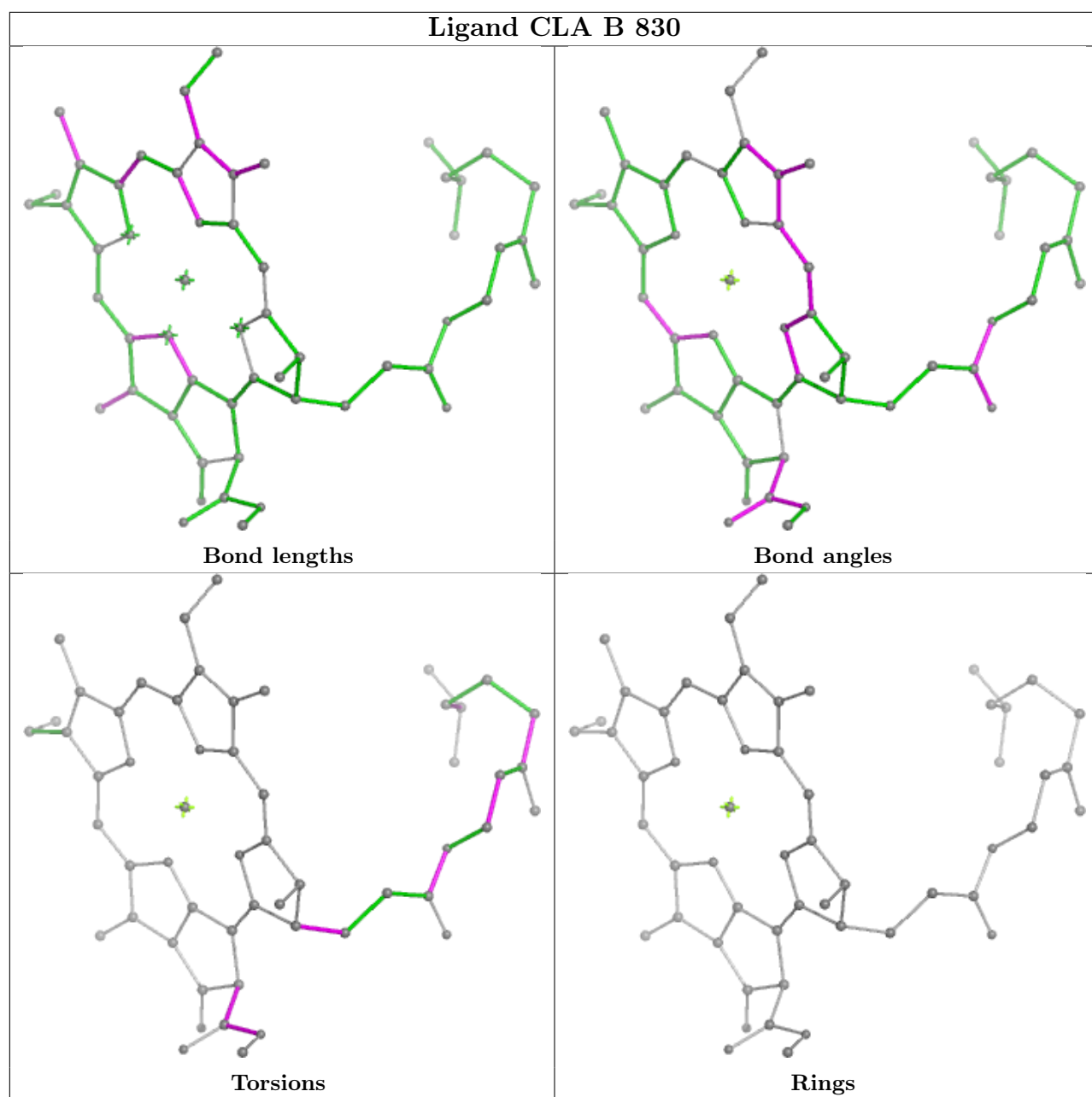
## Ligand CLA B 809



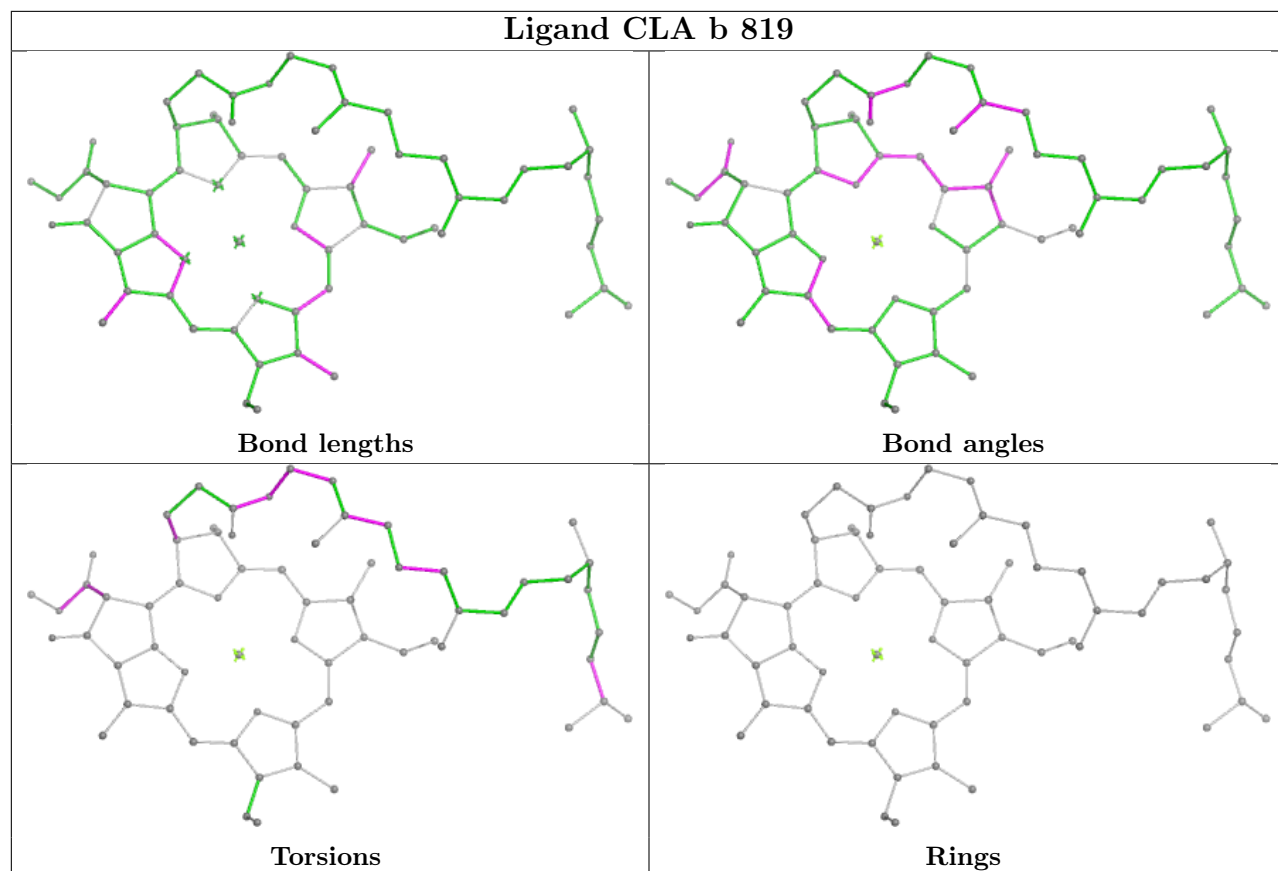


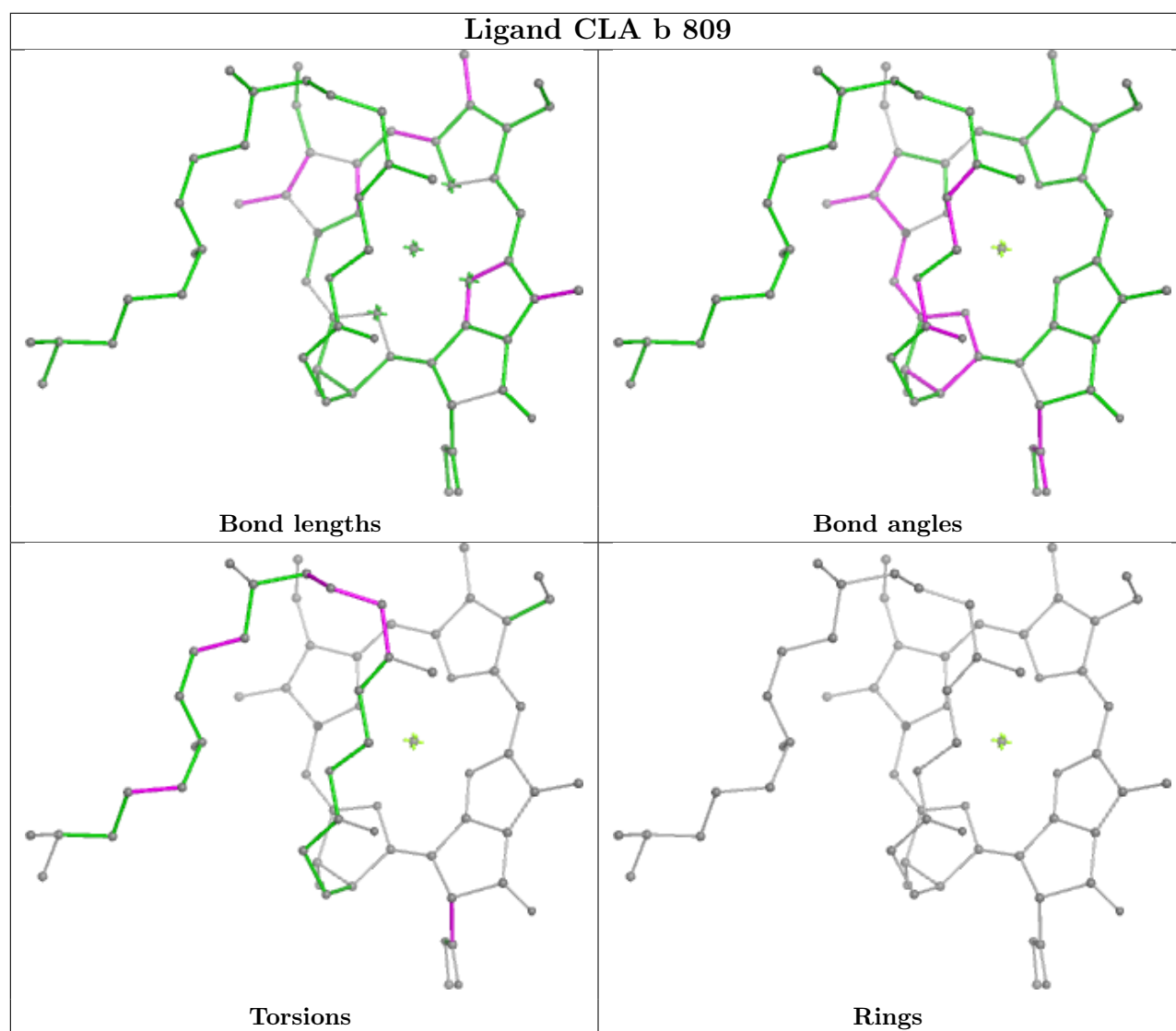




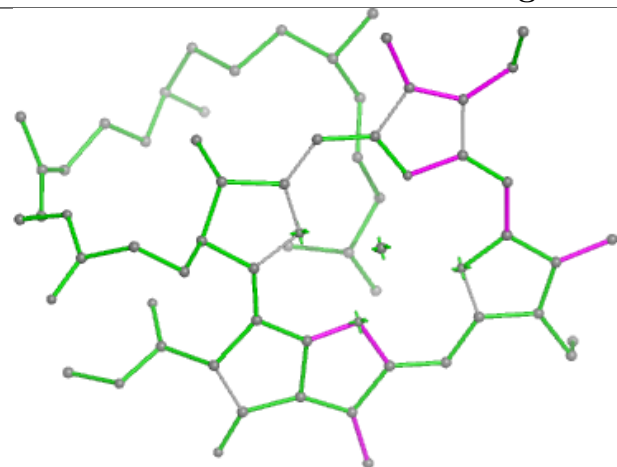


## Ligand CLA b 819

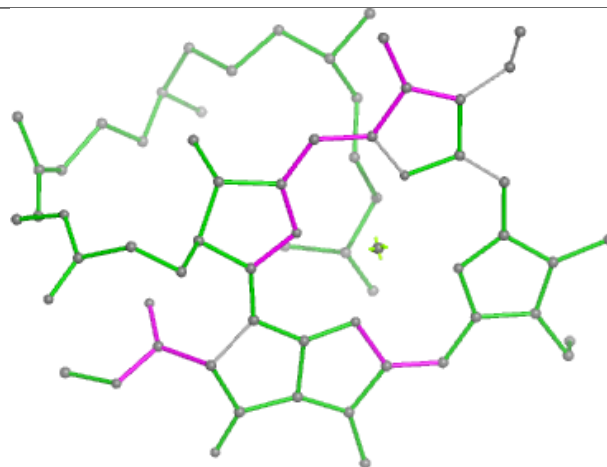




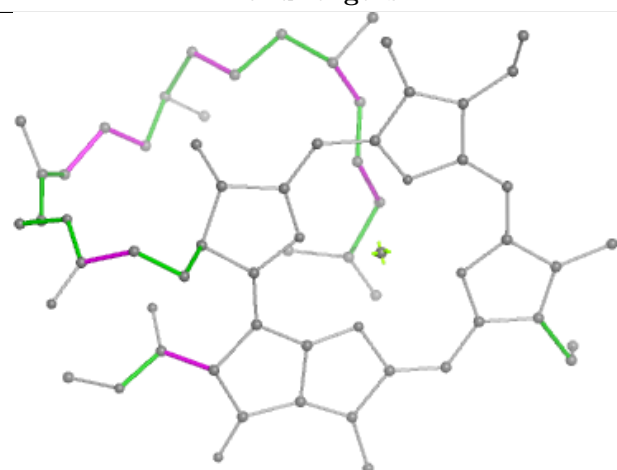
## Ligand CLA B 806



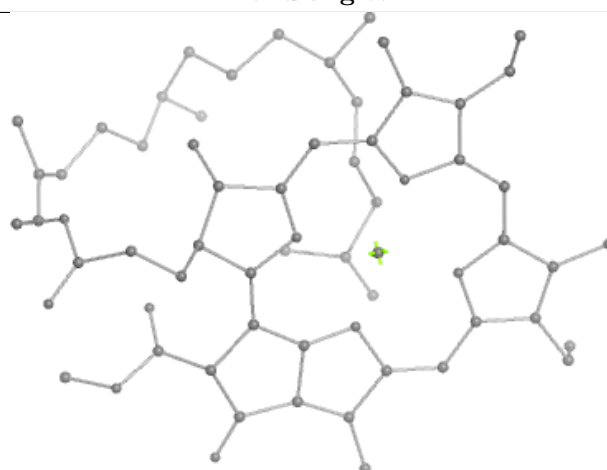
Bond lengths



Bond angles

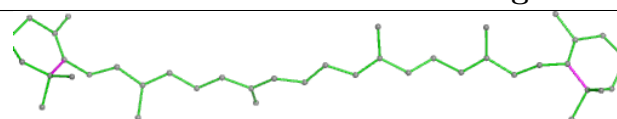


Torsions

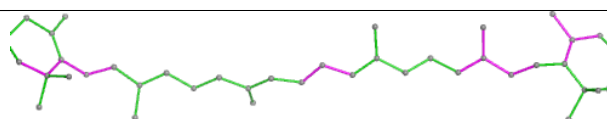


Rings

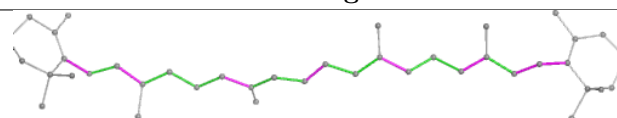
## Ligand BCR 1 1648



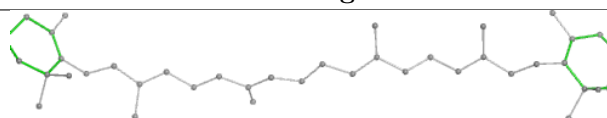
Bond lengths



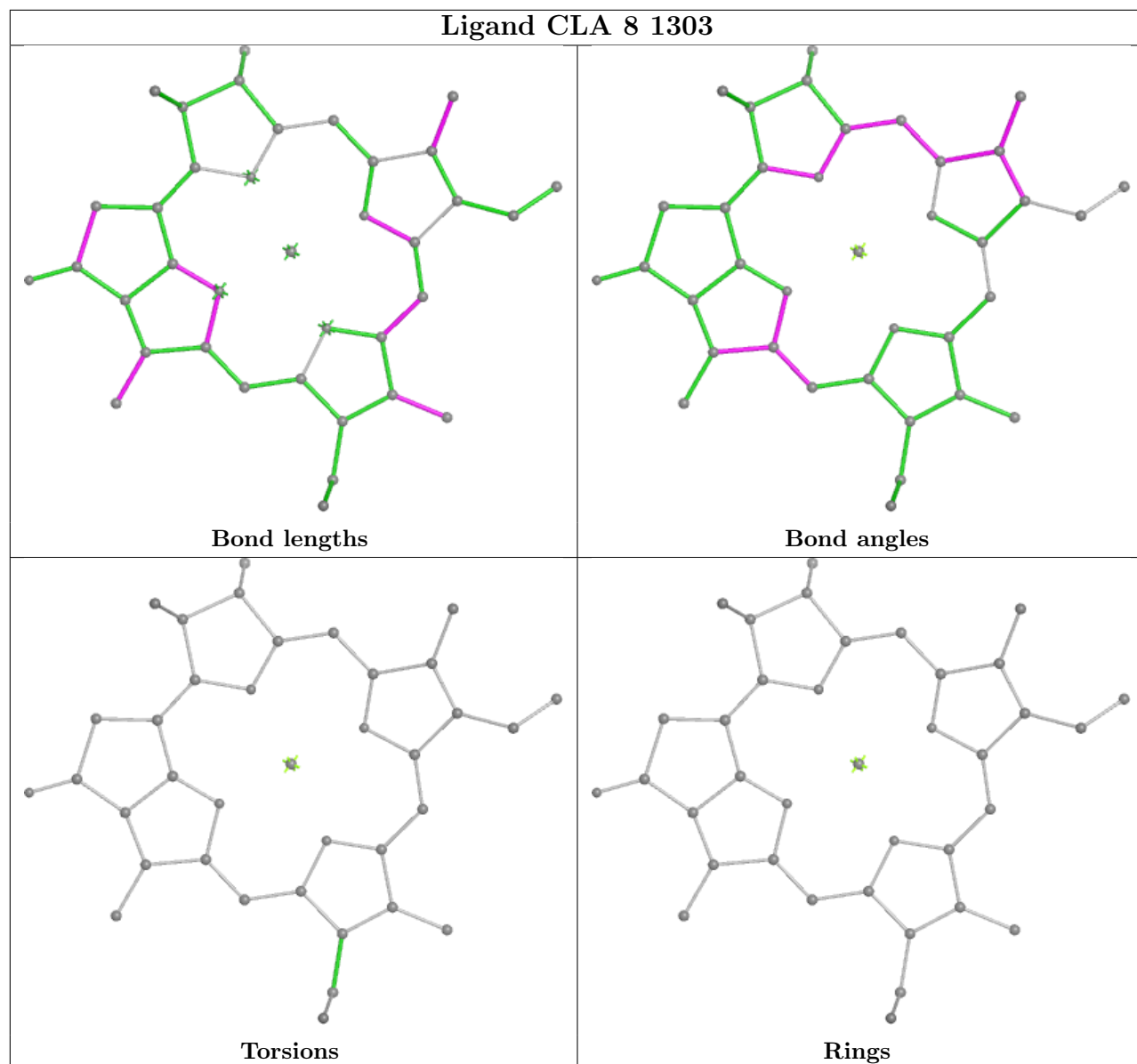
Bond angles

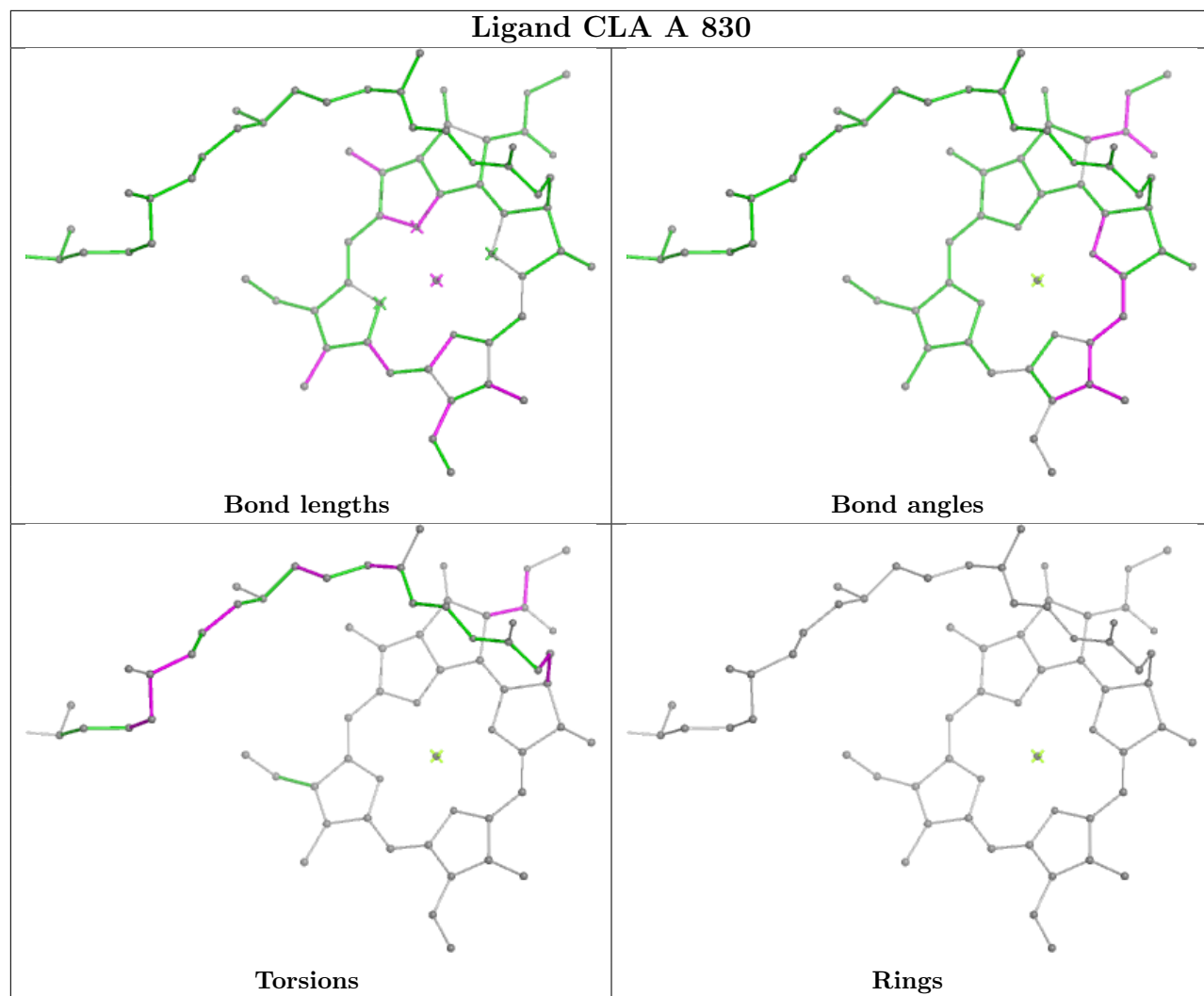


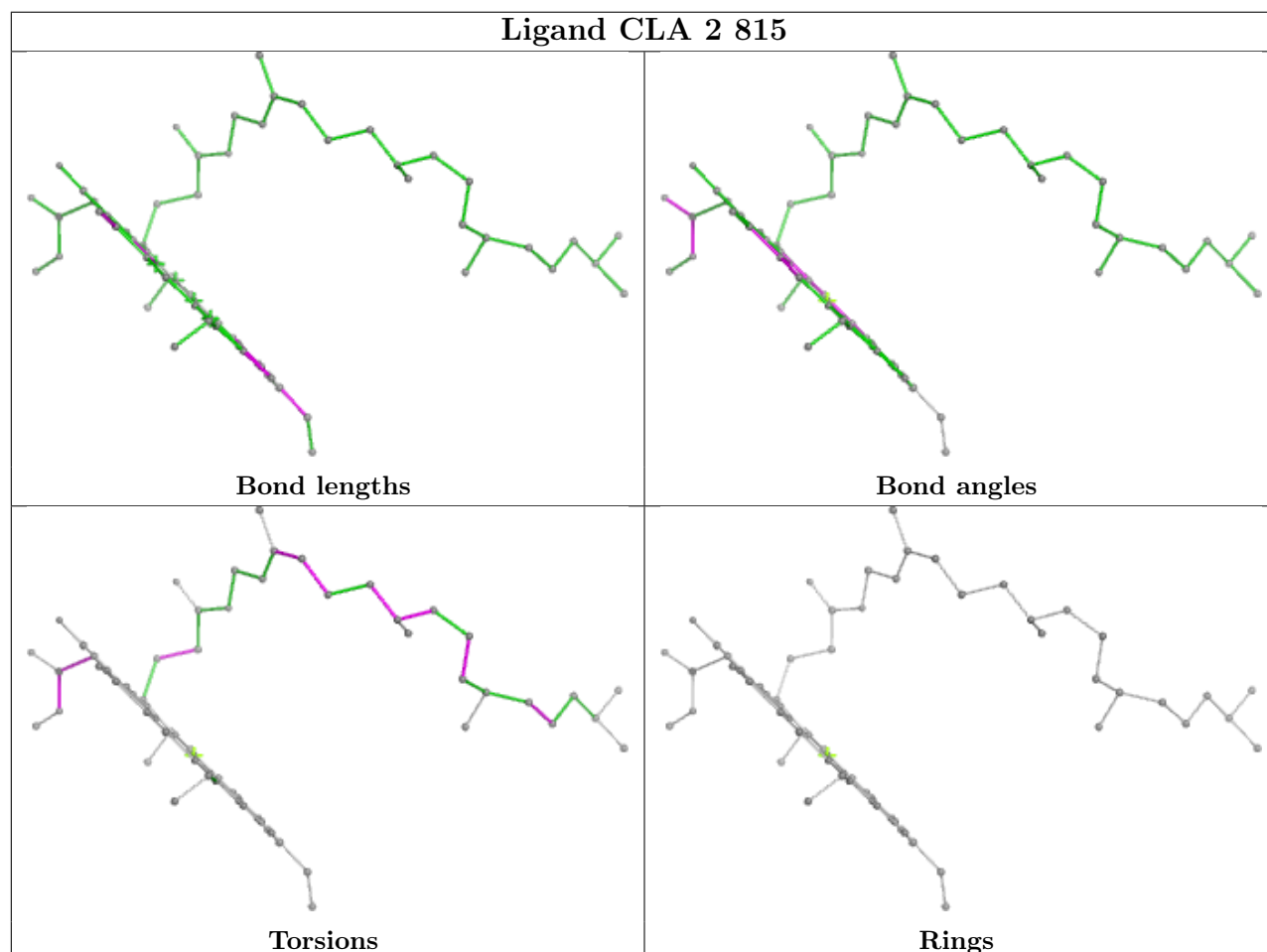
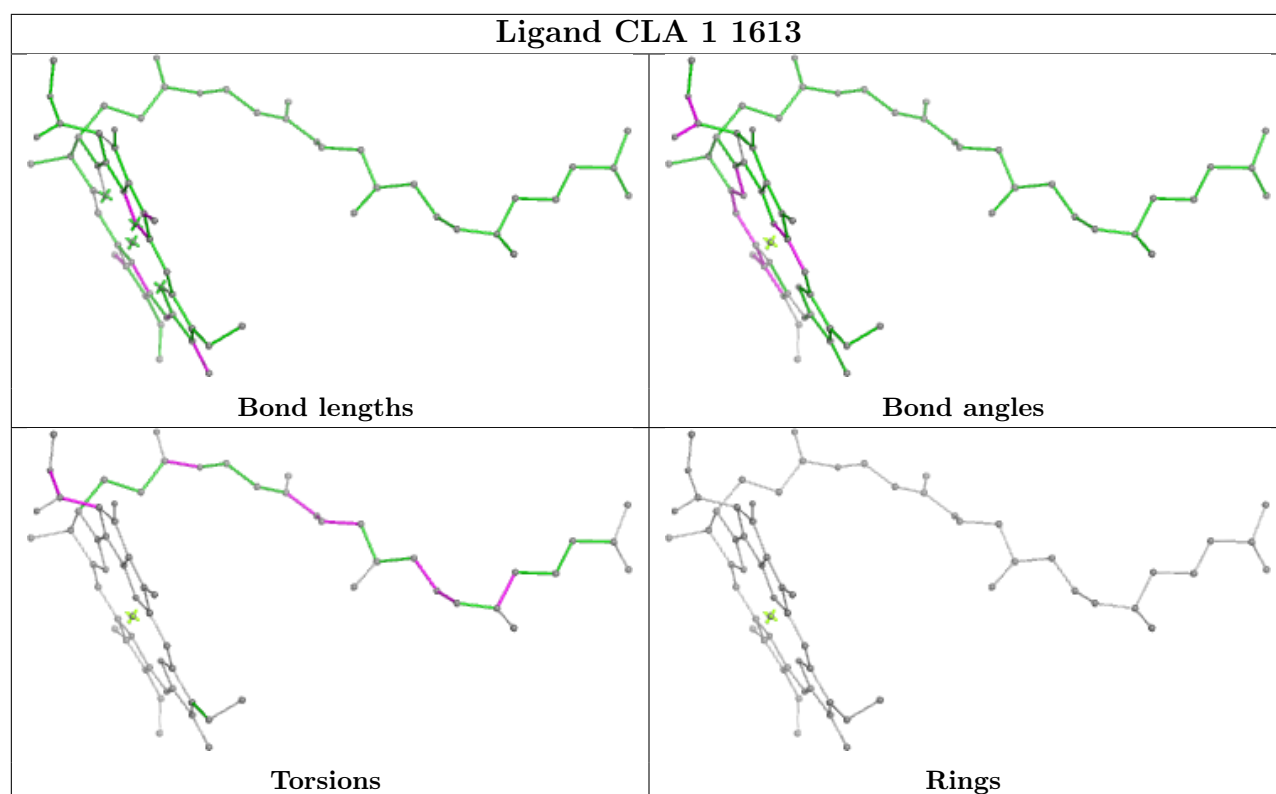
Torsions



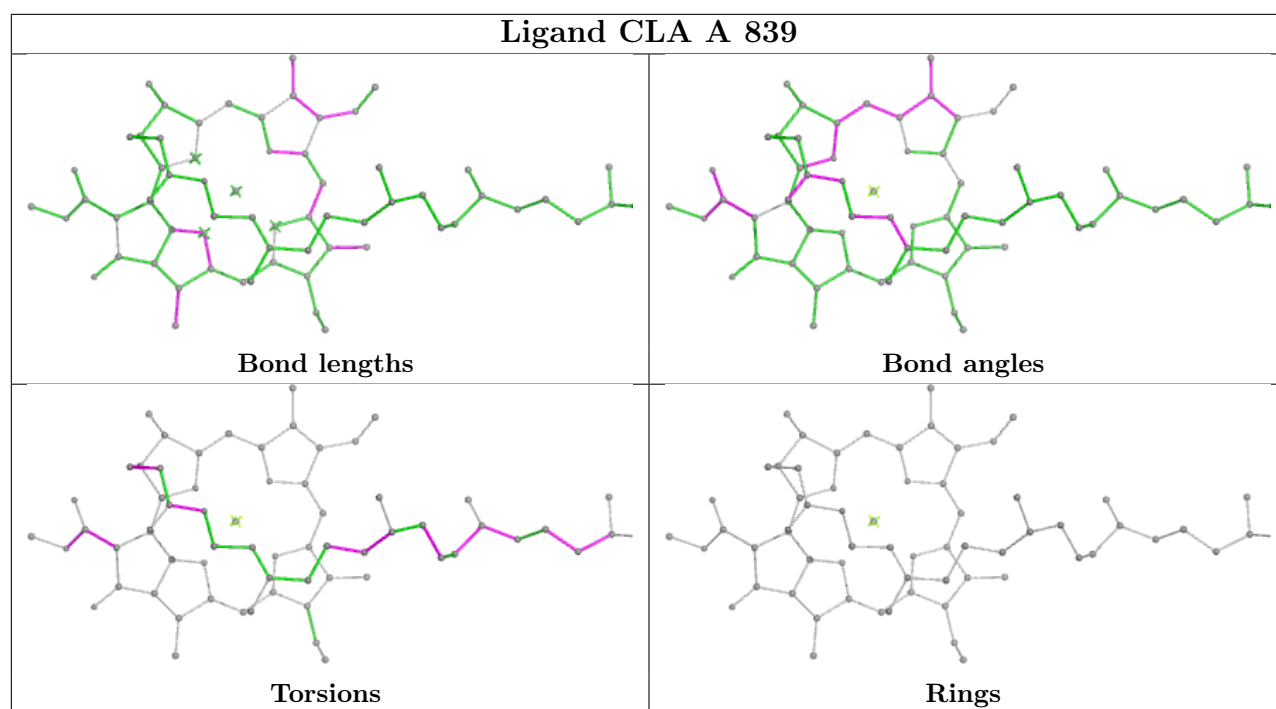
Rings

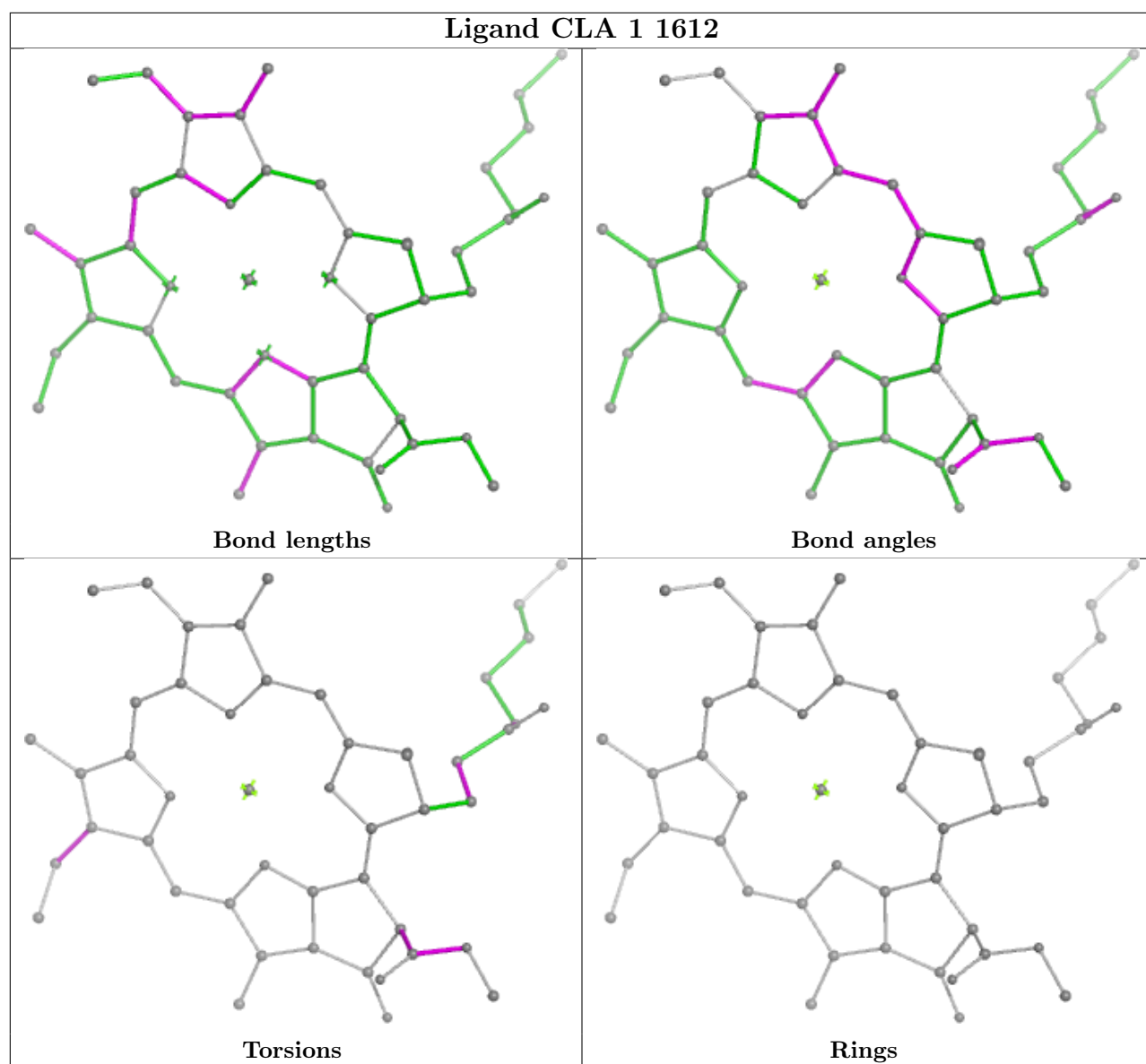




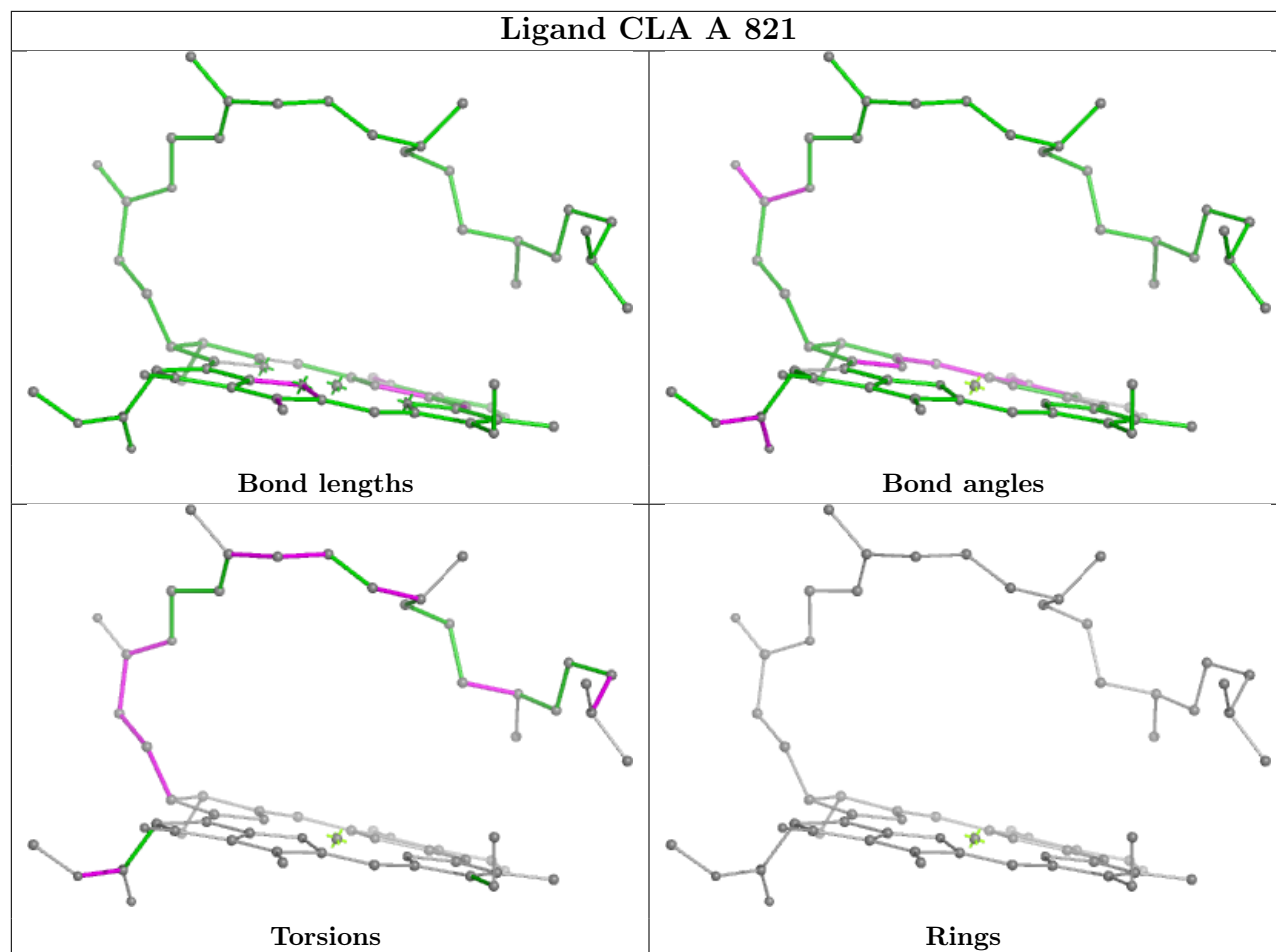




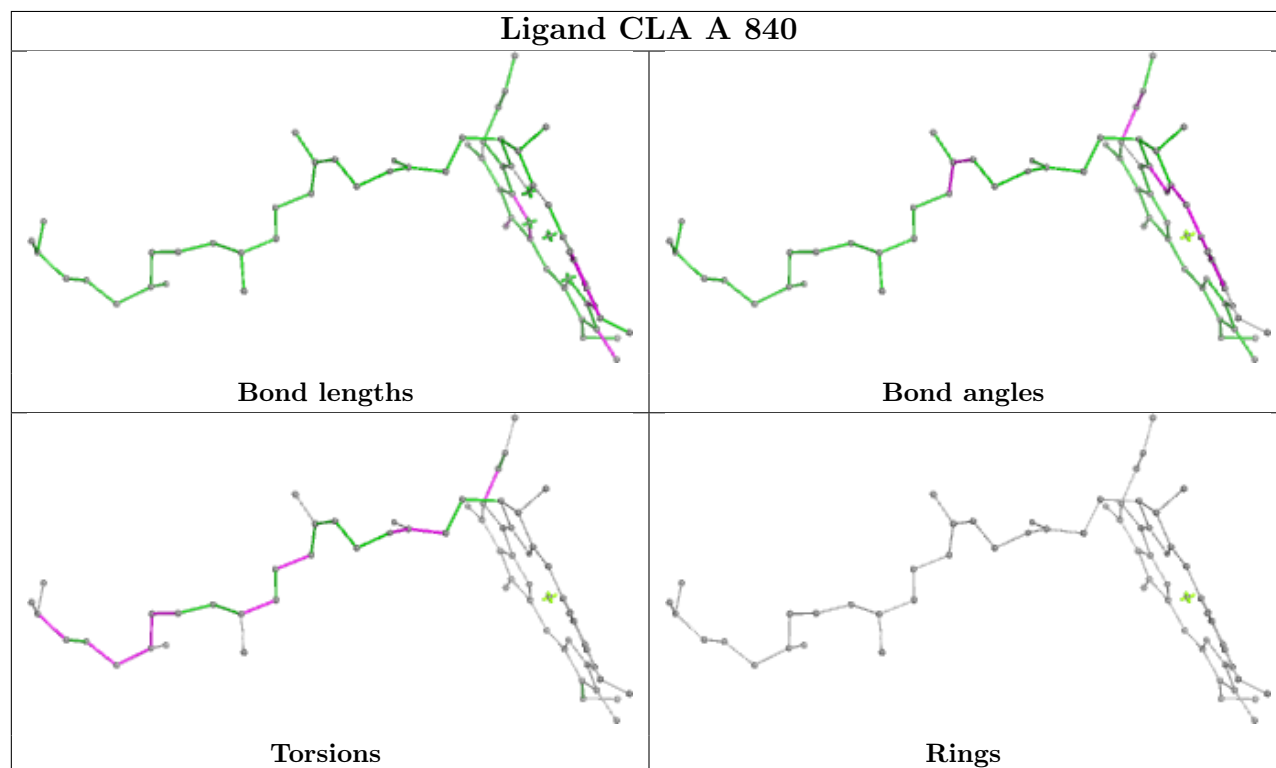


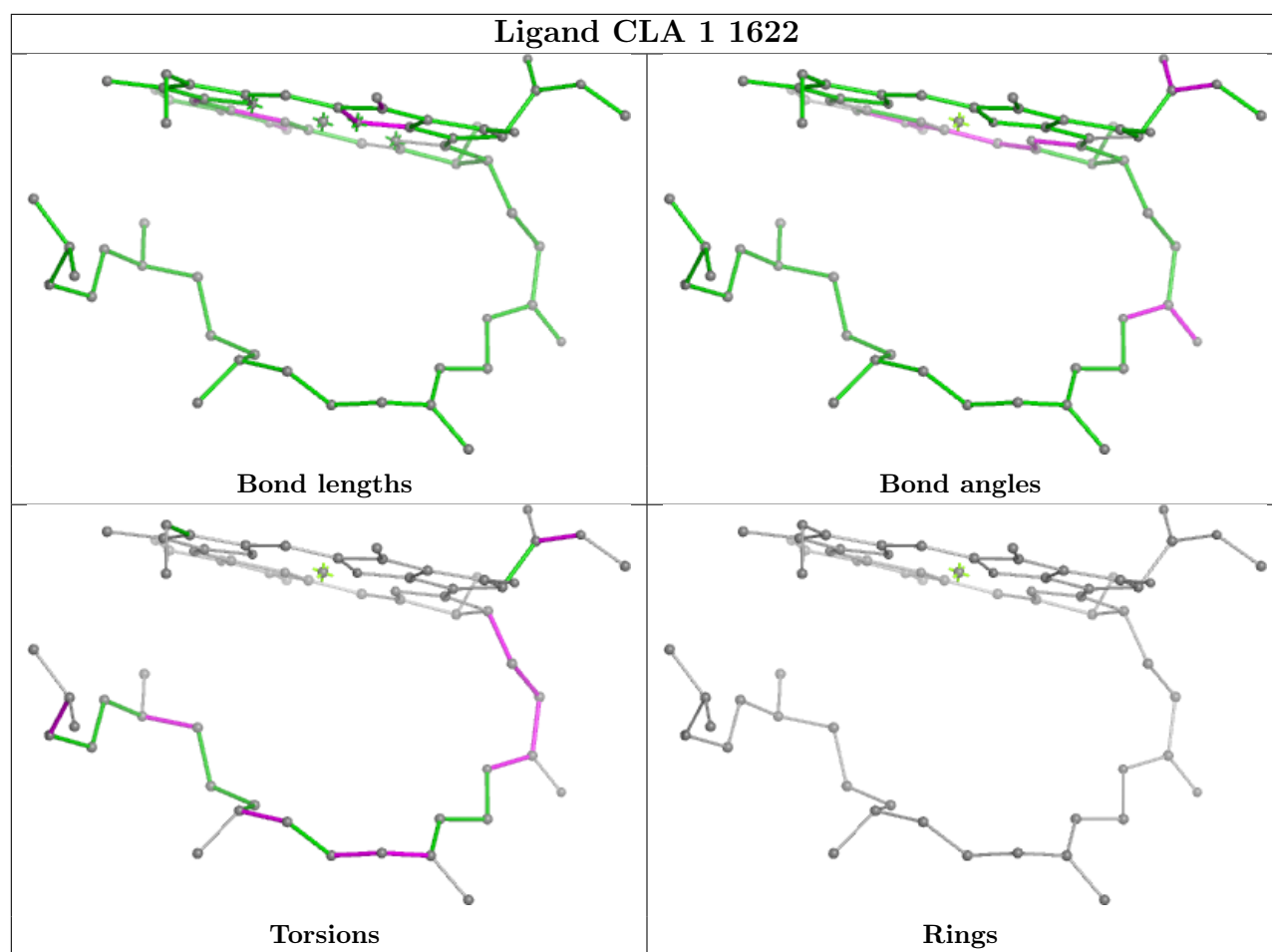


## Ligand CLA A 821

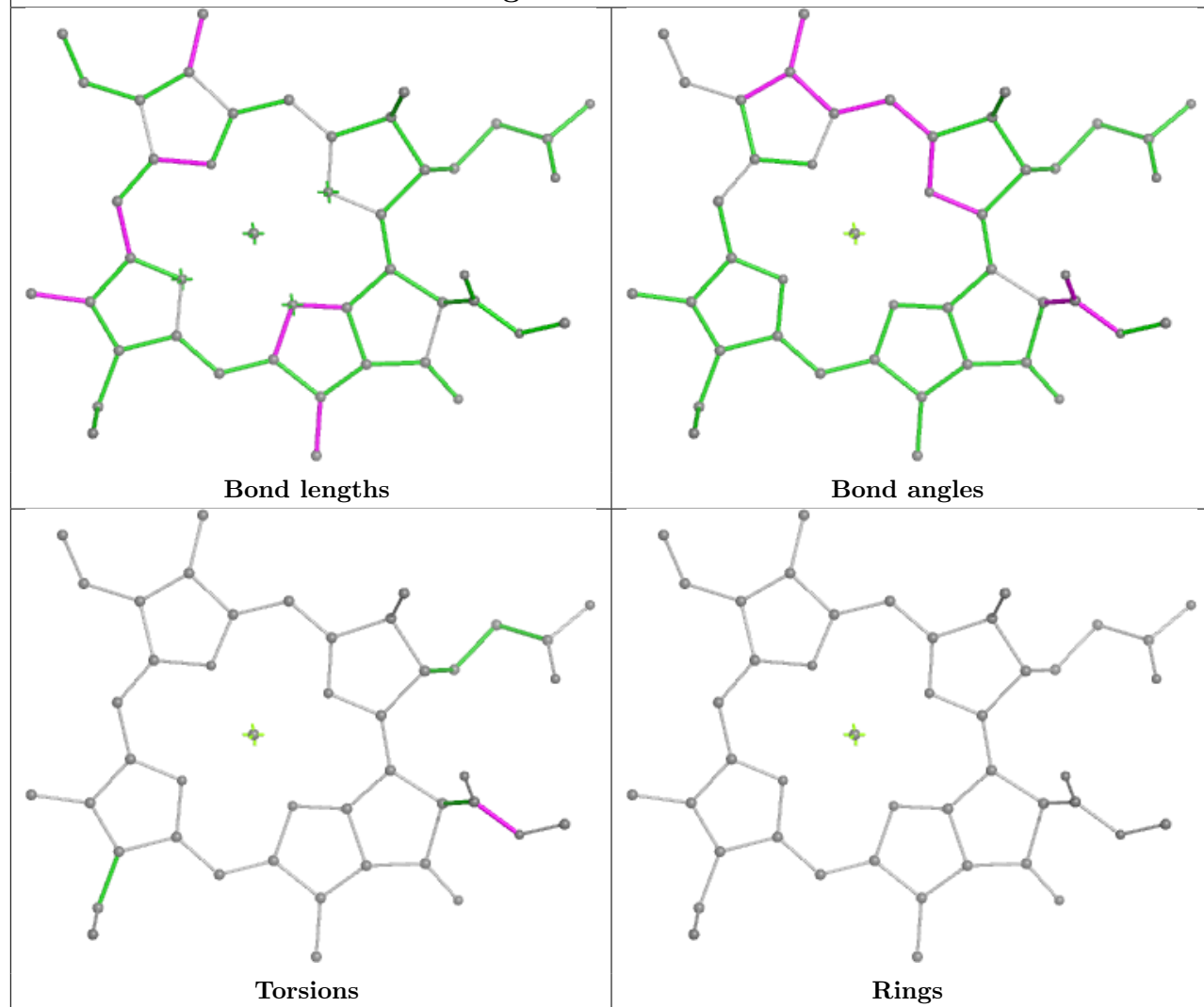


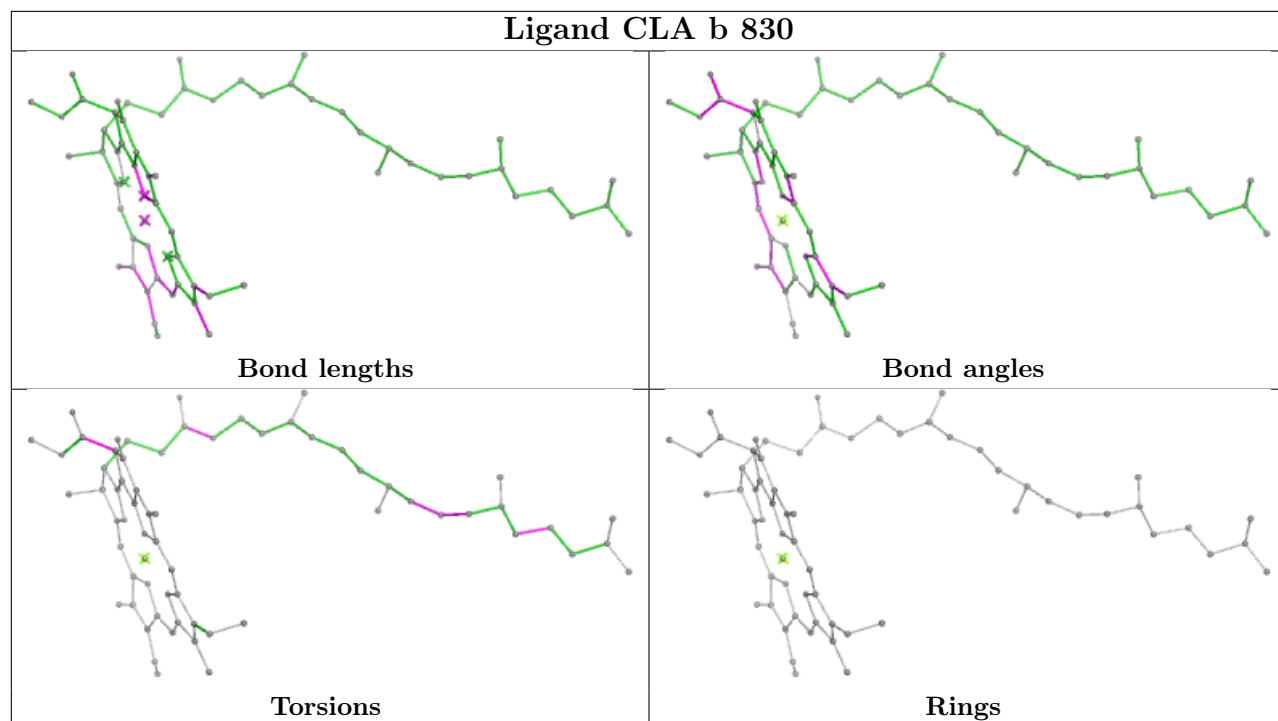
## Ligand CLA A 840



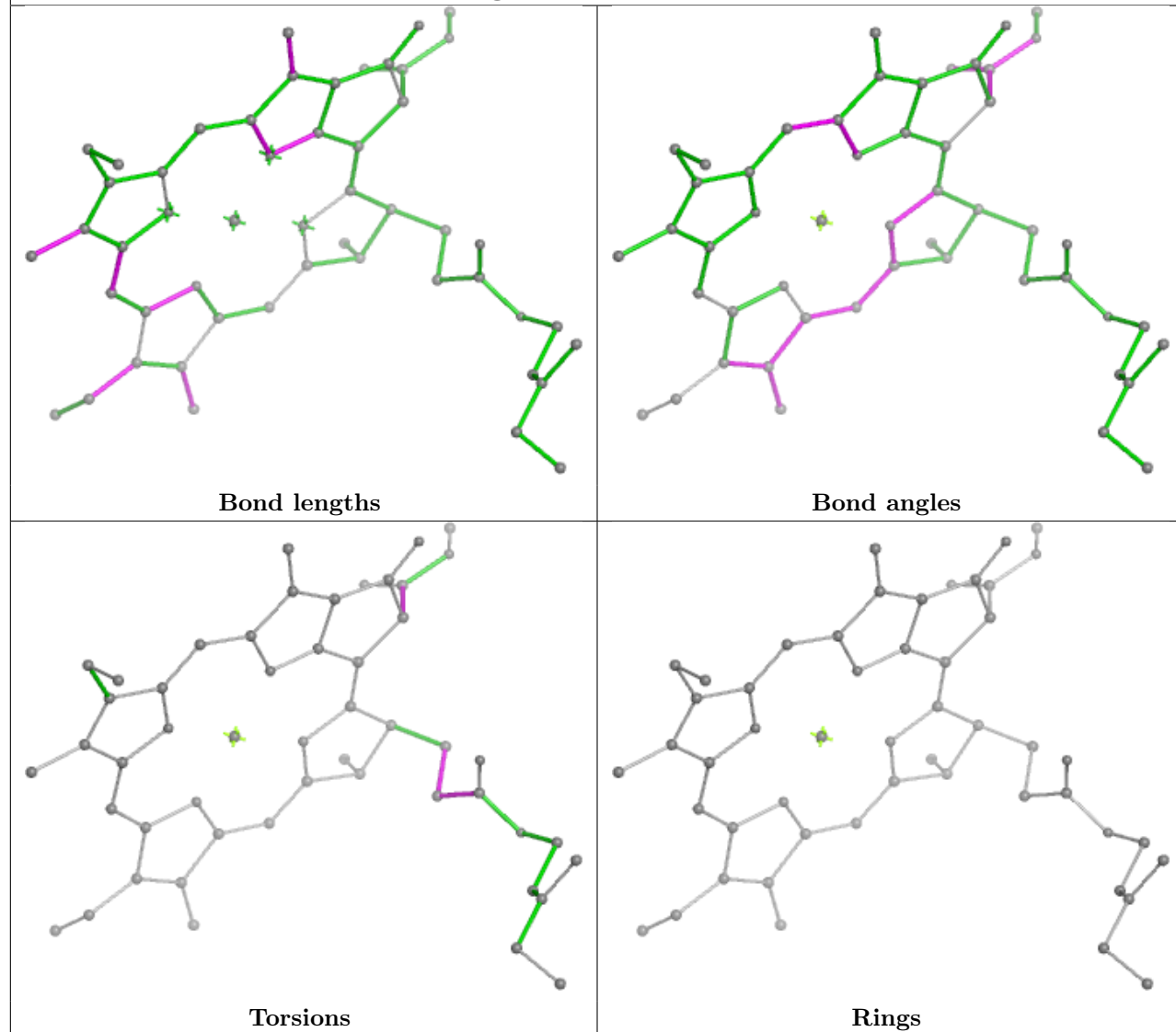


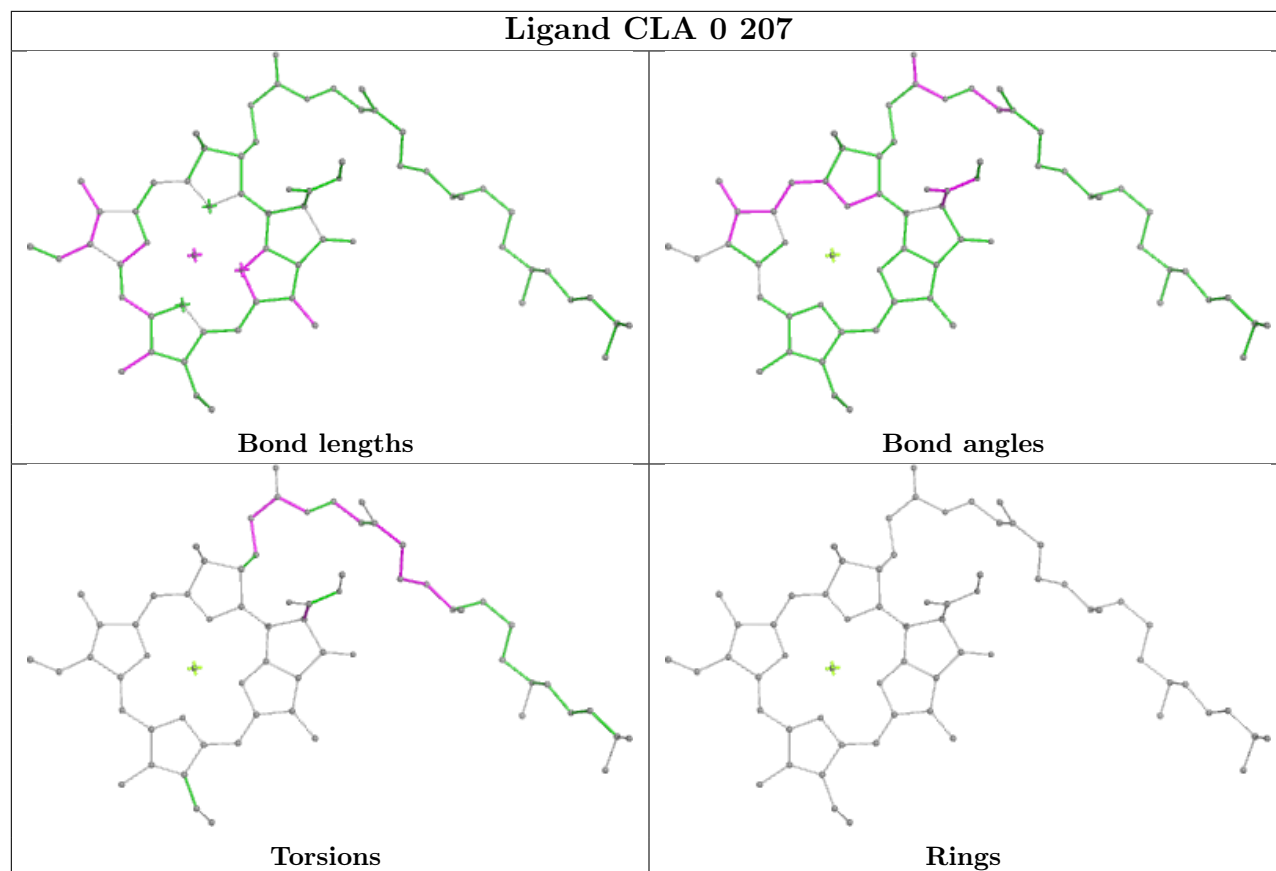
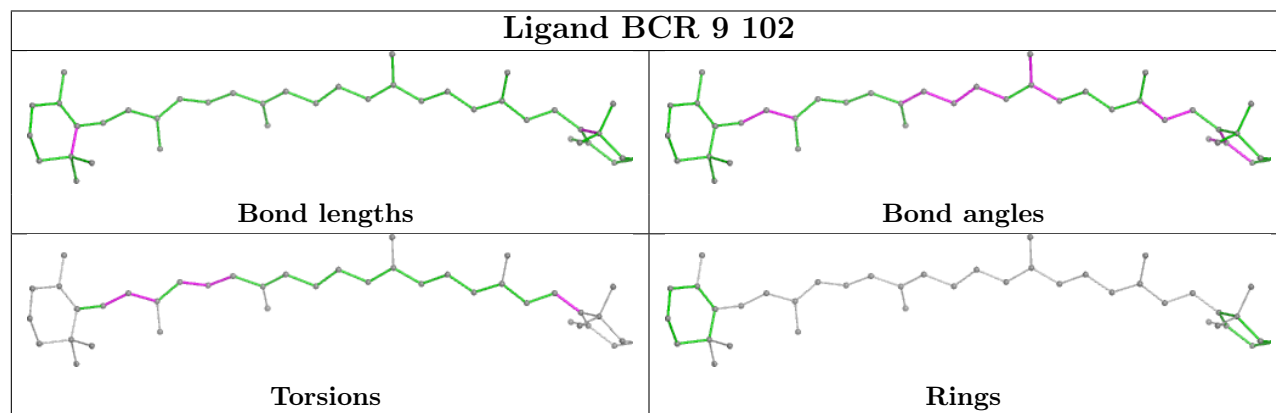
## Ligand CLA F 203





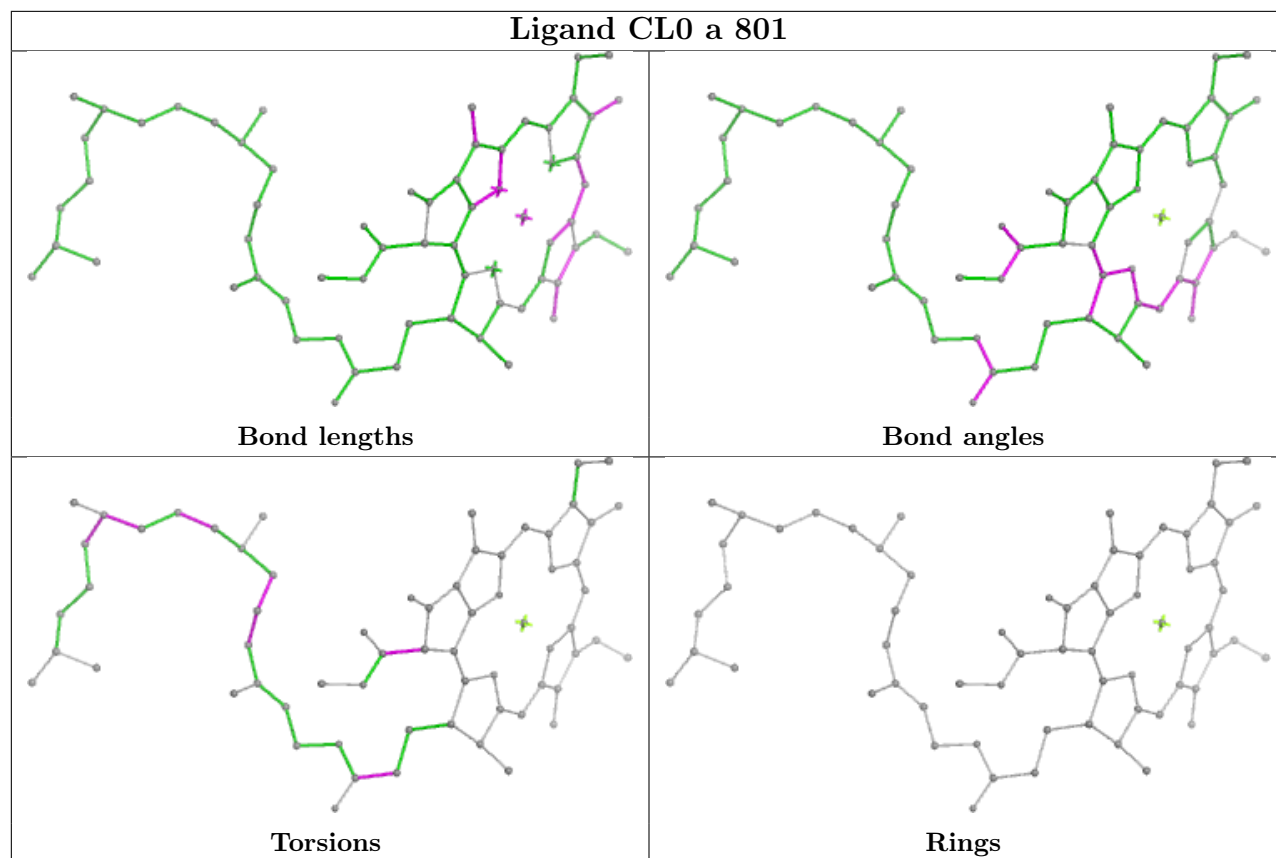
## Ligand CLA A 808



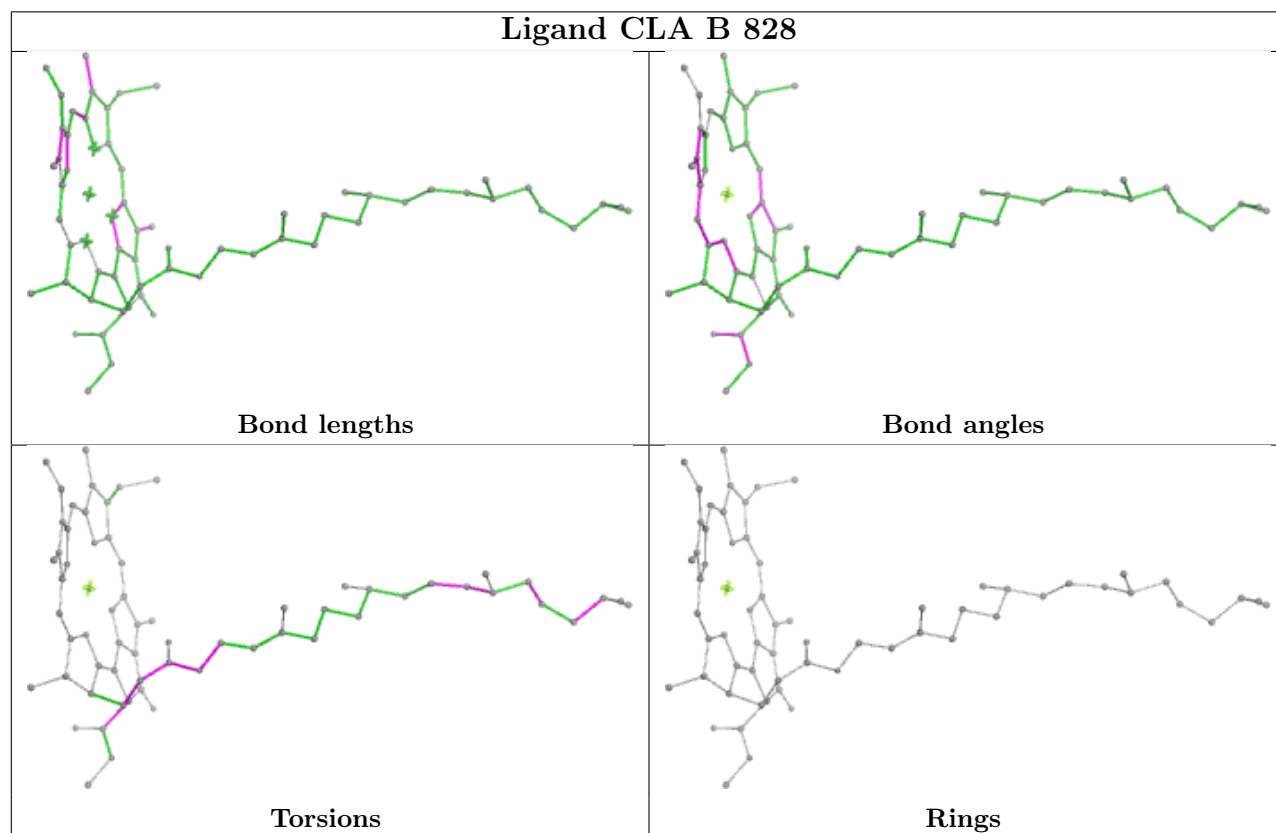
**Ligand CLA 0 207****Ligand BCR 9 102**

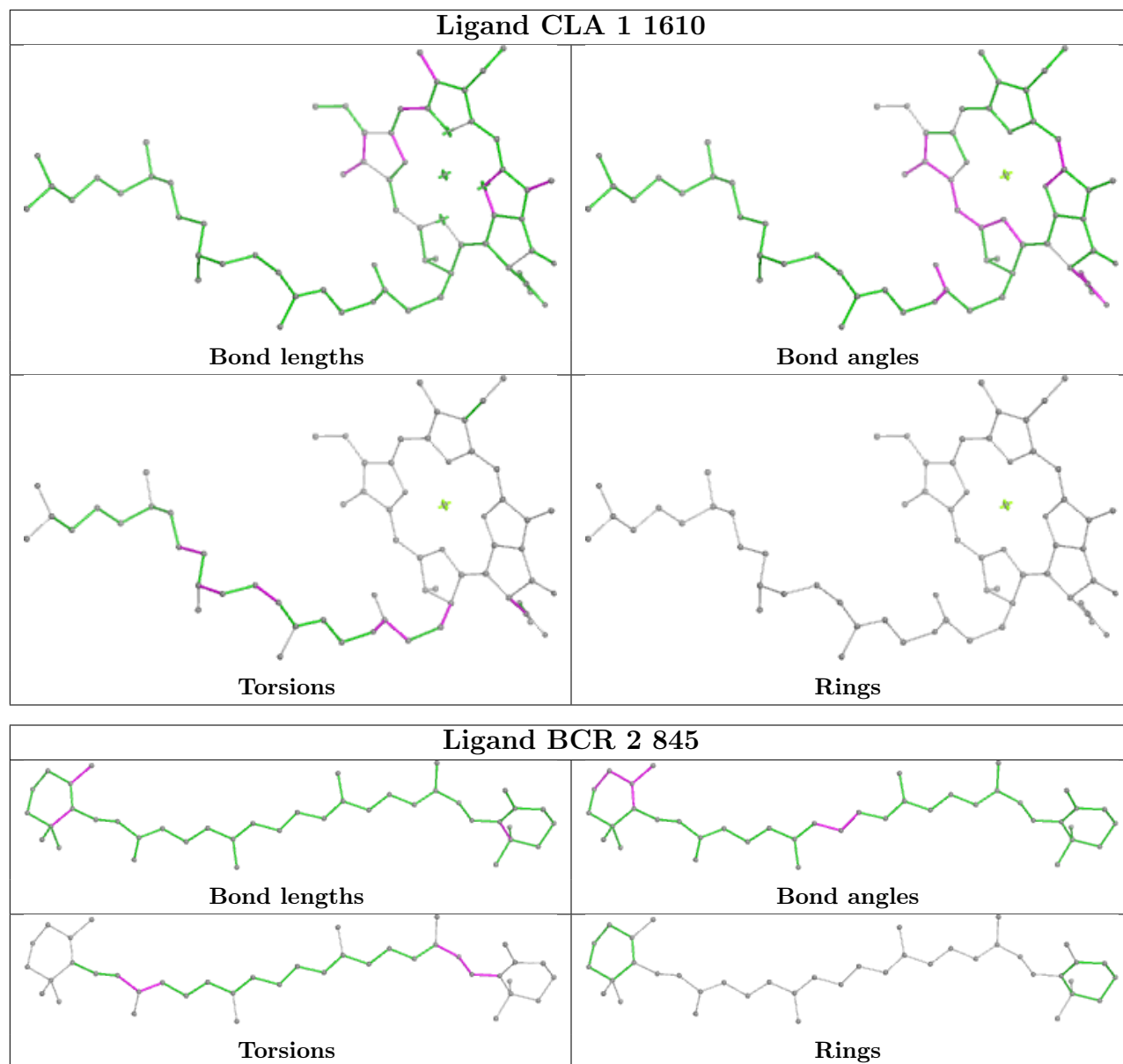


## Ligand CL0 a 801

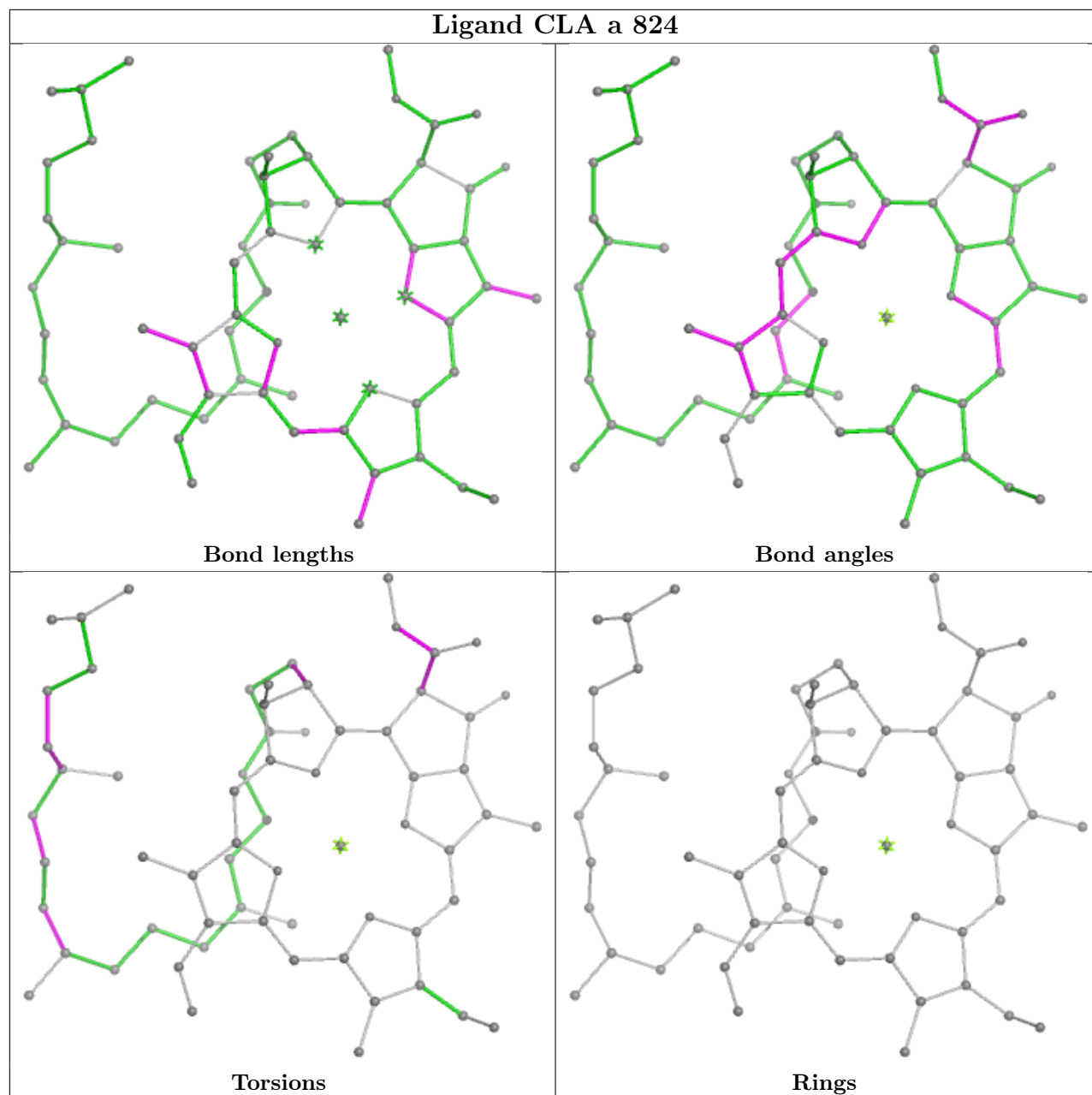


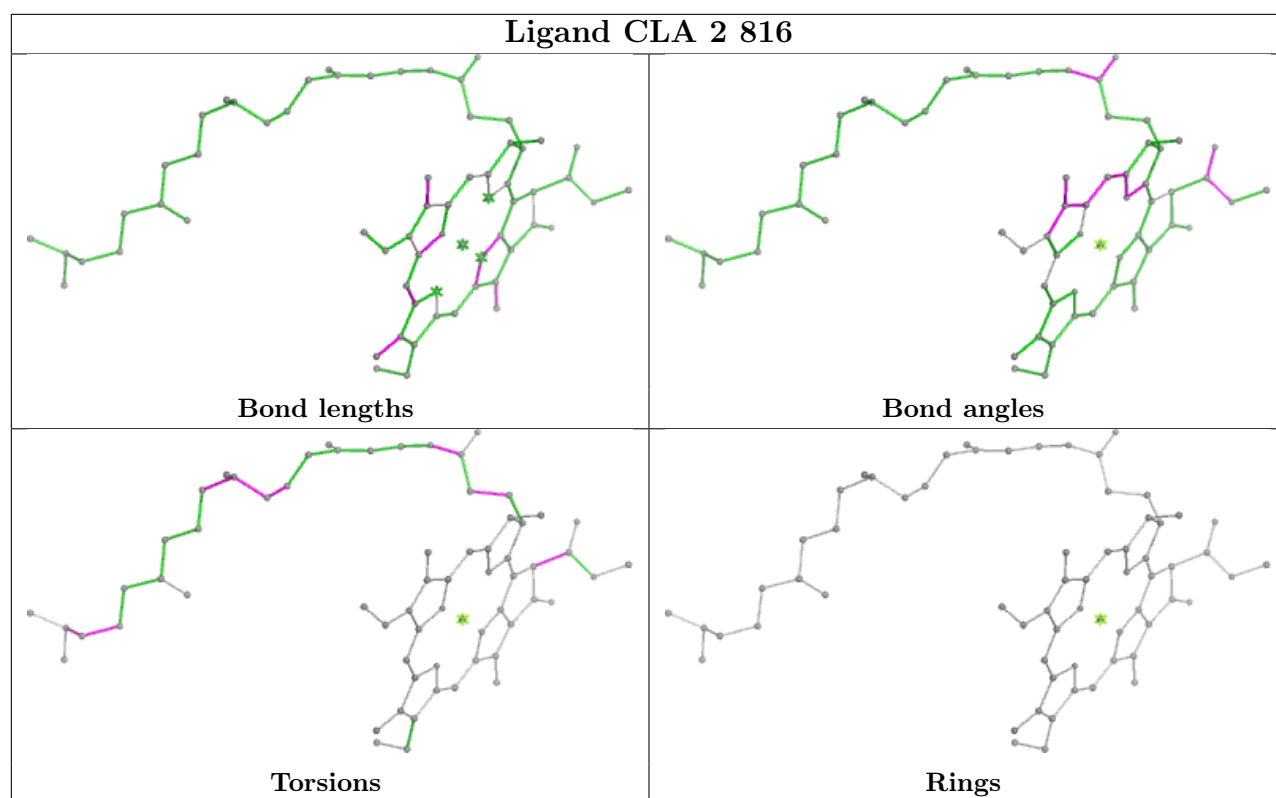
## Ligand CLA B 828

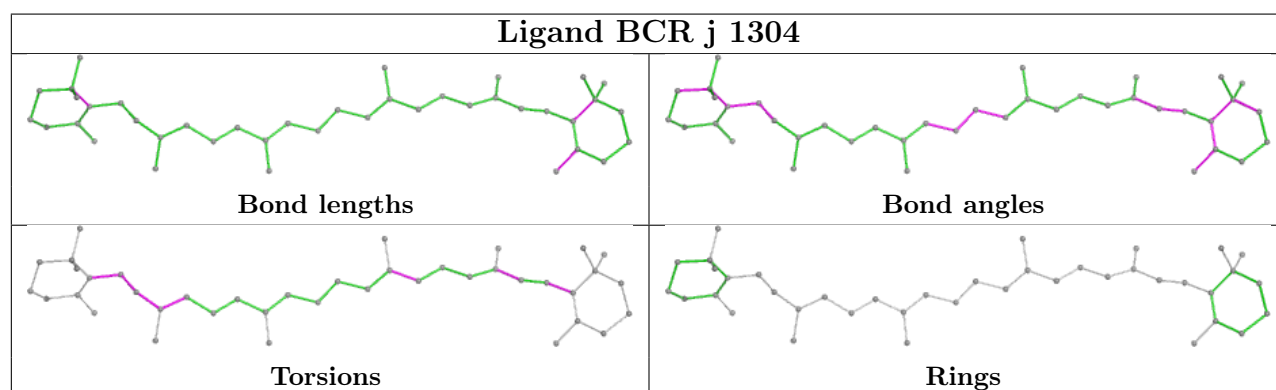
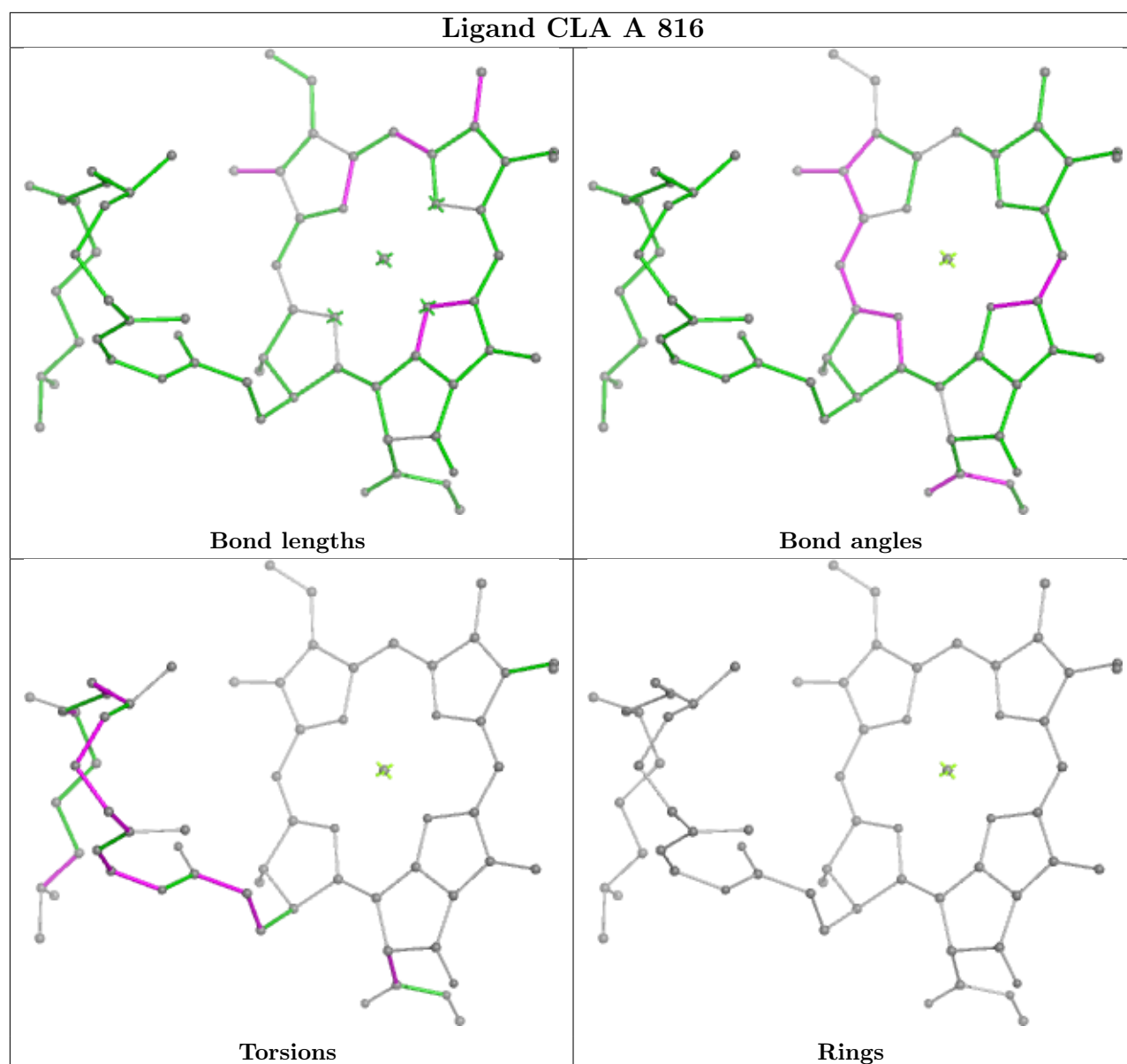


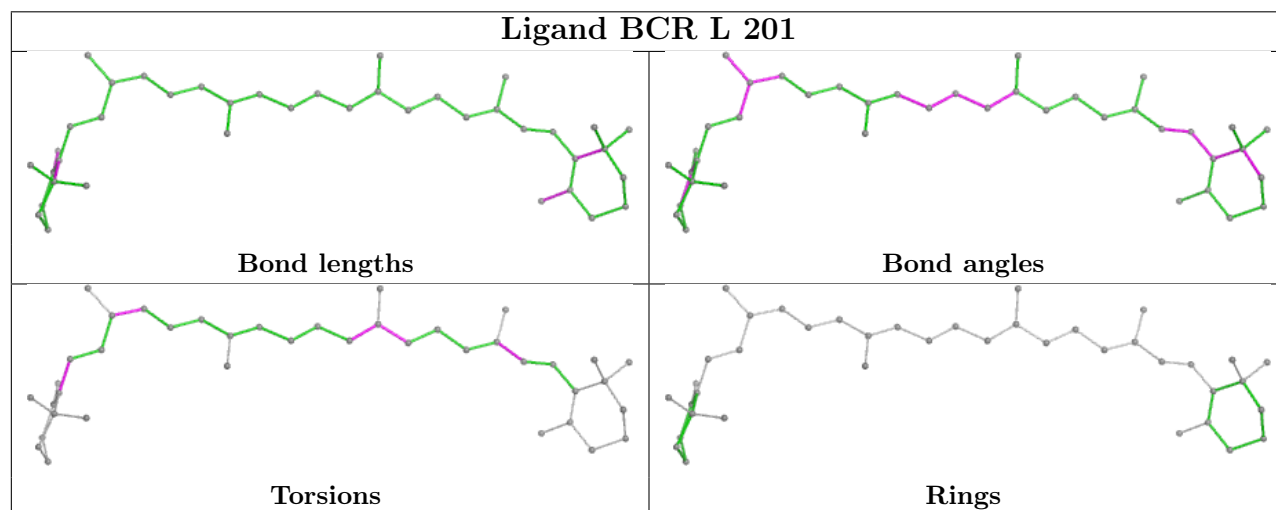
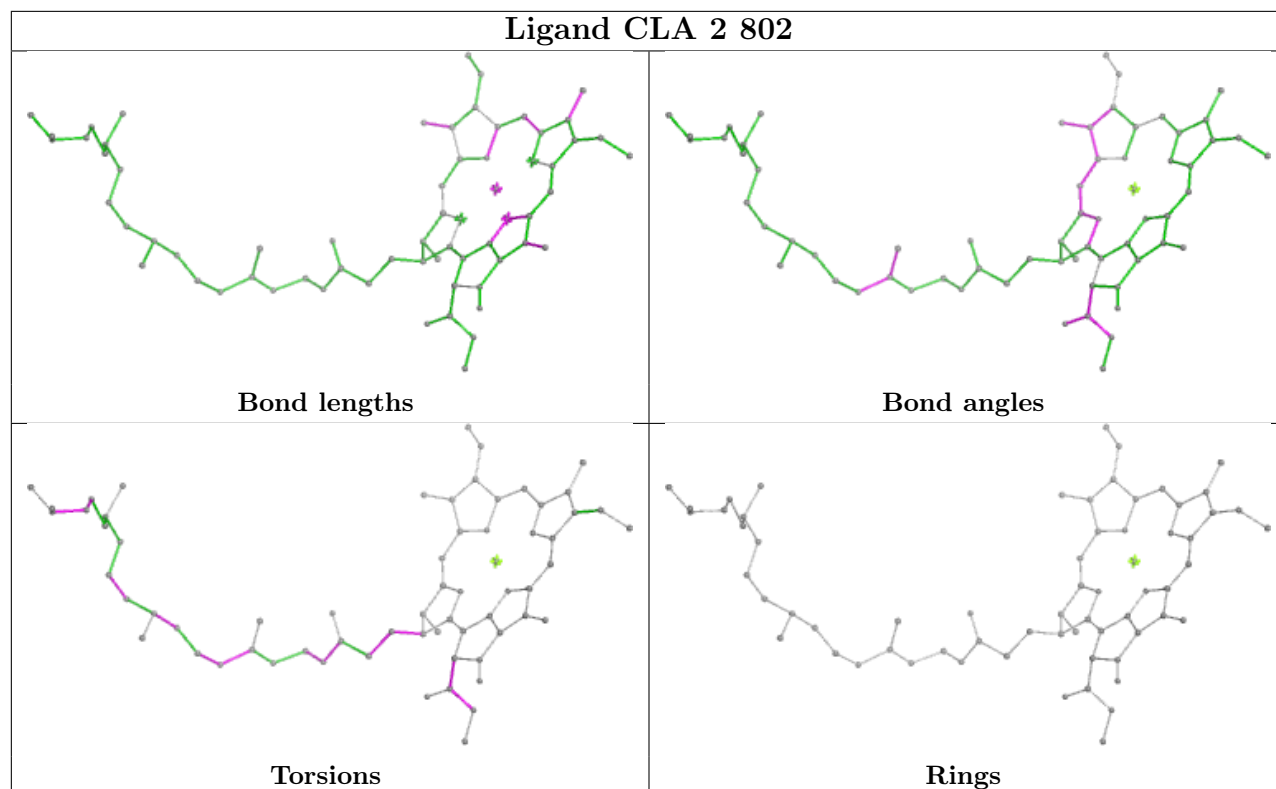


## Ligand CLA a 824

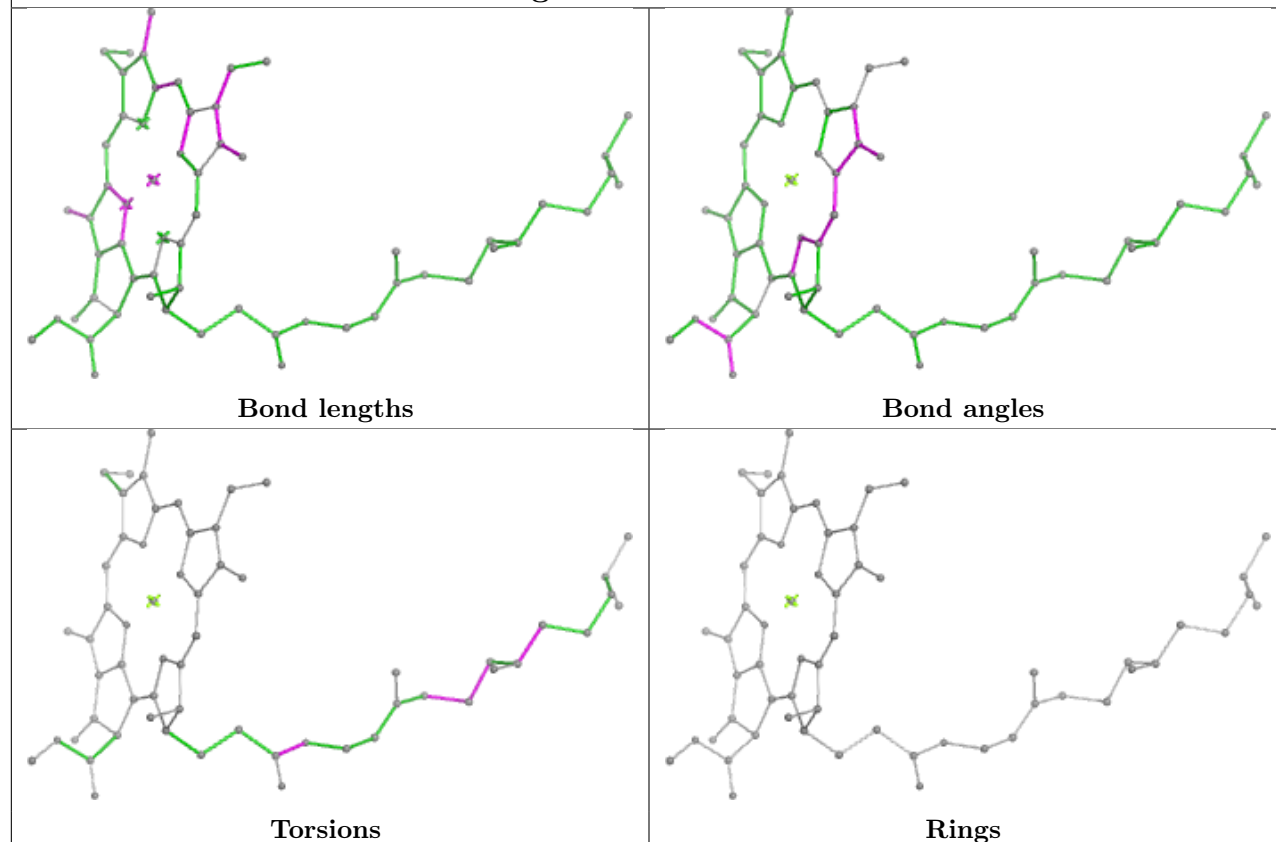




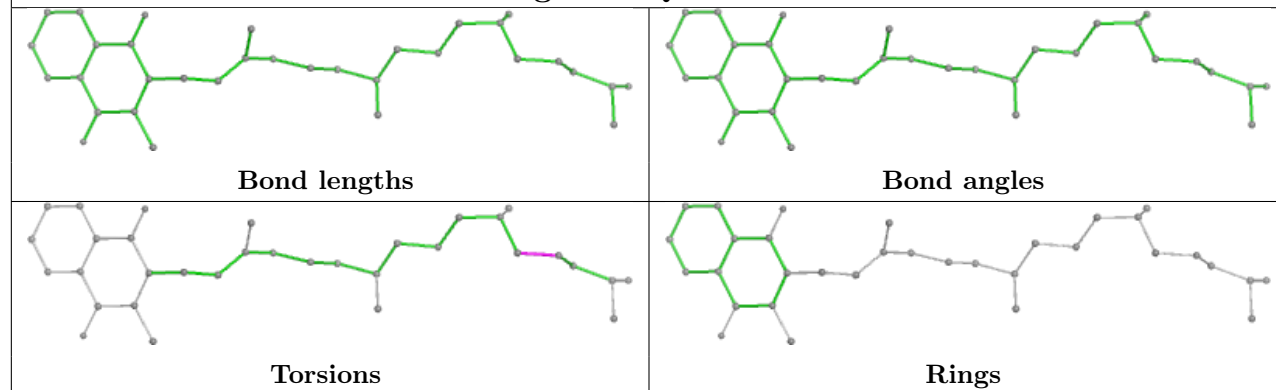




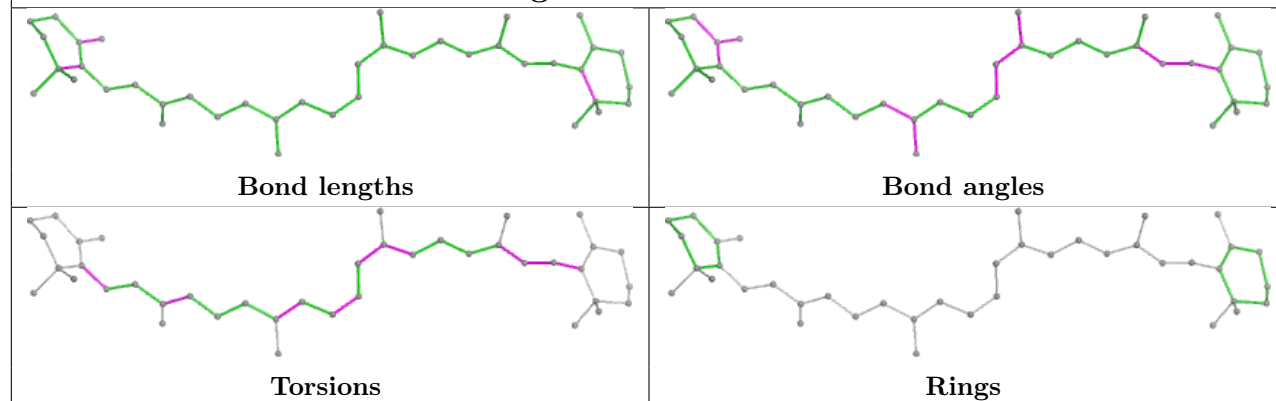
## Ligand CLA A 832

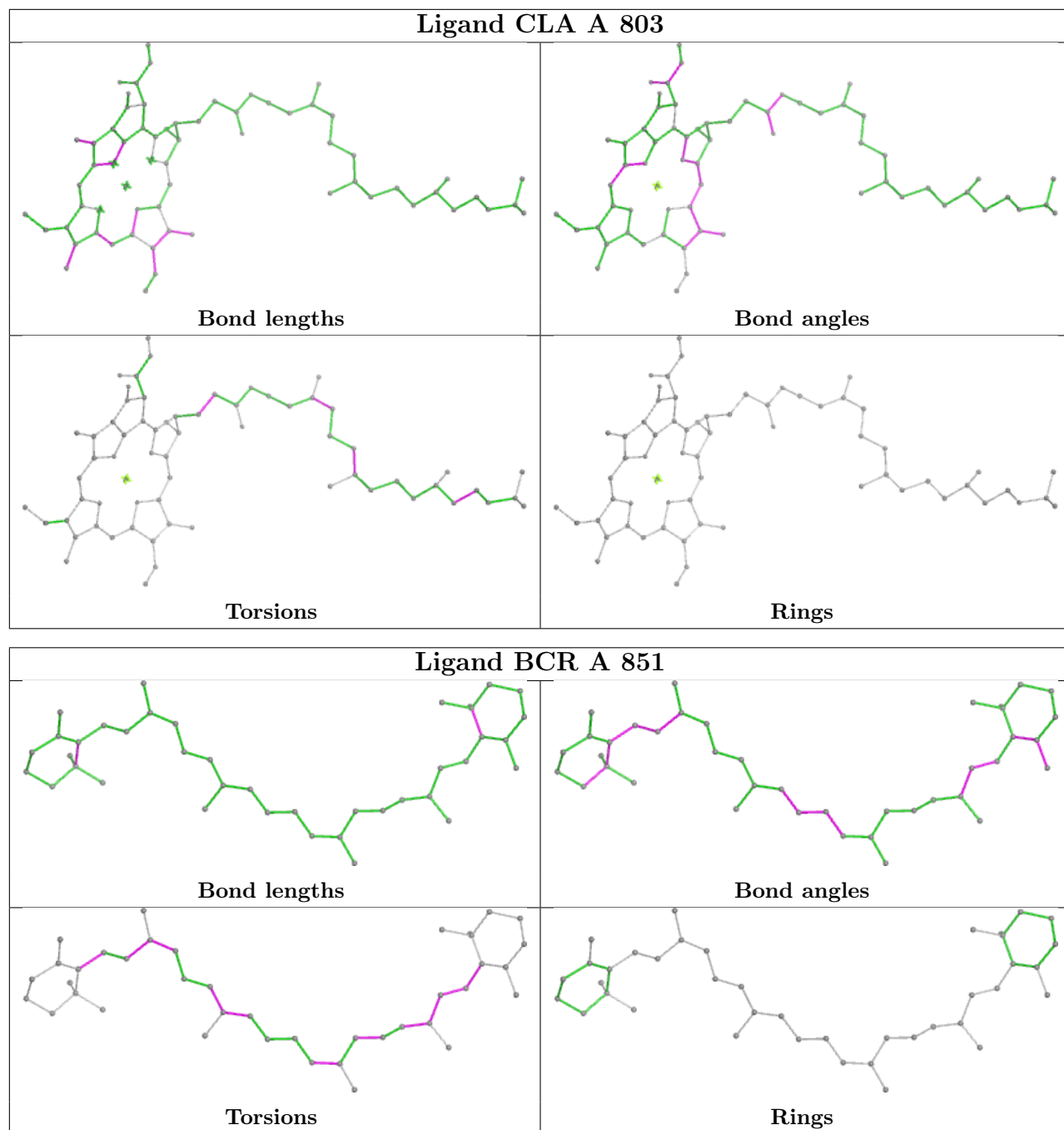


## Ligand PQN a 845



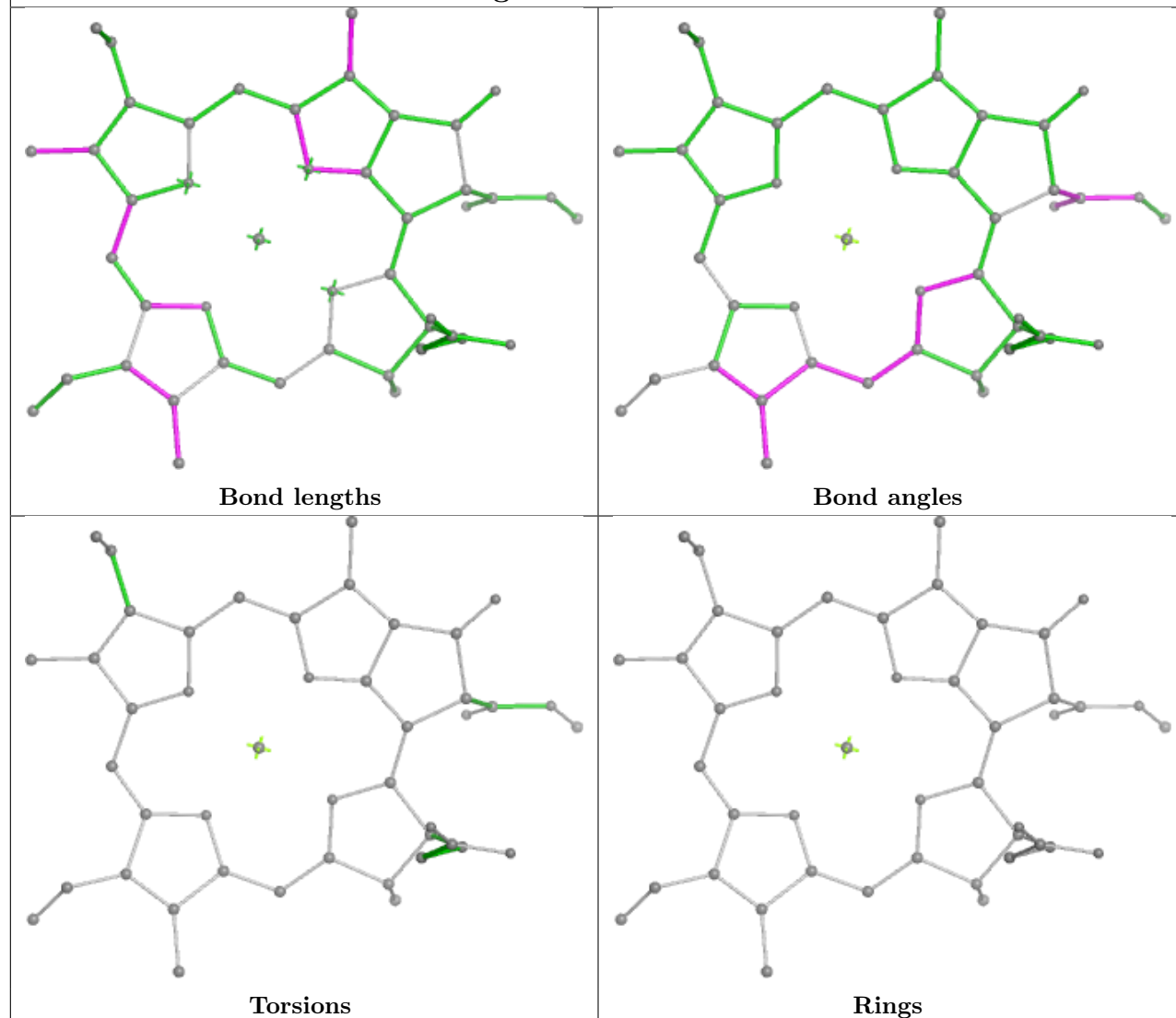
## Ligand BCR B 846



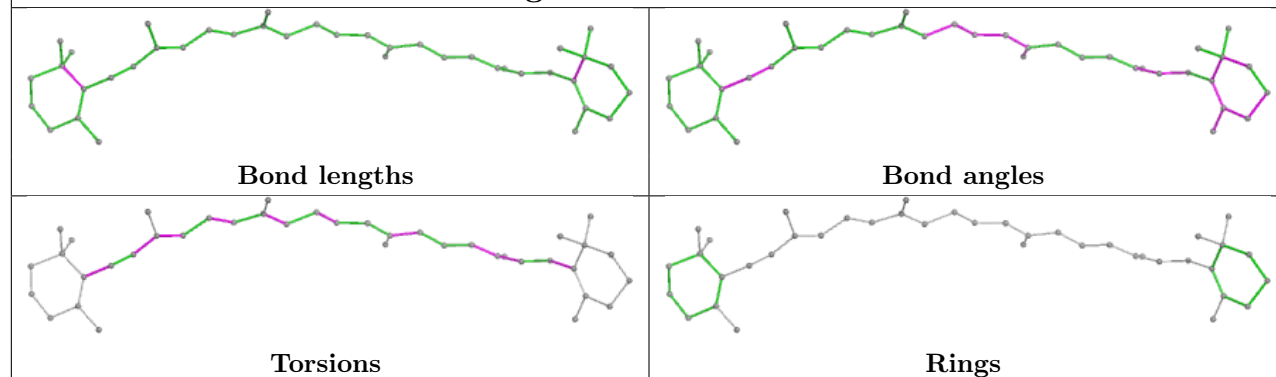


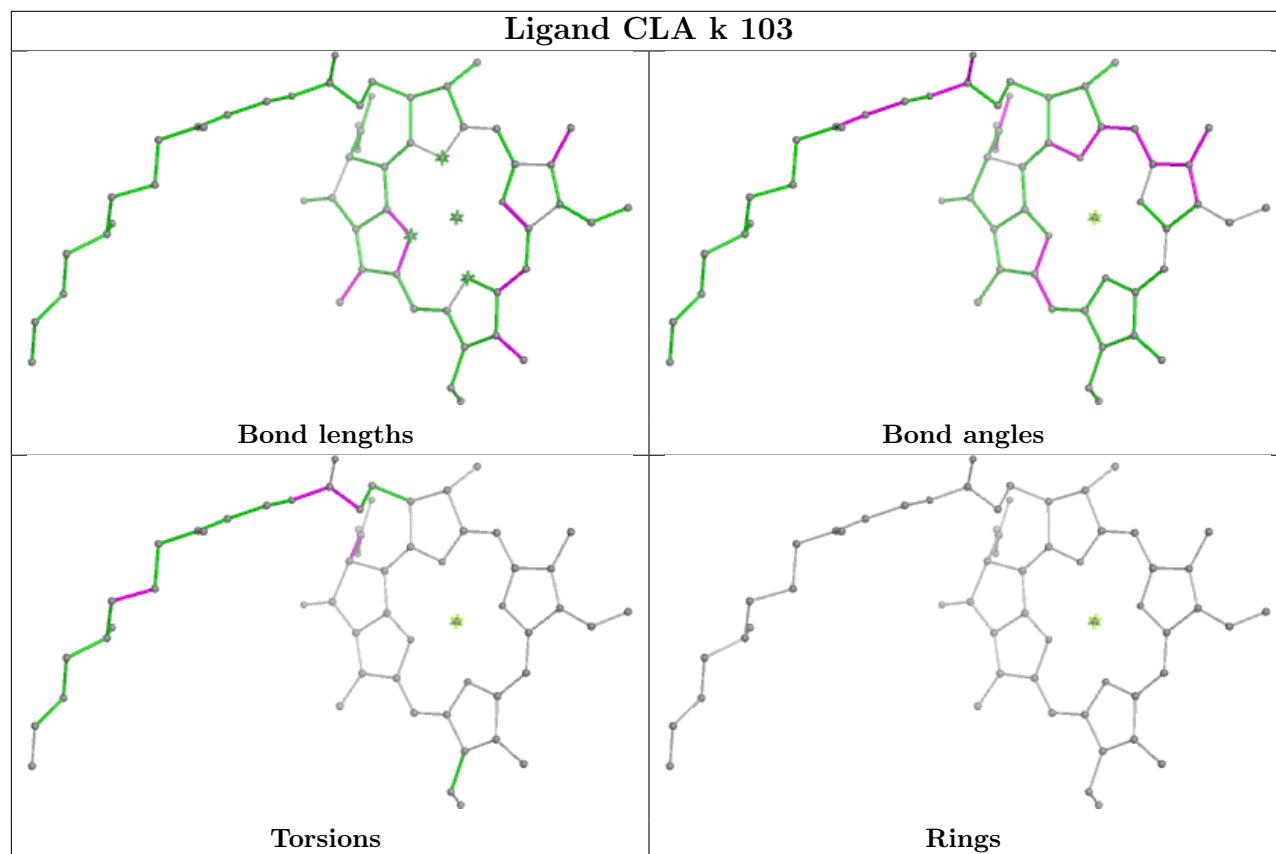


## Ligand CLA b 813

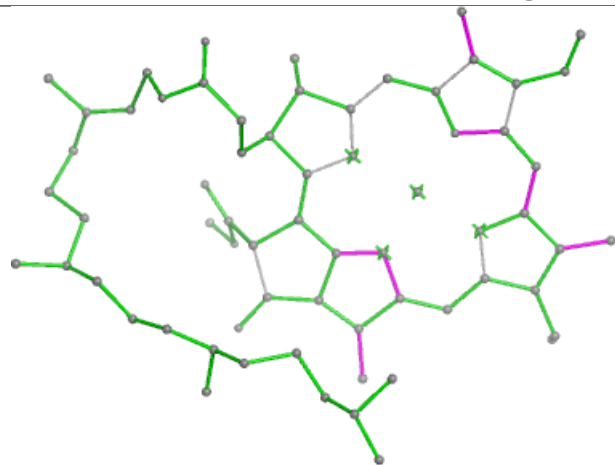


## Ligand BCR 8 1305

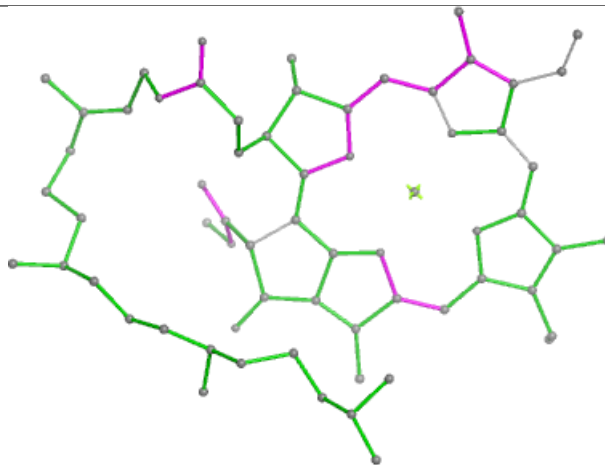




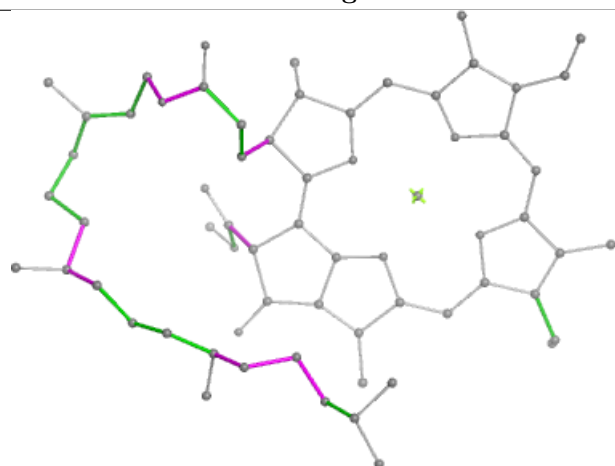
## Ligand CLA 2 806



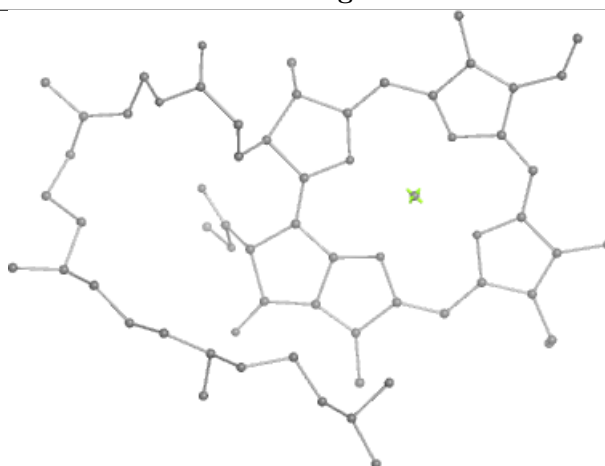
Bond lengths



Bond angles

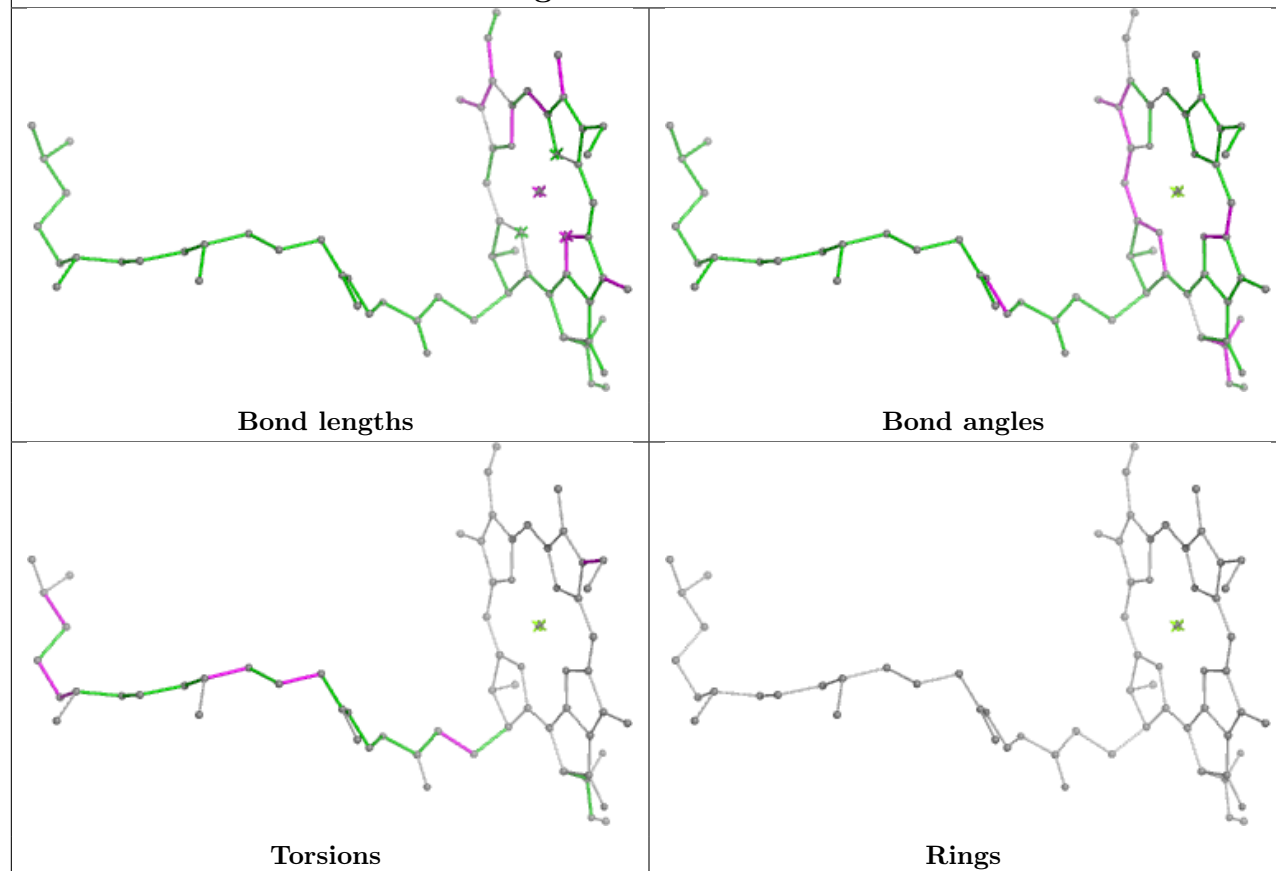


Torsions

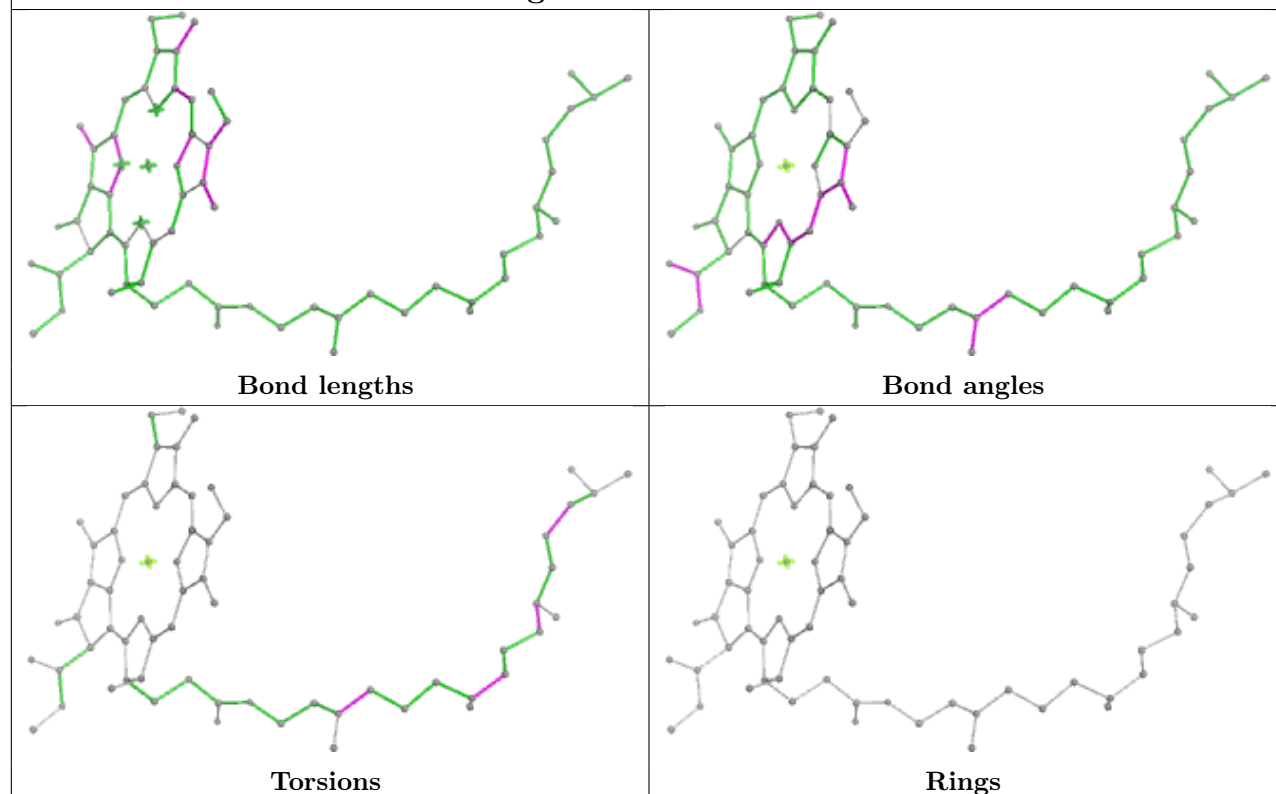


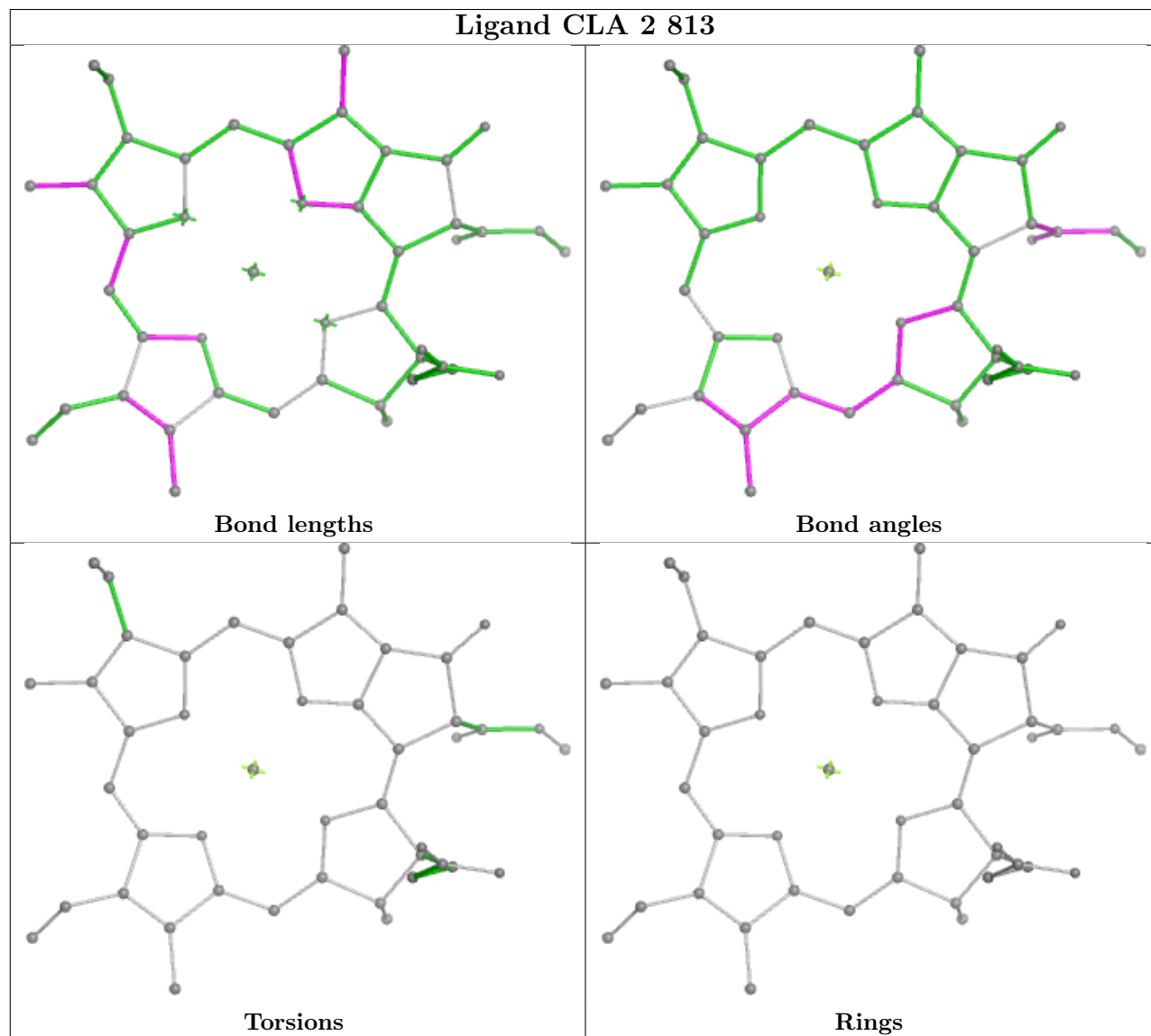
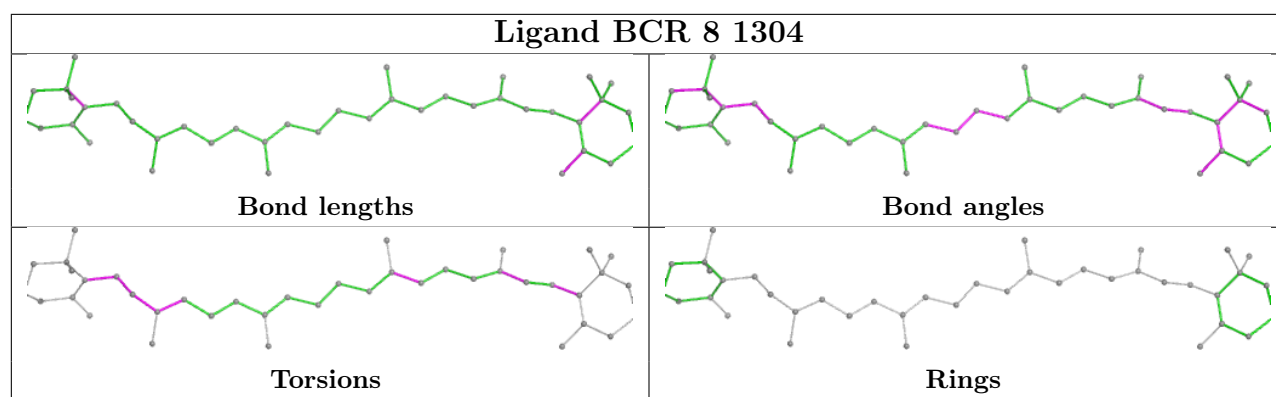
Rings

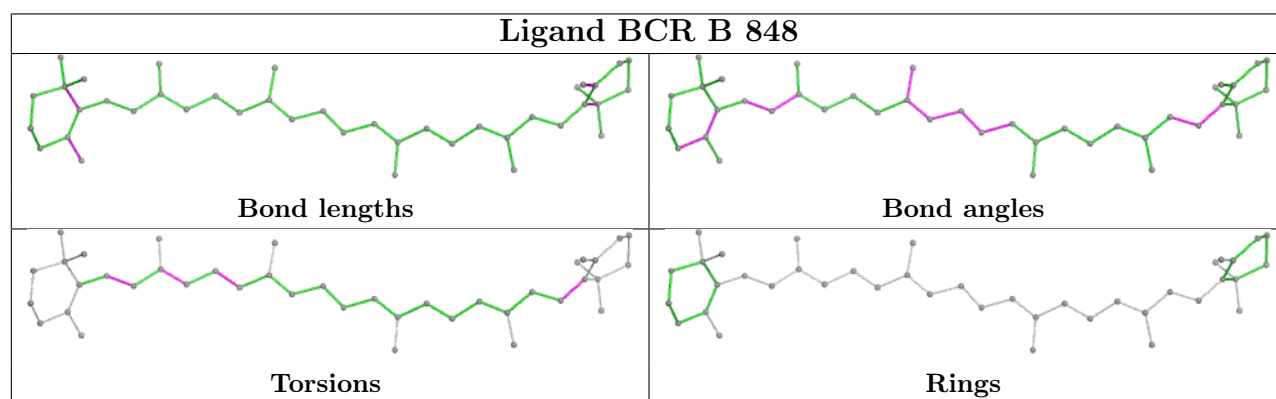
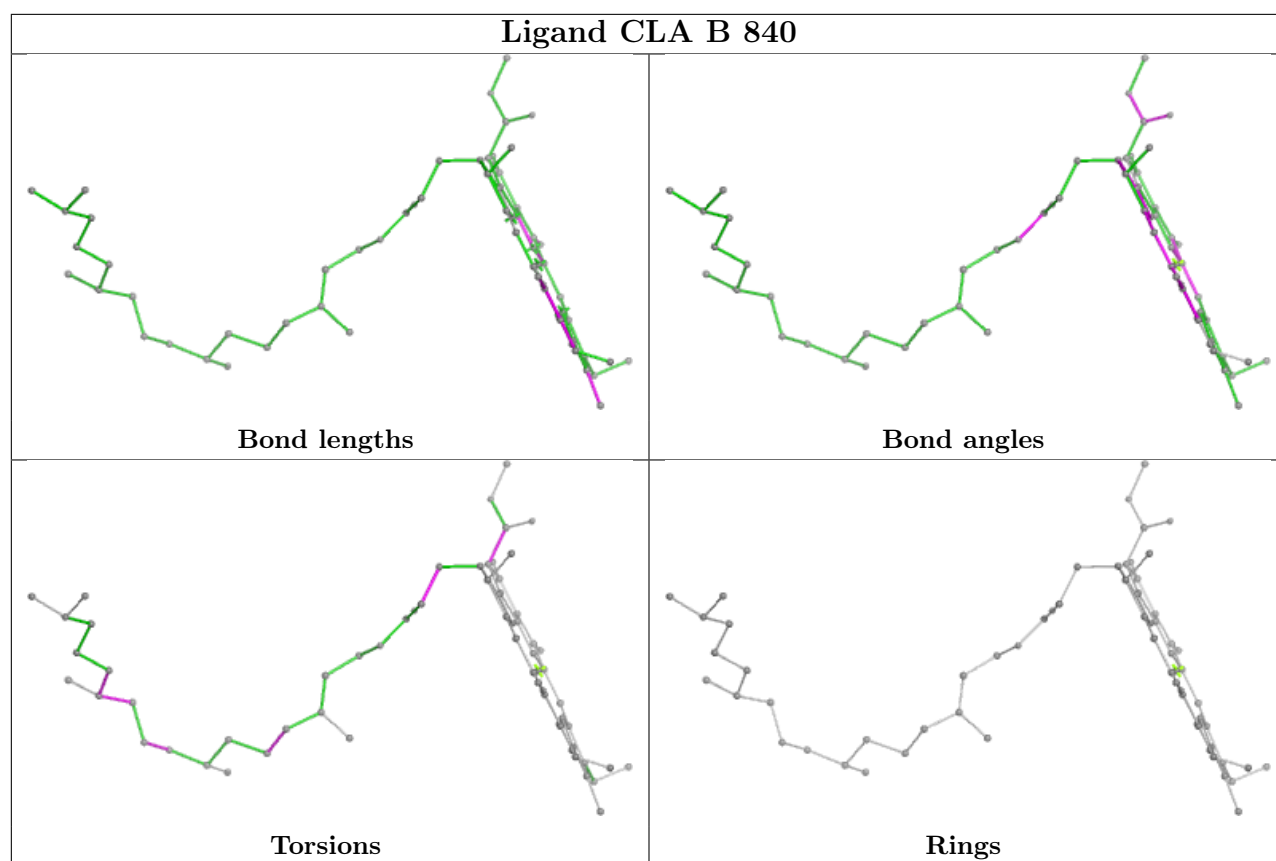
## Ligand CLA L 204



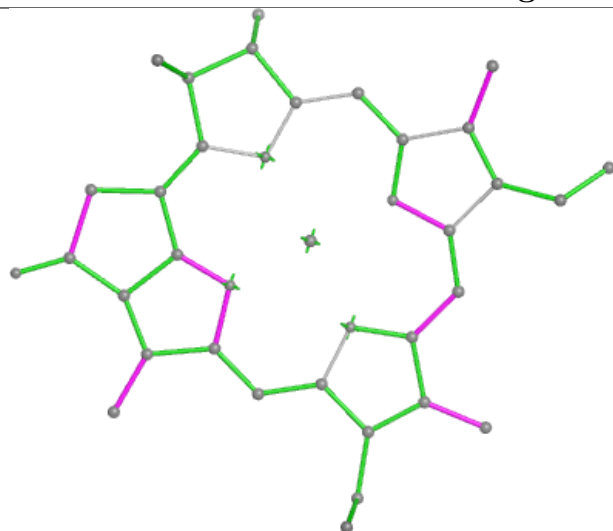
## Ligand CLA 1 1637



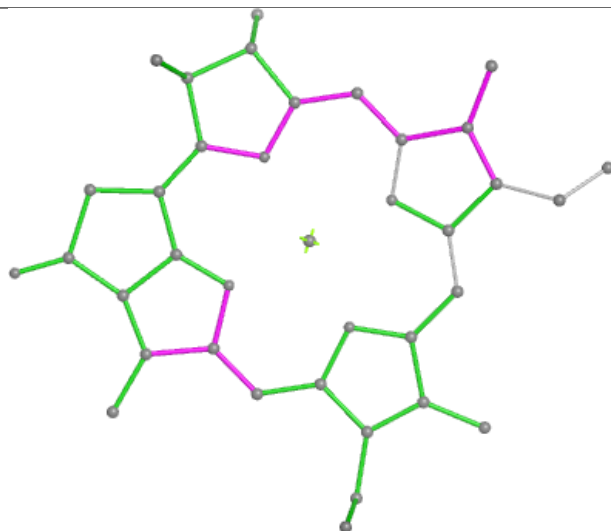




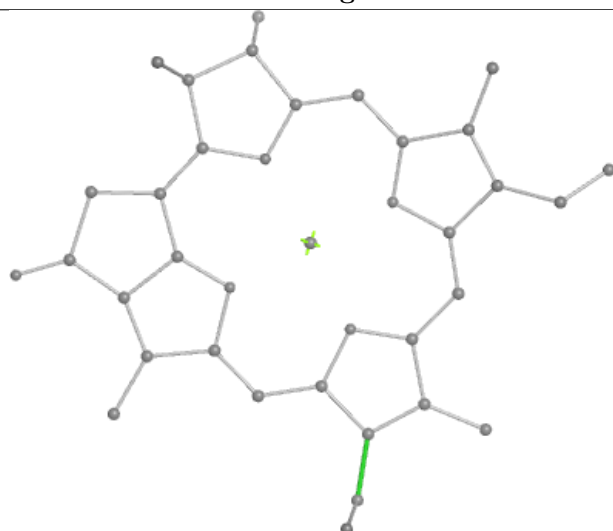
## Ligand CLA J 102



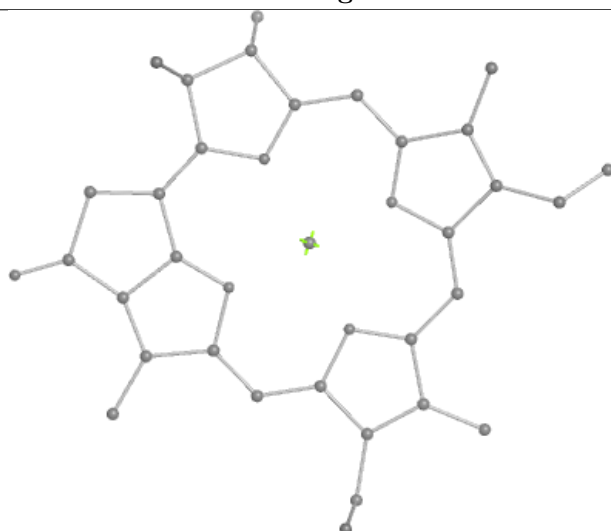
Bond lengths



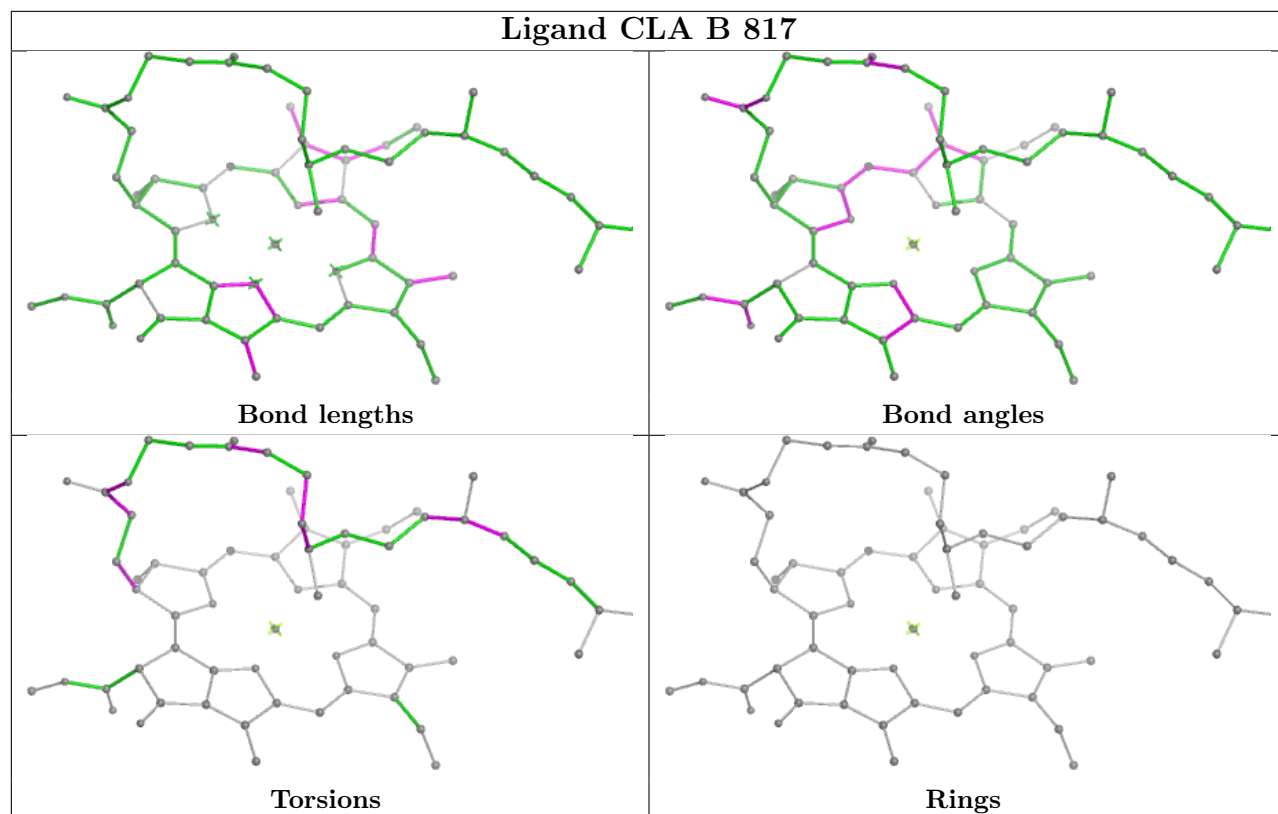
Bond angles



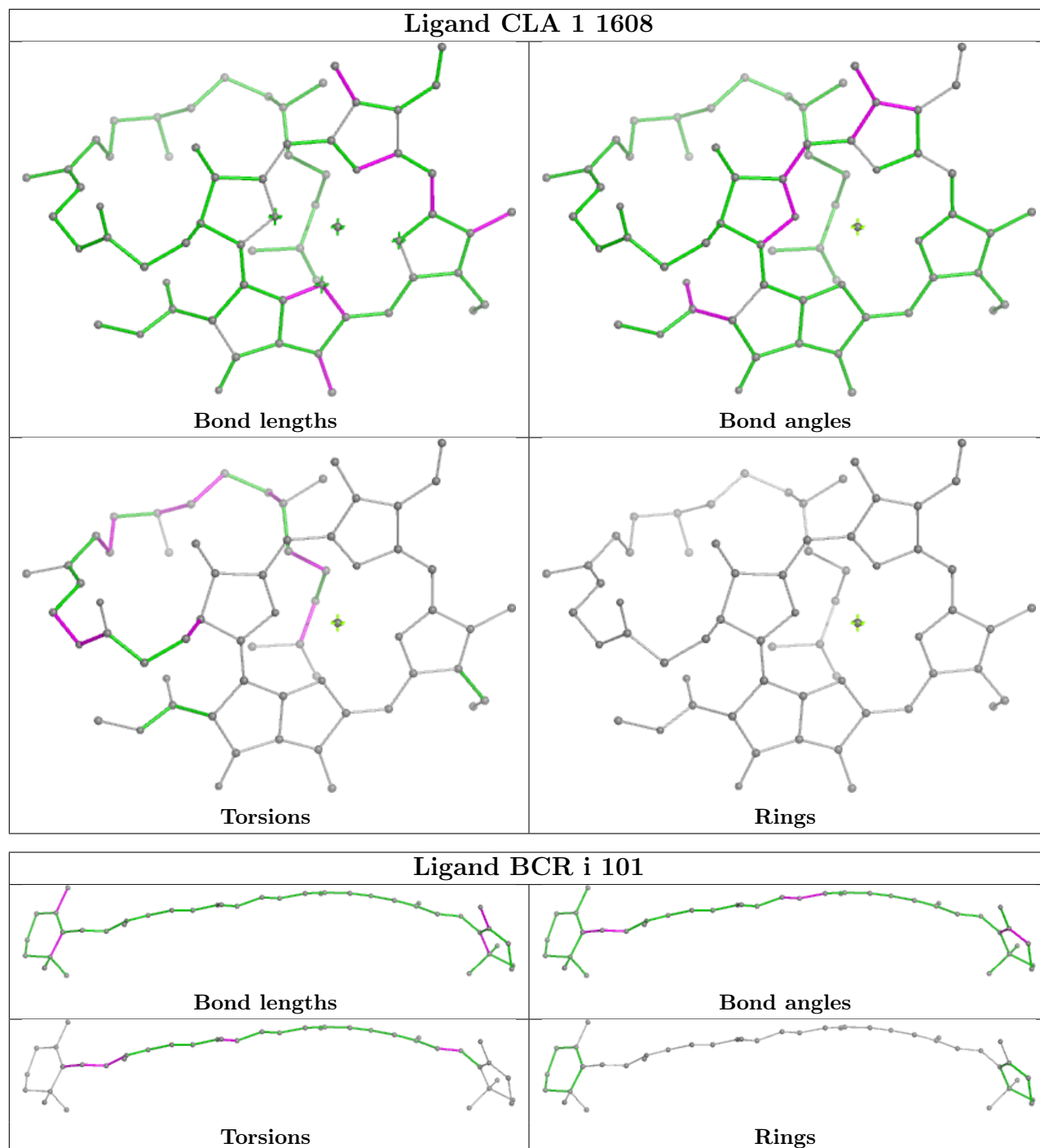
Torsions

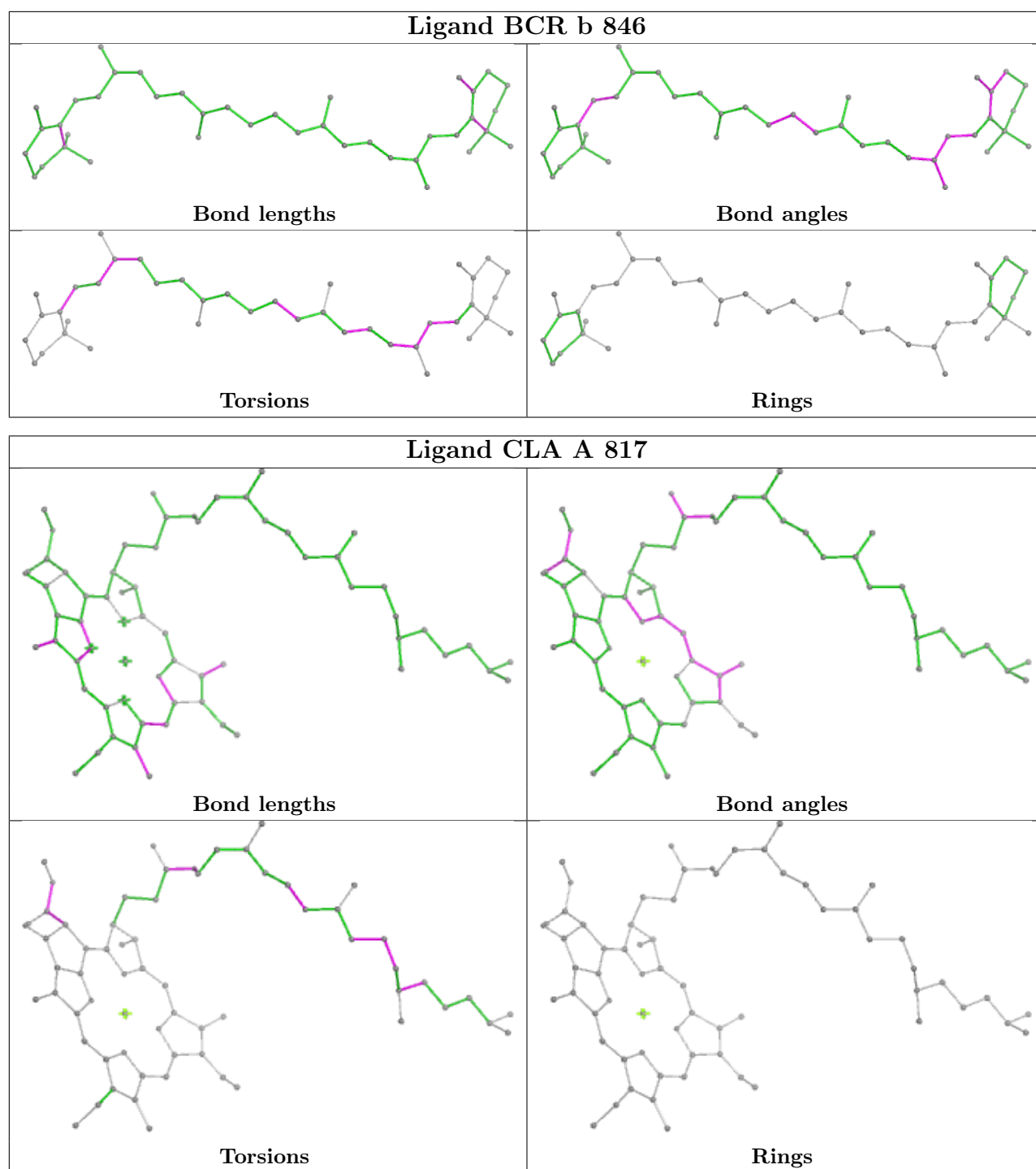


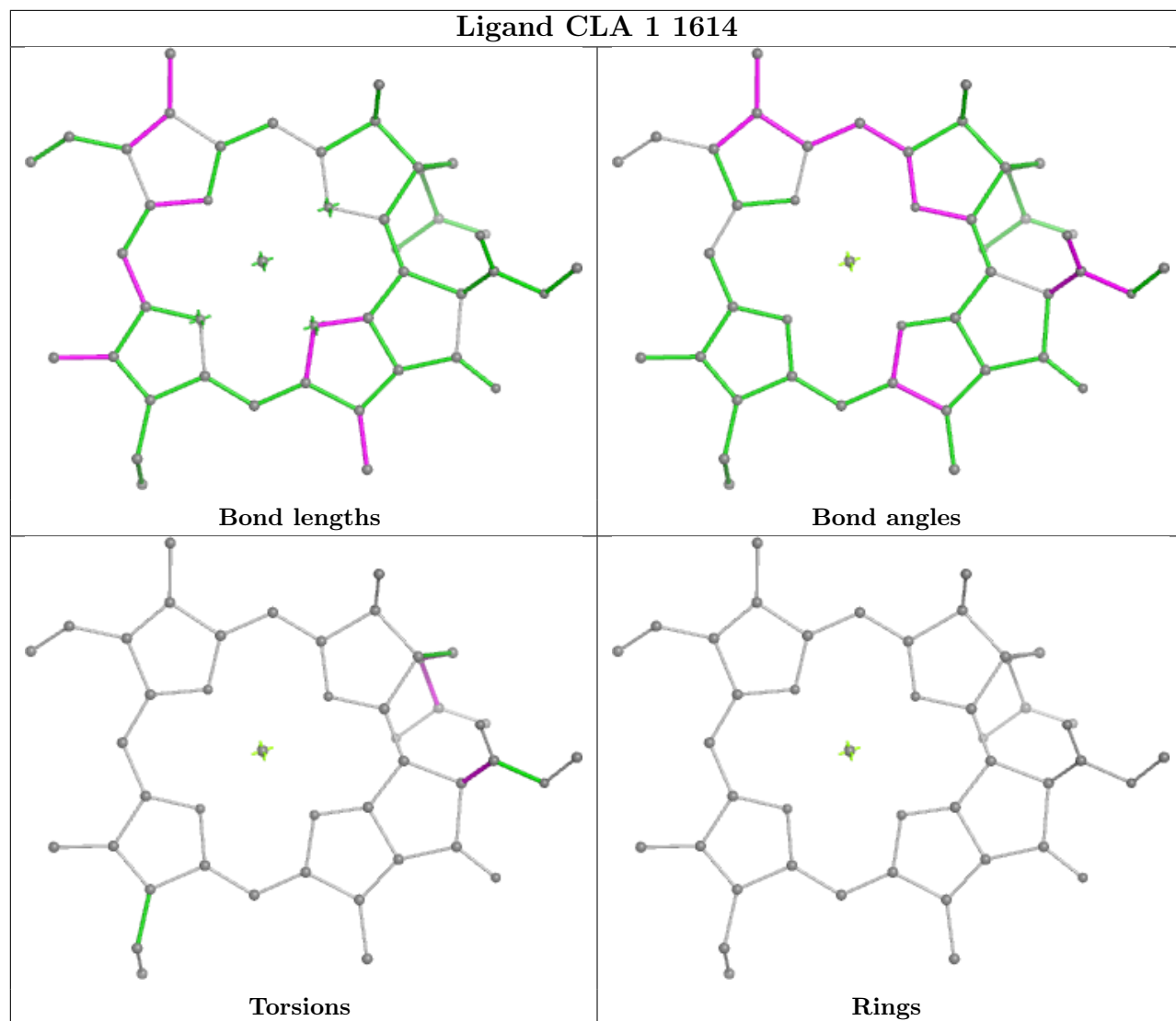
Rings

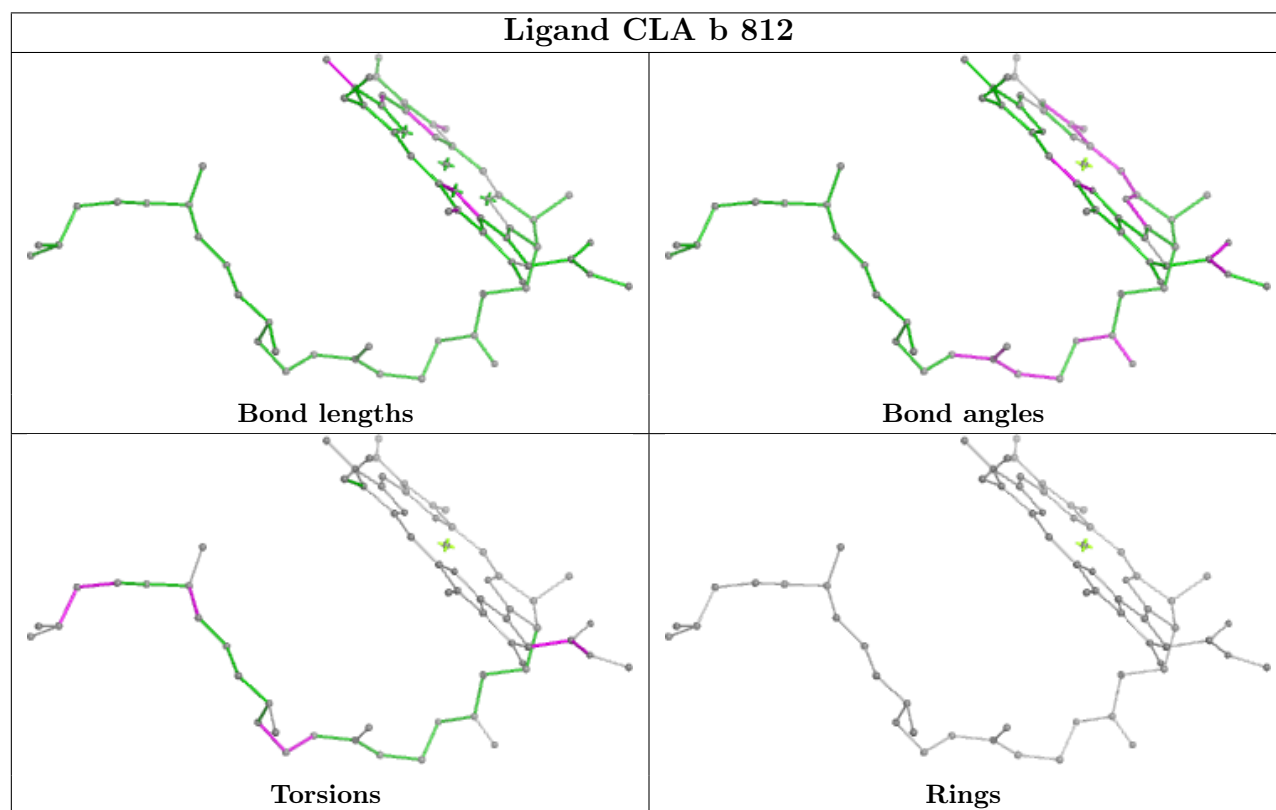
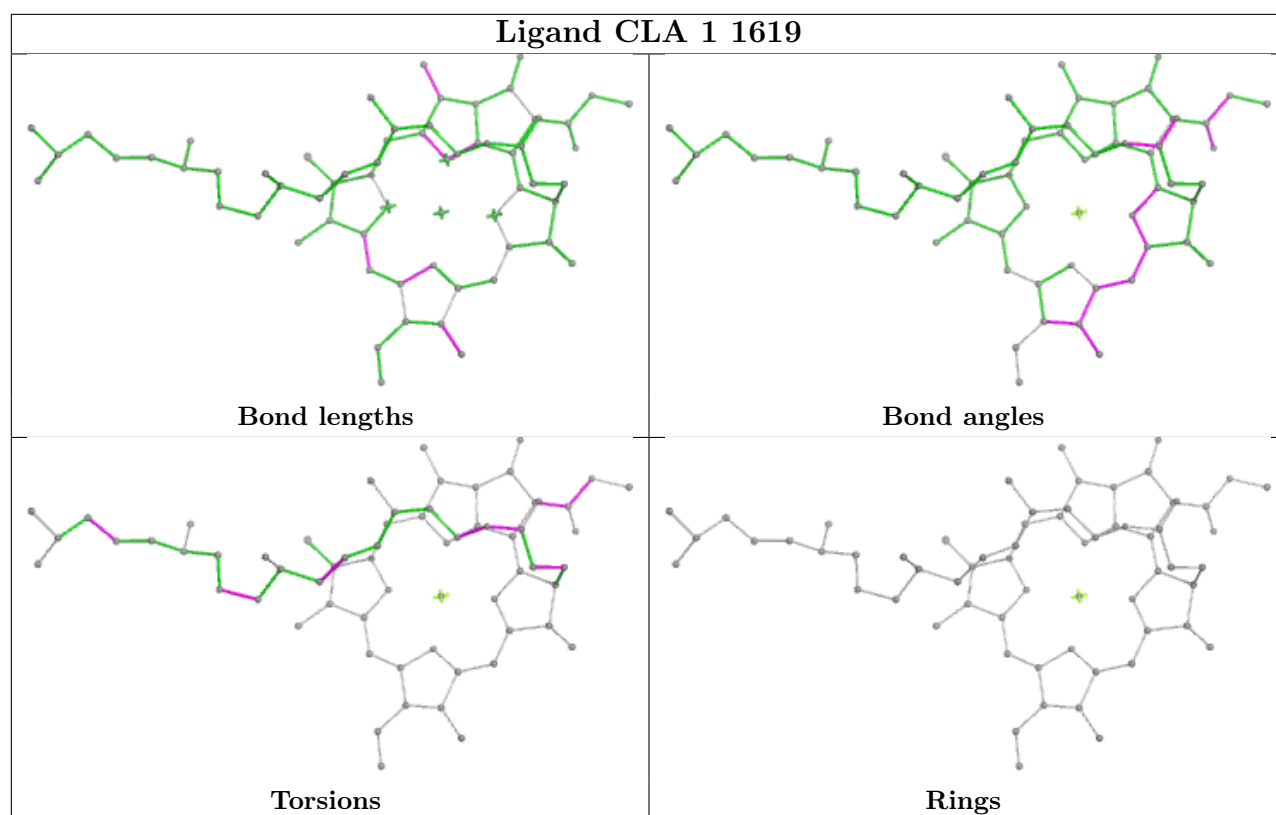


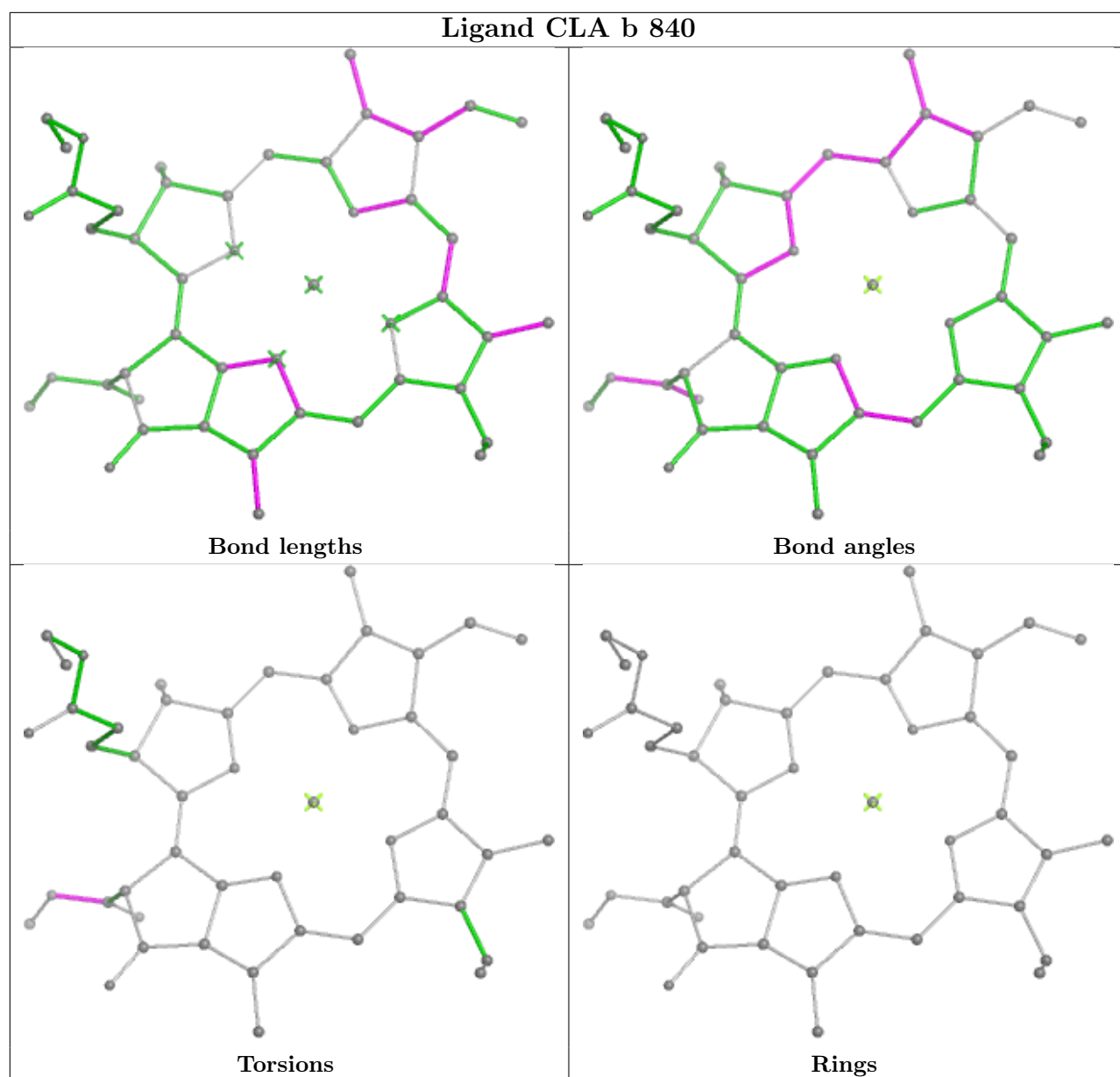


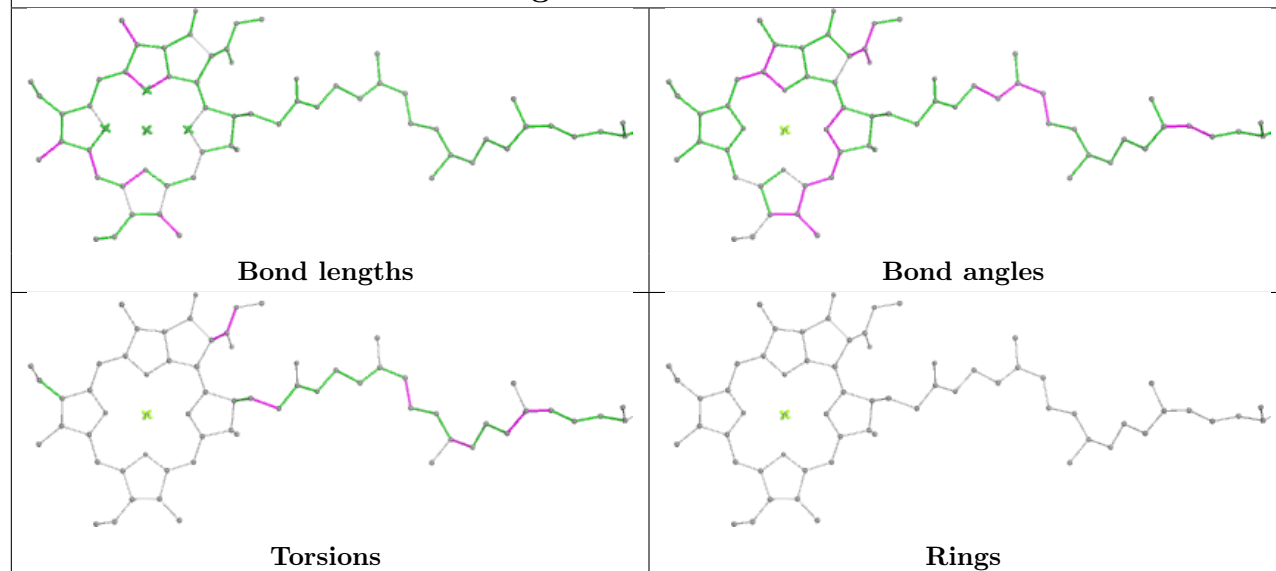
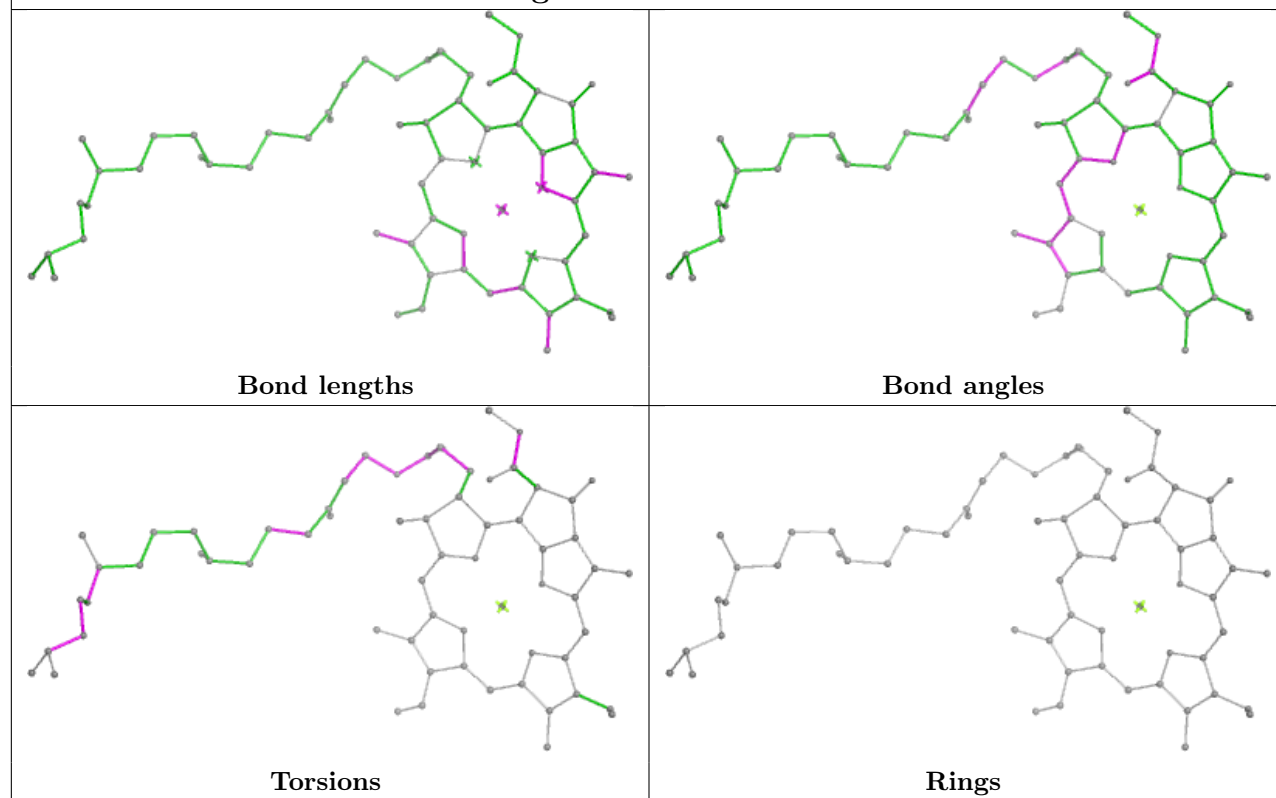


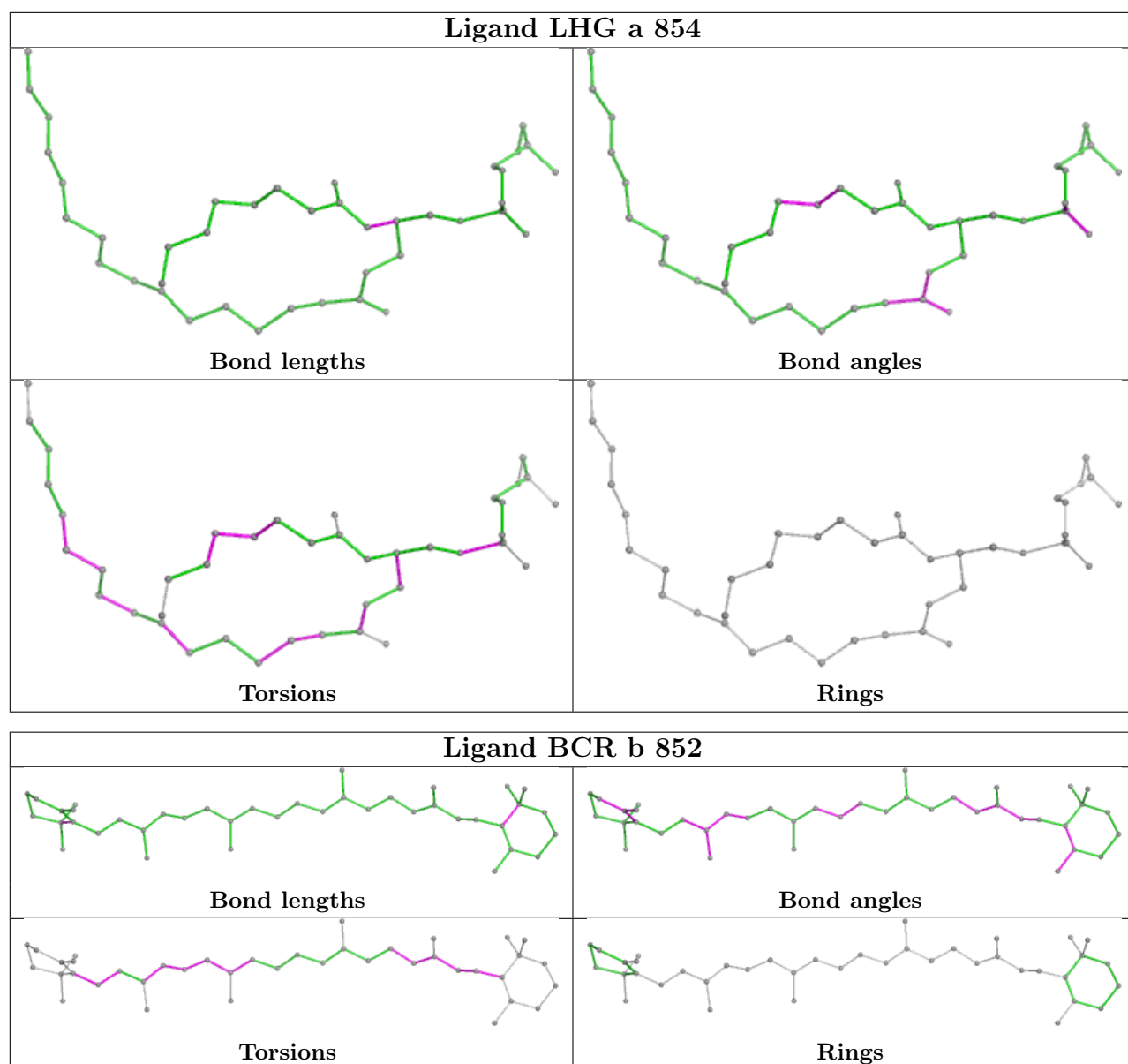


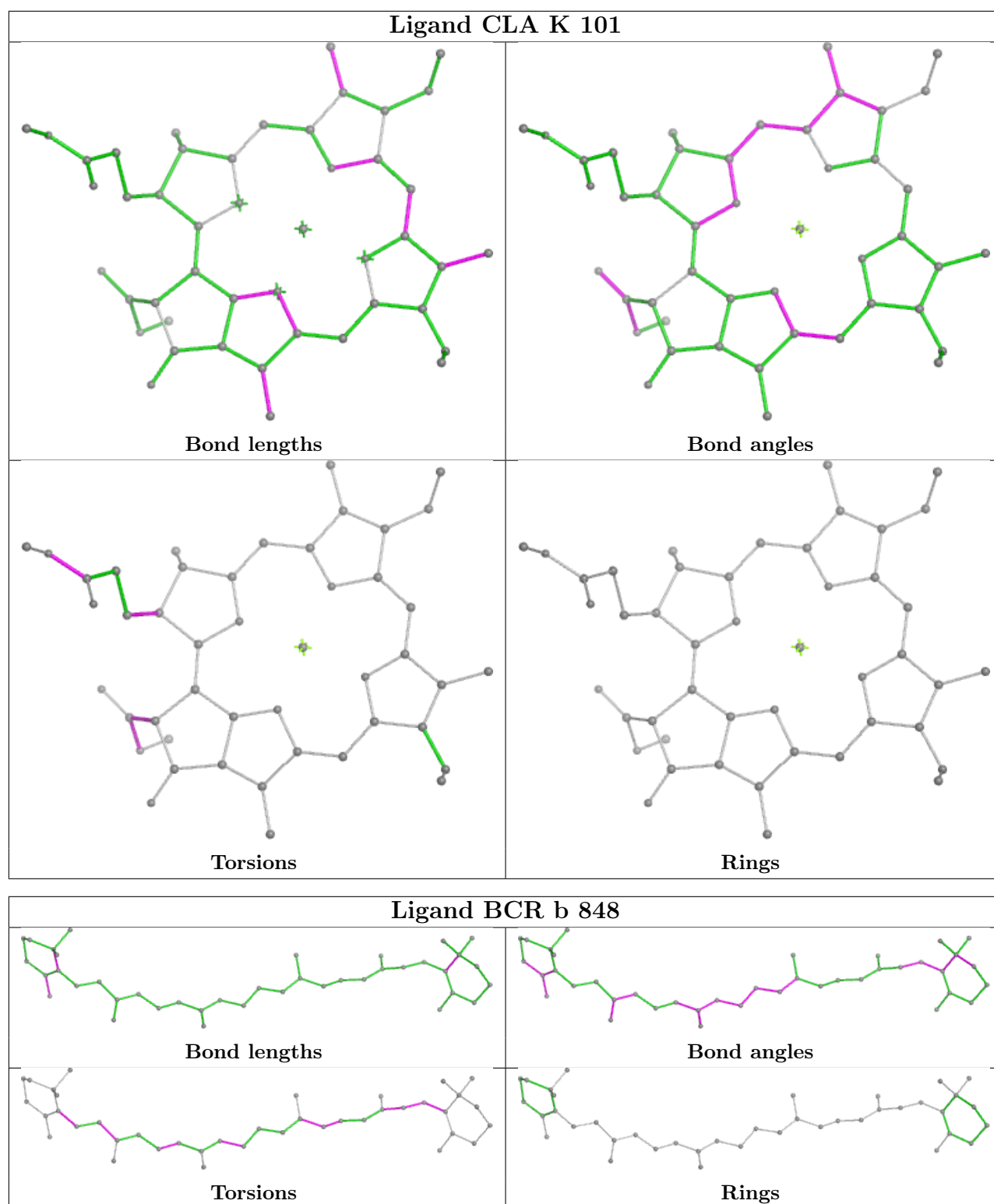






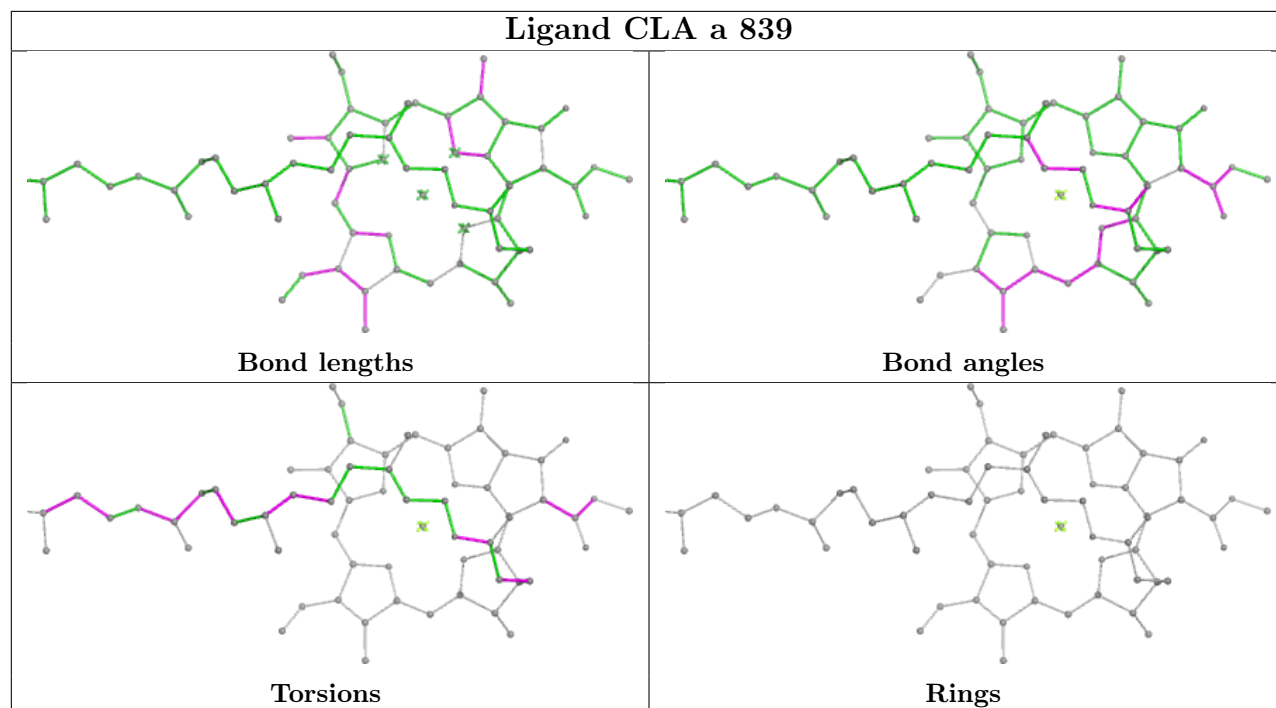
**Ligand CLA A 834****Ligand CLA A 802**



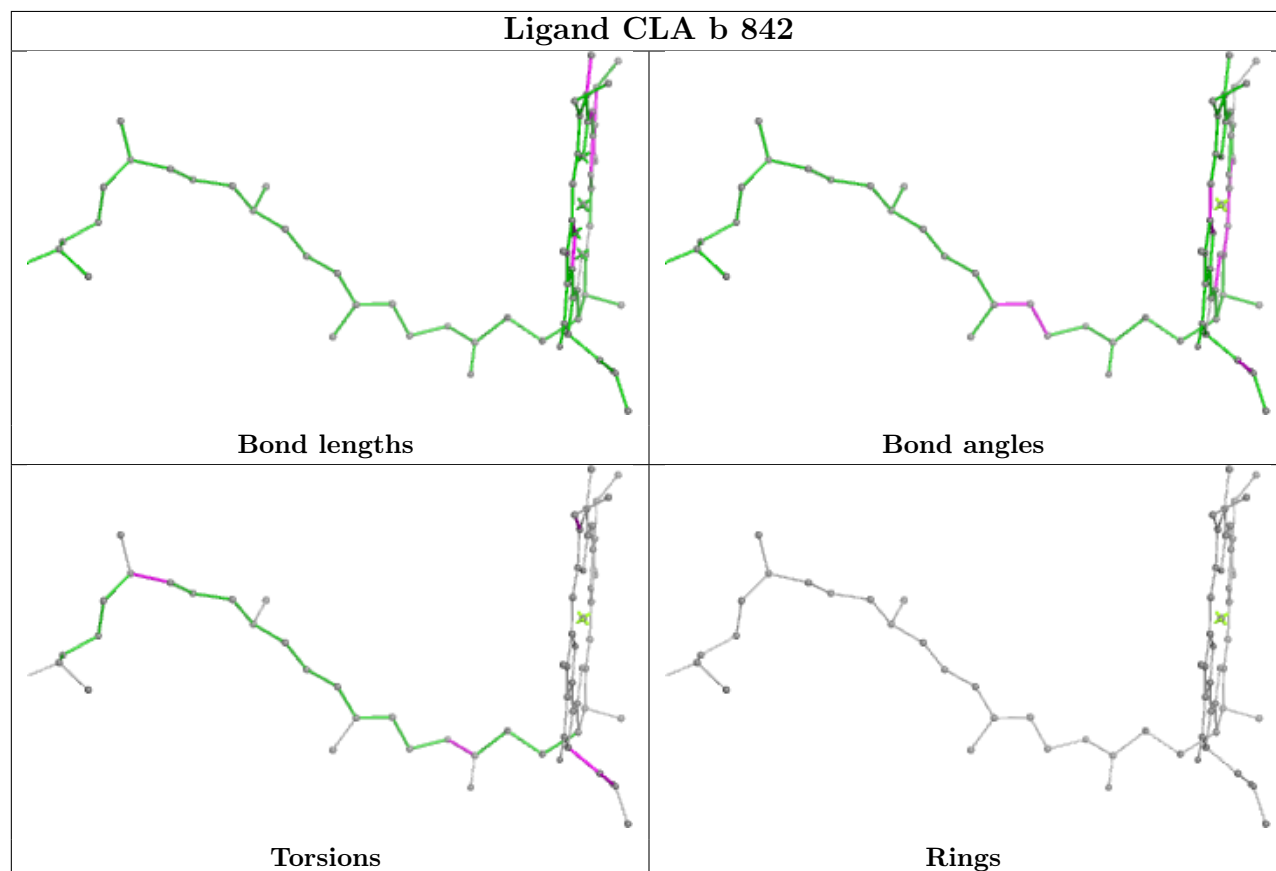


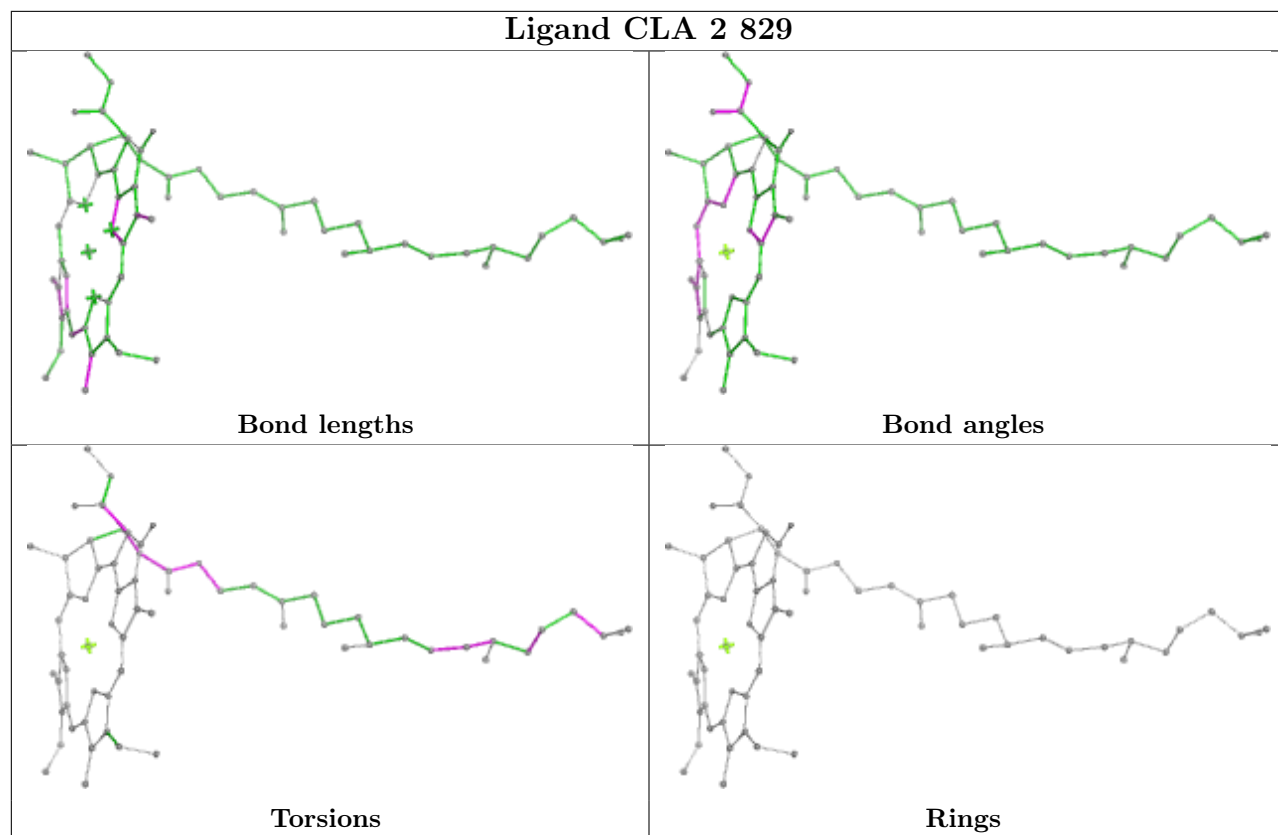


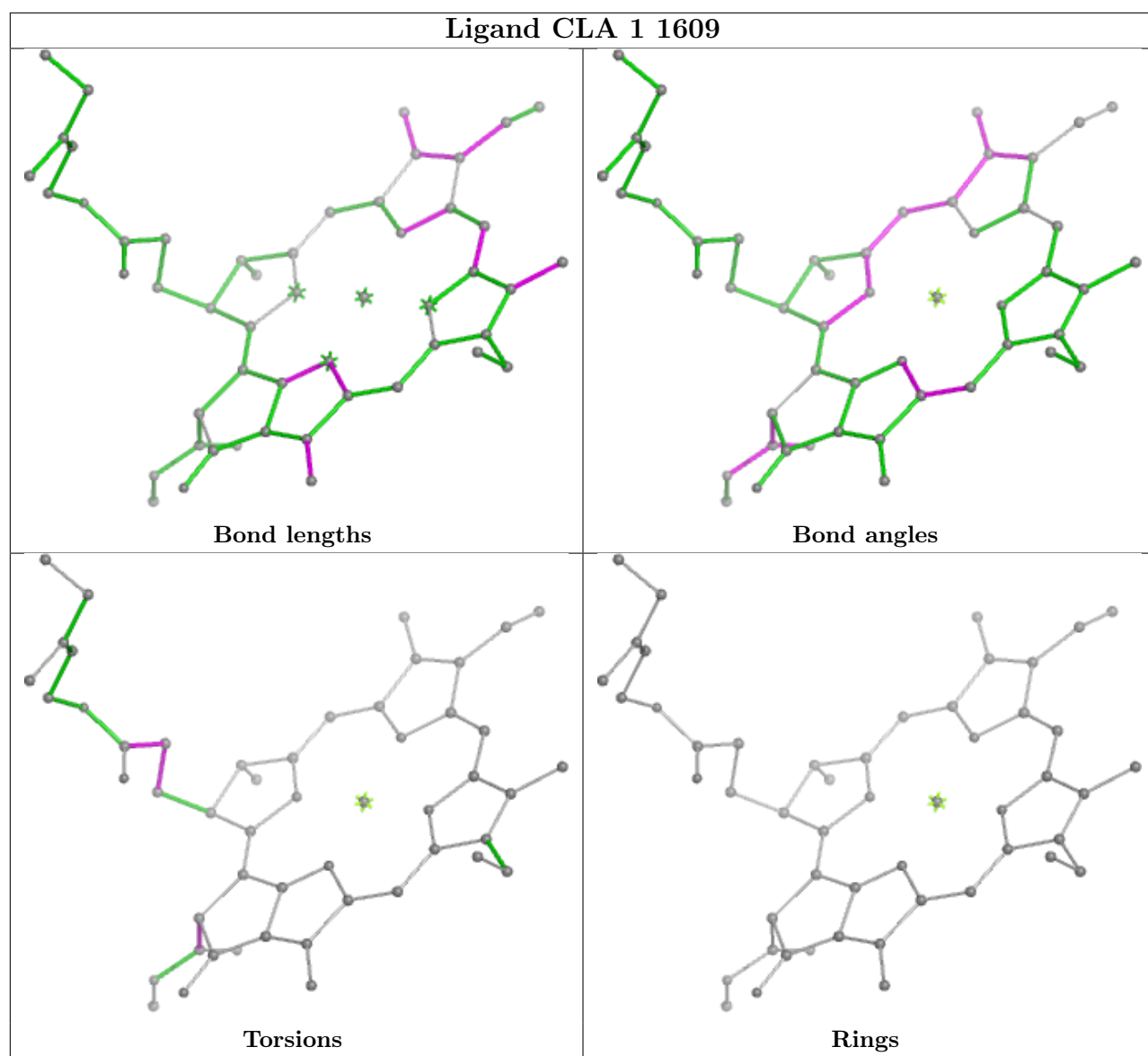
## Ligand CLA a 839

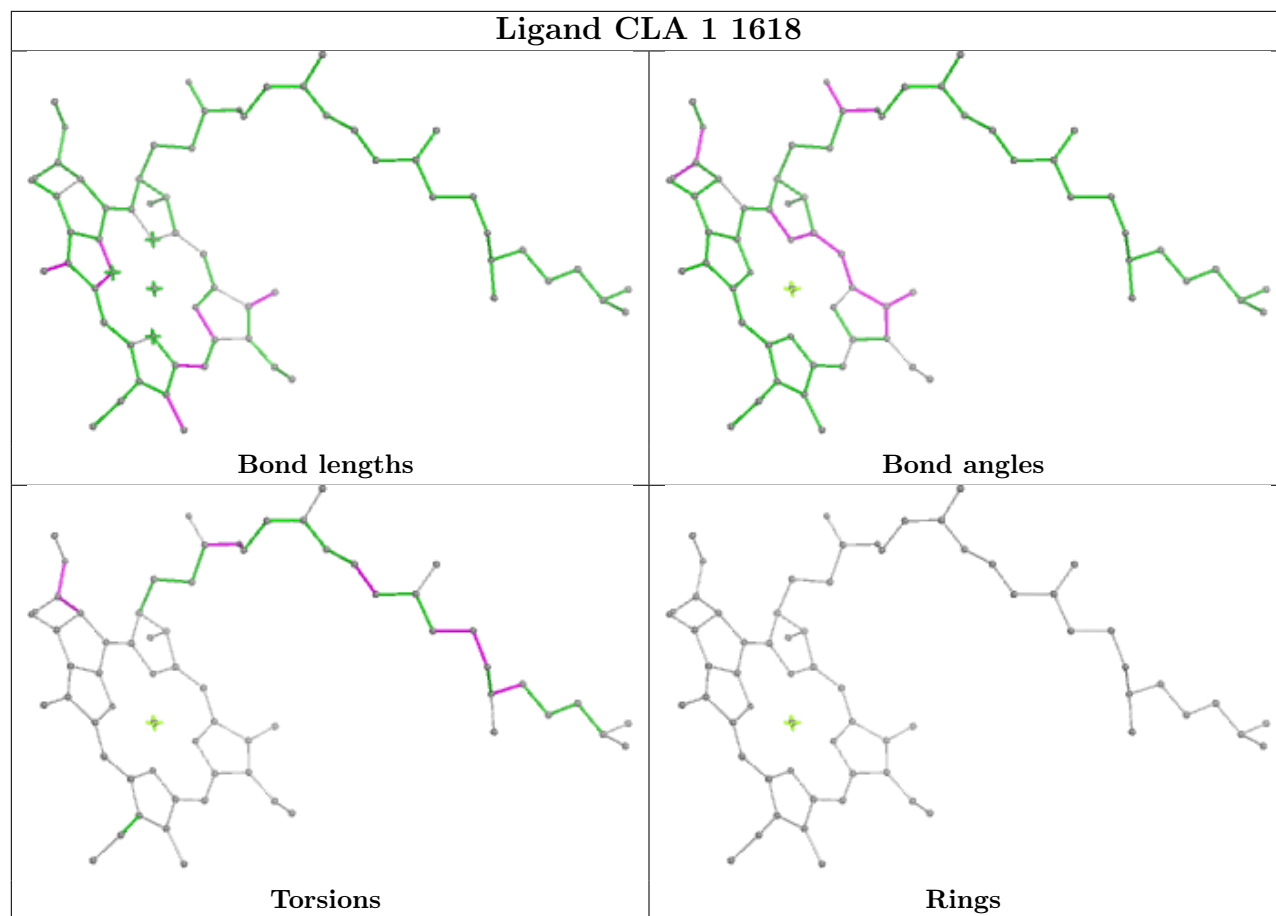


## Ligand CLA b 842

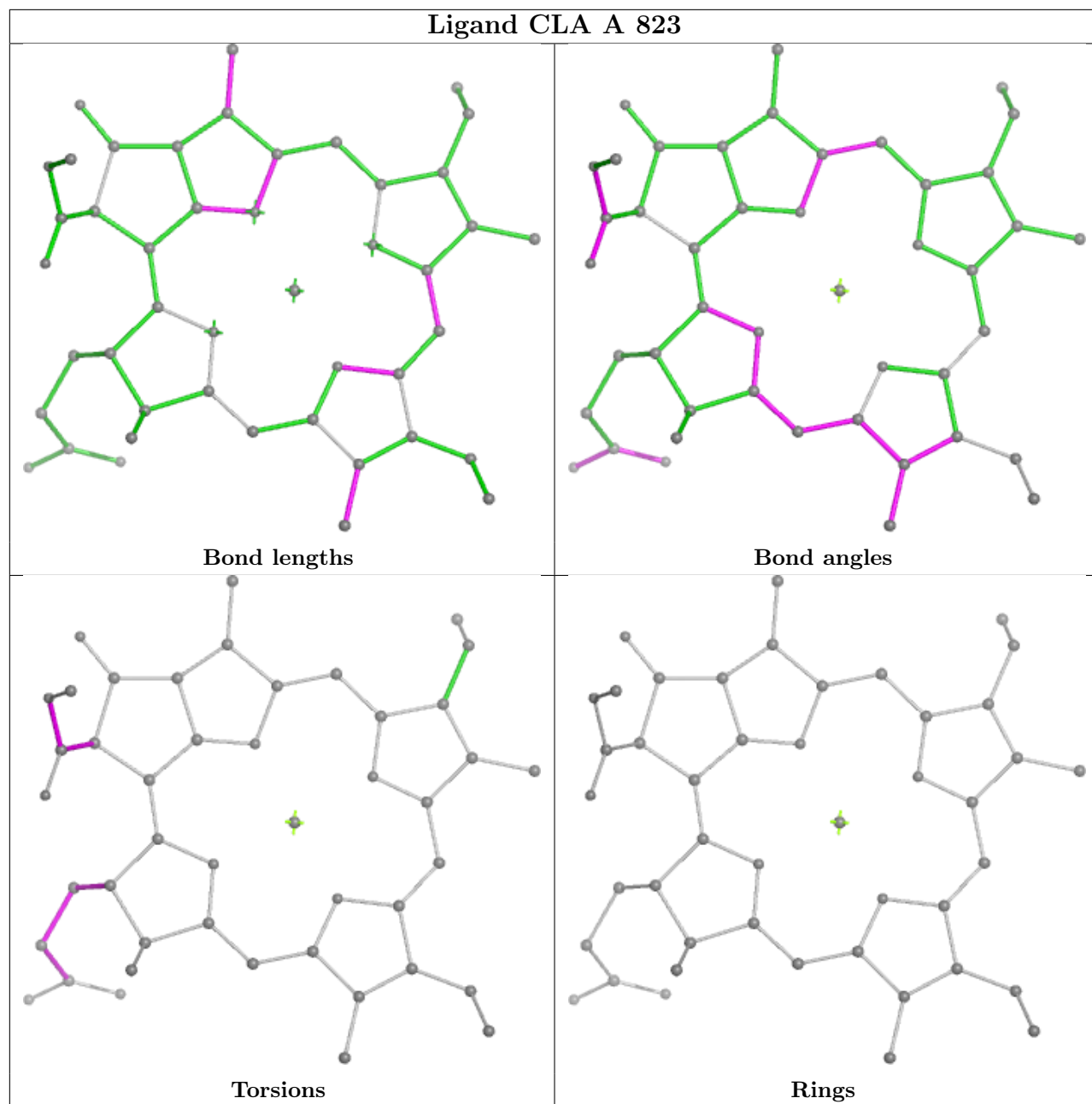


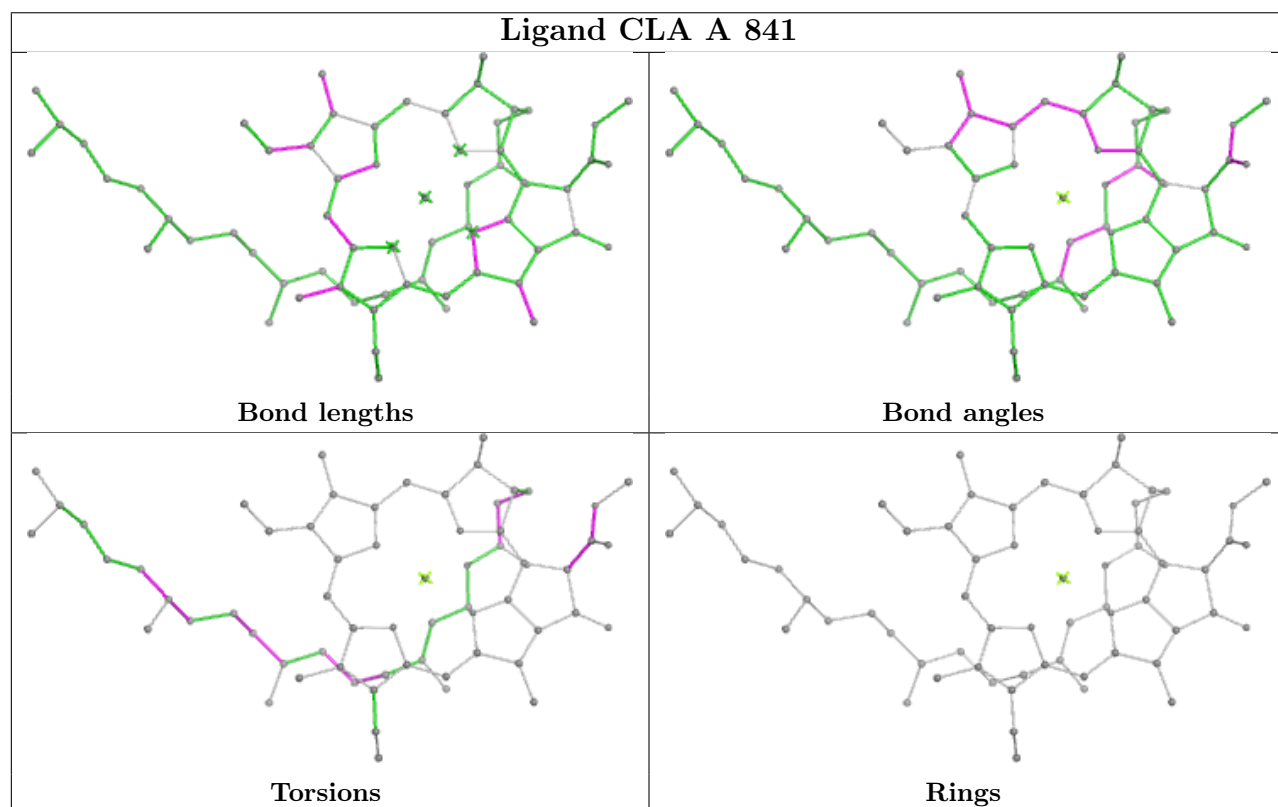
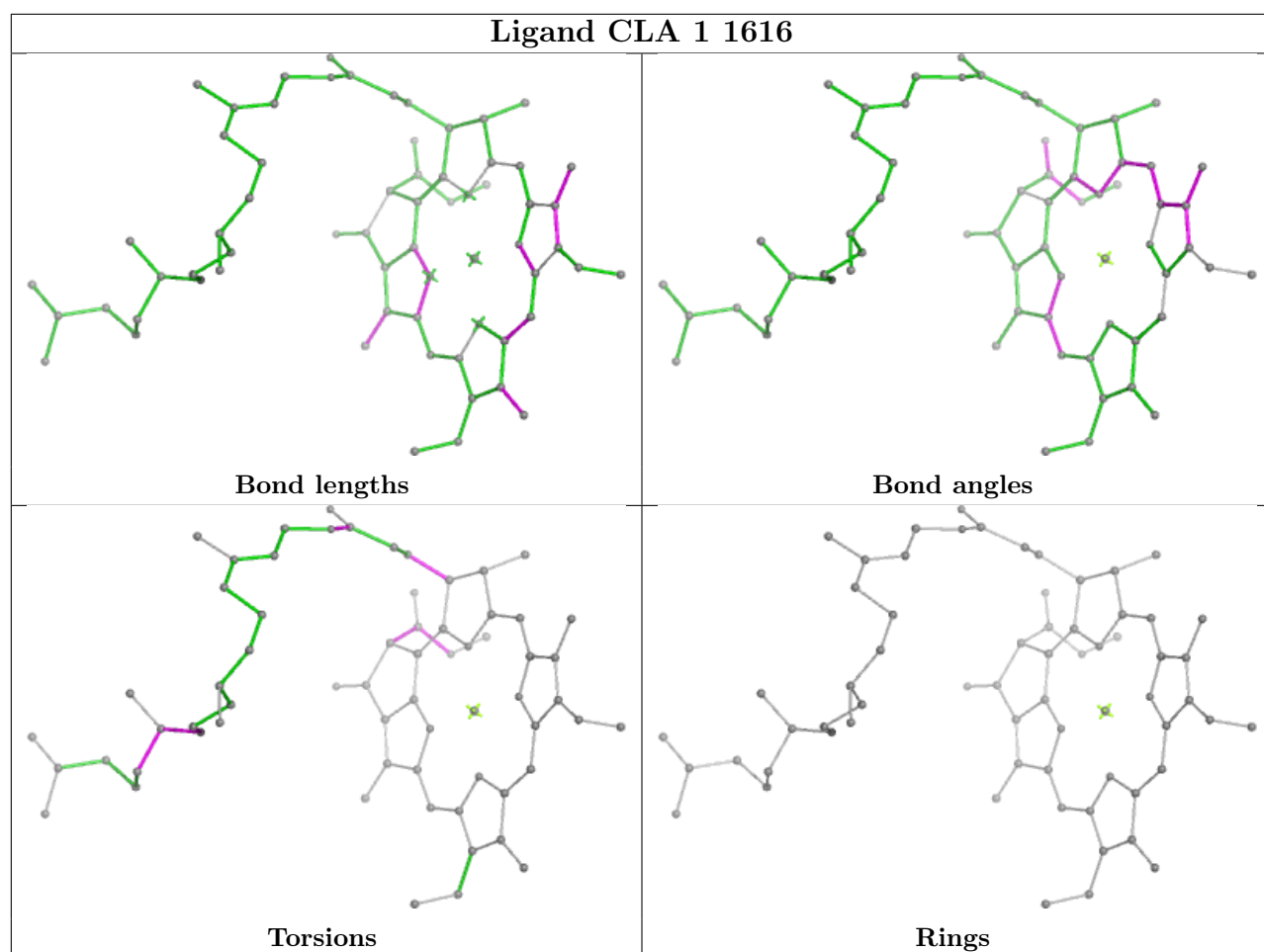




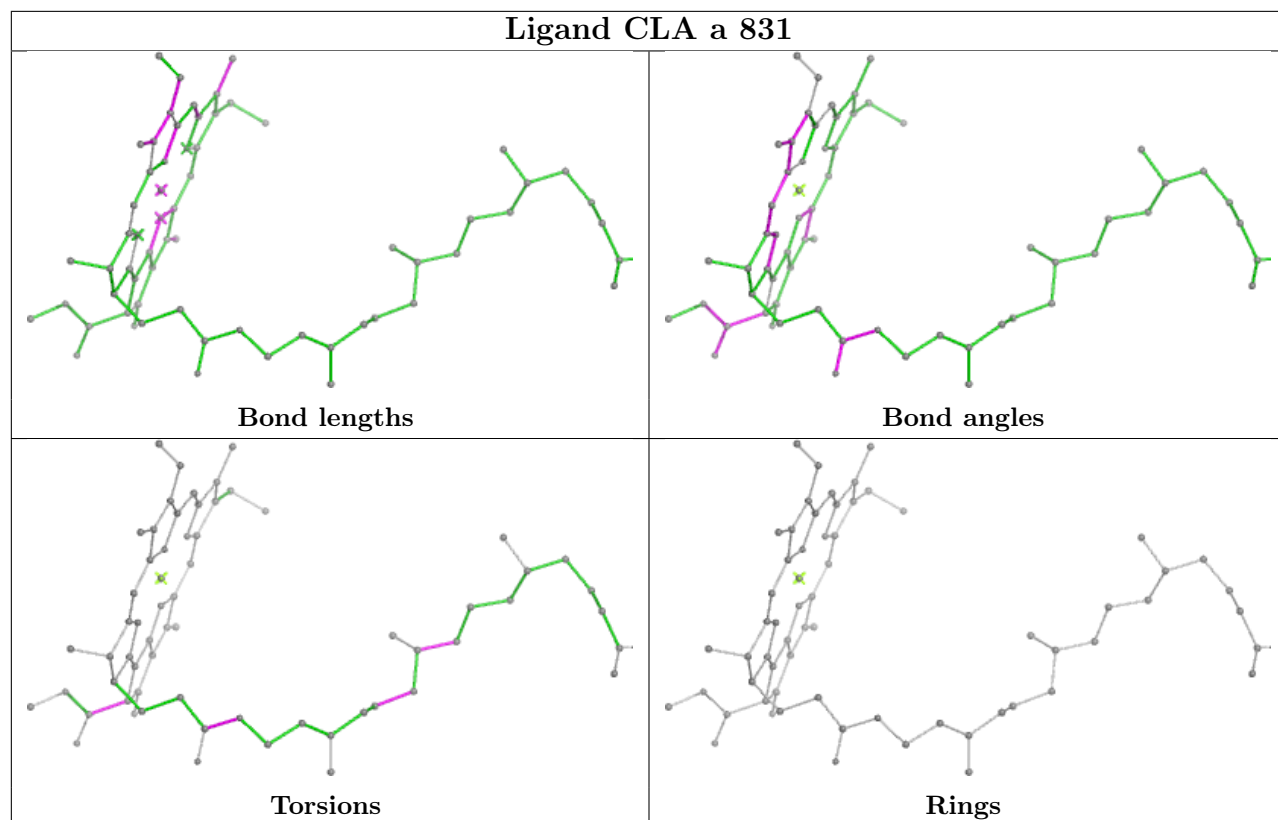


## Ligand CLA A 823

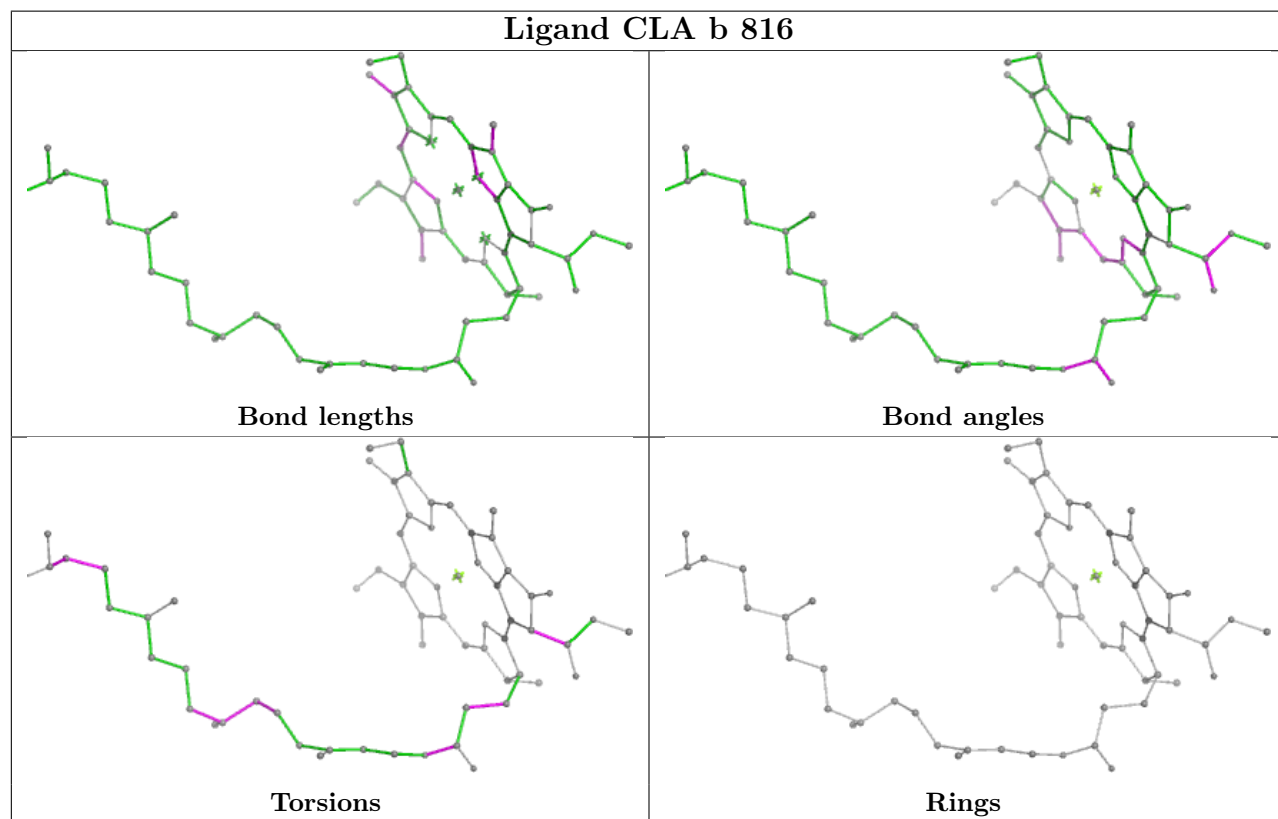




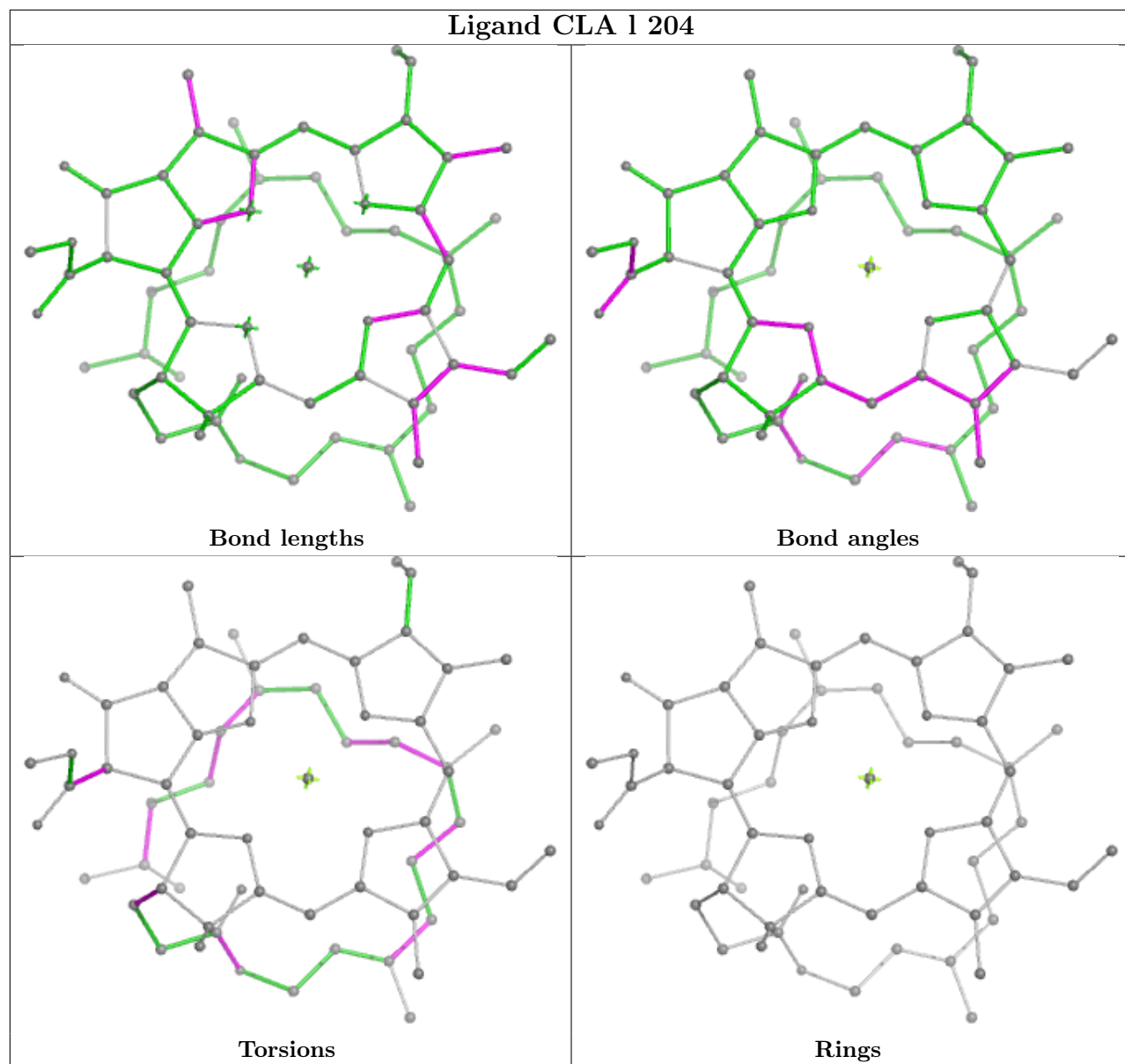
## Ligand CLA a 831



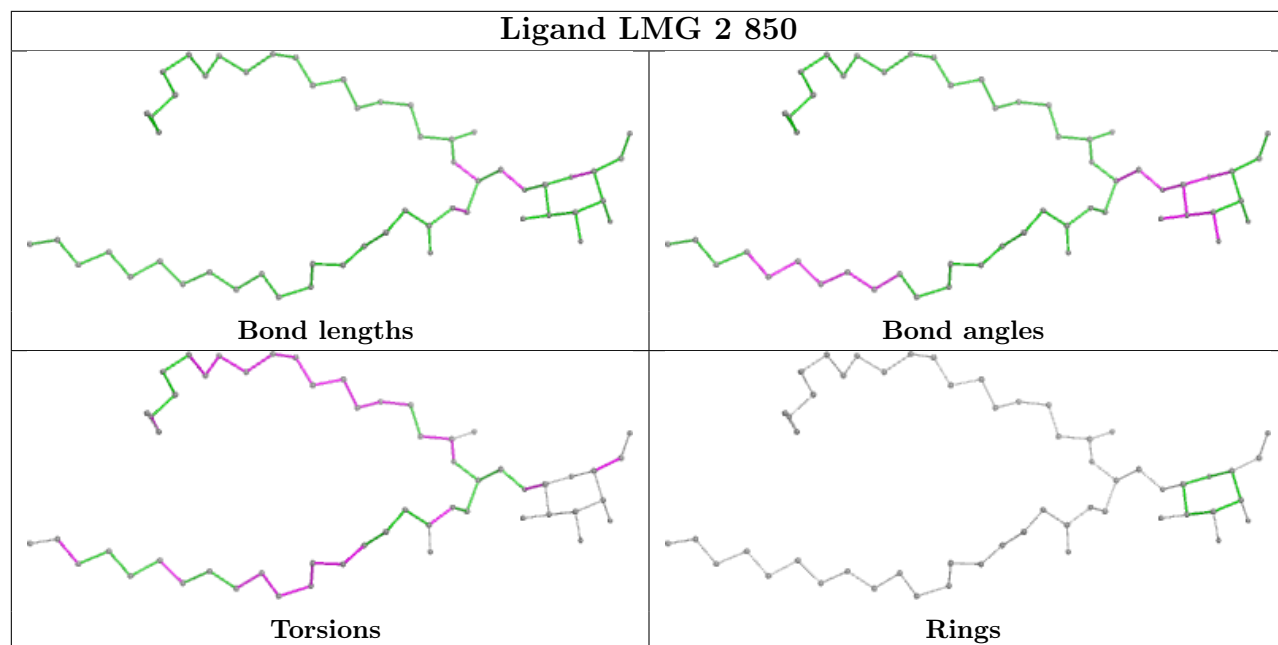
## Ligand CLA b 816

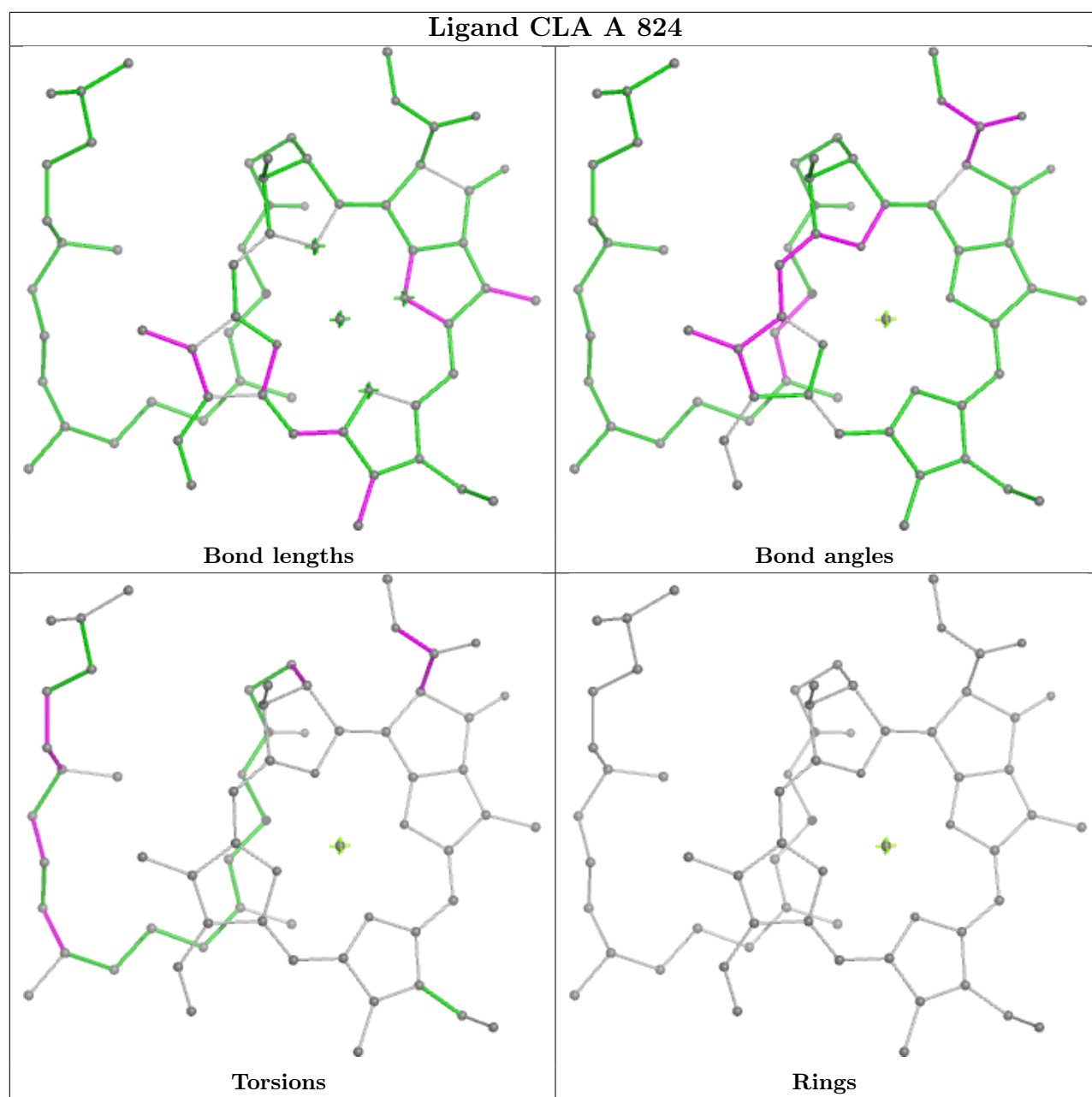


## Ligand CLA 1 204

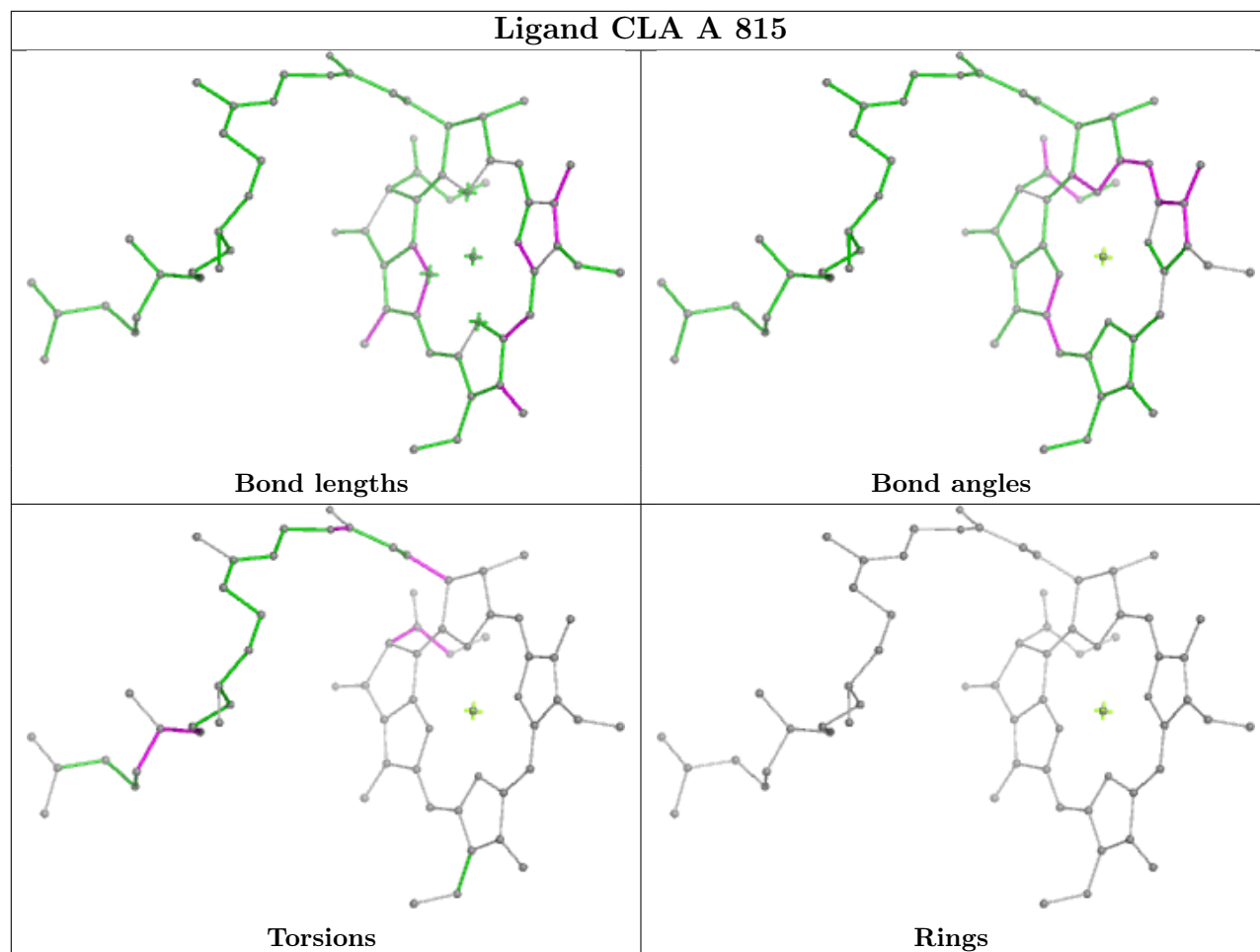




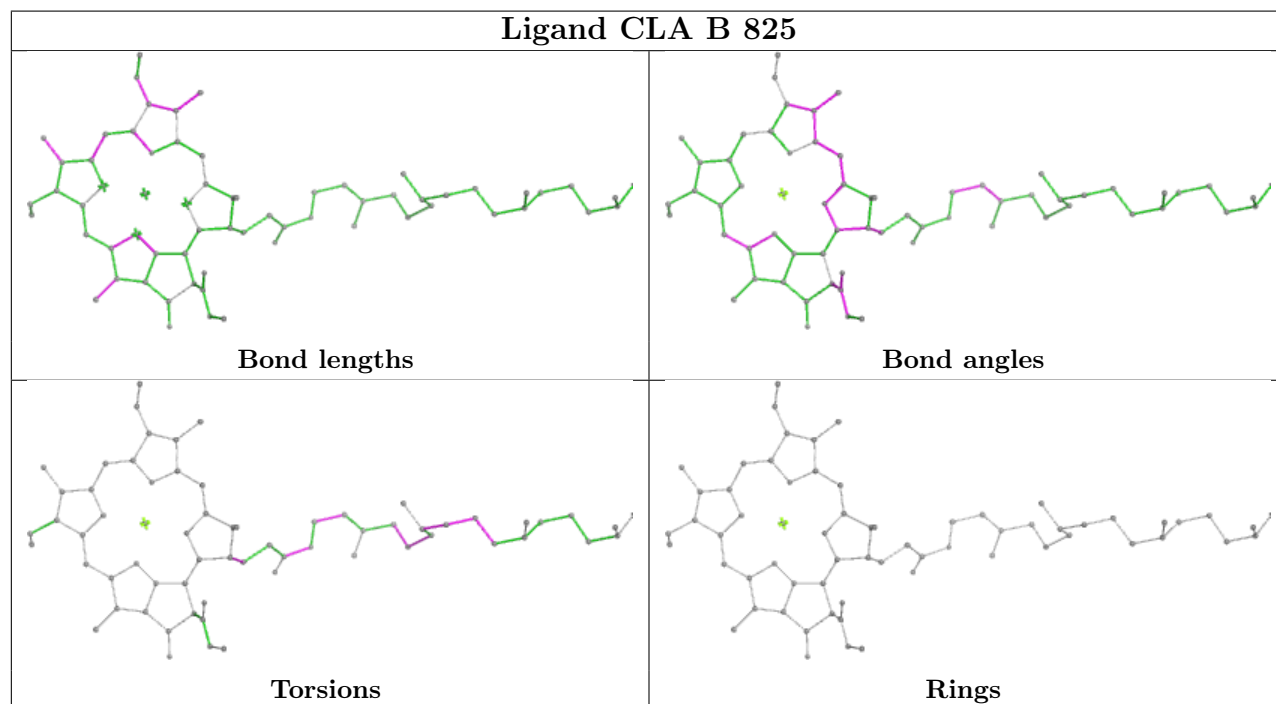


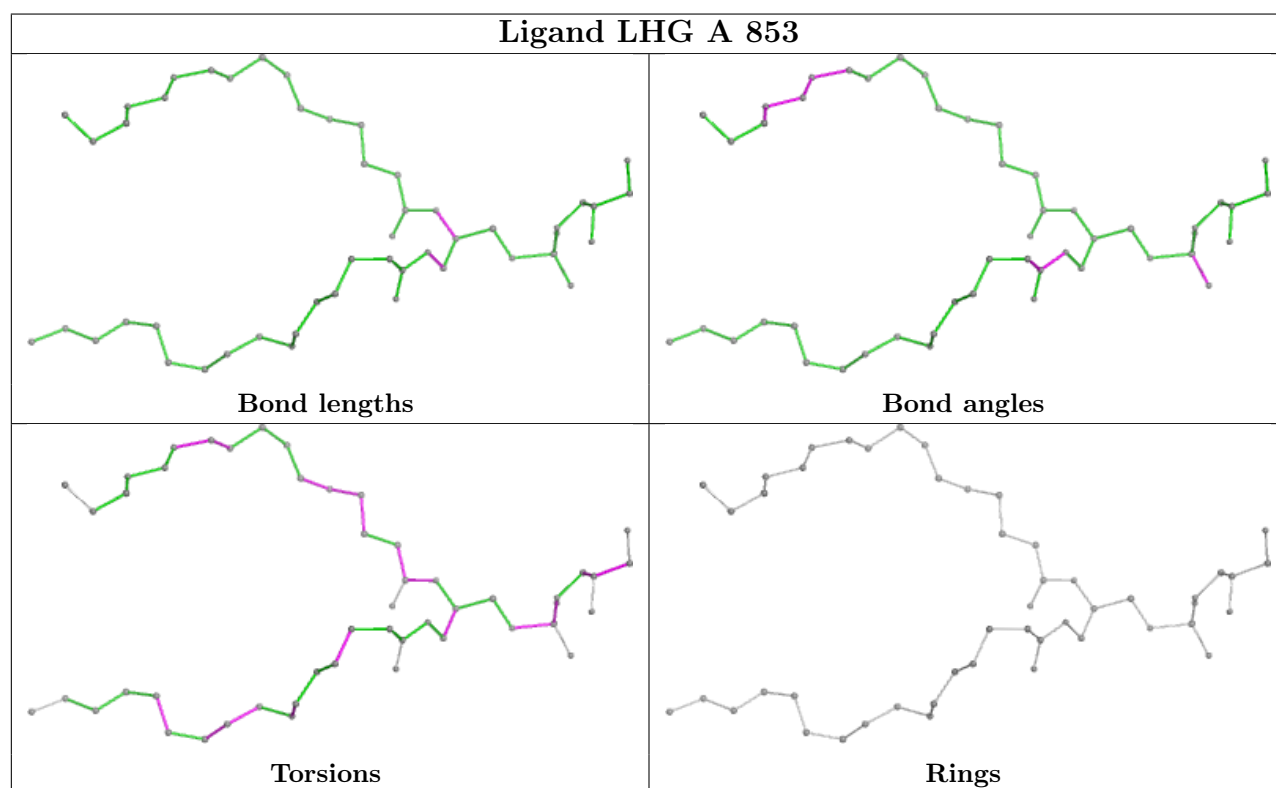
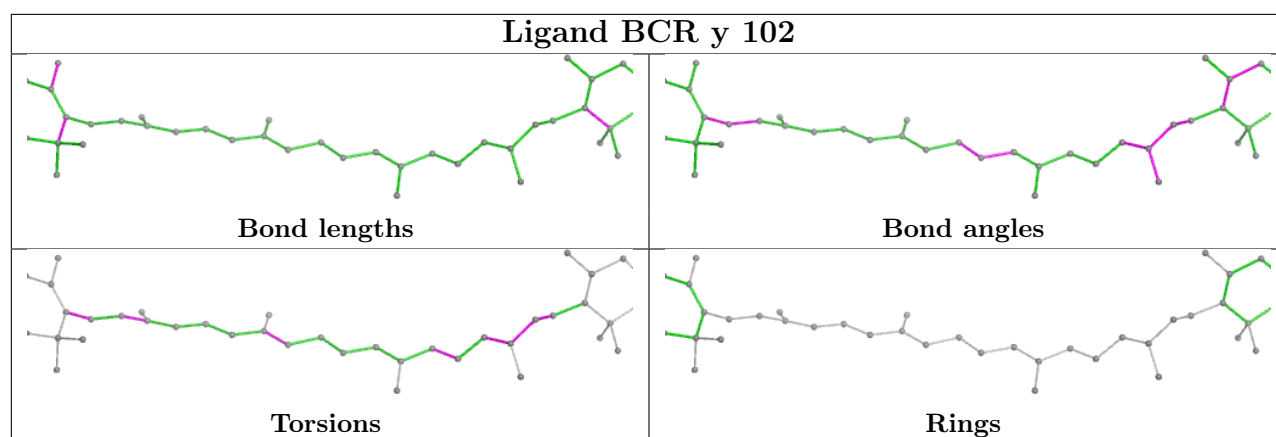


## Ligand CLA A 815

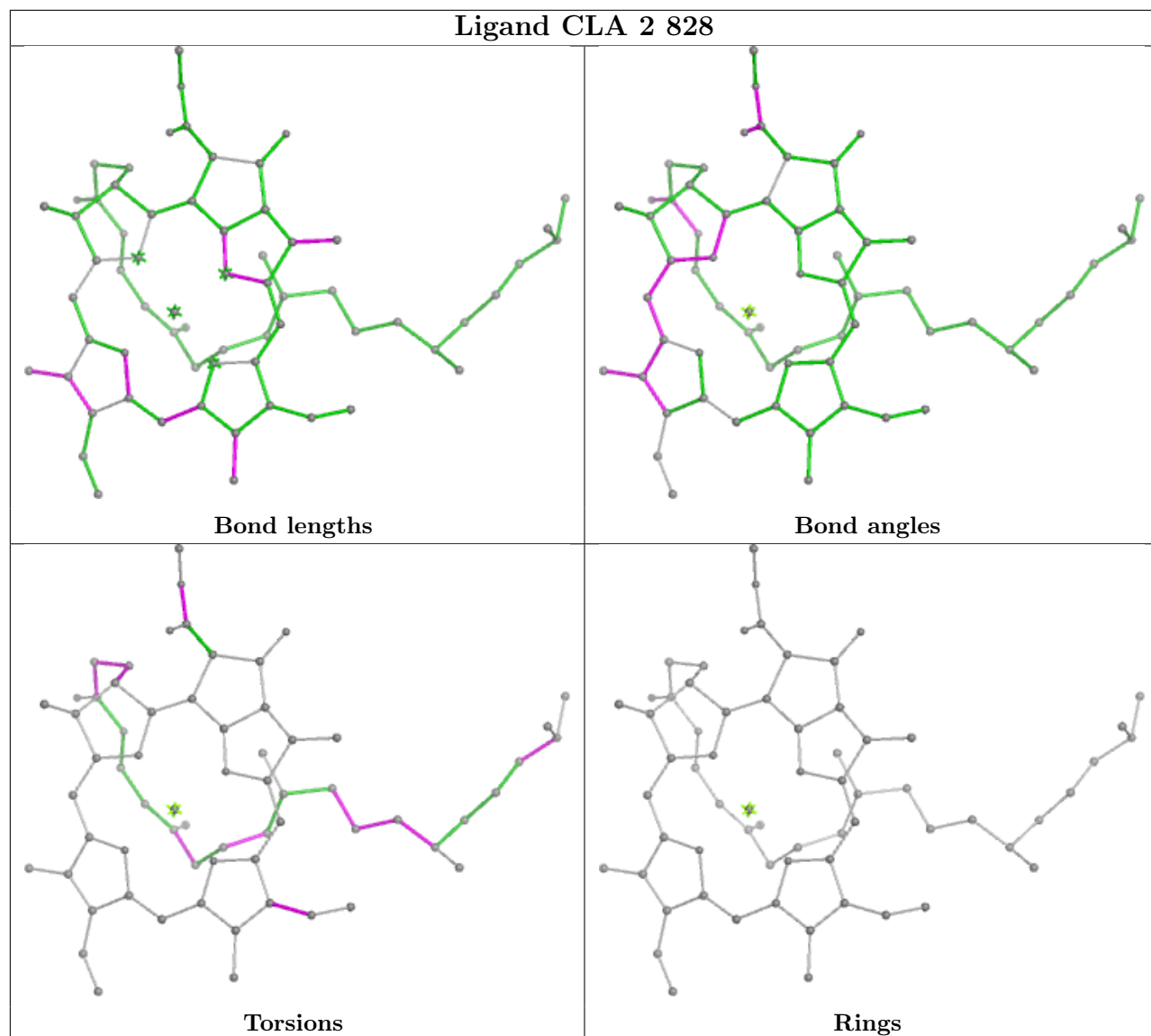


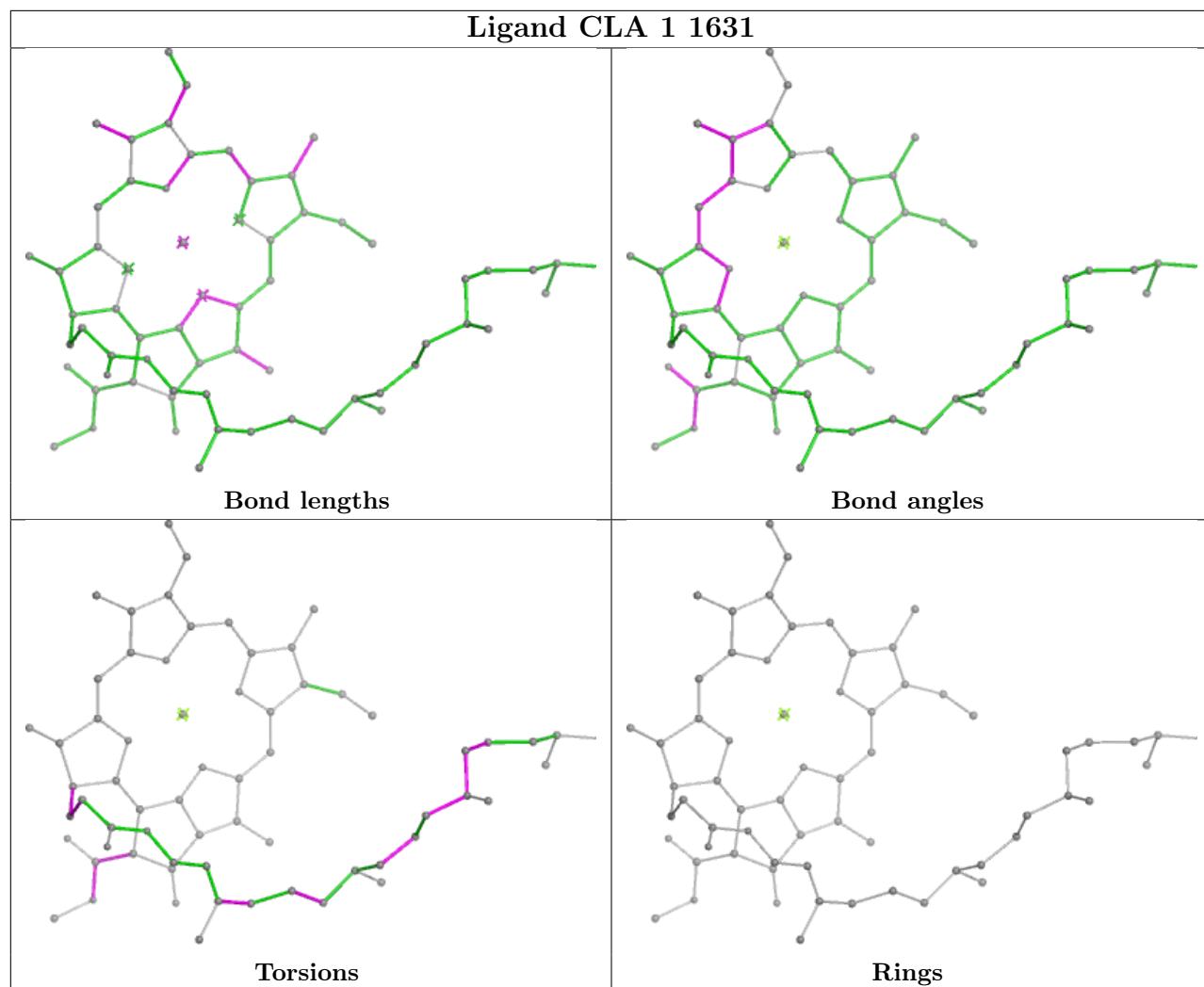
## Ligand CLA B 825

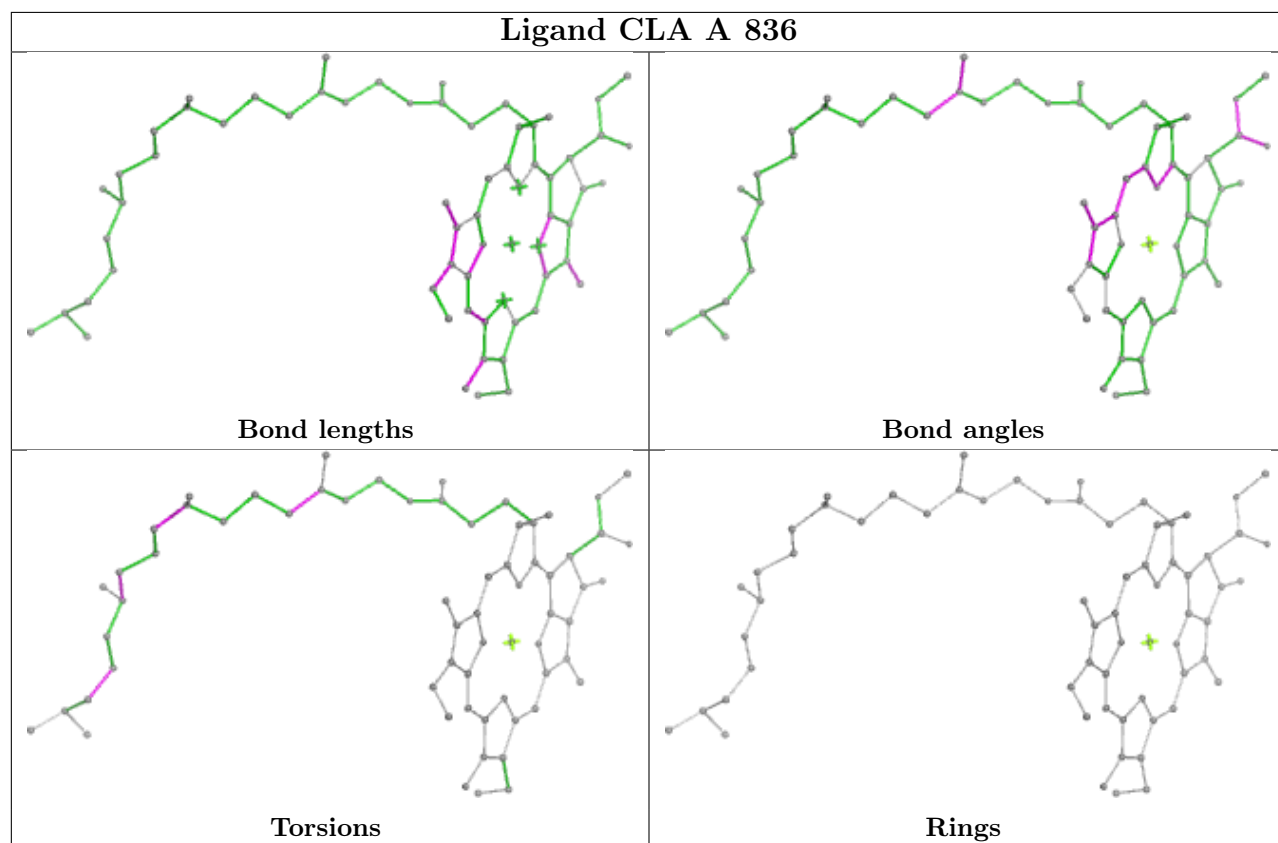
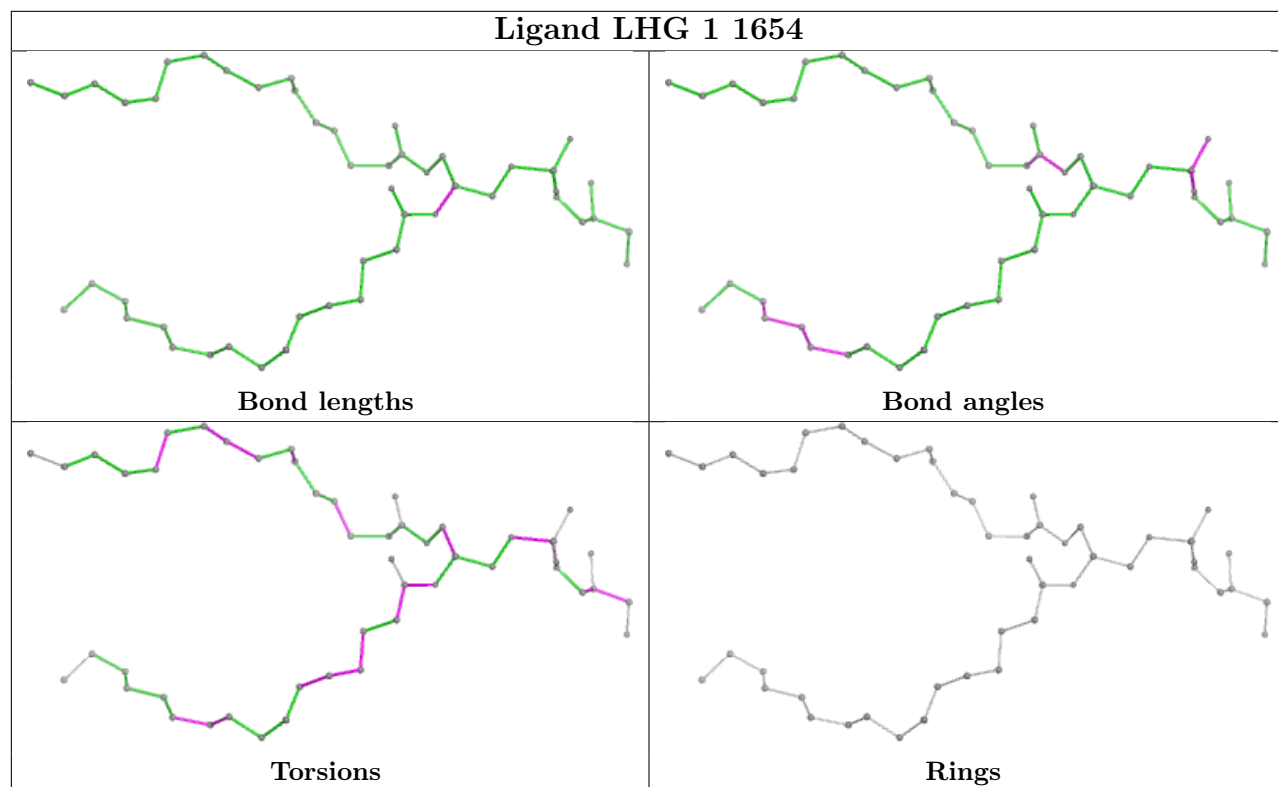




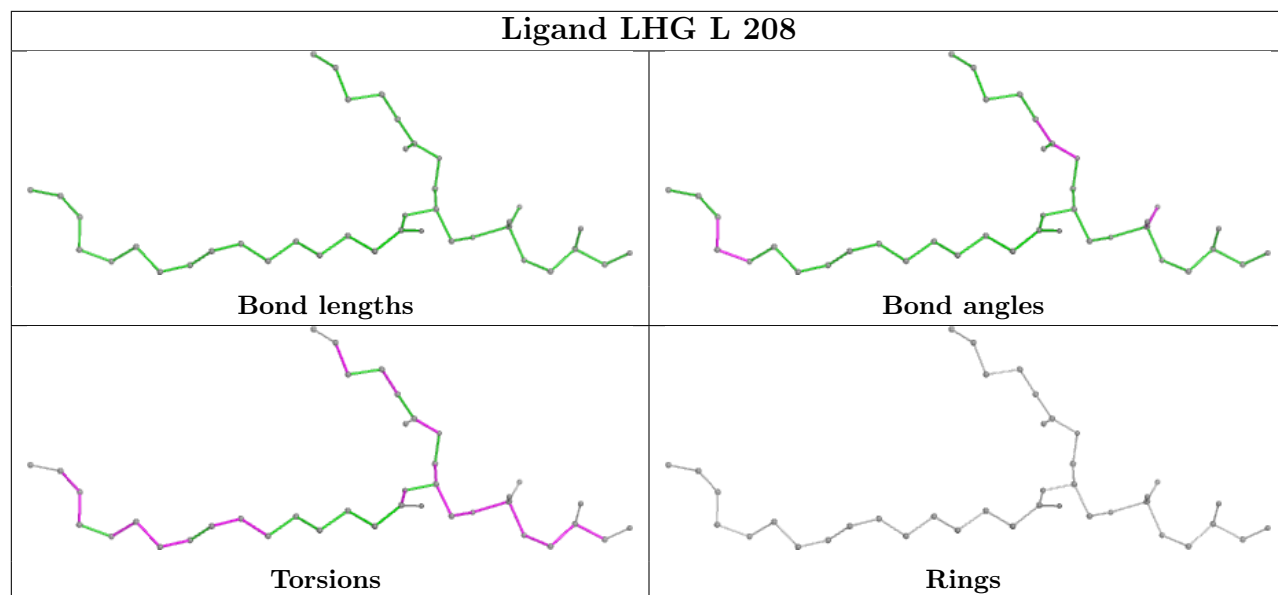
## Ligand CLA 2 828



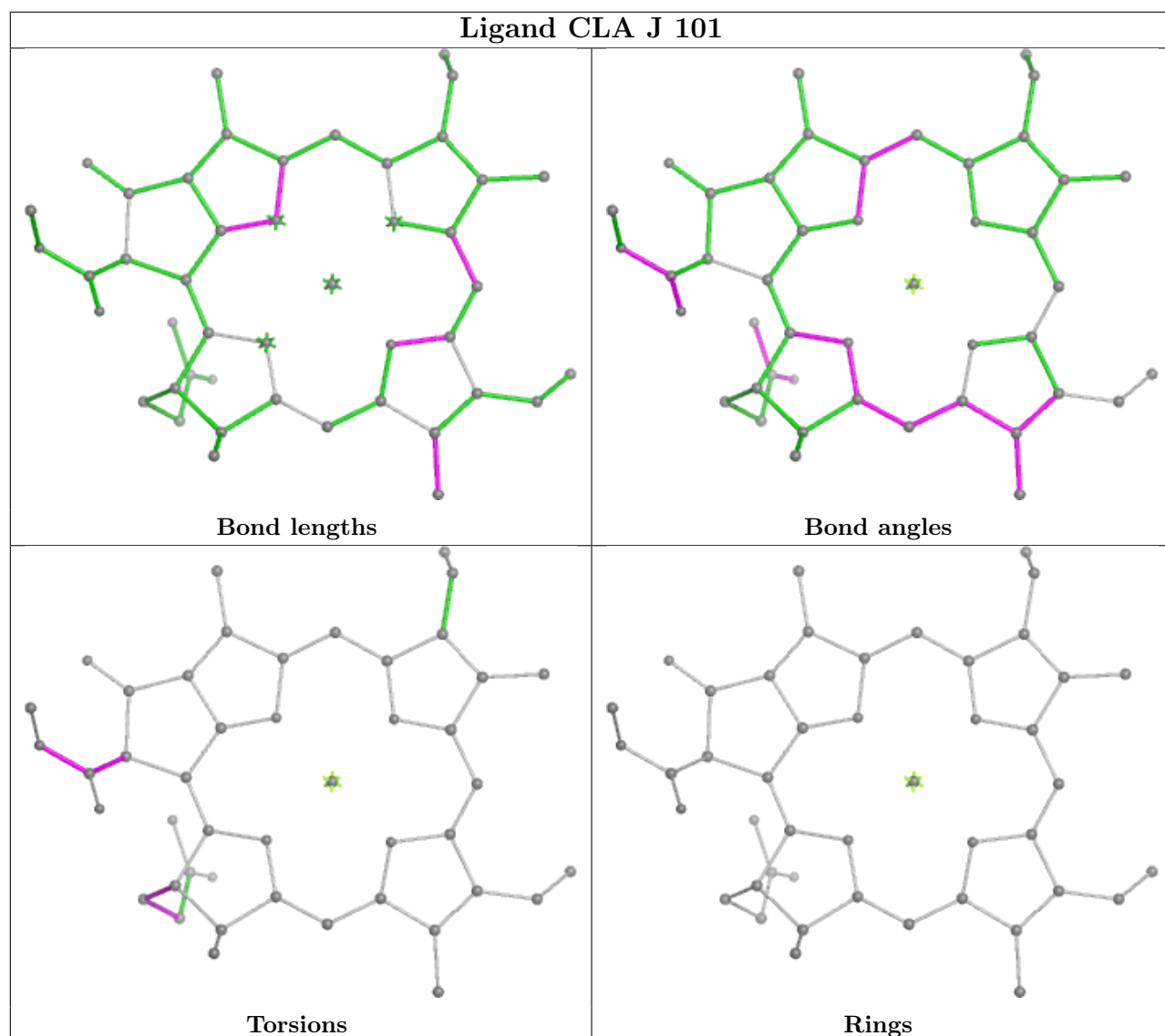




## Ligand LHG L 208

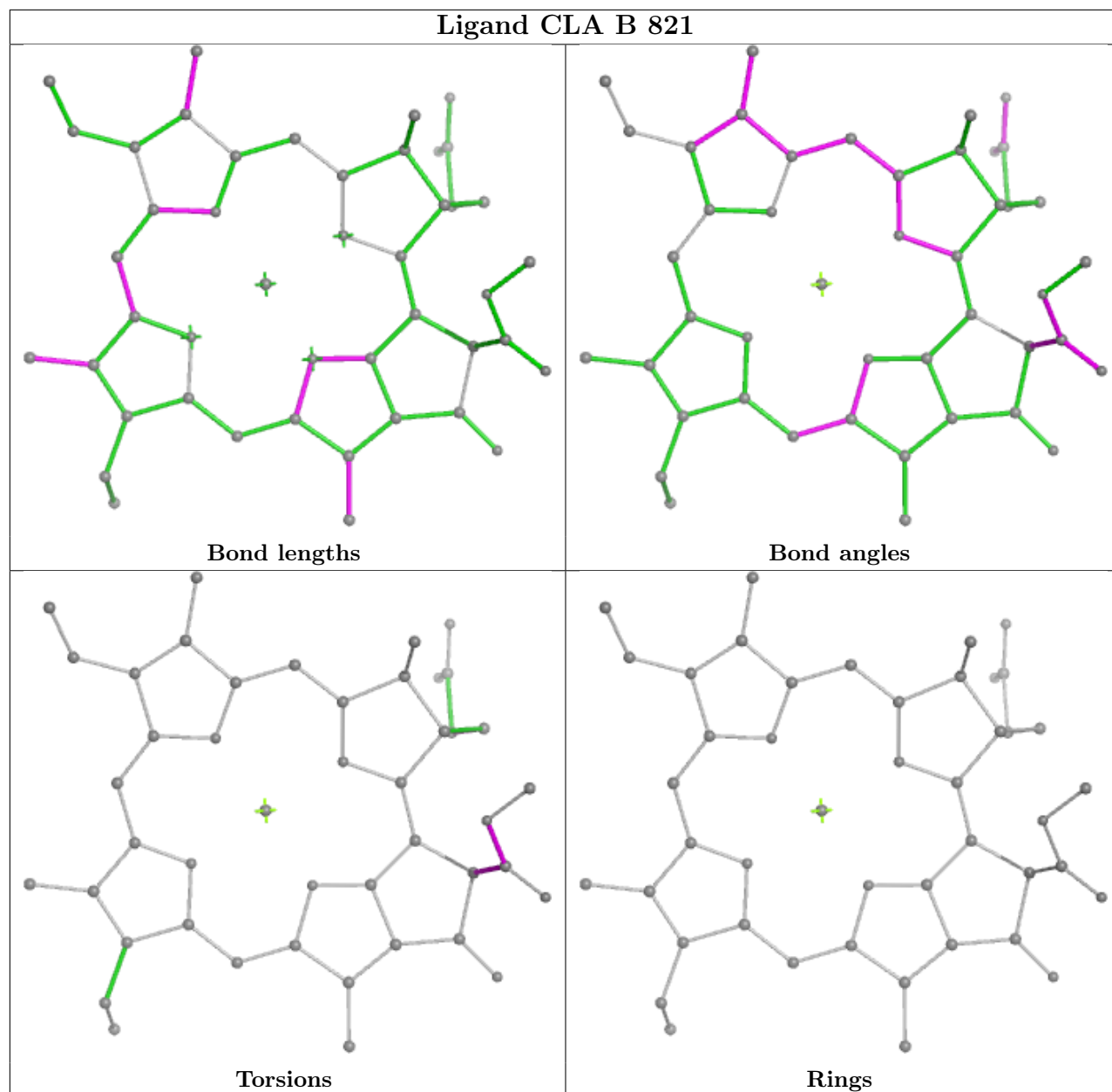


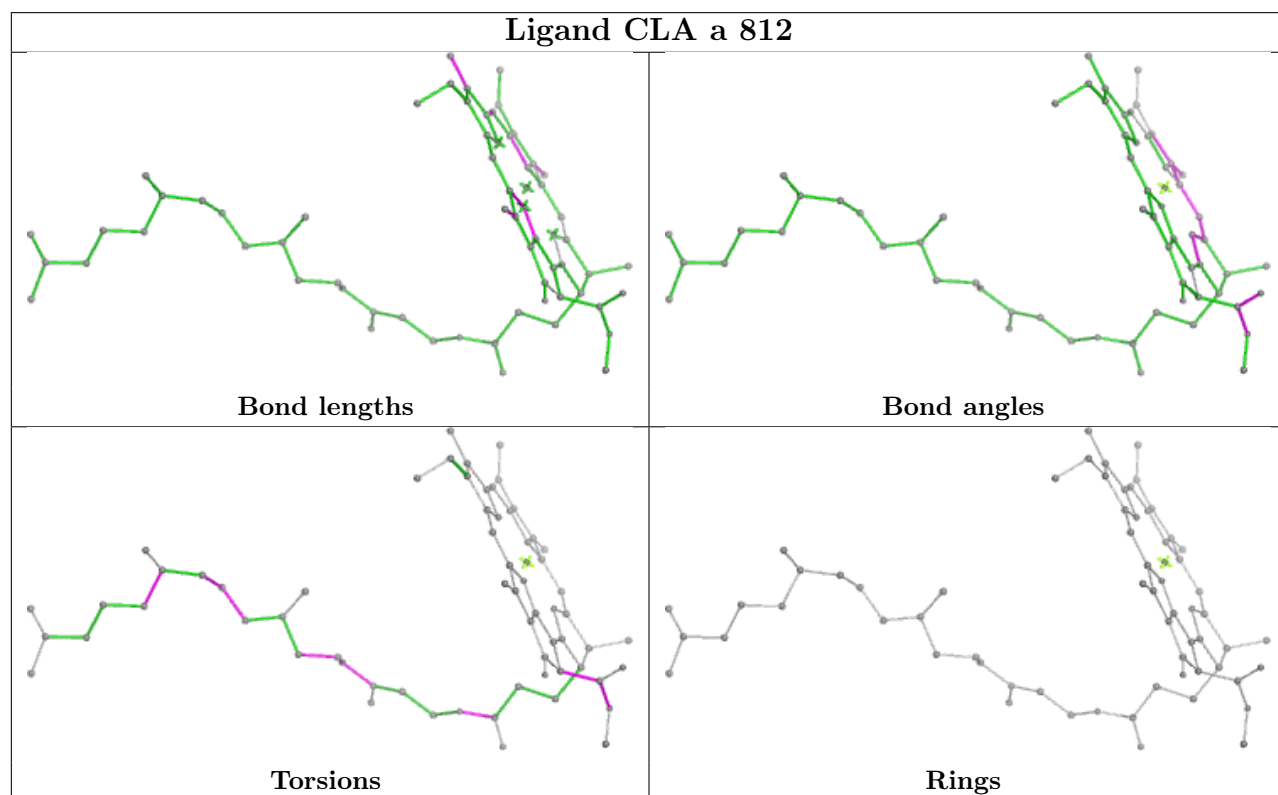
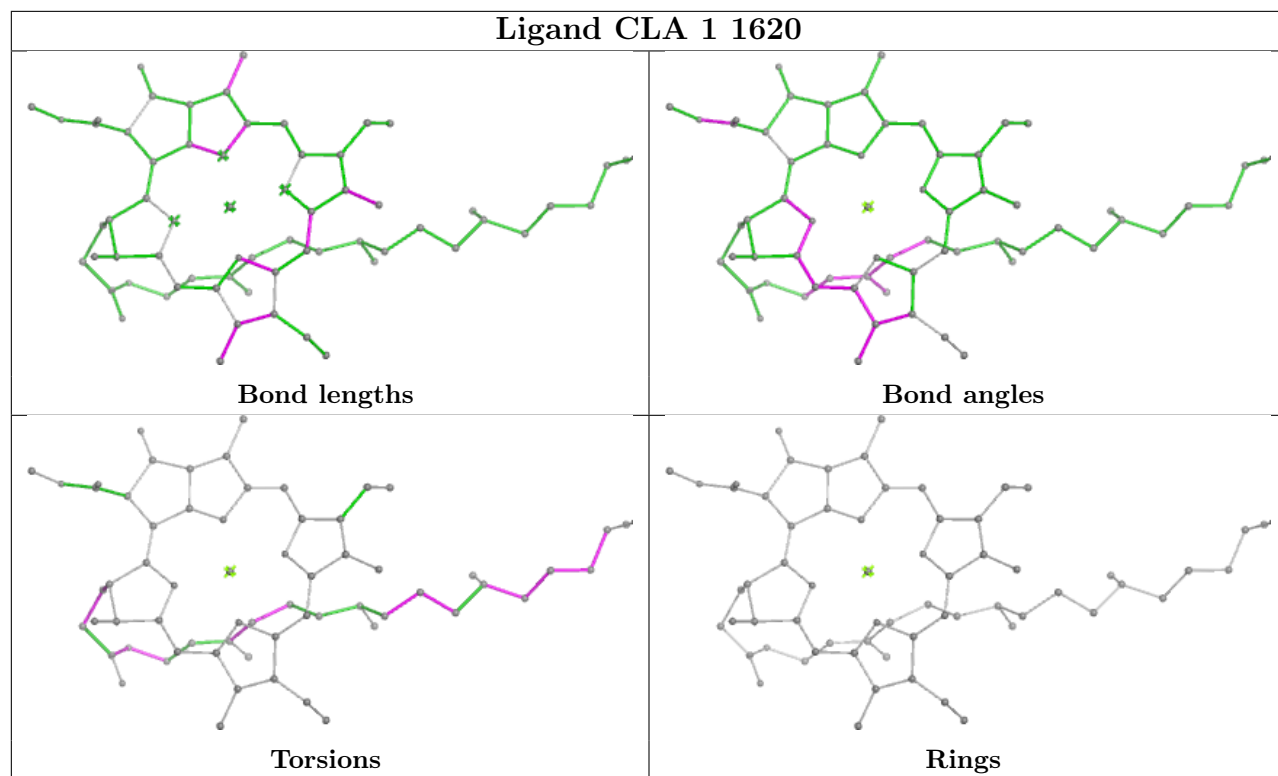
## Ligand CLA J 101

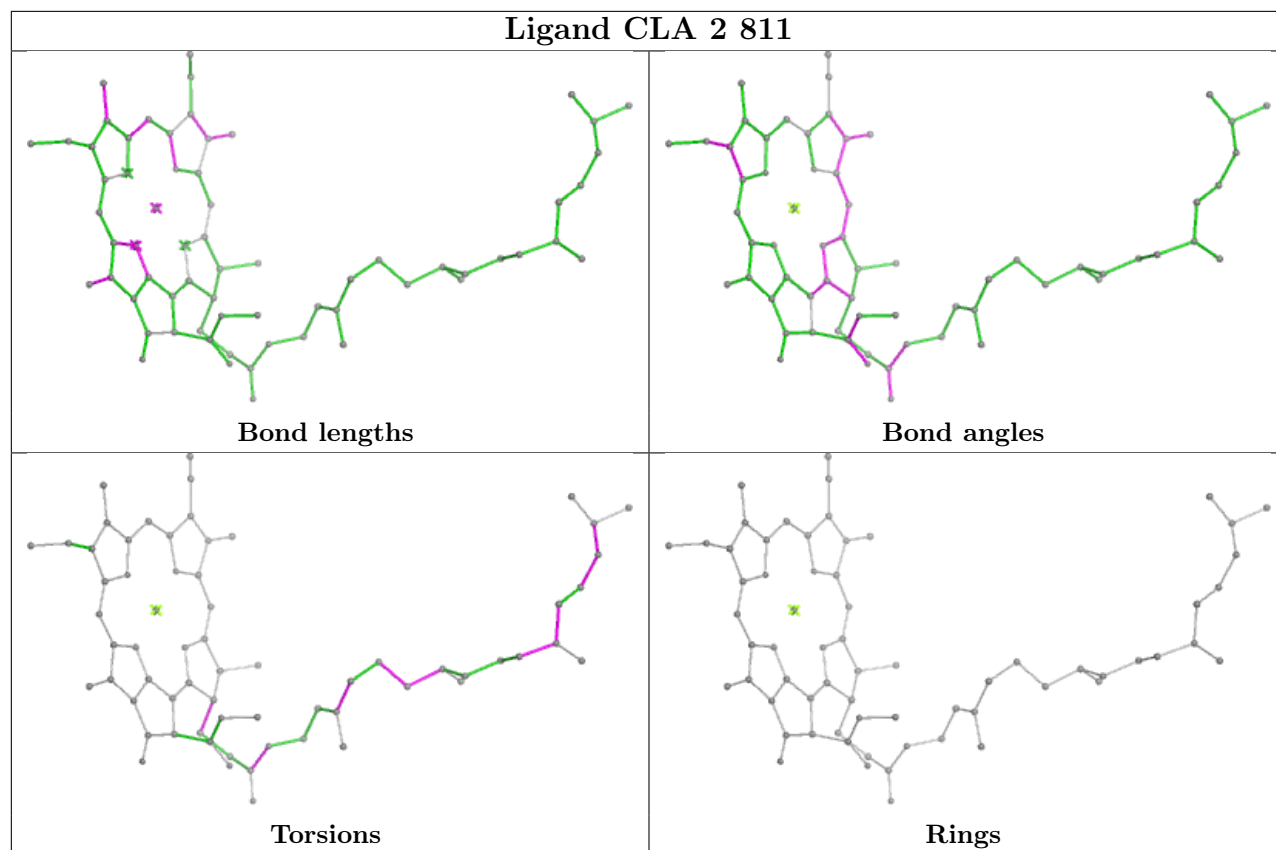




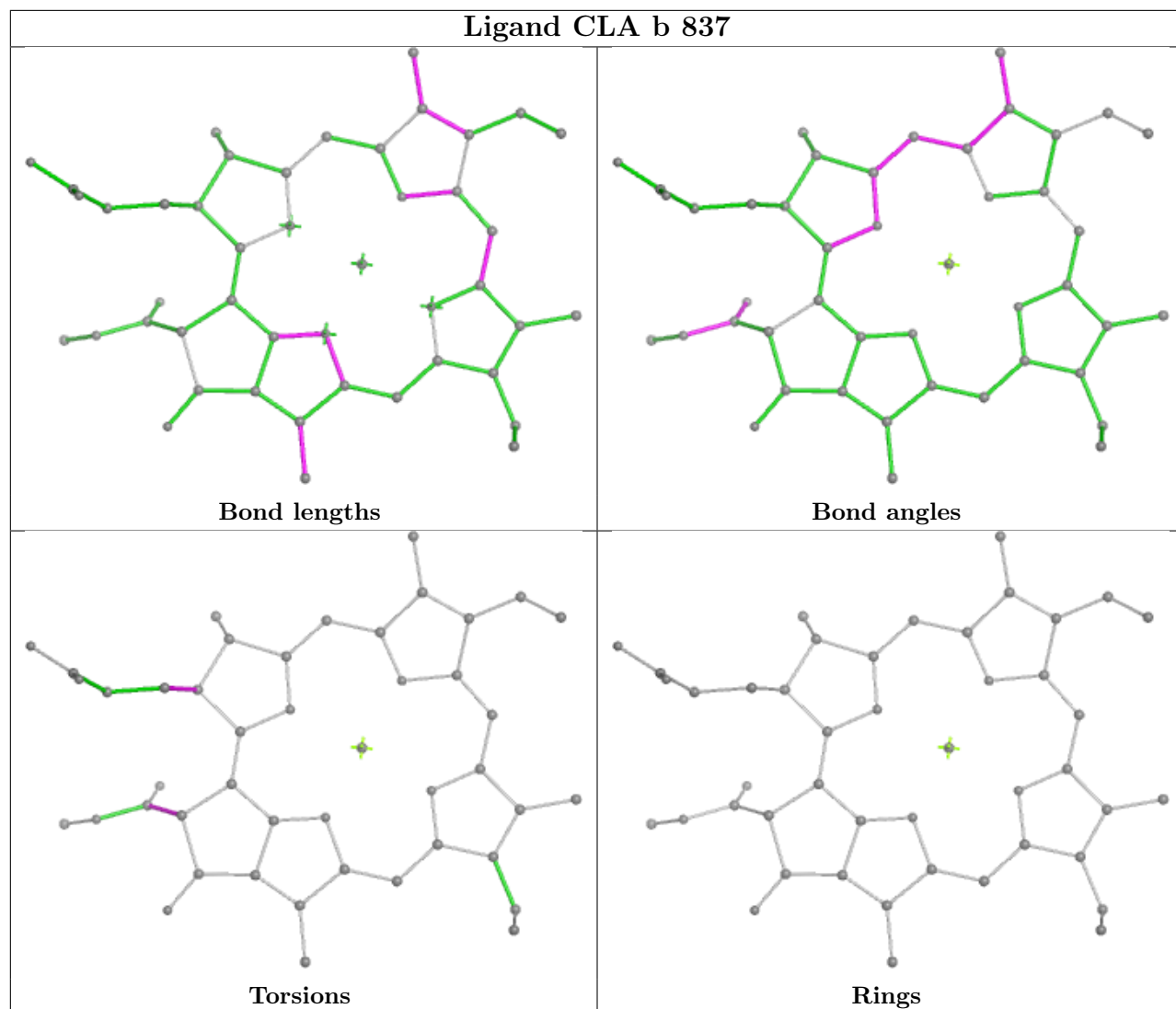
## Ligand CLA B 821

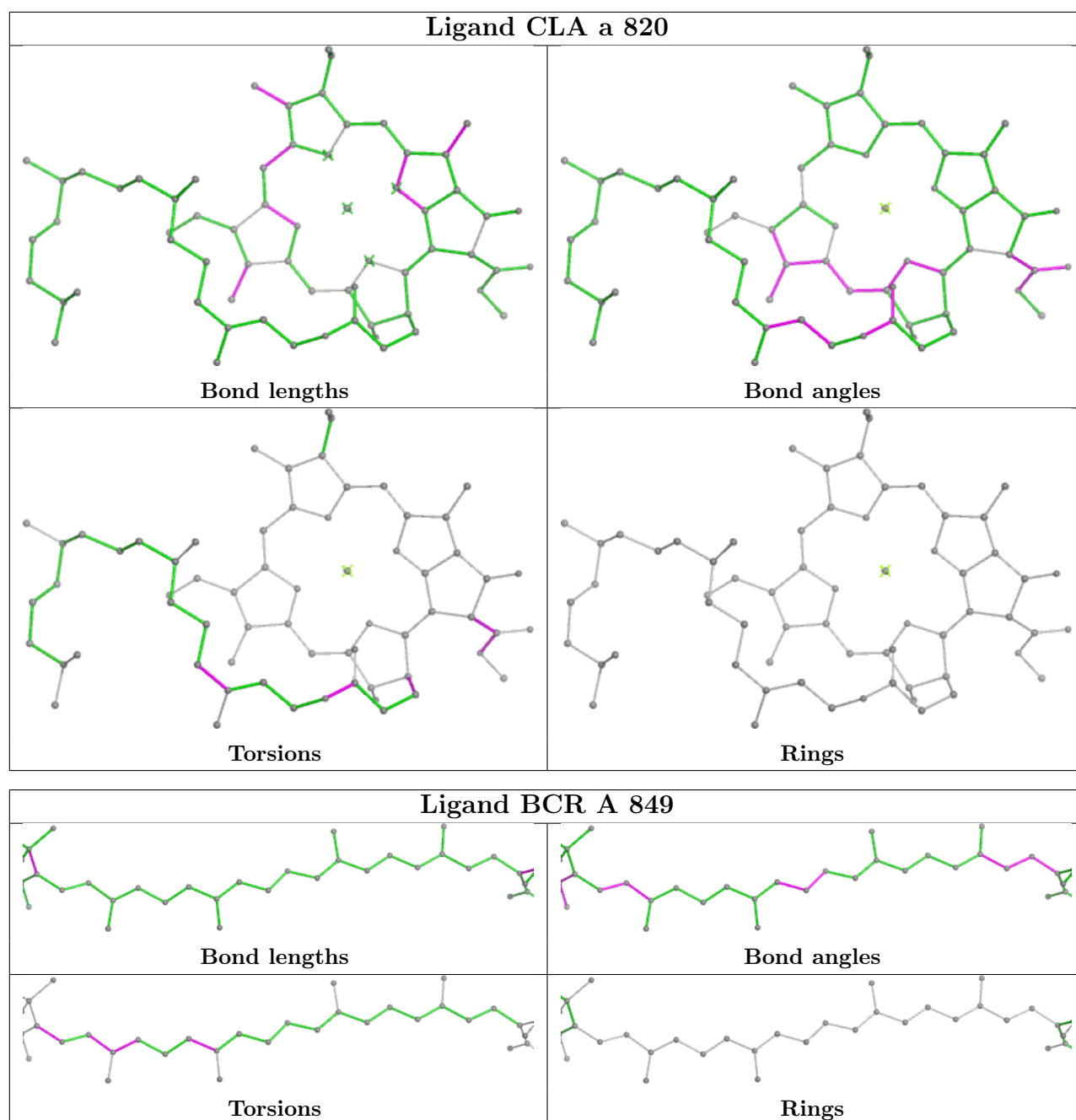




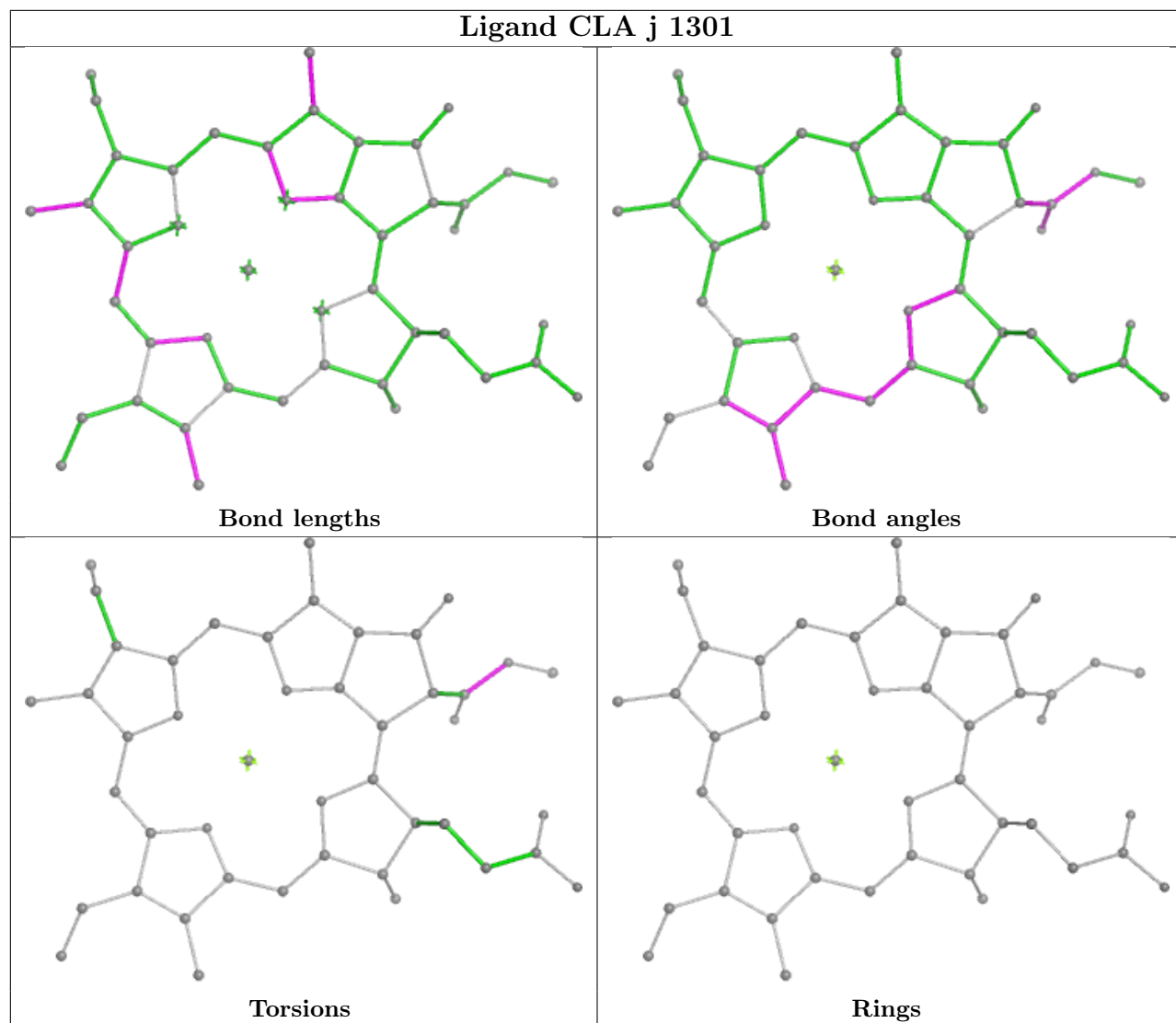


## Ligand CLA b 837

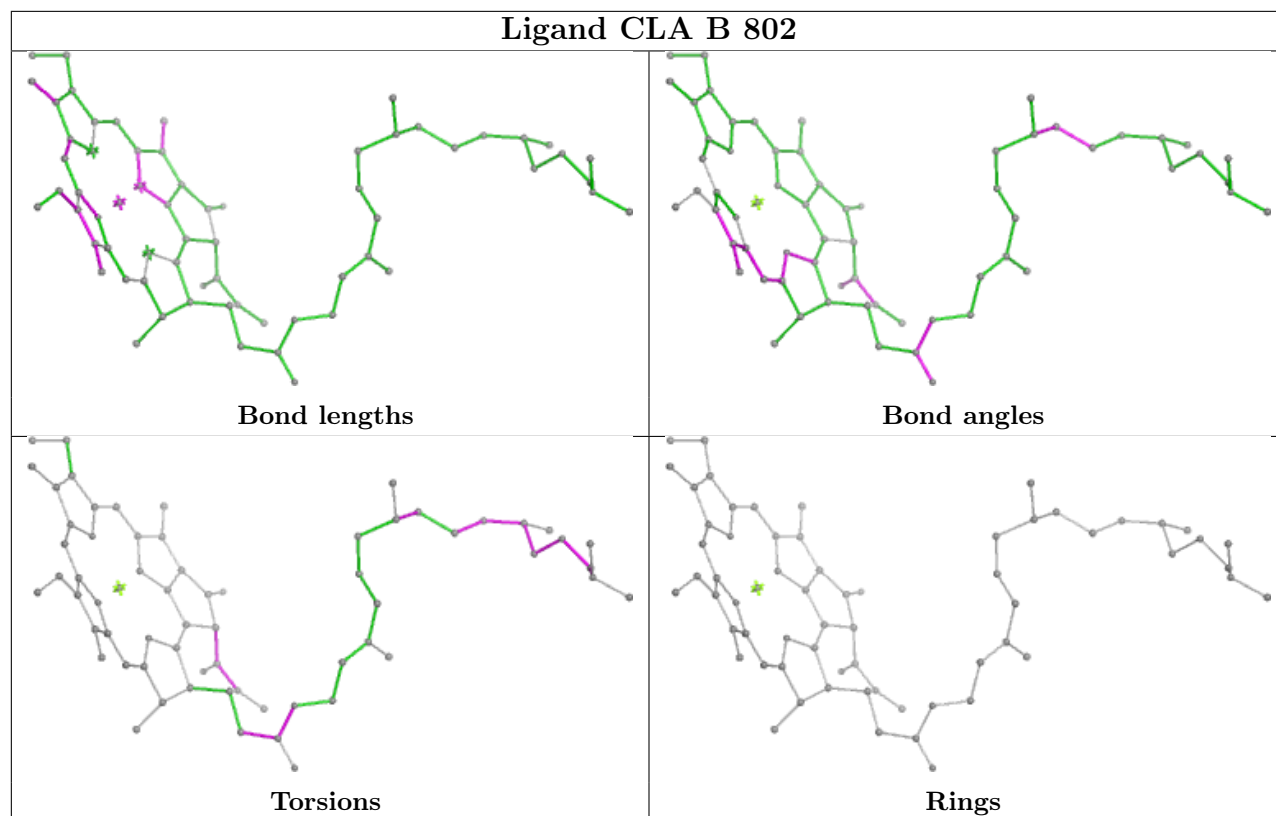




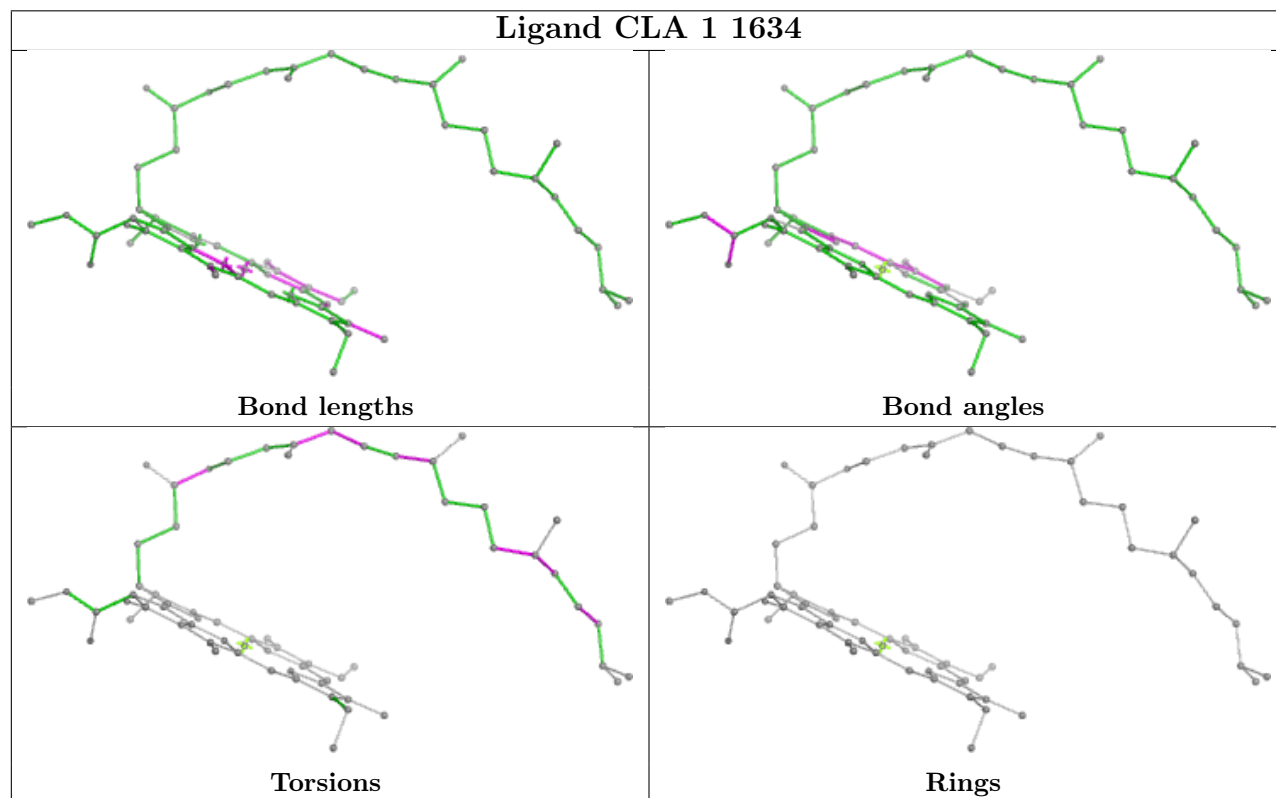
## Ligand CLA j 1301

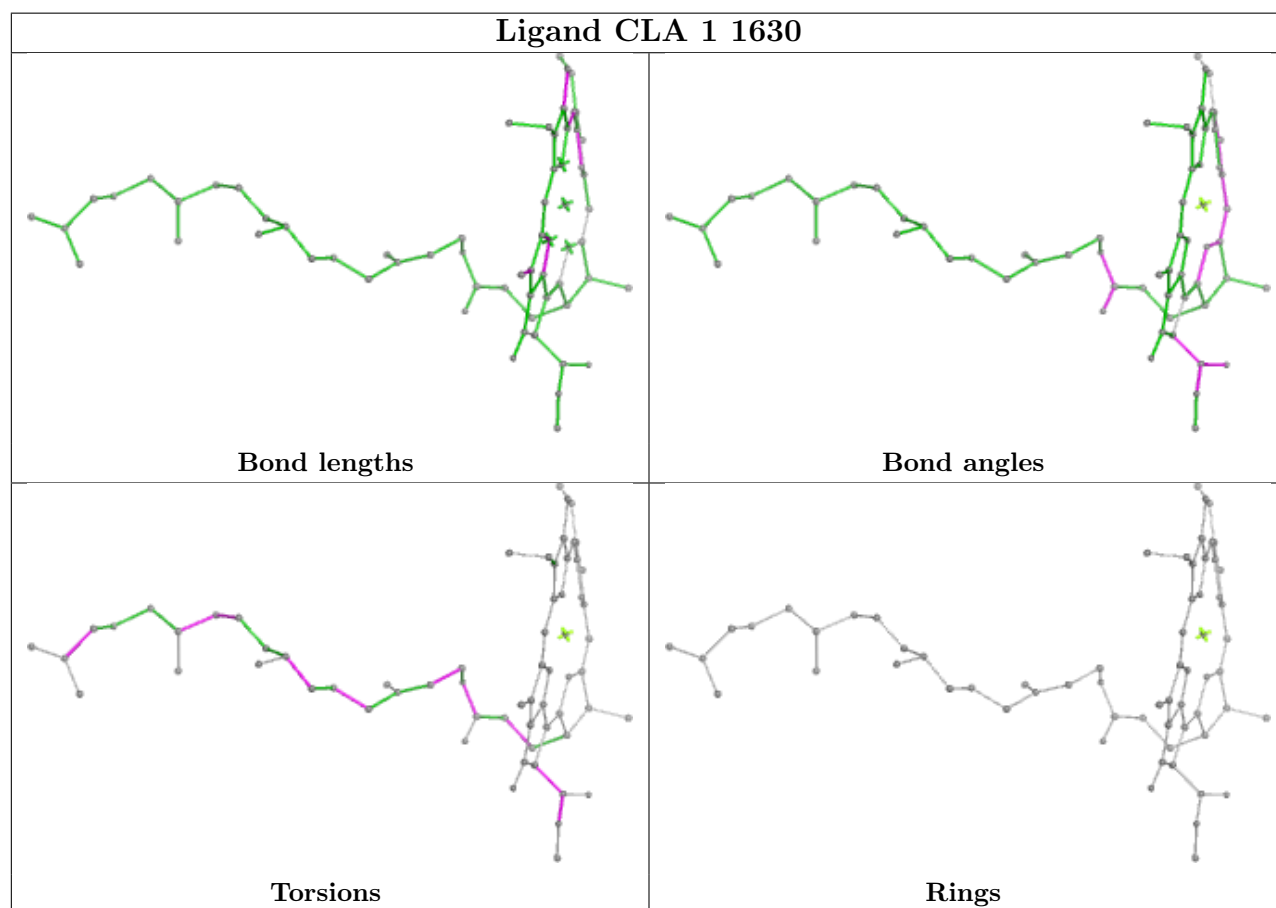
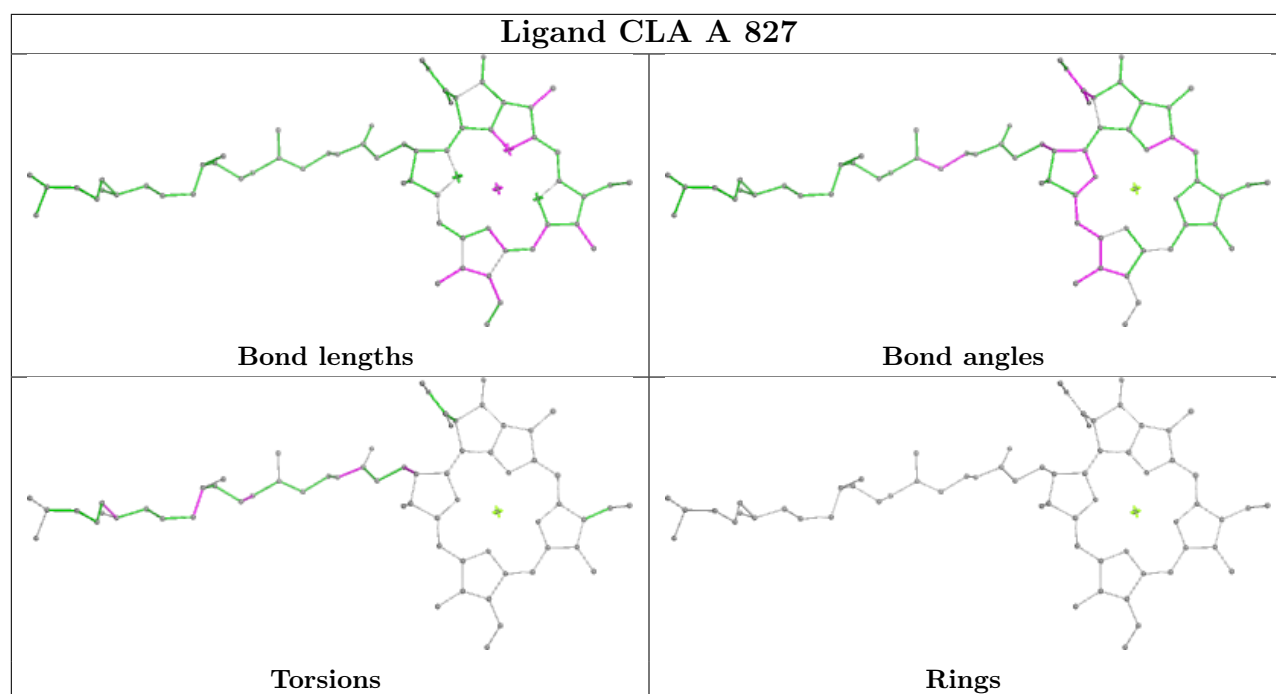


## Ligand CLA B 802

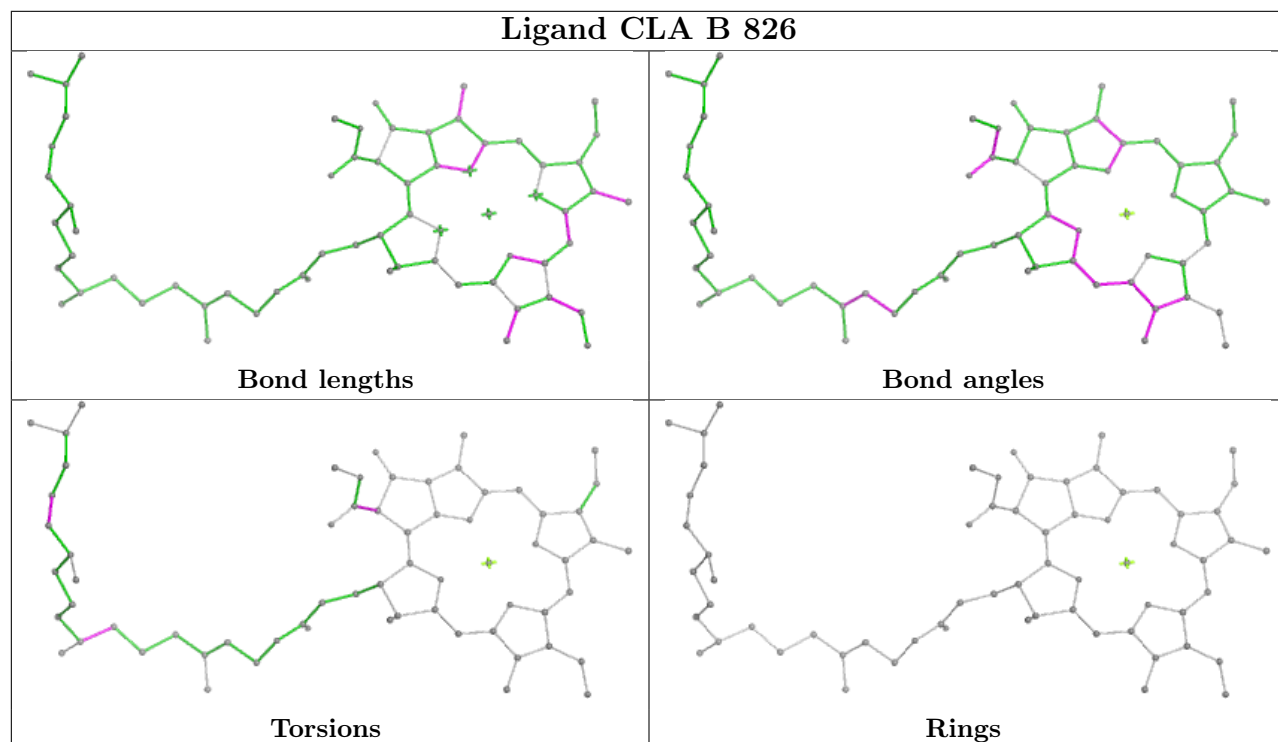
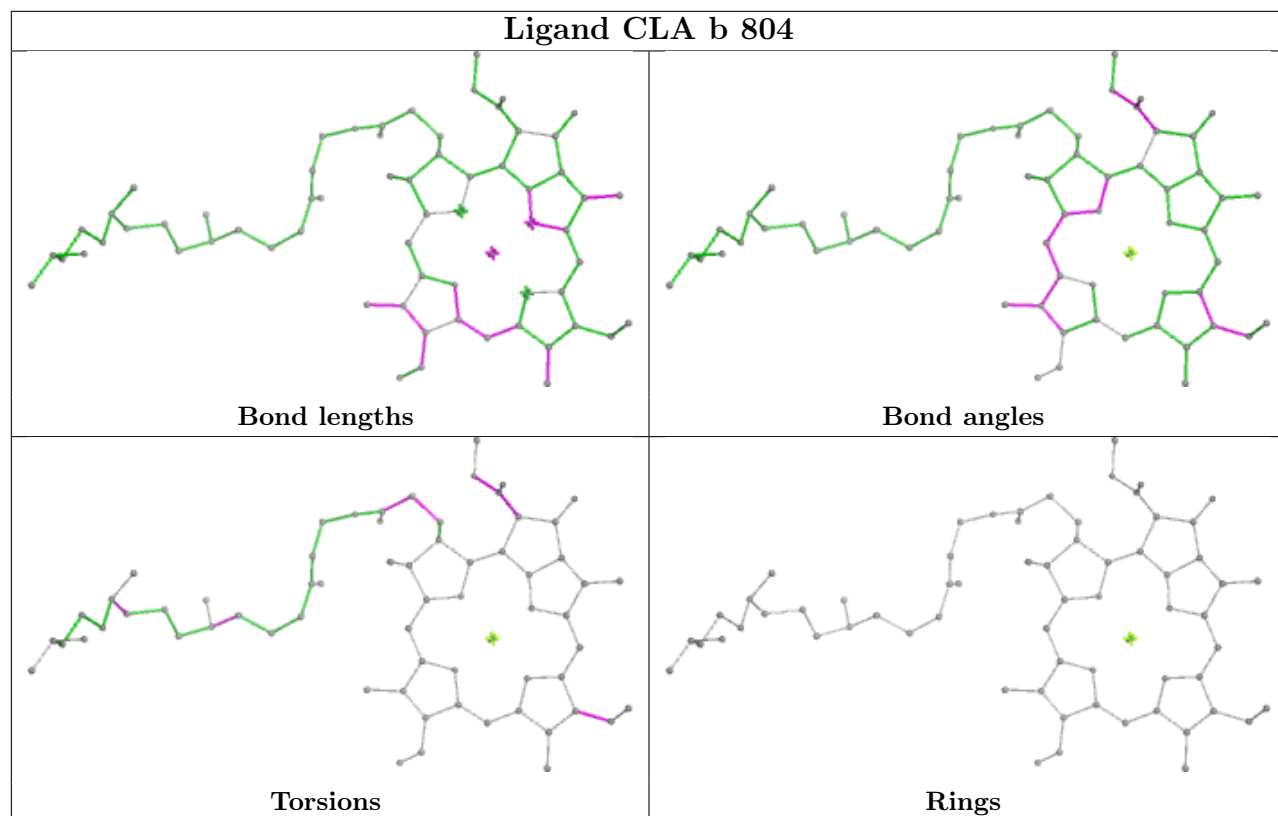


## Ligand CLA 1 1634

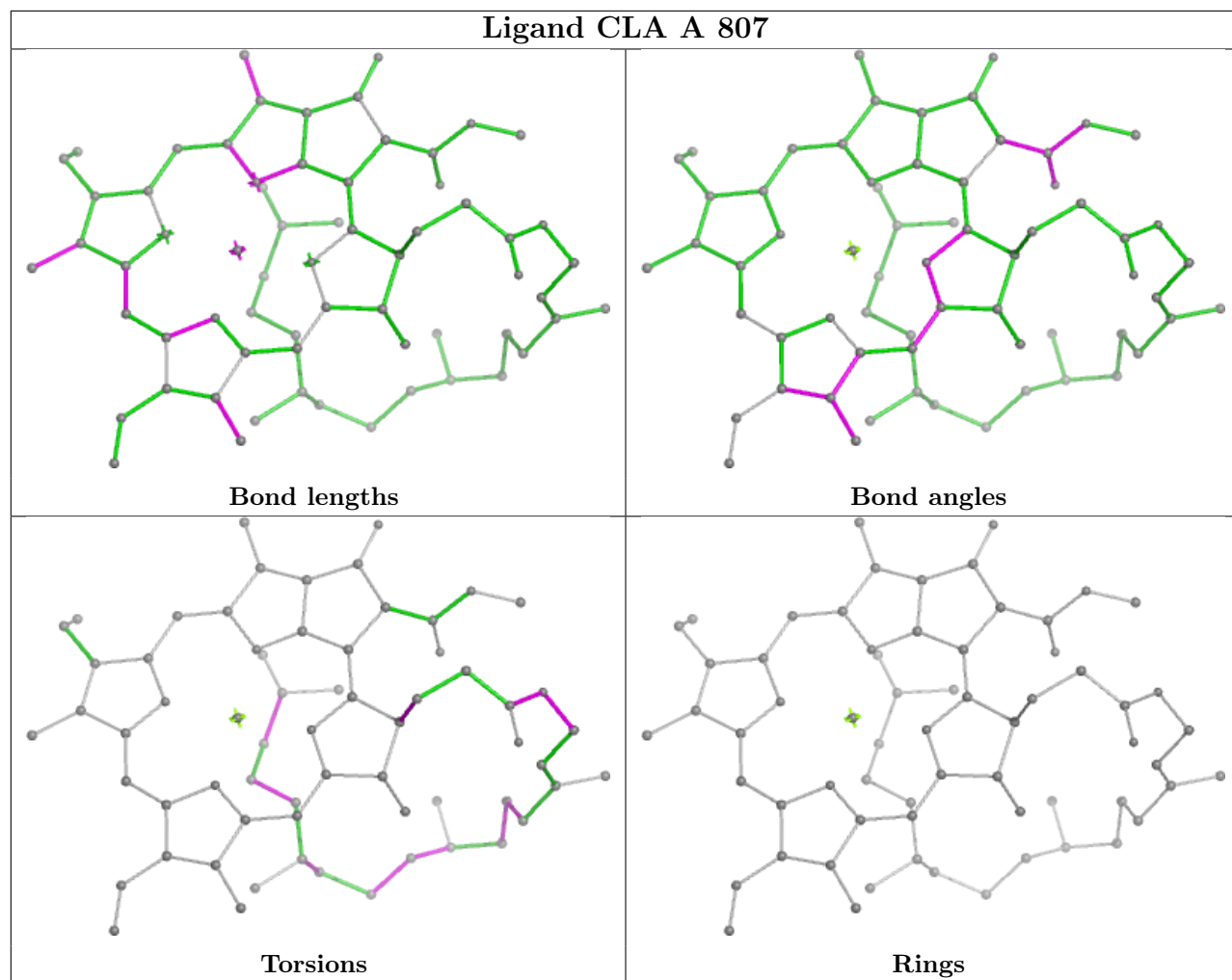




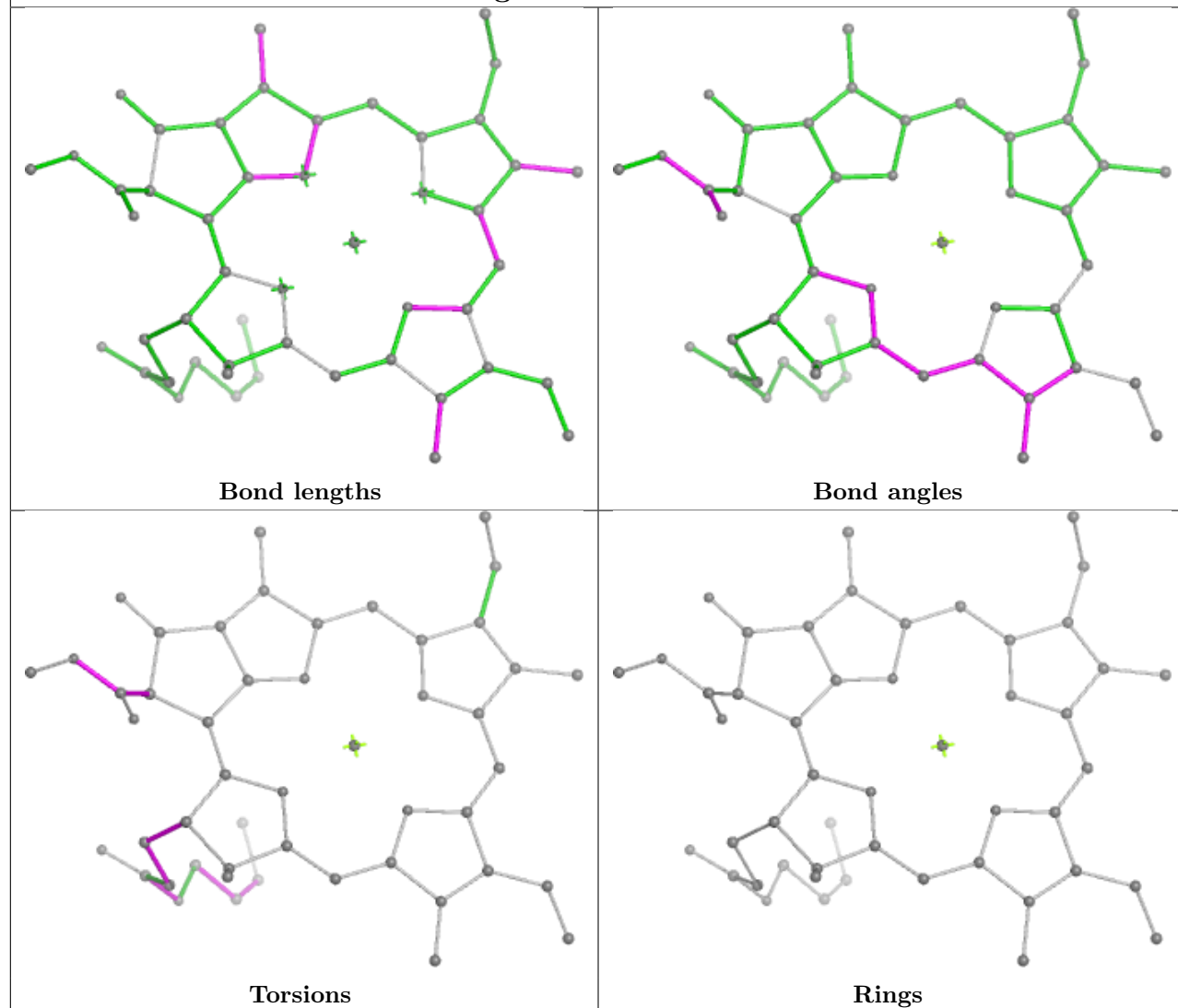




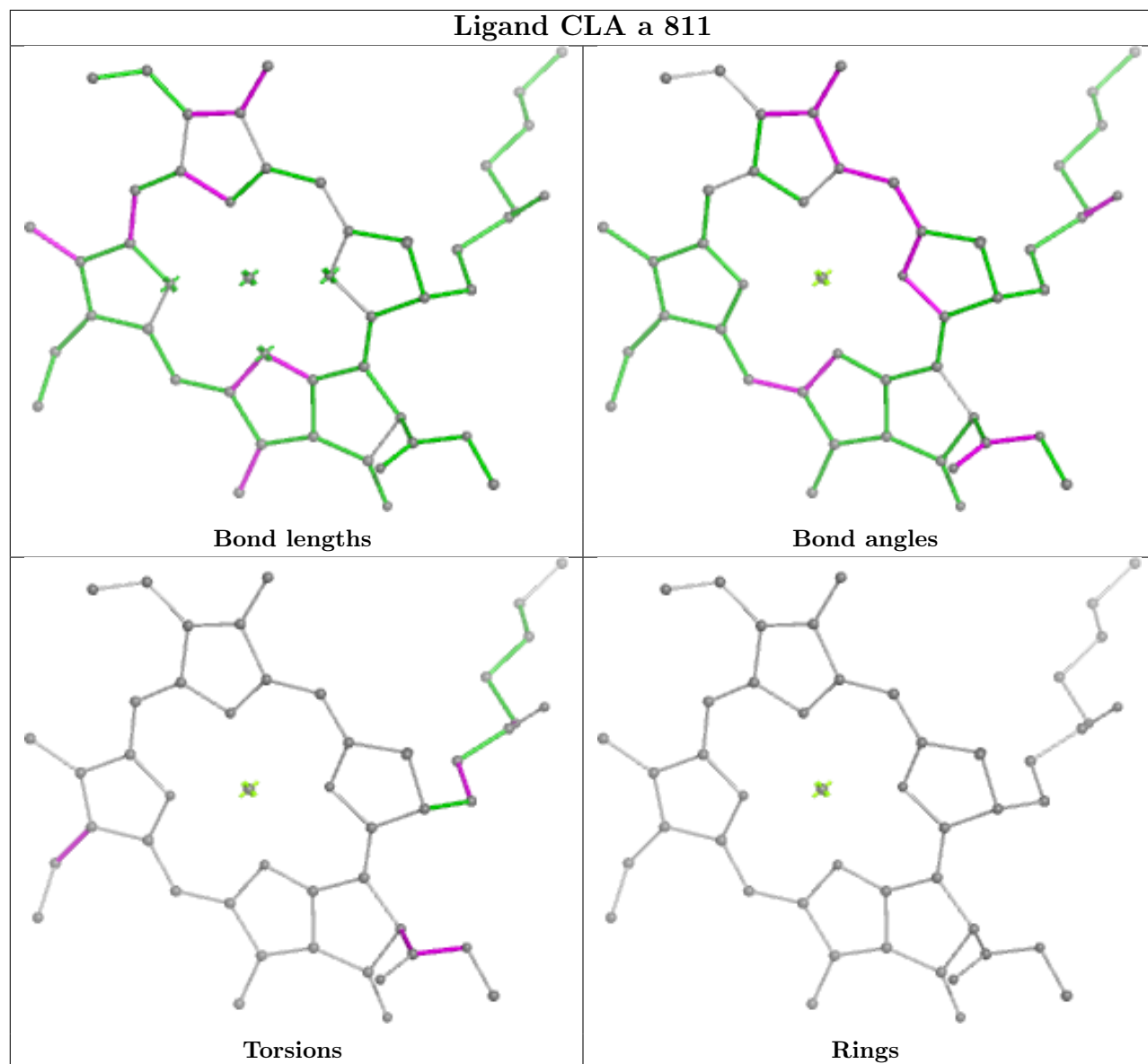
## Ligand CLA A 807

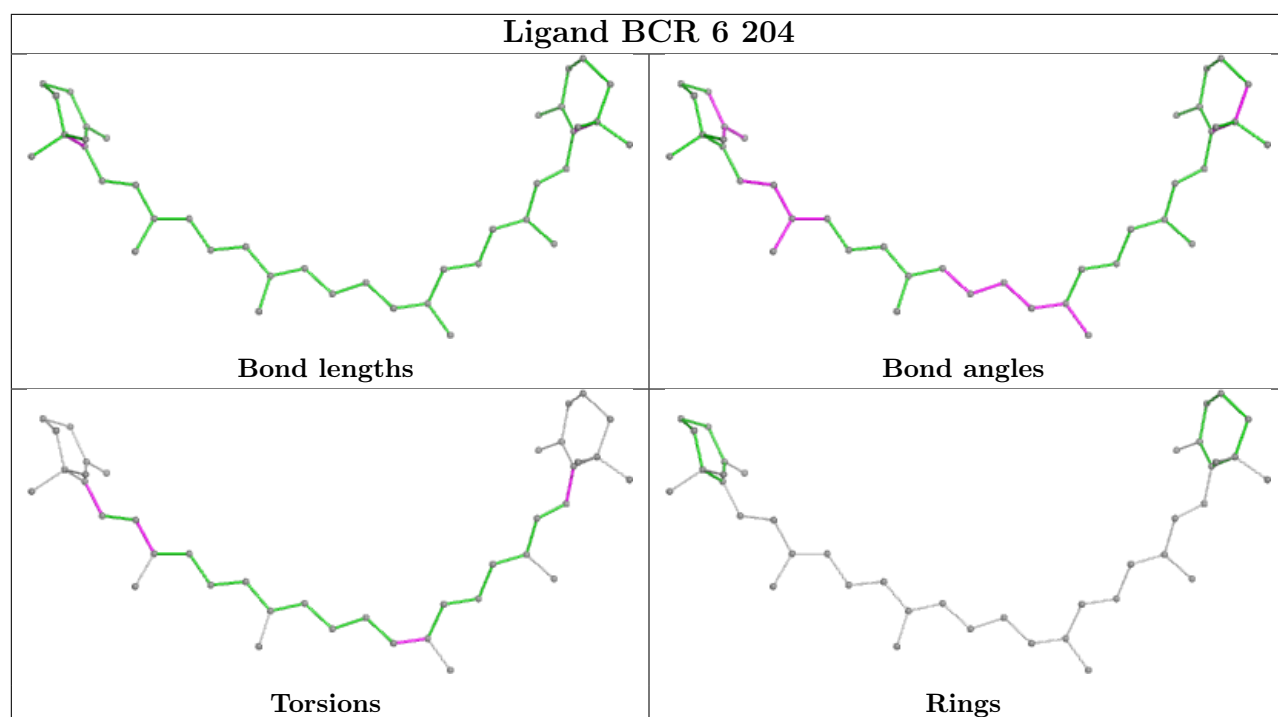


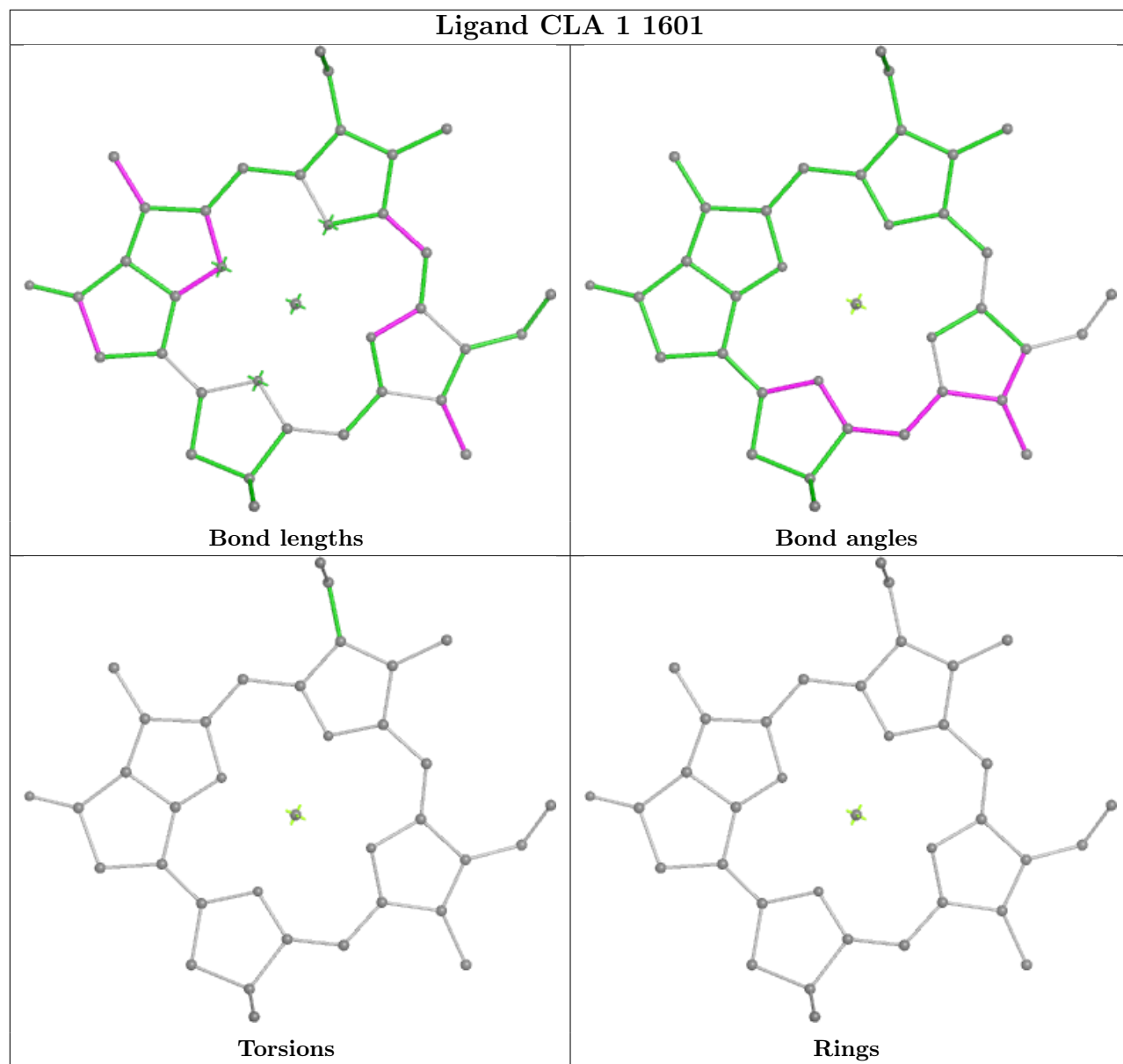
## Ligand CLA 2 832

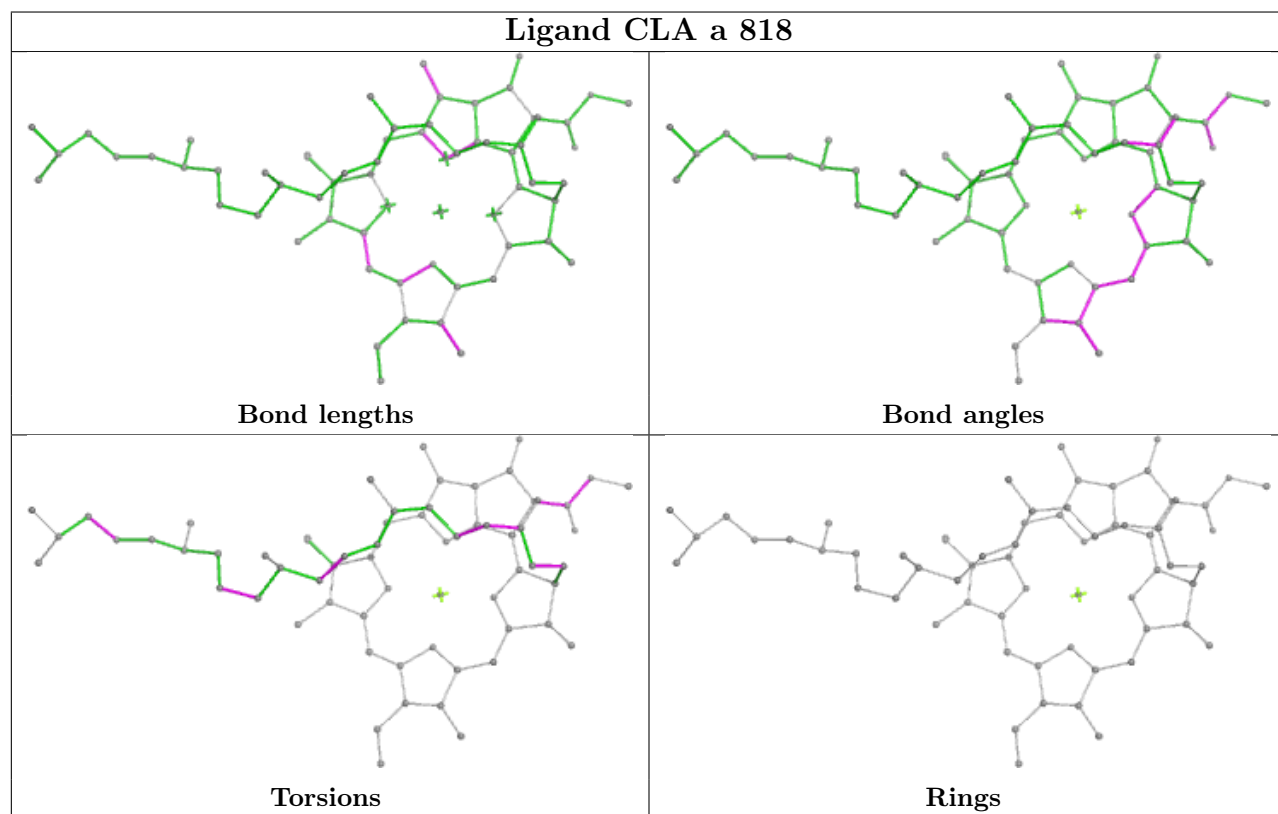
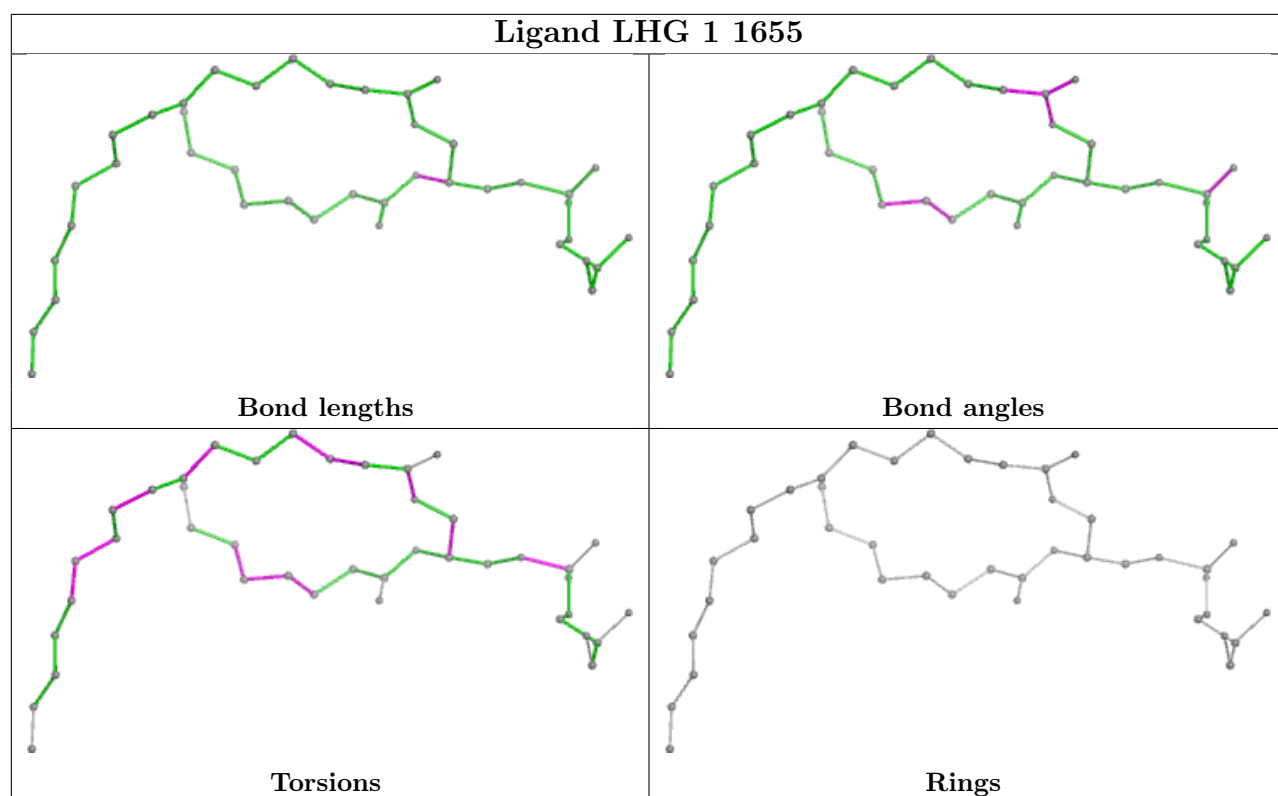


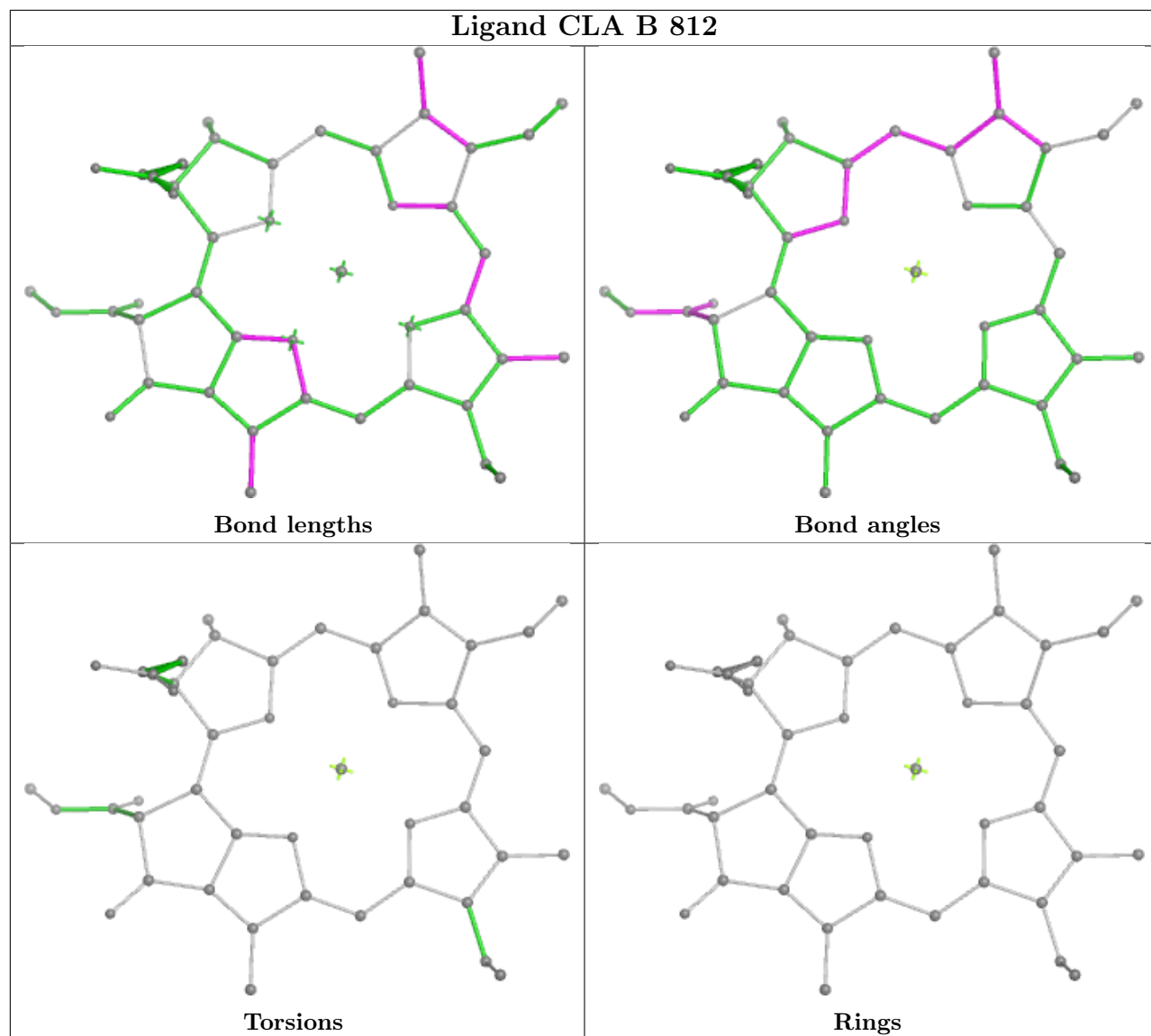
## Ligand CLA a 811





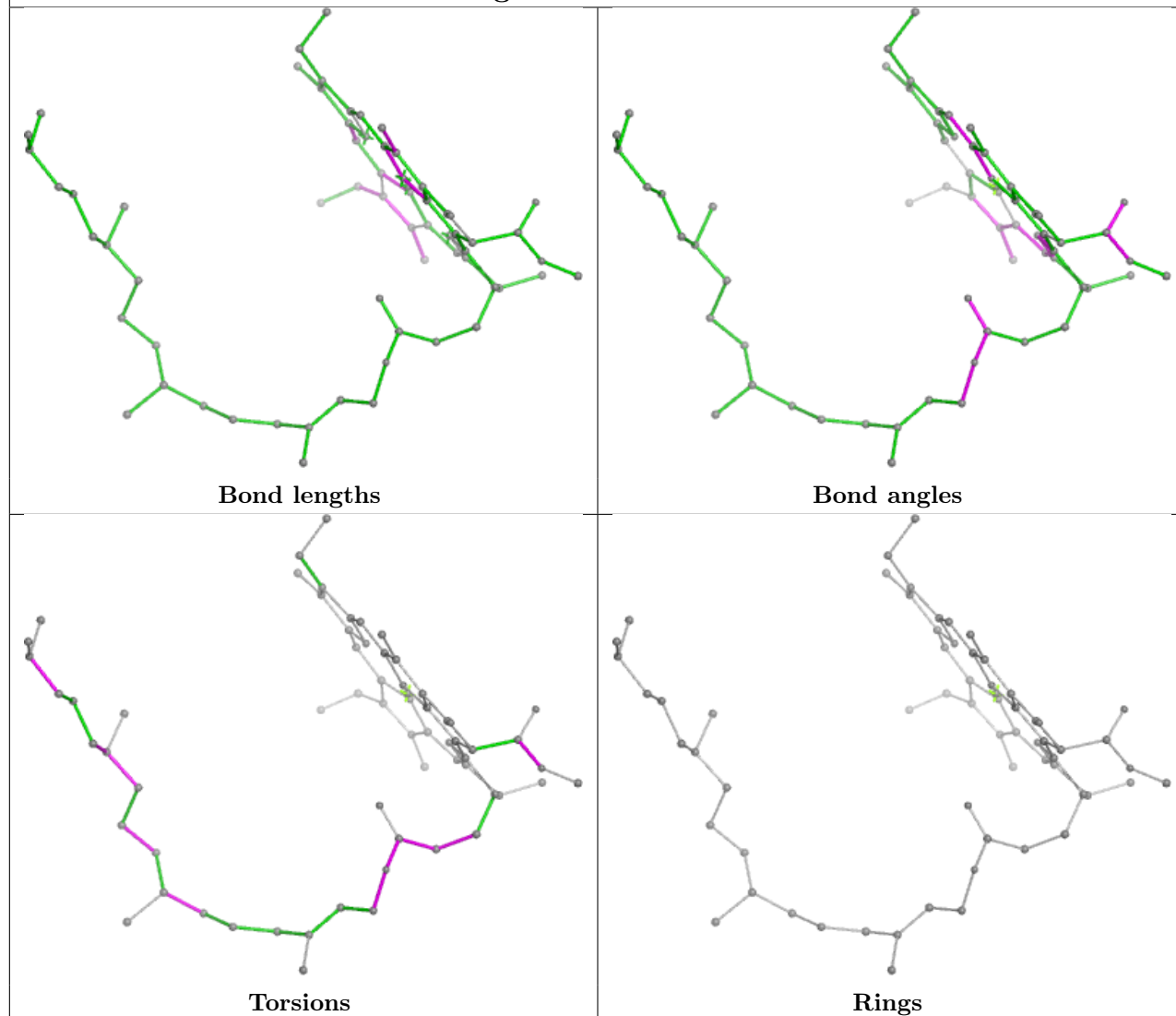




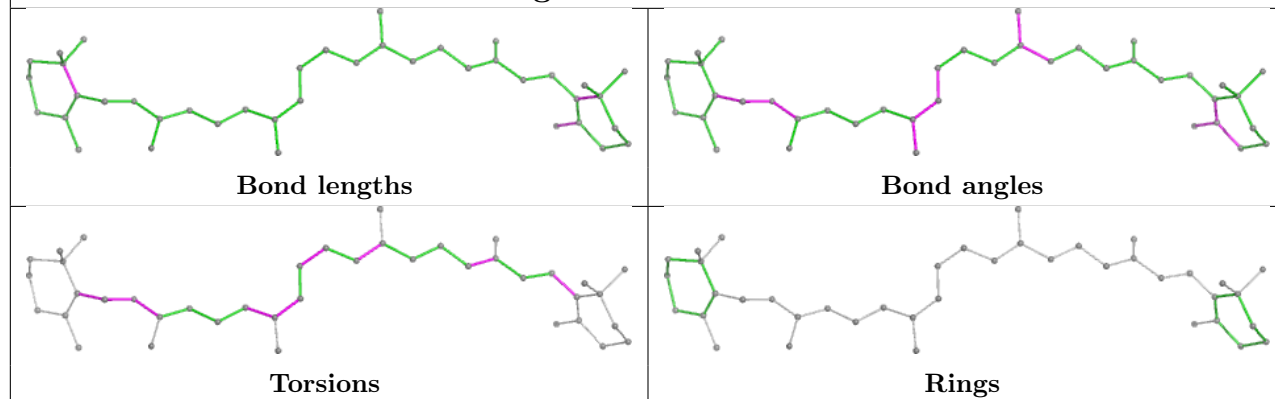


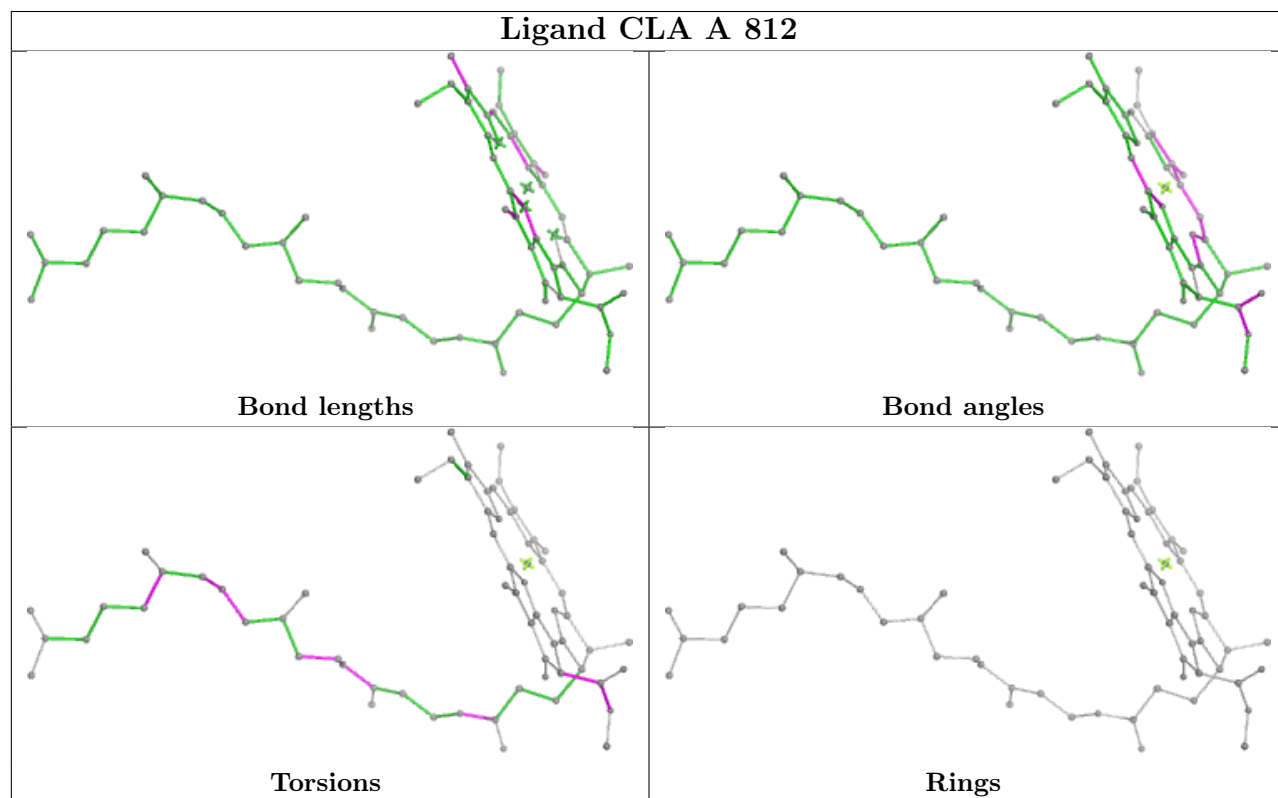
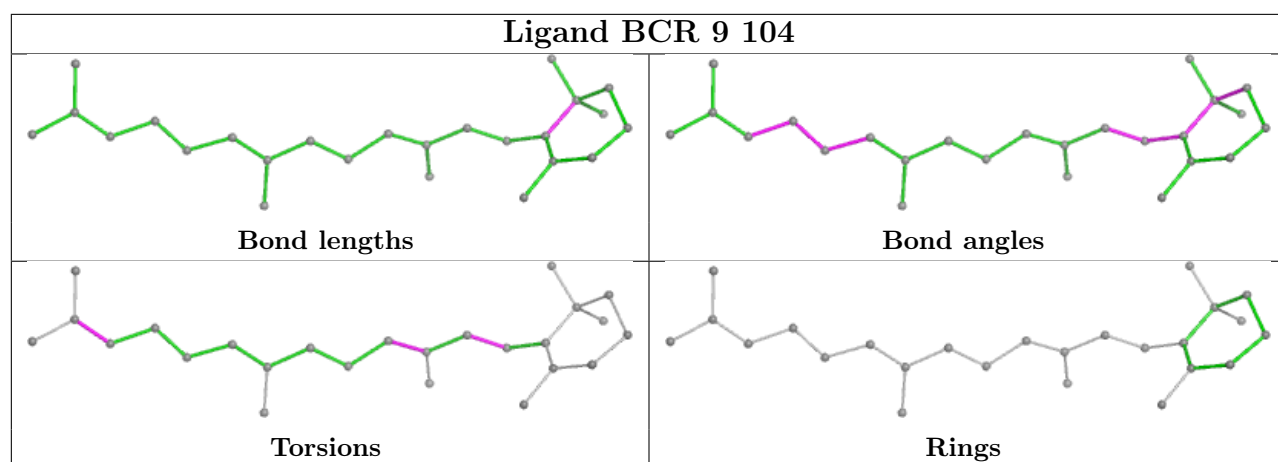


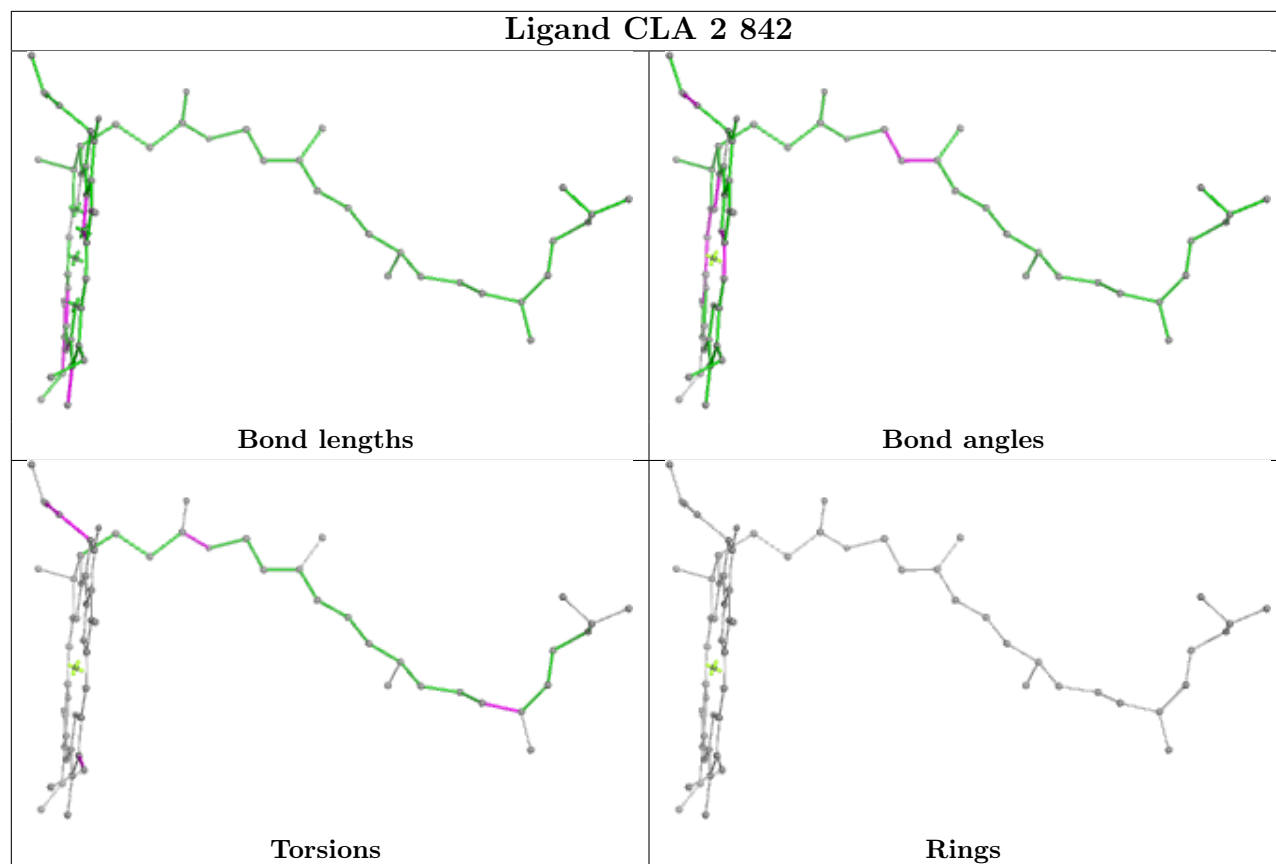
## Ligand CLA 2 820



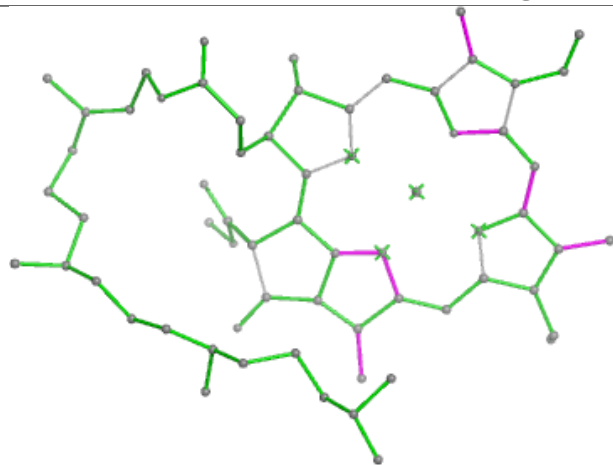
## Ligand BCR 2 847



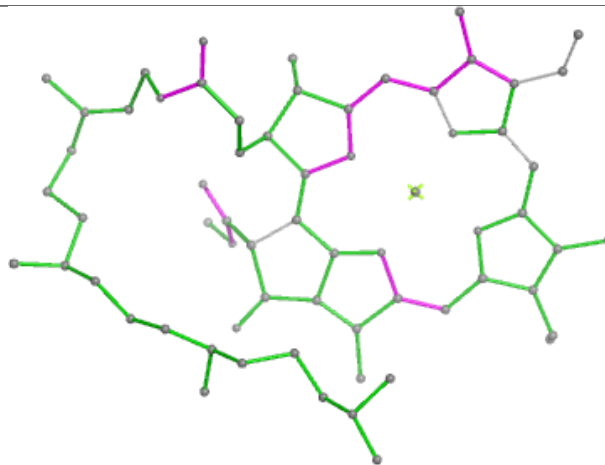




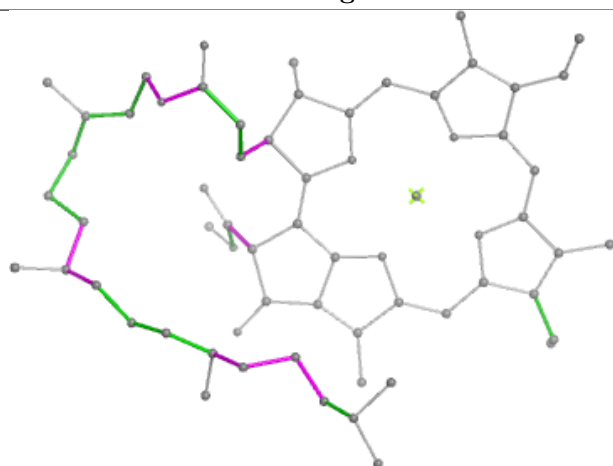
## Ligand CLA b 806



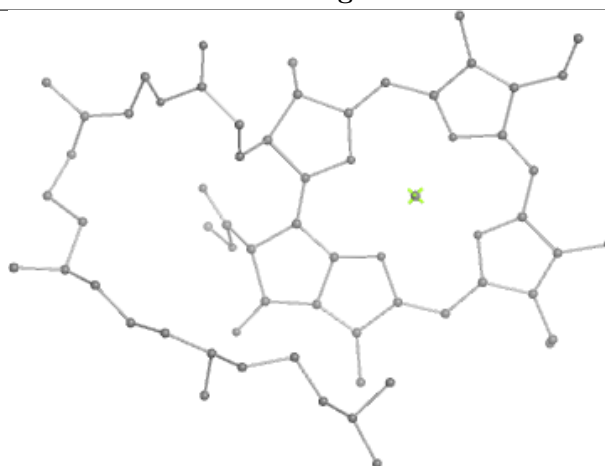
Bond lengths



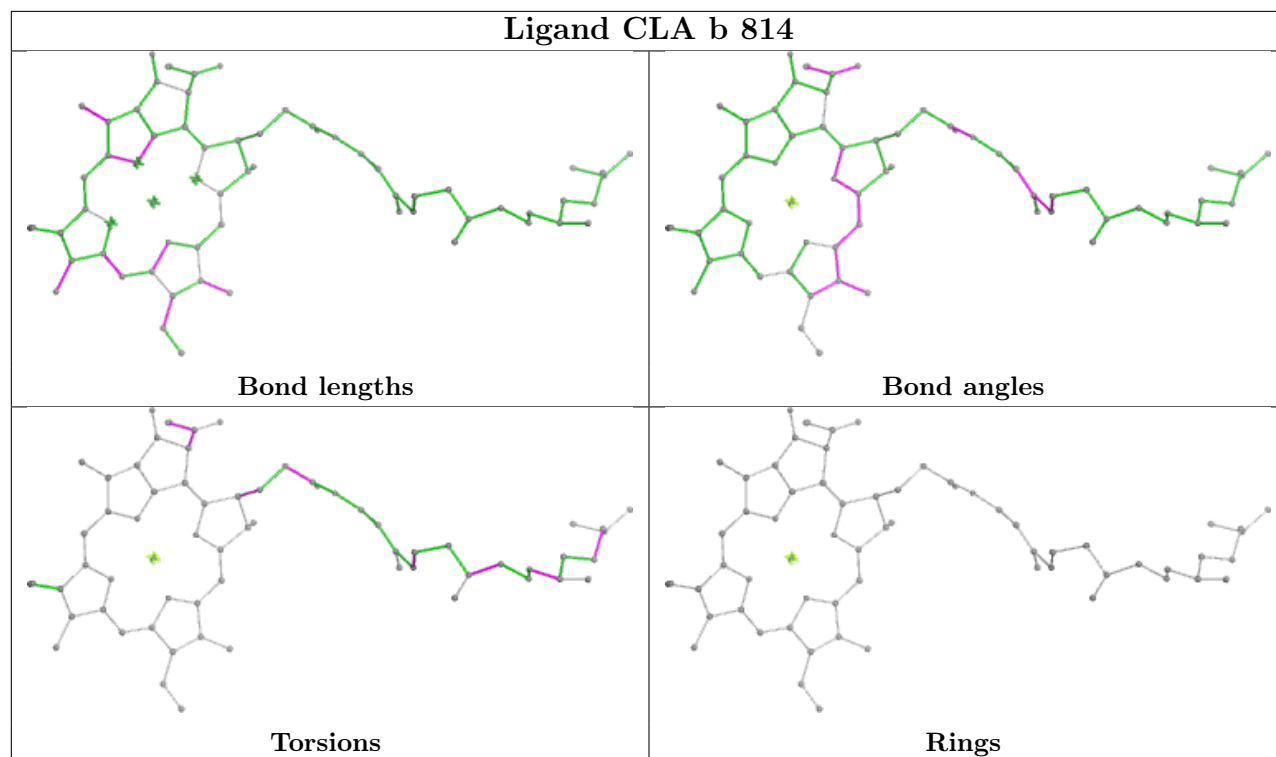
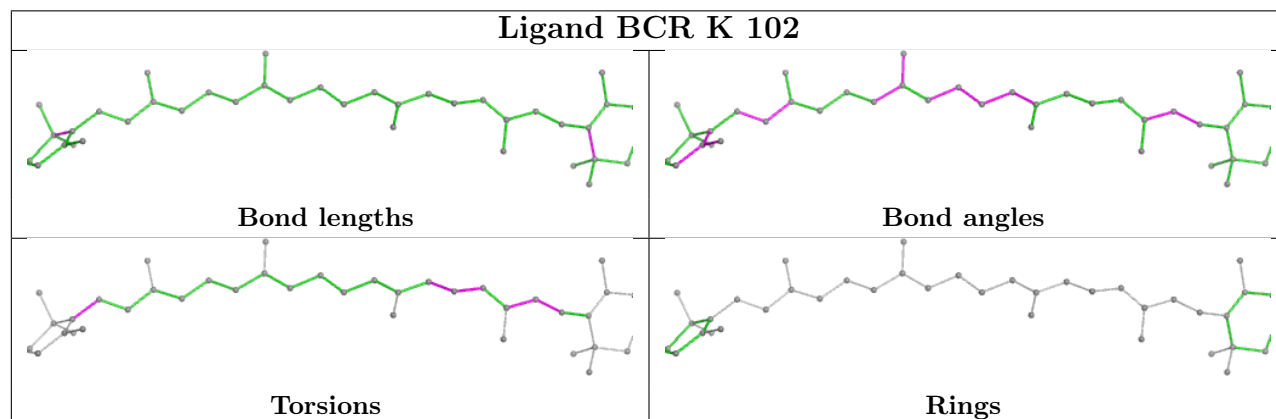
Bond angles



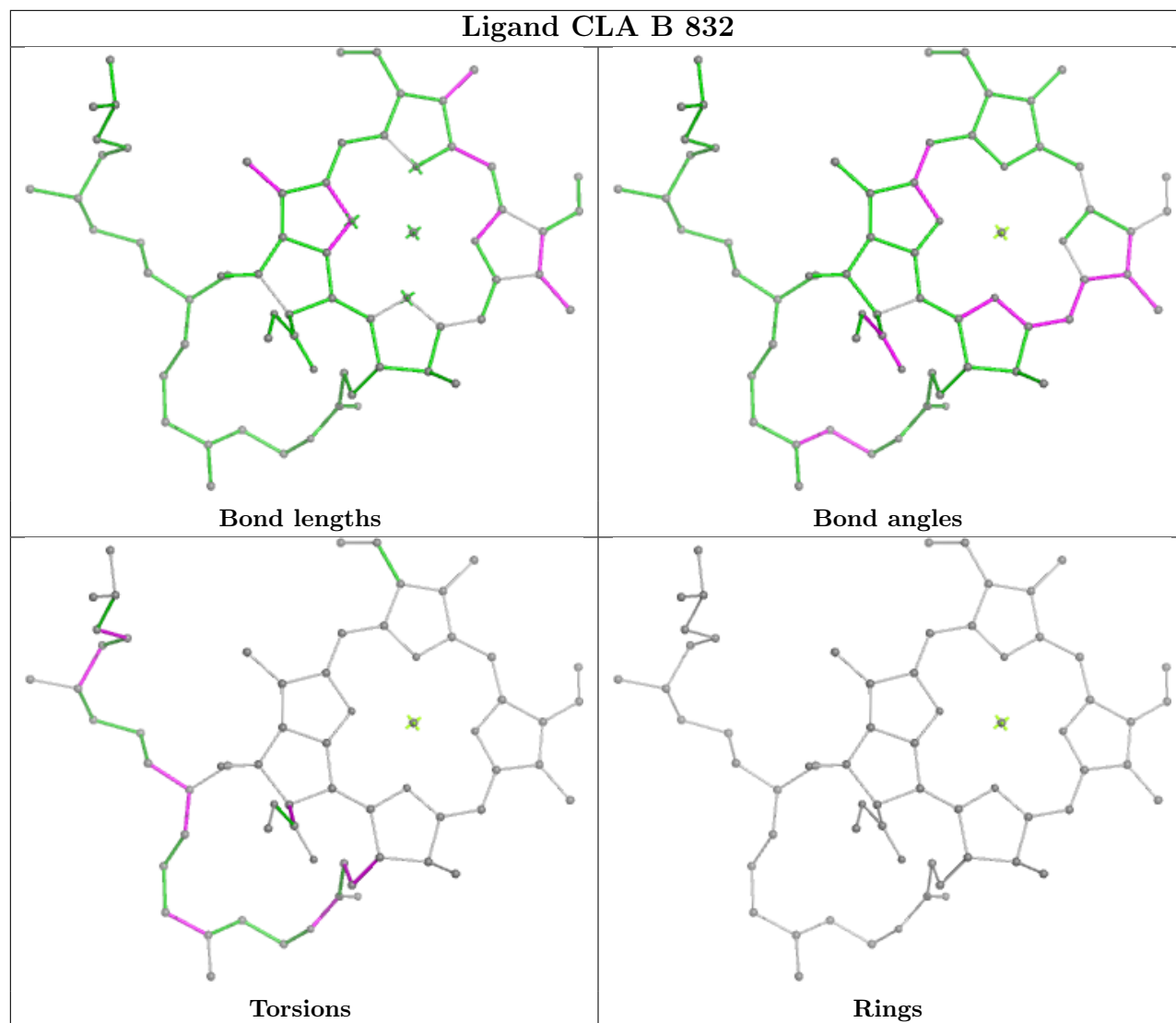
Torsions



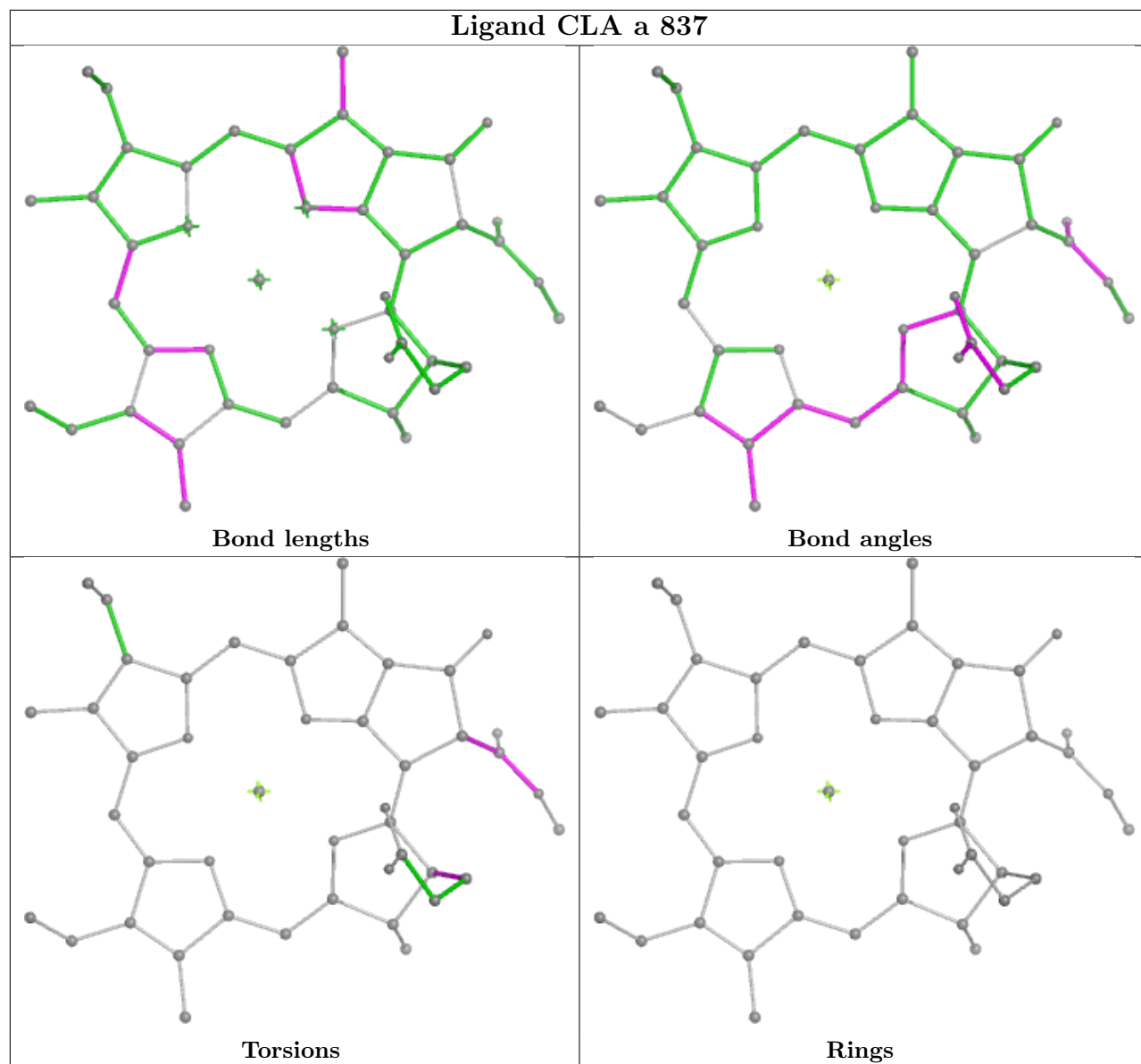
Rings

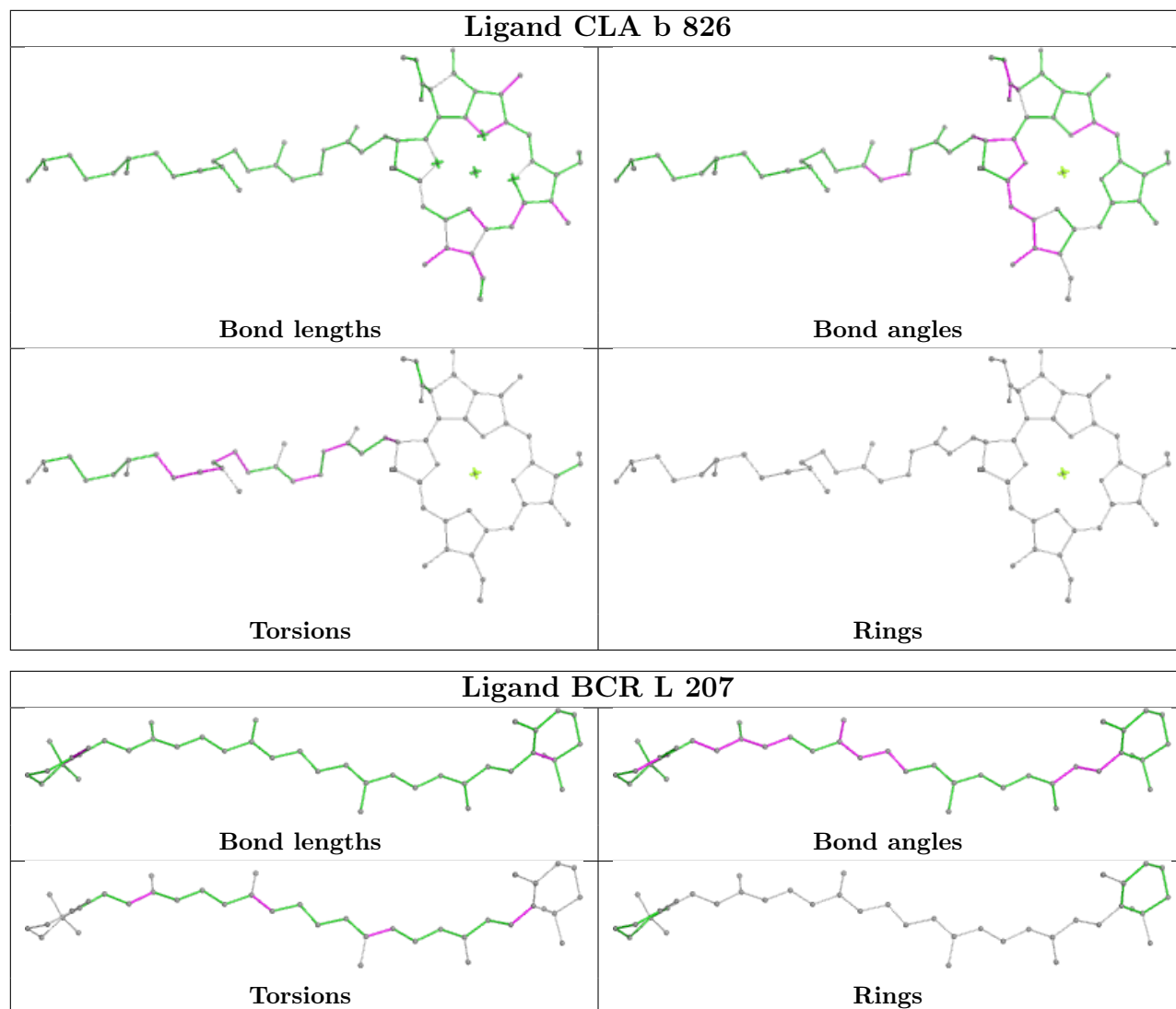
**Ligand CLA b 814****Ligand BCR K 102**

## Ligand CLA B 832



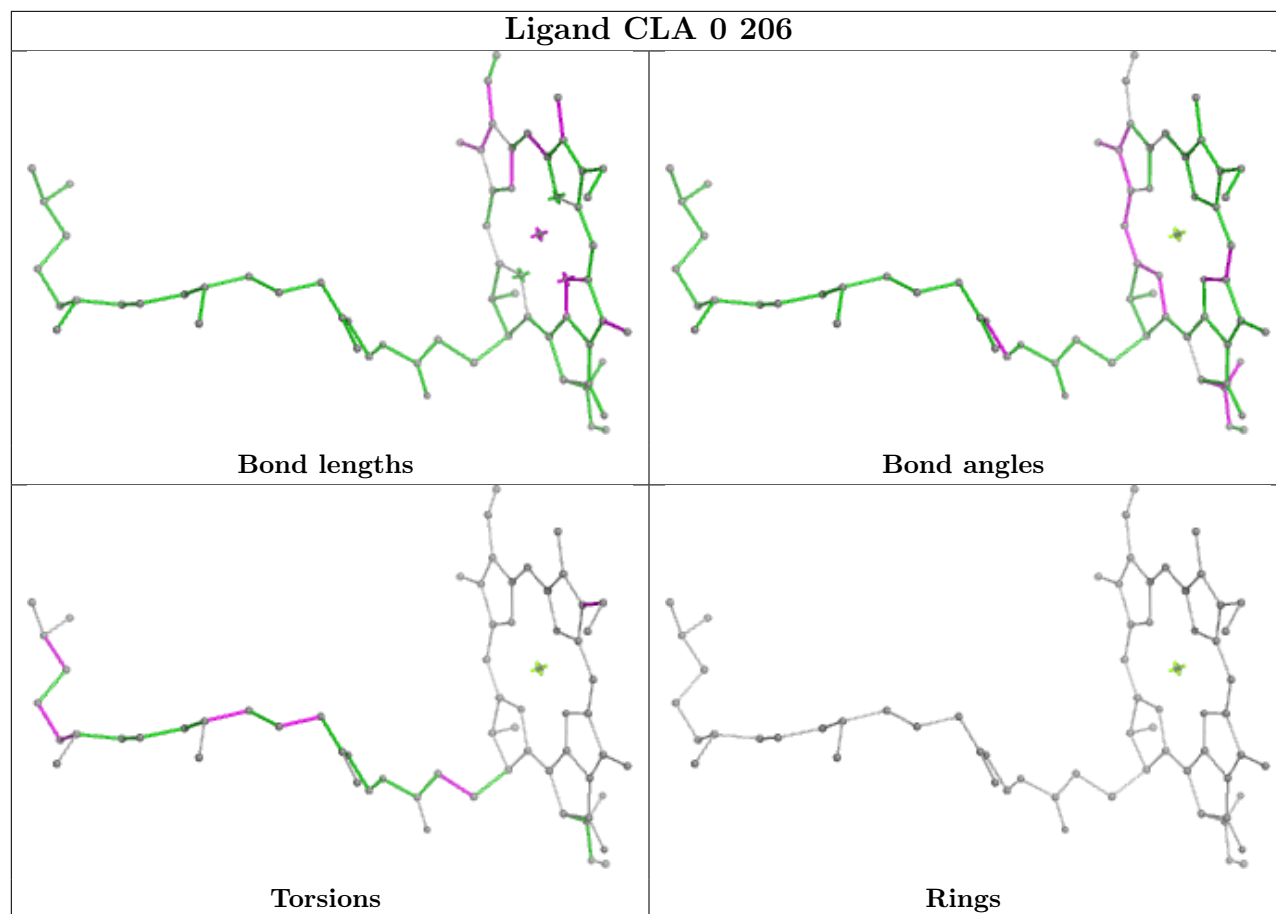
## Ligand CLA a 837



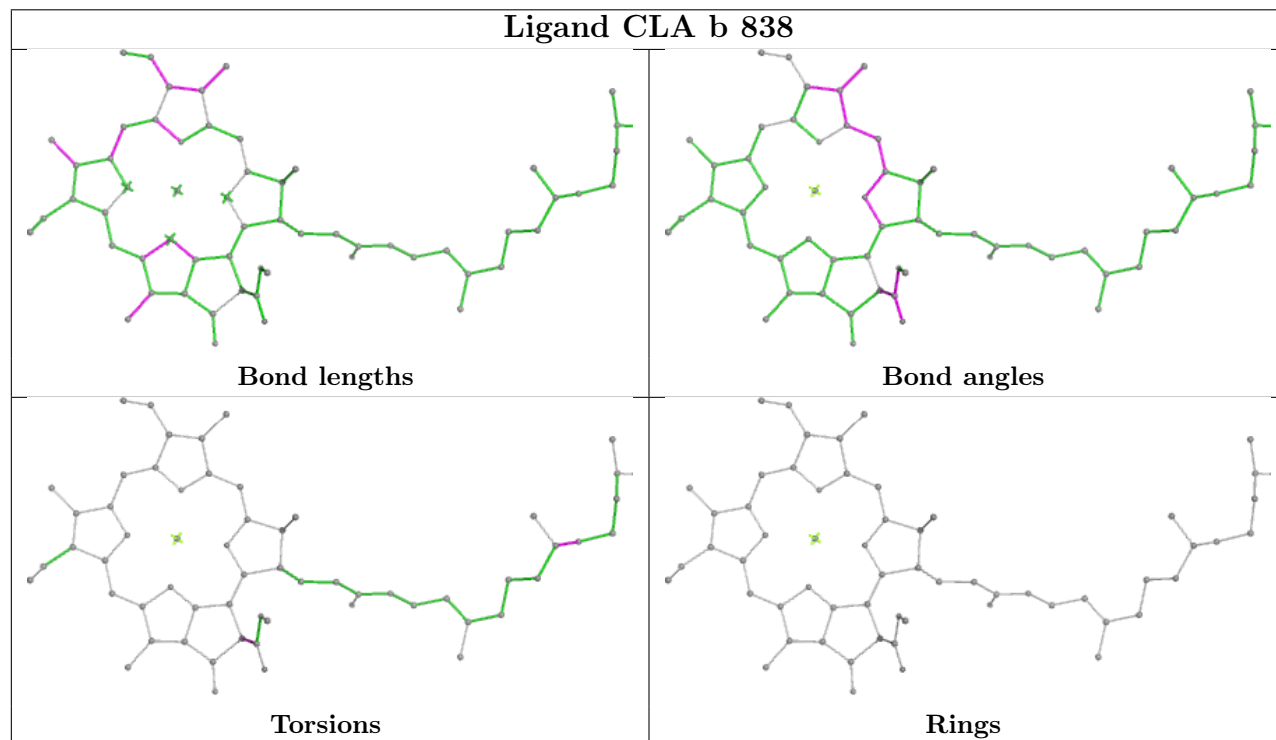




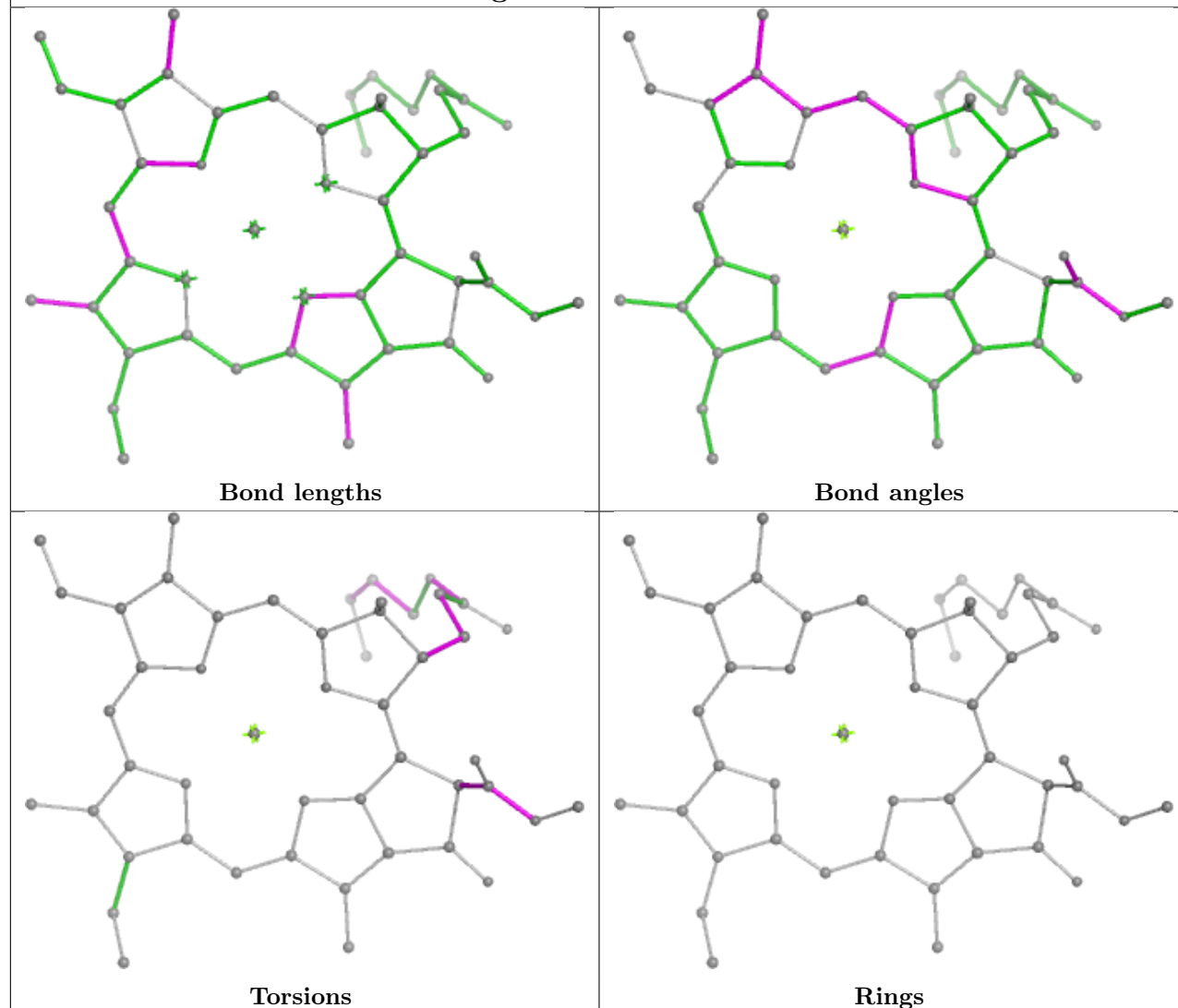
## Ligand CLA 0 206



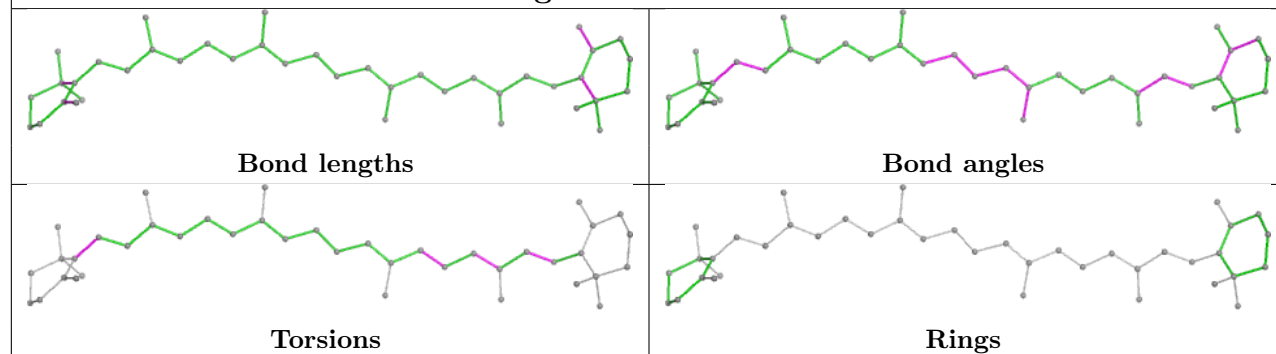
## Ligand CLA b 838

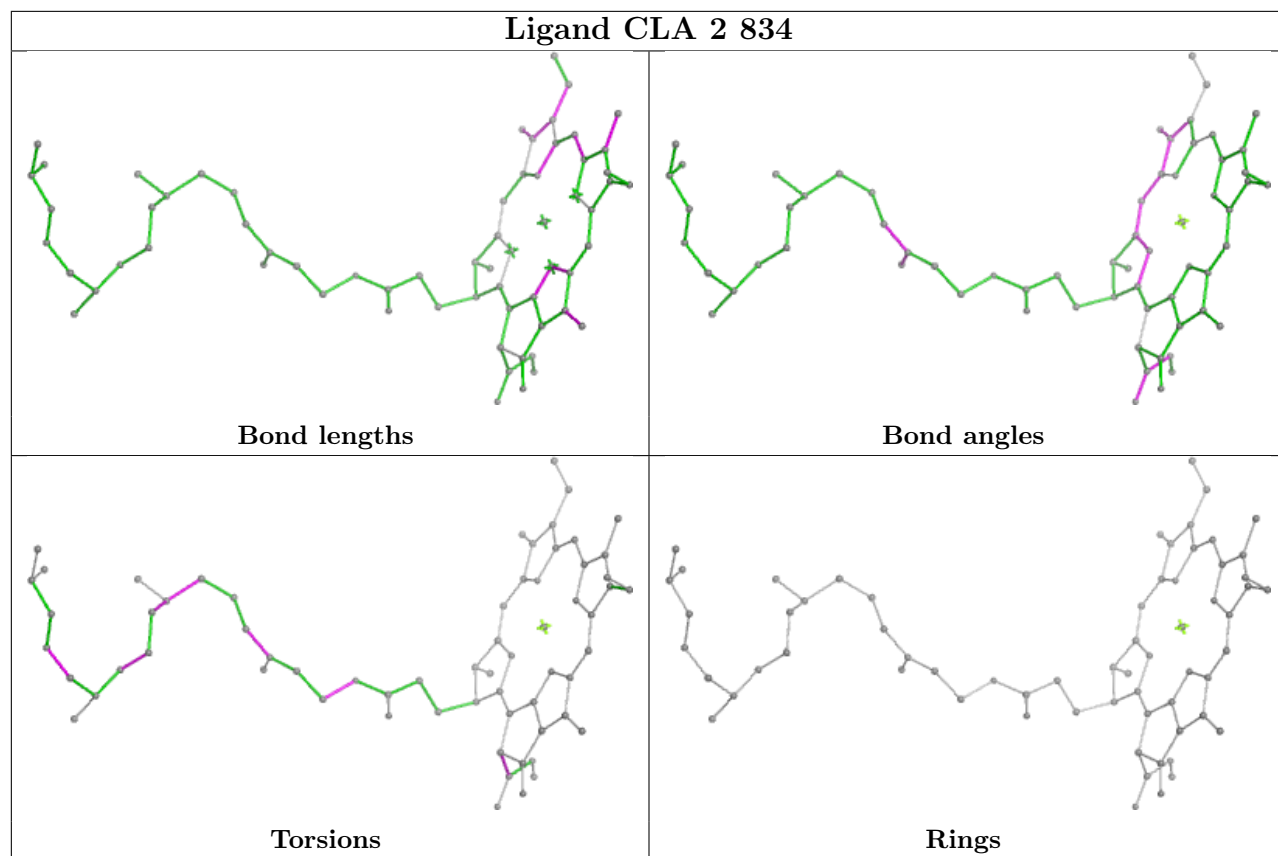


## Ligand CLA B 831

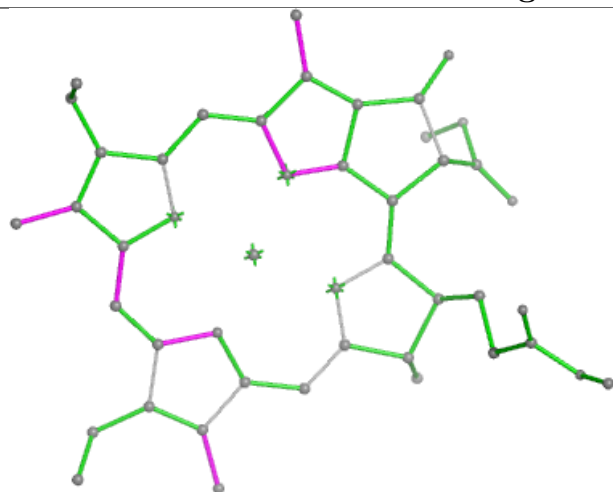


## Ligand BCR 2 849

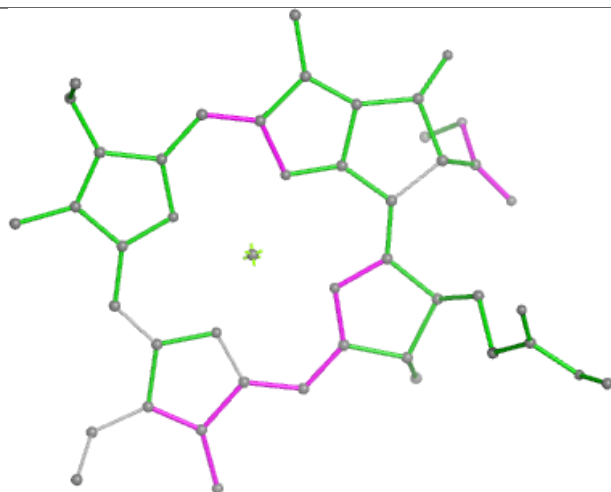




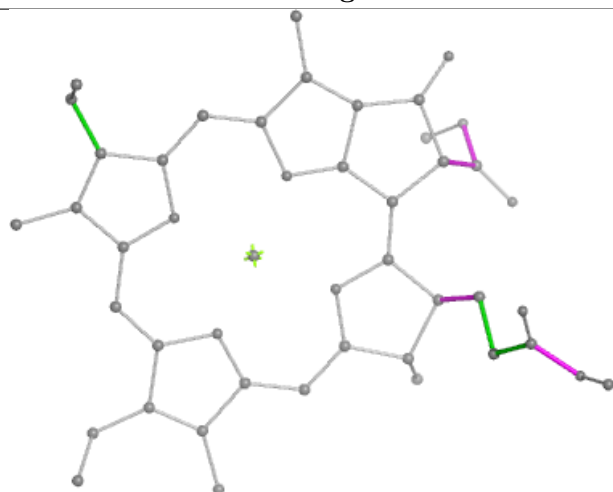
## Ligand CLA 9 101



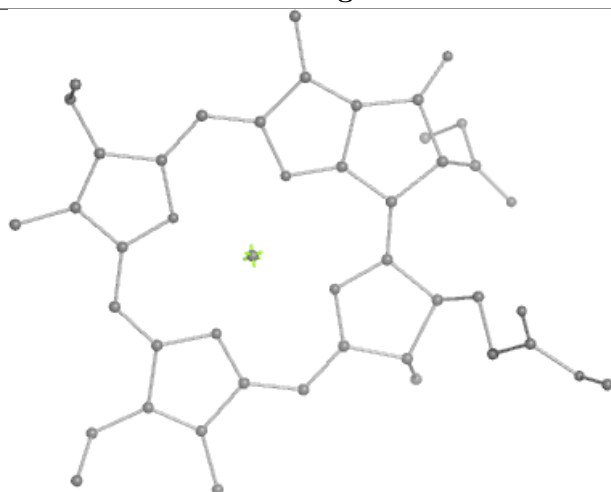
Bond lengths



Bond angles

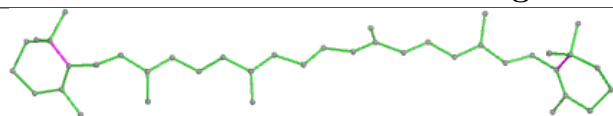


Torsions

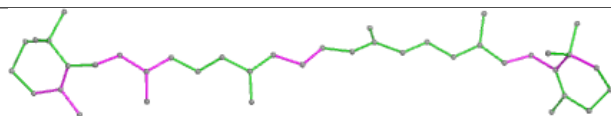


Rings

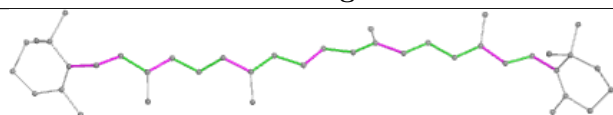
## Ligand BCR A 847



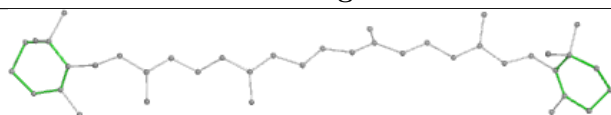
Bond lengths



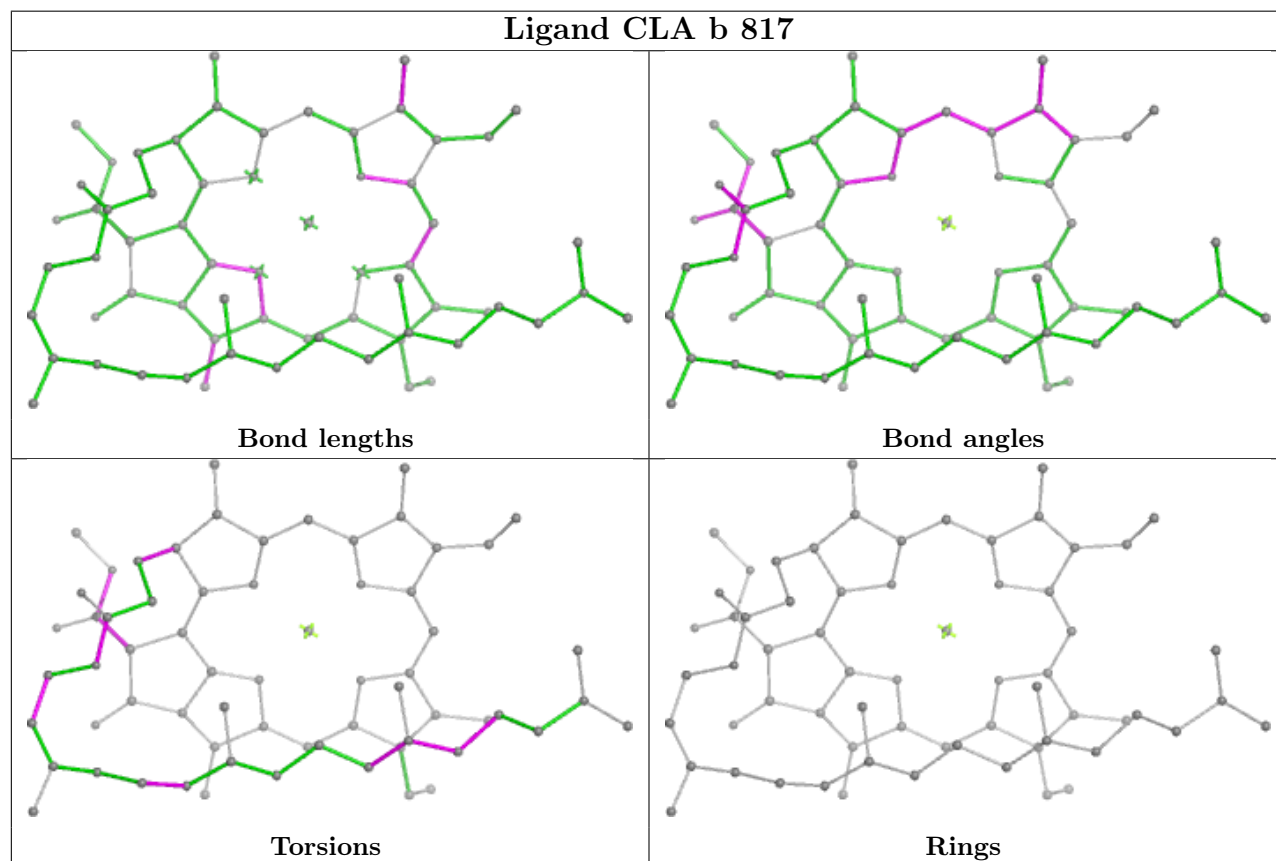
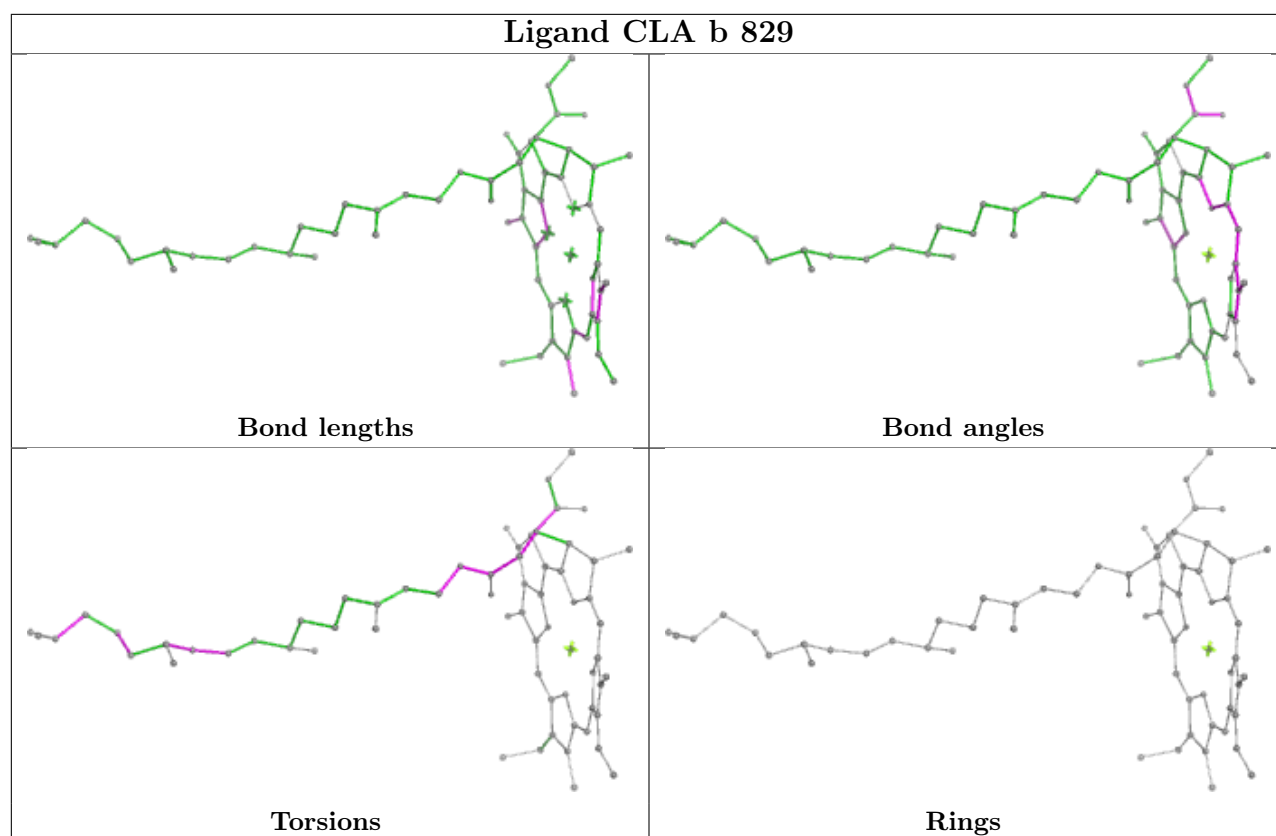
Bond angles

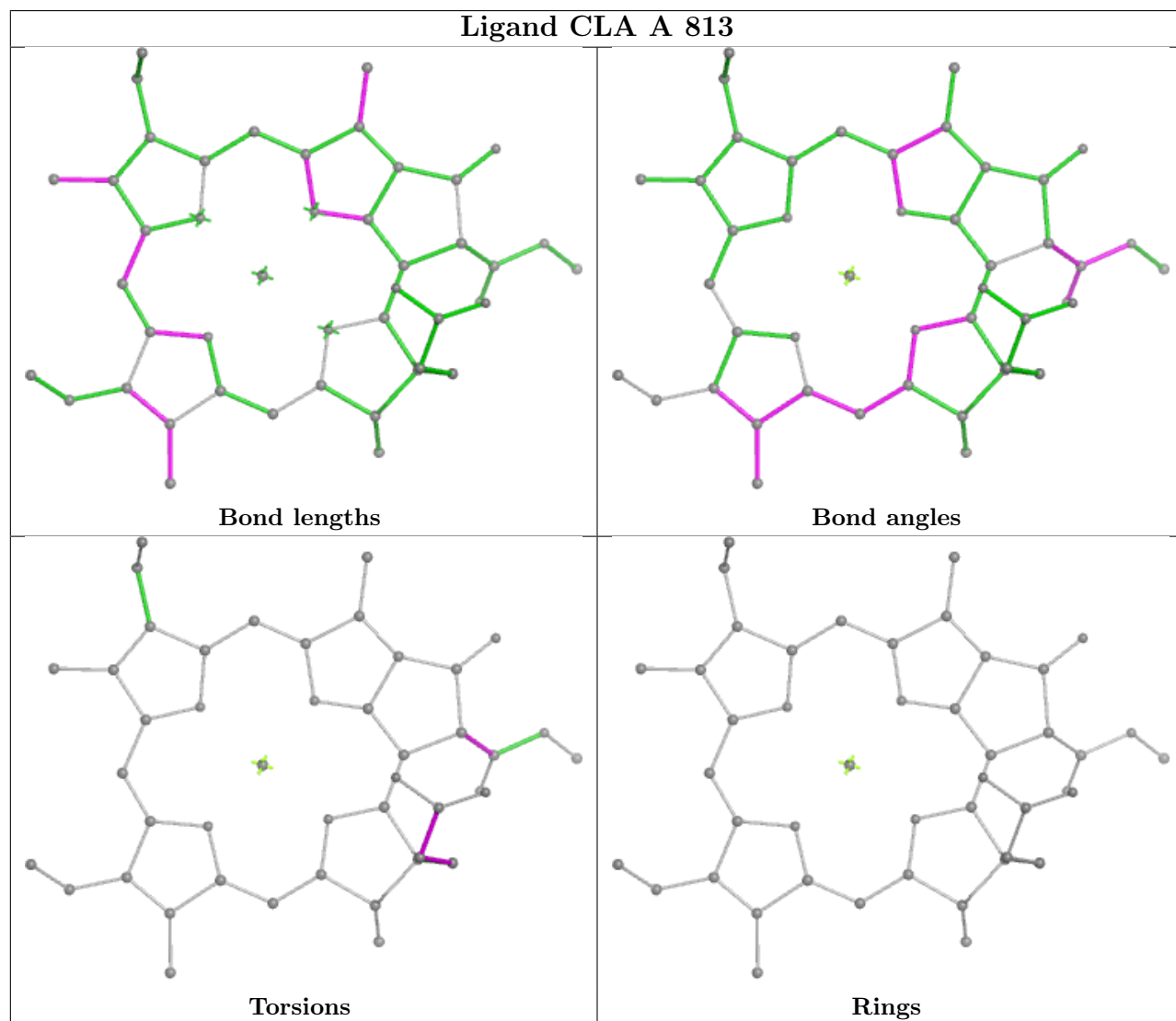
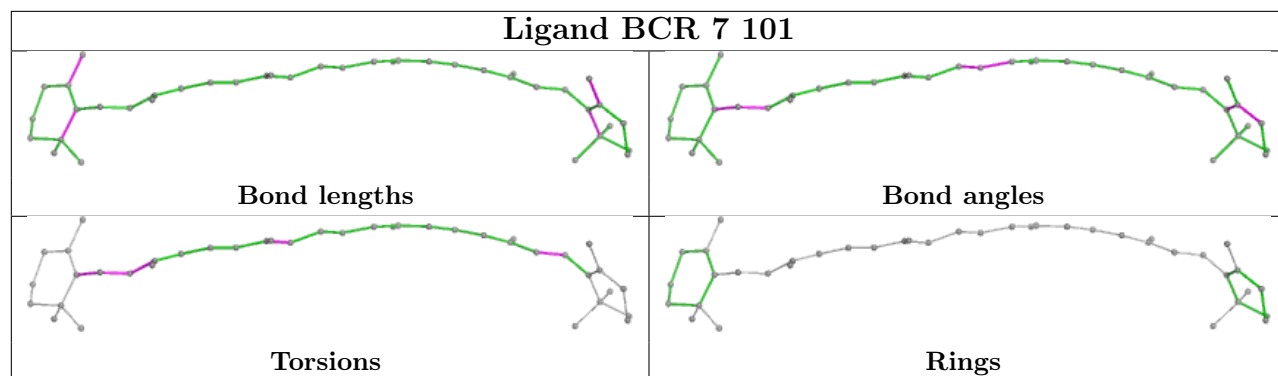


Torsions

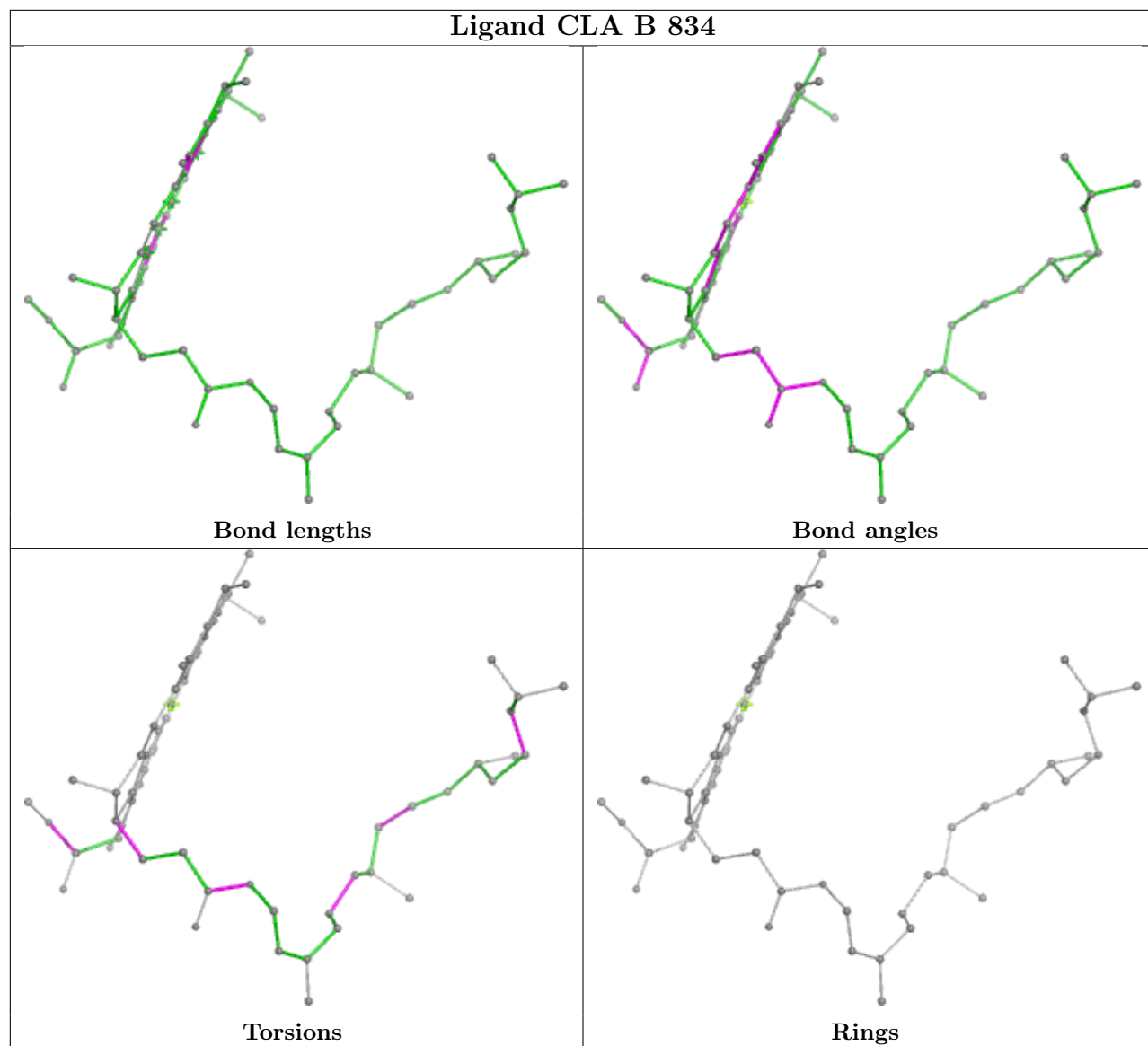


Rings

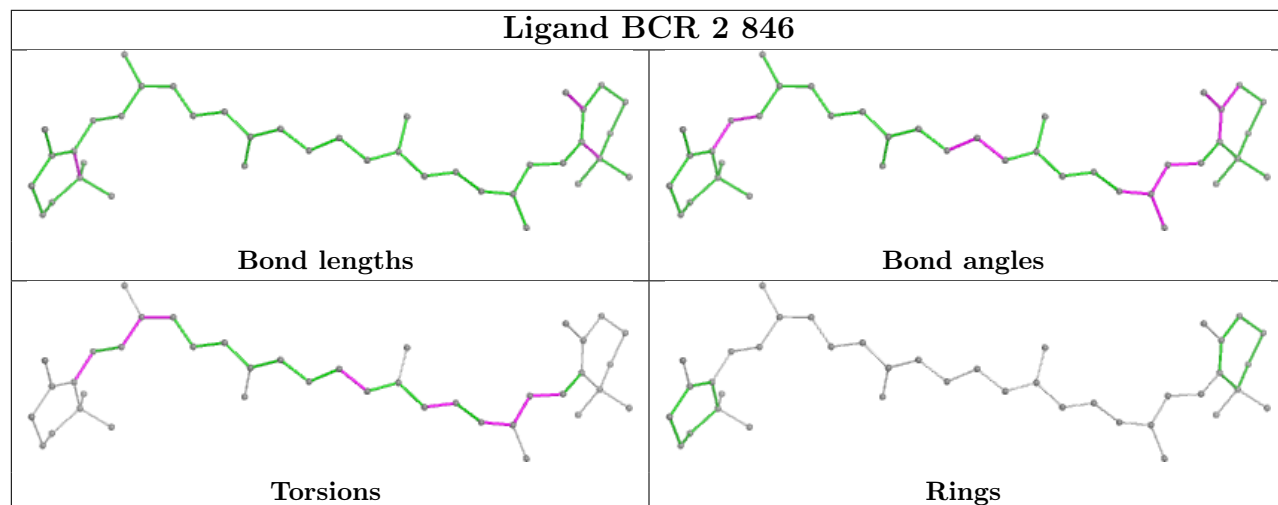




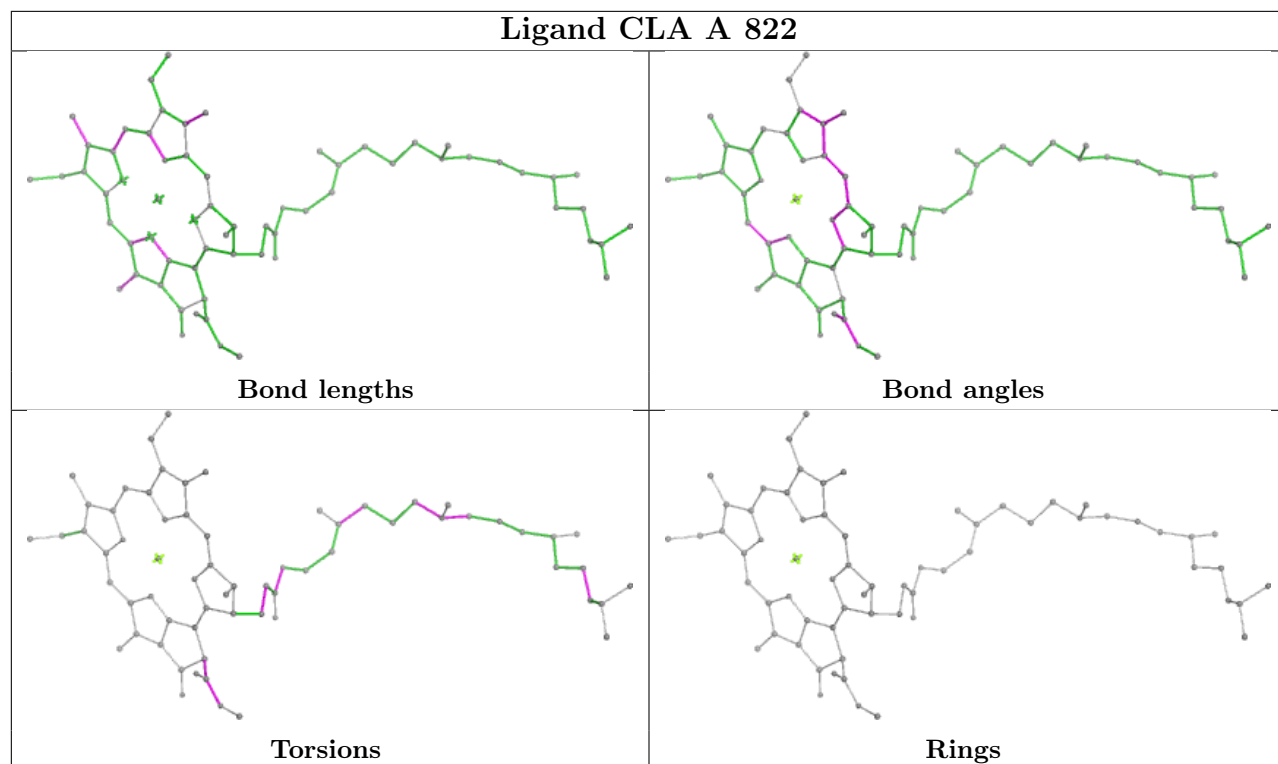
## Ligand CLA B 834



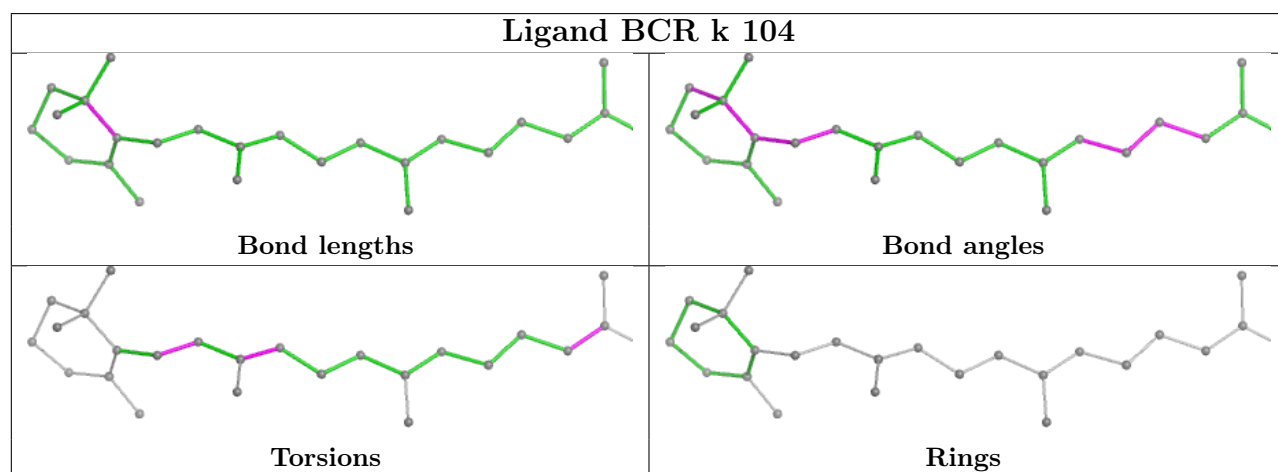
## Ligand BCR 2 846



## Ligand CLA A 822

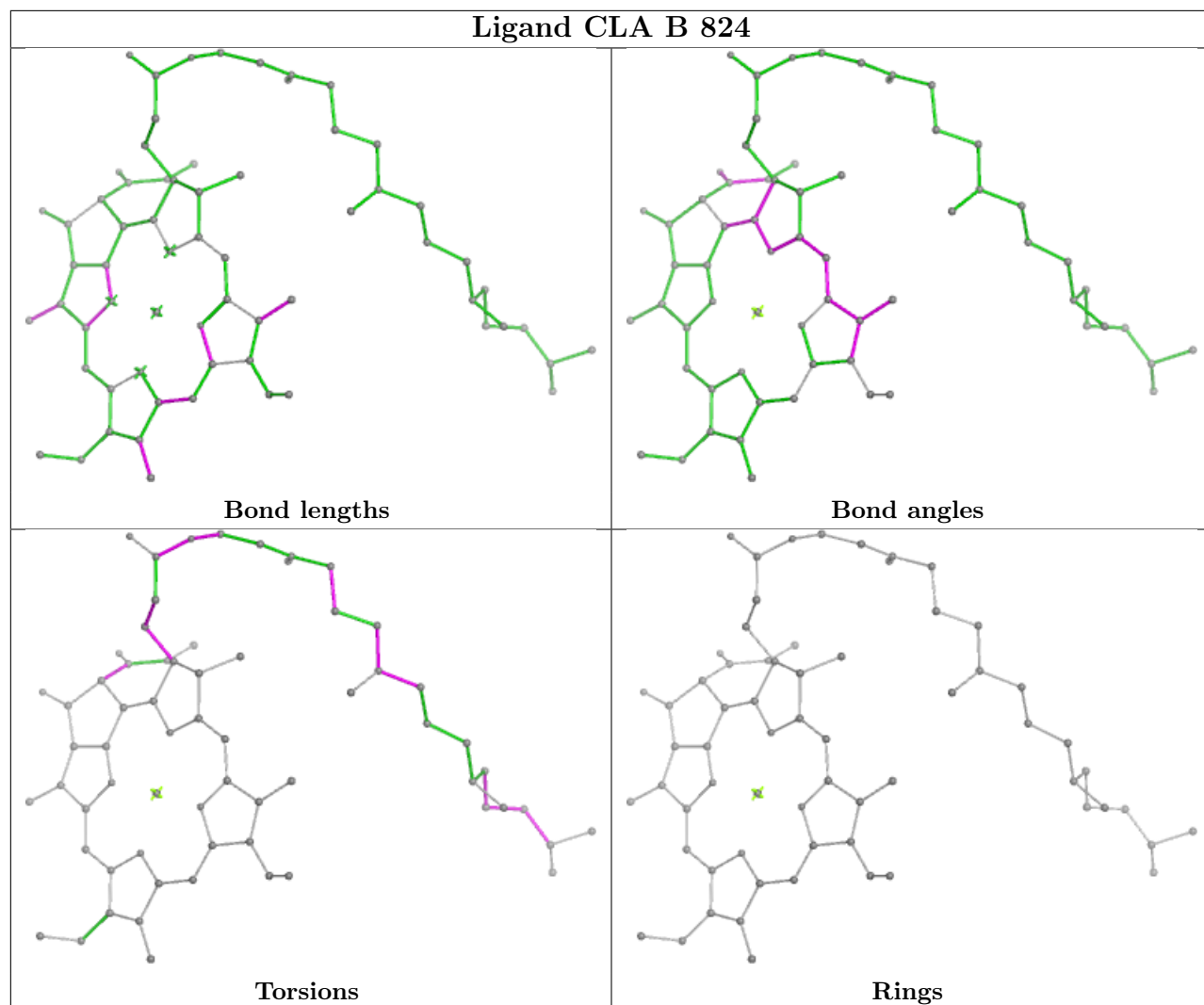


## Ligand BCR k 104

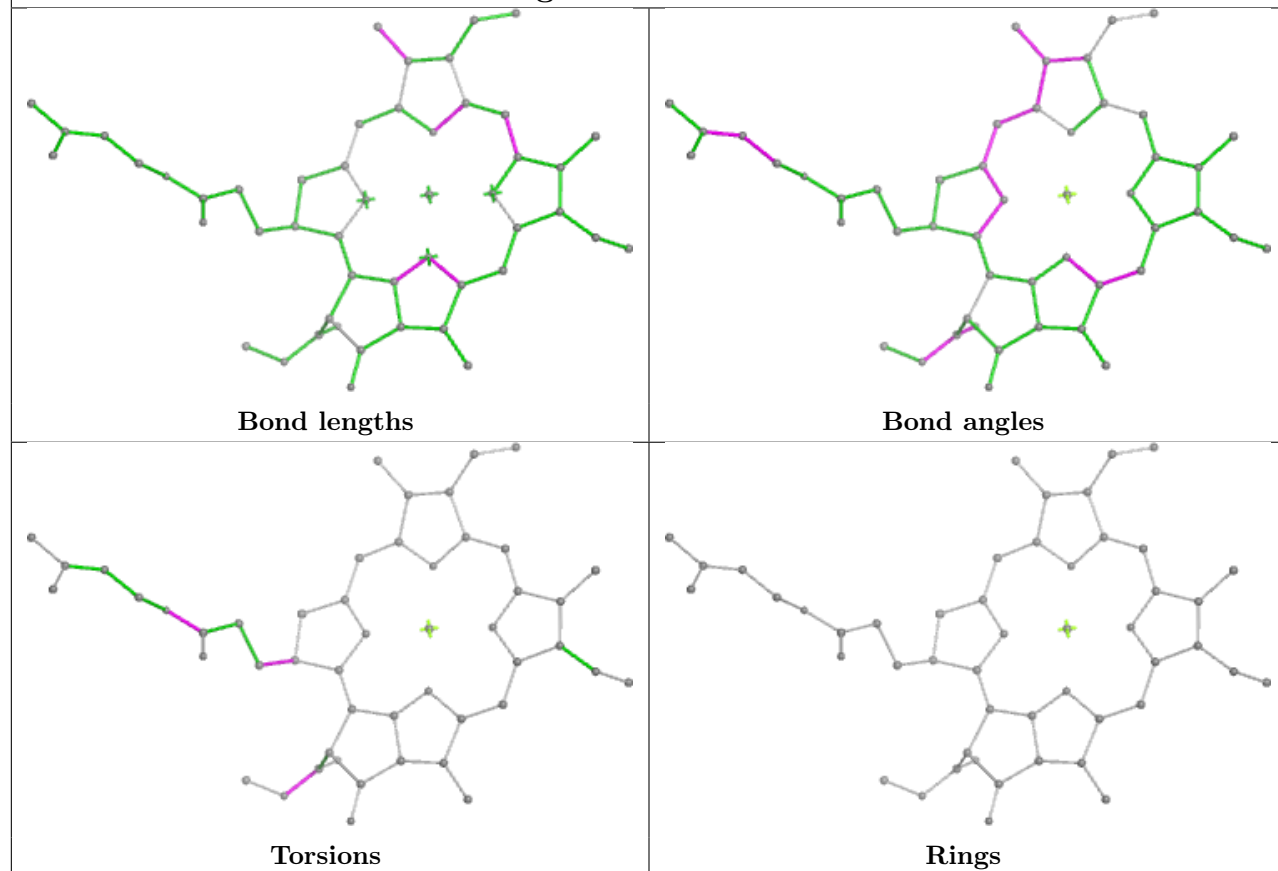




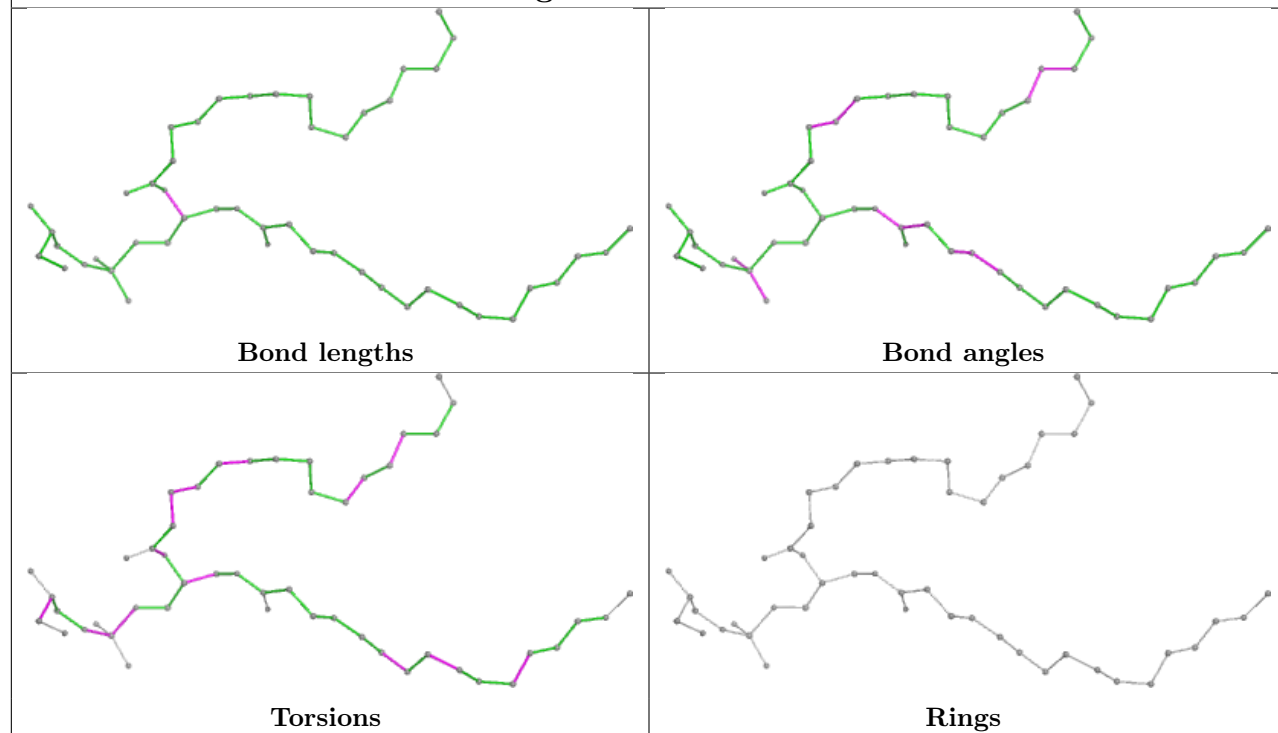
## Ligand CLA B 824

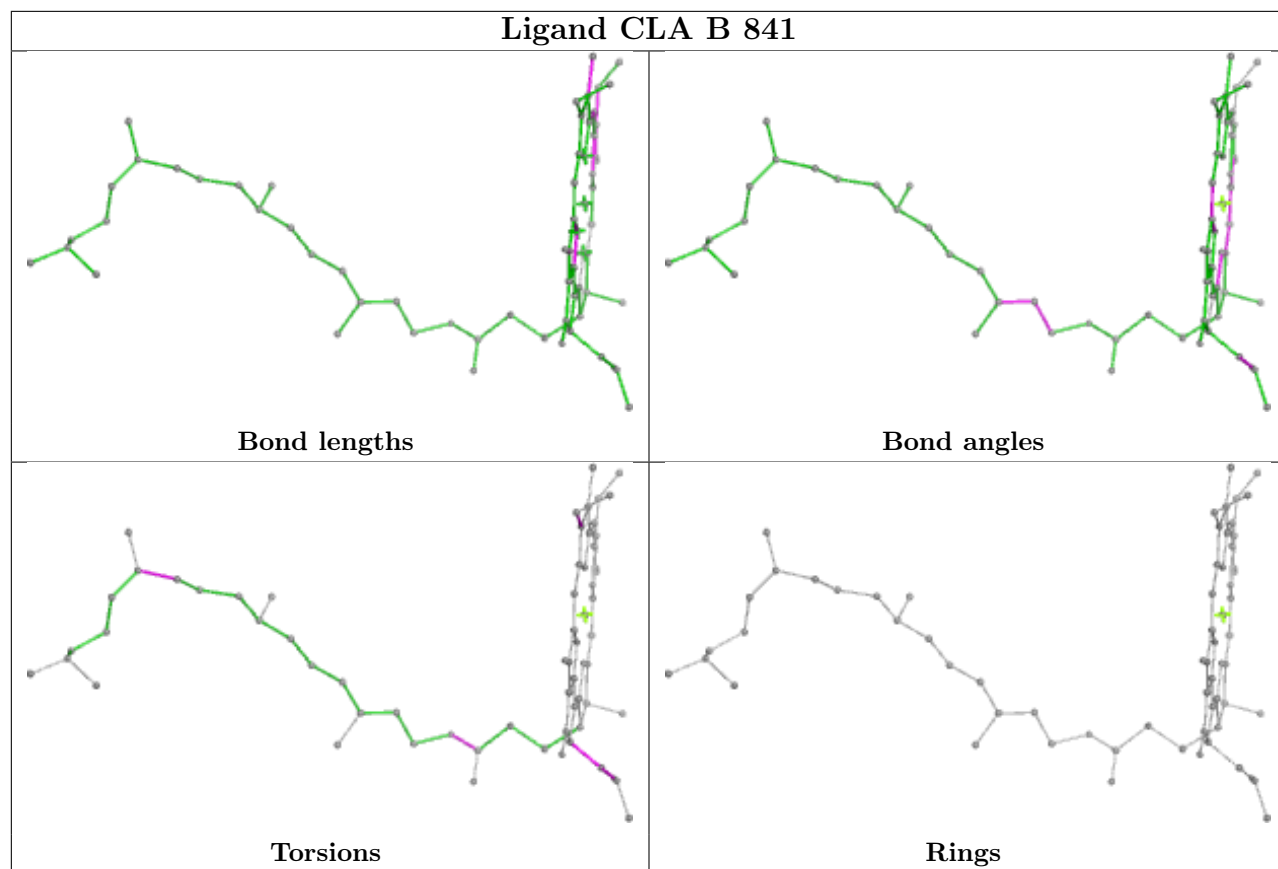


## Ligand CLA 6 203

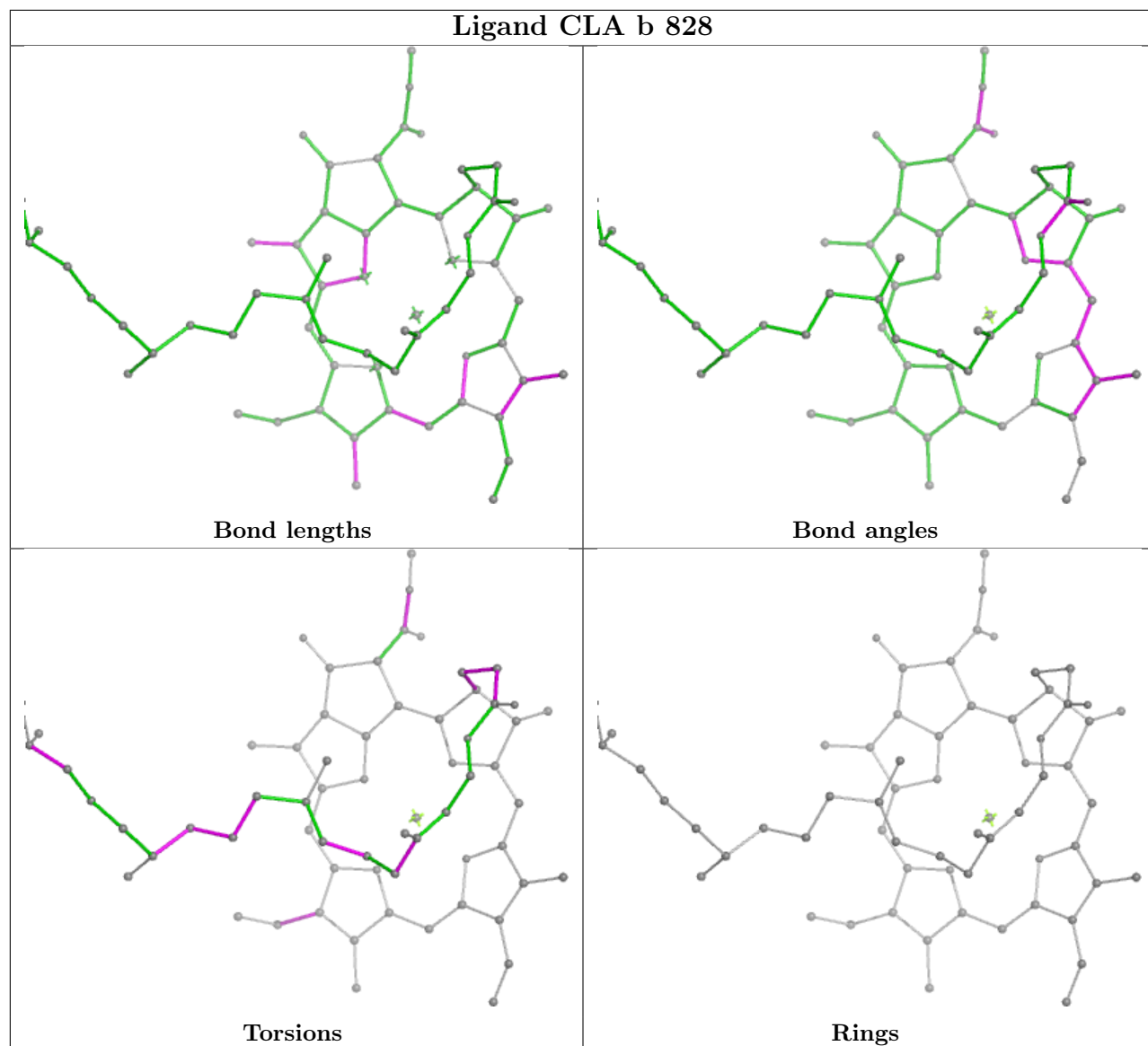


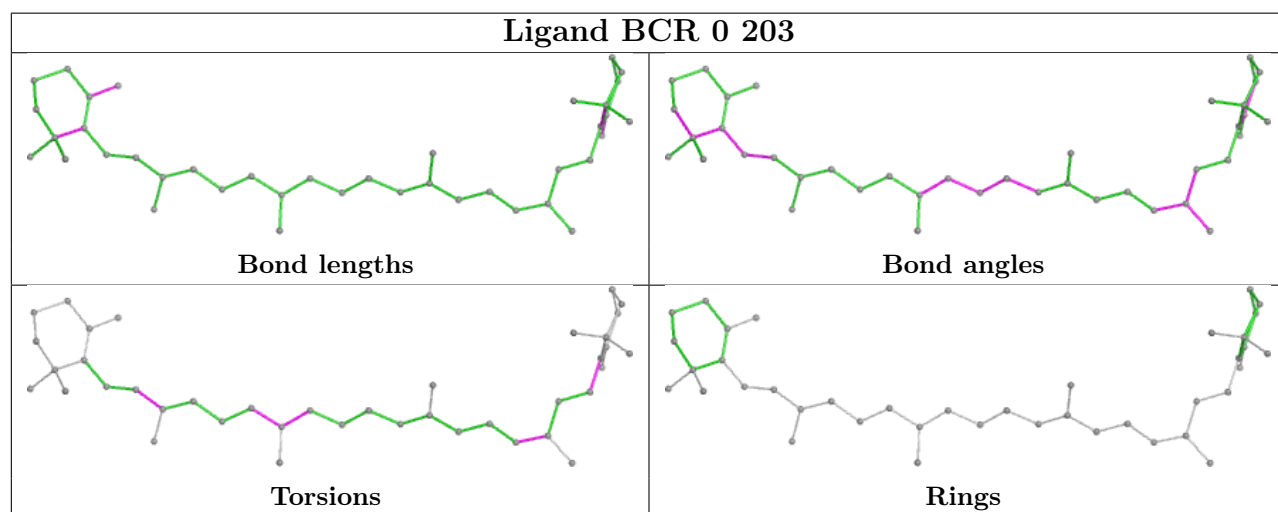
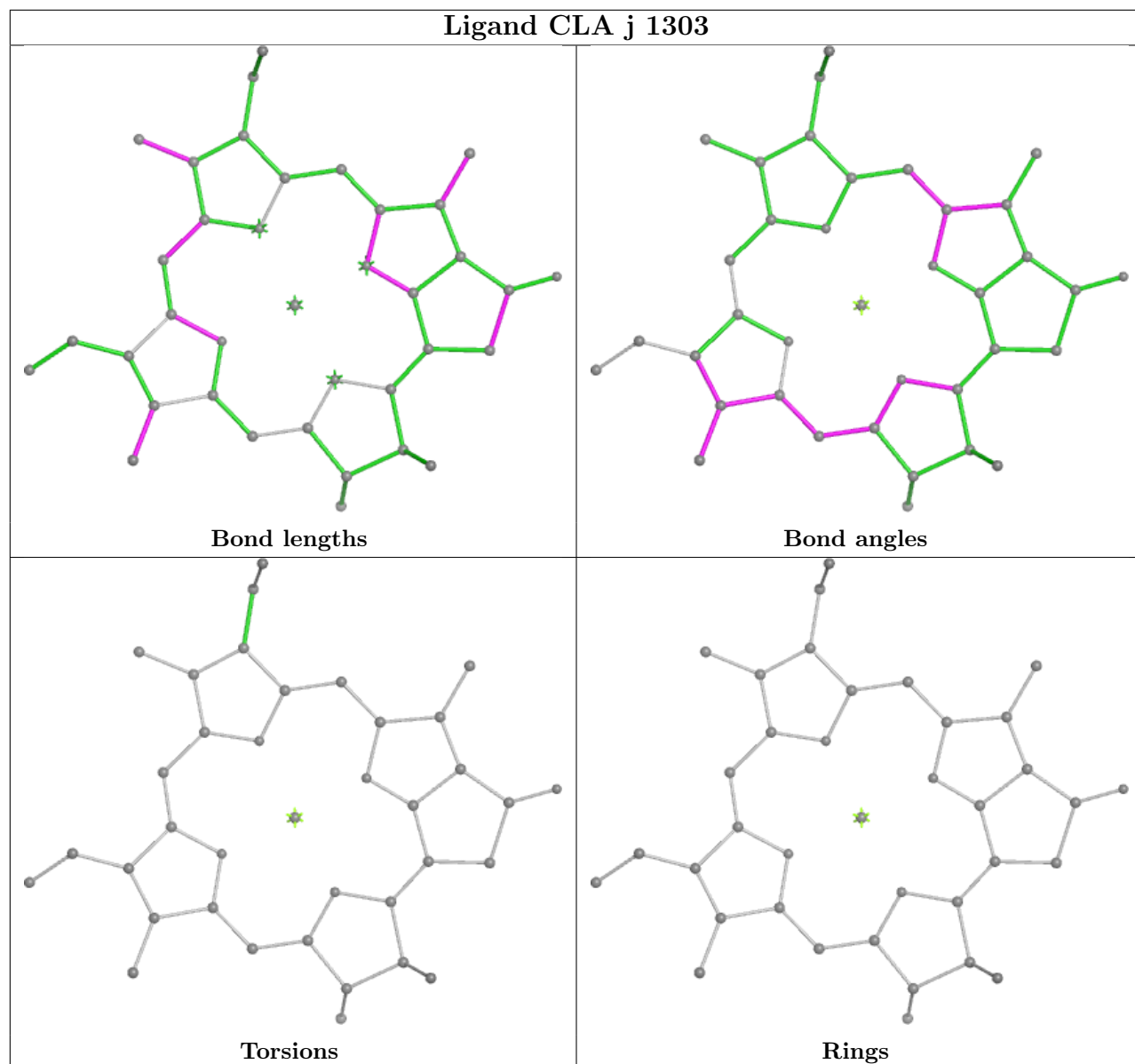
## Ligand LHG z 101

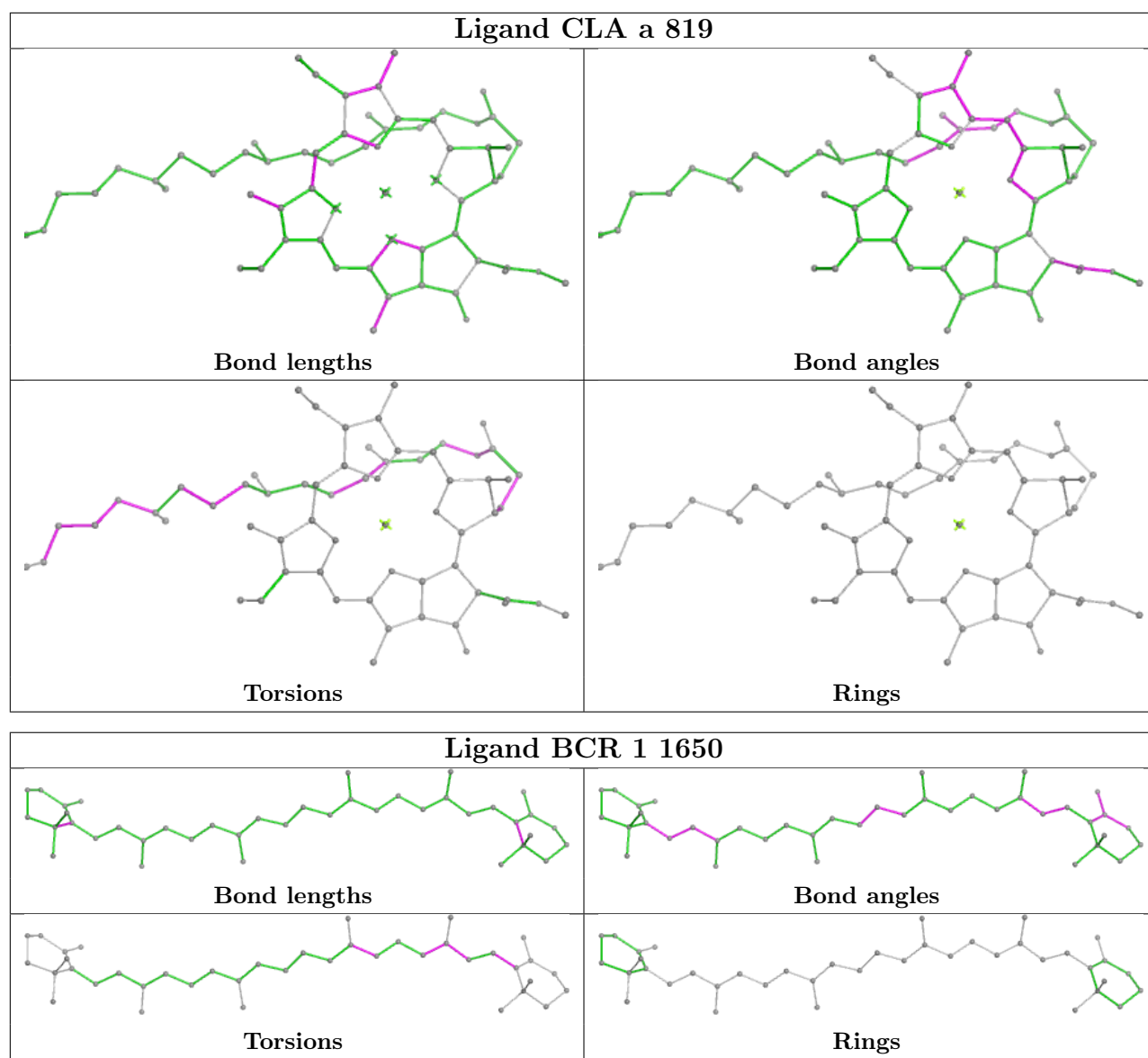




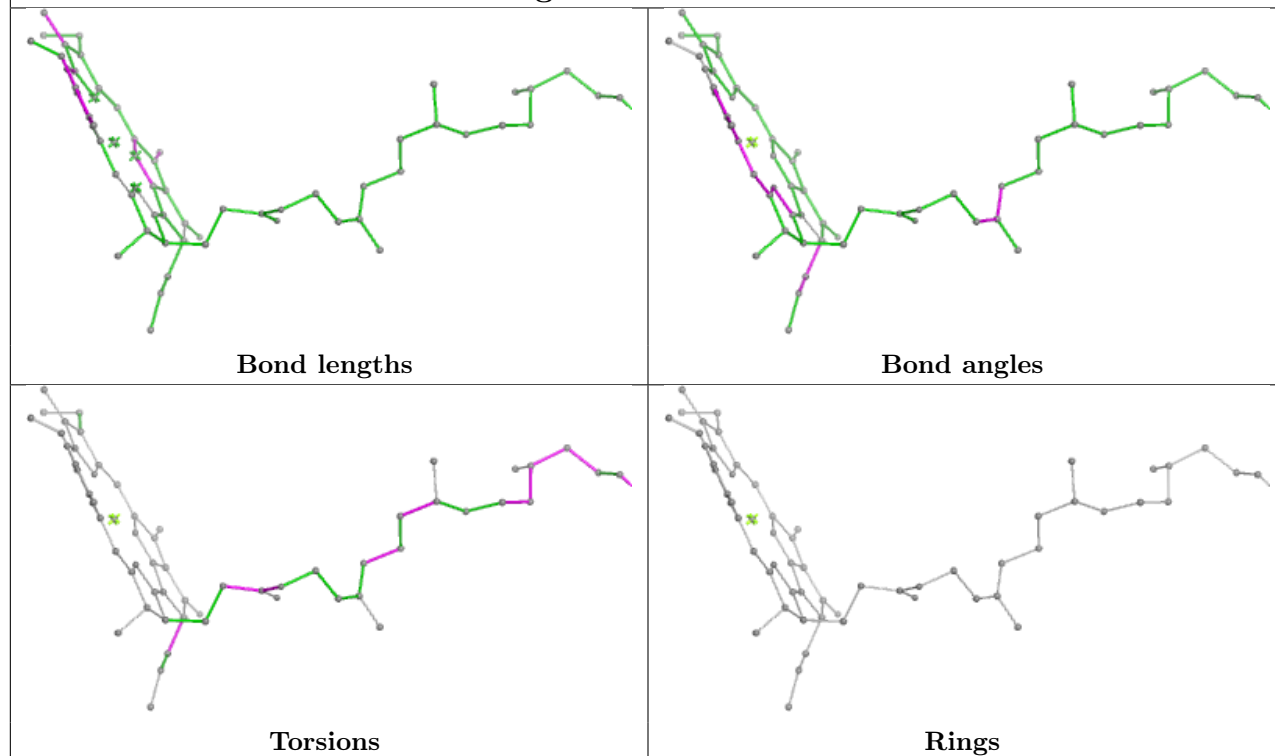
## Ligand CLA b 828



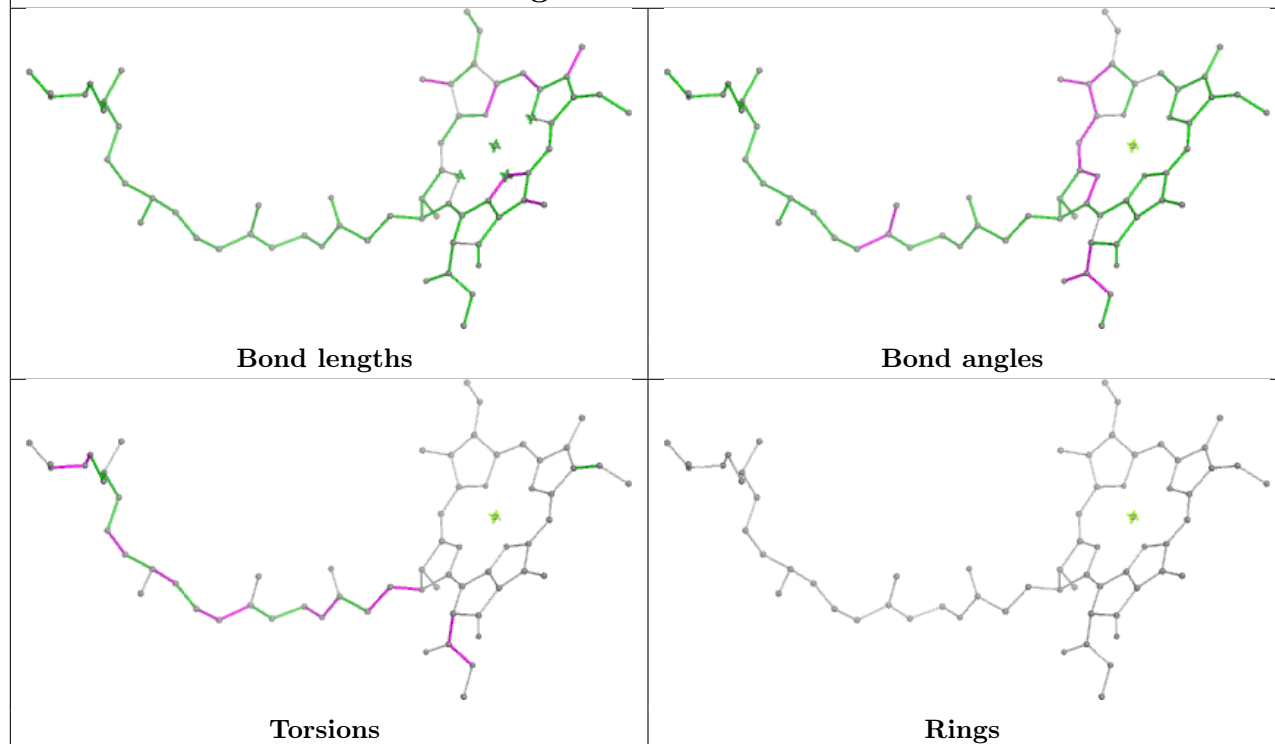


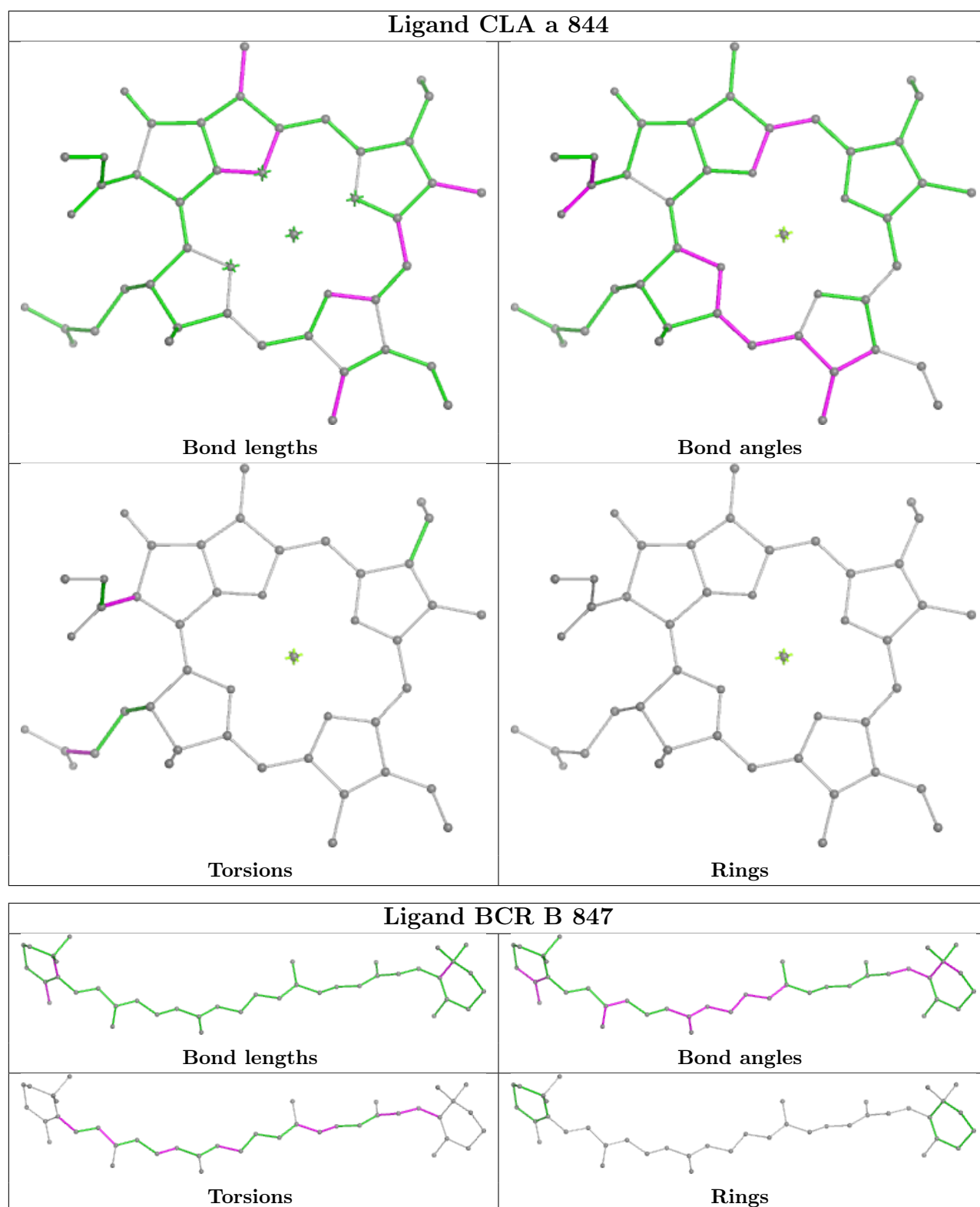


## Ligand CLA a 840



## Ligand CLA A 855





## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10559. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

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

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 Mask visualisation

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

## 7 Map analysis ⓘ

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

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit

This section was not generated.